Abstract

We present *-CFQ (“star-CFQ”): a suite of large-scale datasets of varying scope based on the CFQ semantic parsing benchmark, designed for principled investigation of the scalability of machine learning systems in a realistic compositional task setting. Using this suite, we conduct a series of experiments investigating the ability of Transformers to benefit from increased training size under conditions of fixed computational cost. We show that compositional generalization remains a challenge at all training sizes, and we show that increasing the scope of natural language leads to consistently higher error rates, which are only partially offset by increased training data. We further show that while additional training data from a related domain improves the accuracy in data-starved situations, this improvement is limited and diminishes as the distance from the related domain to the target domain increases.

1 Introduction

Intuitively, if you see a lot of examples of natural language questions about TV shows, it ought to also help understand similar syntax in questions about movies, or in questions that refer to both movies and TV shows together. Ideally, the training examples from the related domain should strictly improve performance, not hurt it. If you can satisfy that property, then you have at least a chance at eventually achieving arbitrarily robust performance across a range of domains, given sufficient training data in aggregate.

How and to what extent current machine learning (ML) approaches can be made to robustly solve natural language understanding (NLU) at the scale of arbitrary natural language across domain – with or without access to large quantities of training data – remains, however, an open question.

On one hand, research into the scaling behavior of deep learning systems has found generalization loss to decrease reliably with training size and model size in a power law or related logarithmic relationship across a range of architectures and tasks, from image classification with convolutional neural networks (Cho et al. 2015) to language modeling with Transformers (Rosenfeld et al. 2019; Kaplan et al. 2020; Brown et al. 2020). Recent results in an i.i.d. setting show this pattern to persist across many orders of magnitude, with no established upper limit (Kaplan et al. 2020).

At the same time, it has been shown that current ML systems continue to struggle to achieve robust performance in classes of tasks that require compositional generalization (Keysers et al. 2020) – an ability that has been argued to be crucial to robust language understanding (Fodor, Pylyshyn et al. 1988; Lake and Baroni 2018; Battaglia et al. 2018; Hupkes et al. 2019).

In this paper, we combine these two lines of research by investigating the effect of training size on error rates in the context of a compositional task. Specifically, we derive a suite of extended datasets based on the Compositional Freebase Questions (CFQ) semantic parsing benchmark (Keysers et al. 2020). We then use the compositional structure of each example to construct controlled experiments that measure the error rates when increasing training size in settings requiring compositional generalization and in settings simulating scaling to a broader scope of natural language. We apply these experiments to analysis of Transformers (Vaswani et al. 2017) in a setting of fixed computational cost – that is, of fixed model size and fixed training steps – and demonstrate key limits to their scalability in this setting.

Our contributions are the following:

- We present *-CFQ (“star-CFQ”): a suite of large-scale datasets and corresponding canonical splits, designed to enable principled investigation of the scalability of ML systems in a realistic compositional task setting. The datasets and splits follow the same setup as the original CFQ, but span a range of data sizes, rule scopes, and compound divergences with the largest consisting of 76% more rules, 41x as many examples, 14x as many question patterns, 53x as many SPARQL patterns, and covering a 32x larger domain than CFQ (Section 3).

- We confirm that under conditions of fixed computational cost, error rates for Transformers plateau at large training sizes. Moreover, targeting larger scopes of natural language leads to consistently higher error rates which are only partially offset by increased training data (Section 4).

- We demonstrate that compositional generalization remains a challenge at all training sizes, but that increases in training size continue to reap benefits in situations requiring compositional generalization, even when error rates
would seem to have plateaued in the i.i.d. case (Section 5).

- We show that while access to additional training data from a related domain improves accuracy in data-starved situations, this improvement is limited and diminishes as the distance from the related domain to the target domain increases (Section 6).

2 CFQ Benchmark

Keysers et al. (2020) introduced the Compositional Freebase Questions (CFQ), which is a simple but realistic and large natural language dataset that is specifically designed to measure compositional generalization. The task of interest is semantic parsing from a natural language question (such as ‘Which art director of [Stepping Sisters 1932] was a parent of [Imre Sándorházi]?’) to a SPARQL query, which can then be executed against the Freebase knowledge base. Named entities are anonymized, which is standard practice and ensures that the models do not have to learn all the entities.

CFQ was constructed using the Distribution-Based Compositional Assessment (DBCA) method. This means that the dataset is automatically generated from a set of rules in a way that precisely tracks which rules (atoms) and rule combinations (compounds) were used to generate each example. Using this information, the authors generate “maximum compound divergence” (MCD) splits, which maximize the compound divergence while guaranteeing a small atom divergence between train and test sets. MCD splits are well suited for assessing compositionality because they are both fair (because the distribution of individual rules is similar) and compositionally challenging (because the distribution of compounds is as different as possible).

The authors release a number of MCD splits for CFQ, and show that there is a strong negative correlation between the accuracy of three standard sequence-to-sequence architectures and the compound divergence. They investigate this for LSTM+attention (an LSTM (Hochreiter and Schmidhuber 1997) with attention mechanism (Bahdanau, Cho, and Bengio 2015)), for Transformer (Vaswani et al. 2017), and for Universal Transformer (Dehghani et al. 2018).

In a follow-up publication, Furrer et al. (2020) show that this negative correlation also applies to architectures that specifically target compositional generalization (such as CGPS (Li et al. 2019) and Neural Shuffle-Exchange Networks (Freivalds, Ozoliņš, and Sostaks 2019)) and cannot be overcome by masked language model pre-training using the Text-to-Text Transfer Transformer (T5) (Raffel et al. 2019).

3 *-CFQ

We present here *-CFQ4, a suite of datasets building on the same overall structure and base rule set as CFQ, but with two key differences intended to facilitate investigation of the scalability of solutions to the semantic parsing task:

- Increased data size: The datasets span a range of data sizes, with the largest 41x the size of CFQ.

Table 1: Statistics of the largest of the *-CFQ datasets, in comparison with the original CFQ. “Question pattern” here corresponds to “Query patterns (mod entities and properties)” from Keysers et al. (2020), while “Query pattern” corresponds to “Query patterns (mod entities and properties)”.

• Expanded rule set: The datasets span a range of rules scopes, based on grammar extensions to support additional Freebase types and properties (via new leaf rules) and additional syntactic constructs (via non-leaf rules).

All datasets in the suite include detailed instrumentation of the compositional structure of each example, in a similar format to that used in CFQ.

3.1 Increased Data Size

The *-CFQ datasets are generated following the algorithm described in Keysers et al. (2020) using rule sets closely related to the CFQ rules, but with sampling run at a larger scale in order to generate significantly larger datasets. As in Keysers et al. (2020), after the initial sampling phase, we apply sub-sampling and then semantic and structural filtering to increase the diversity of rule combinations while maintaining a balance of complexity levels and reducing the number of unnatural-sounding questions. The one difference from Keysers et al. (2020) is that in order to avoid an observed performance bottleneck, we omit the step of grounding the question in Freebase, which means that the generated questions contain only entity placeholders, without the guarantee that an actual set of entities can be found in Freebase that would lead to a non-empty answer to the question. In Appendix C, we show that while omitting the grounding step leads to a higher incidence of semantically implausible questions, the behavior of the baseline ML systems are highly consistent between the grounded and ungrounded datasets, which motivates our choice to use ungrounded datasets as proxies for grounded ones when exploring the behavior of ML systems at larger scales of training data.

We apply this procedure first to a nearly identical rule set as CFQ to generate the large ungrounded dataset u-CFQ (see Appendix D.1 for details). Datasets generated by the same procedure applied to different rule sets are described below in Section 3.3. Table 1 shows summary size statistics of two datasets from *-CFQ compared with CFQ. The size statistics for all the *-CFQ datasets can be found in Appendix C.

3.2 Extended Rule Set

In order to simulate coverage of a greater scope of natural language, we enrich the CFQ grammar to include up to 92%
In which TV program did M1 play
Did M0 direct M2 and marry M1
Who was a crime fiction film’s Indian writer
What was M1’s Anglican art director’s ethnicity
Was the daughter of the brother of M0 M2

Table 2: Examples of newly supported questions.

| Question | Example |
|----------|---------|
| Who was M1’s Australian crime fiction film’s writer? | M1’s writer |
| What was M1’s American crime fiction film’s setting? | M1’s setting |

Table 3: Examples of newly supported question patterns.

| Pattern | Example |
|---------|---------|
| Related to M1 | M1’s Australian crime fiction film’s writer |
| Related to M2 | M2’s American crime fiction film’s setting |

3.3 Rule Set Lattice

As we are interested in exploring the effect of both the number of new rules added and their type (leaf vs. non-leaf), we prepare a suite of rule sets with varying number of leaf and non-leaf rules, which together form a rule set lattice. We then generate separate large-scale dataset corresponding to each rule set in the lattice. For convenience, we will use the same name (e.g., B-CFQ, X-CFQ, etc.) to refer to both the rule set and the largest dataset generated from that rule set.

At the bottom of the lattice is a base rule set which we name B-CFQ, containing the rules shared by all other rule sets in the lattice. This rule set is designed to be as close as possible to U-CFQ, but with some minimal adjustments to enable separate evaluation of the addition of leaf- vs. non-leaf rules (see Appendix D for details).

L-CFQ is a rule set containing the rules of B-CFQ plus all additional leaf rules. N-CFQ consists of the rules of B-CFQ plus all additional non-leaf rules. X-CFQ contains the union of rules from L-CFQ and N-CFQ.

In order to test the effect of adding varying numbers of rules of a similar type, we also provide rule sets half-L-CFQ, half-N-CFQ, and half-X-CFQ, which have only half of the additional rules of the relevant types added.

The main characteristics of the rule sets from the lattice are shown in Table 3 with more details in Appendix D.3.

4 Experiments on Effect of Rule Scope

Increased rule scope yields consistently higher error rates, which are only partially offset by increased training size.

Figure 1 plots error rates vs. training size for a Transformer evaluated on random splits of datasets of increasing rule set scope. In each experiment, the model size and number of training steps (and hence, computational cost) are held constant, with hyperparameters as described in Appendix E.

Previous research has shown a power law relationship between data size and error rates or loss across a variety of deep learning architectures and tasks when model size and data size are increased in tandem (Kaplan et al. 2020; Brown et al. 2020; Rosenfeld et al. 2019; Hestness et al. 2017).

The results shown in Figure 1 are compatible with this previous research in that for all rule scopes, error rates initially vary in a rough power law relationship with training size, while flattening out at higher training sizes. We suspect that the flattening-out is due primarily to the fixed computational cost setting, and that with sufficiently large model sizes the power law relationship would persist longer.

What is most notable in Figure 1 is that as the rule scope increases, the asymptotic value of the error rate increases consistently, such that X-CFQ plateaus at an error rate roughly 3 times that of B-CFQ. This suggests a notable scalability implication for the Transformer architecture, in that, despite the fact that every dataset in the *-CFQ suite is fully described by a small set of rules, the moderately-sized Transformer fails to fully capture the rules regardless of the number of training examples provided, and training data alone is insufficient to fully offset the increased error rates that result from even modest increases to the rule scope.

It is also notable that adding non-leaf rules impacts error rate more than adding leaf rules, as evidenced by the error rates for N-CFQ being considerably higher than L-CFQ – in fact, nearly matching the error rates of the combined rule set X-CFQ. As shown in Appendix E this is despite the fact that the L-CFQ rule set describes a much larger space of possible questions than that described by N-CFQ. This suggests that Transformers struggle more with generalizing to new complex rule combinations than with generalizing to “primitive substitutions” (Li et al. 2019; Russin et al. 2019; Gordon et al. 2020), in which one leaf element is replaced by another within a question pattern observed in training.

5 Experiments on Effect of Compound Divergence

Compound divergence dramatically affects error rates at all training sizes. Large increases in training data yield greater benefit, however, at high compound divergence than at low.
Table 3: A list of the new CFQ-based rule sets with characteristics.

| Rule set | Description | # Grammar rules |
|----------|-------------|-----------------|
|          |             | (Non-leaf) | (Leaf) | (Total) |
| CFQ      | Original CFQ rule set from Keysers et al. (2020) | 54 | 157 | 211 | 443 |
| u-CFQ    | Rule set for ungrounded version of CFQ | 54 | 158 | 212 | 444 |
| b-CFQ    | Base CFQ | 55 | 137 | 192 | 412 |
| N-CFQ    | Base CFQ + additional non-leaf rules | 70 | 139 | 209 | 455 |
| half-N-CFQ | Base CFQ + half the additional non-leaf rules | 62 | 139 | 201 | 447 |
| L-CFQ    | Base CFQ + additional leaf rules | 59 | 324 | 383 | 738 |
| half-L-CFQ | Base CFQ + half the additional leaf rules | 59 | 236 | 295 | 597 |
| X-CFQ    | Base CFQ + both types of additional rules | 74 | 331 | 405 | 799 |
| half-X-CFQ | Base CFQ + half of both types of additional rules | 66 | 238 | 304 | 602 |

Keysers et al. (2020) observe that as the compound divergence between a train set and test set increases— that is, as the need for compositional generalization increases—the accuracy of a Transformer on the CFQ task decreases dramatically from over 98% at compound divergence 0 (a random split) to less than 20% at compound divergence 0.7 when training size is around 100k examples. In their Appendix H they also present preliminary results of the effect of training size on this performance gap—specifically, that the performance gap is even wider at smaller training sizes (e.g., around 10k examples) and shrinks as training size increases. This leaves open the question as to whether further increasing the training size beyond 100k could at some point narrow the performance gap sufficiently that the systems can be said to have effectively learned to compositionally generalize.

We investigate this question by reproducing the experiments of Keysers et al. (2020) across a wider range of training sizes, from around 10k up to nearly 900k examples. As seen in the results in Figure 2 compositional generalization remains a challenge, with even a moderate compound divergence of 0.2 yielding error rates an order of magnitude higher than those at compound divergence 0 even at the largest training sizes. Similarly to results on random splits, error rates vary in a rough power law relationship with training size in ranges of moderately large training data, while presumably plateauing at very large training sizes. However, a noticeable warm-up period can be observed, in which error rates decrease at a much slower rate, with the warm-up period persisting longer, the greater the compound divergence. Also, while in Figure 1 error rates on random splits consistently begin to flatten out starting at around 100-300k training examples (with the plateau even more pronounced in Figure 1 for the compound divergence 0 split), at the higher compound divergence levels, the plateau is yet to be seen for training sizes up to 1M. This suggests that greater benefit can be reaped from very large training sizes in scenarios requiring compositional generalization than in i.i.d. settings. Further experiments at larger training sizes would be required to verify how much compound divergence affects the final asymptotic error level.

A more detailed comparison of our investigation with that of Keysers et al. (2020) is covered in Appendix G.

6 Experiments on Effect of Data from Related Domain

While the experiment results from Section 5 show a clear trend of increasing error rate as rule scope increases, this trend can be seen as the combined effect of multiple simultaneously changing factors, which we may group roughly into test set effects and train set effects.

While increasing rule scope affects the test set on one hand in the obvious way of increasing its breadth, there may be more subtle effects that could lead to either an increase or decrease in inherently “easy” or “hard” examples in the test set, depending on which existing rules the newly added rules tend to compose most easily with. From the perspective of investigating the scalability of ML systems, these test set effects are of limited interest, as they largely represent artifacts of the specific data generation and sampling algorithm.

Of greater interest are the train set effects. On one hand, we expect increasing the rule scope to dilute the train set, in that, from the perspective of any given test example, the pro-
portion of train examples directly relevant to it (e.g., which use a large fraction of the rules or combinations of rules that appear in it) will decrease as the rule scope covered by the train set increases. At the same time, however, increasing the rule scope may increase the diversity of contexts in which each rule is seen, which may improve generalization [Hill et al., 2019]. A key question governing how well ML systems can scale to larger scopes of natural language is indeed how much benefit the system can derive from these training examples that are only partially or indirectly relevant to any given subset of test examples.

To better answer this question while minimizing interference from test set effects, we shift our focus to the following experiment setup. We choose as point of reference a fixed test set $W^{TEST}$, which is randomly sampled from some limited-scope target domain $W$ – specifically, here we will use the B-CFQ dataset. We then suppose we have access to a limited set $W^{TRAIN}$ of $n_{in}$ training examples drawn from the identical distribution as $W^{TEST}$, plus a potentially larger supplementary set $W^{TRAIN}_{sup}$ of $n_{sup}$ training examples sampled from a related domain $V$ that is related to $W$ through some overlap in the rule sets used to generate them. $V$ might consist, for example, of other movie-related questions that are not present in $W$. Of questions that follow a similar syntax but include words referring to different Freebase properties and types (i.e., different leaf rules). In both cases, we investigate, for various choices of supplementary domain $V$ and values of $n_{in}$ and $n_{sup}$, the degree to which blending the supplementary data set $W^{TRAIN}_{sup}$ into the train set improves or harms performance on the original test set $W^{TEST}$.

In each case, we use as supplementary domain $V$ one of the datasets from the *-CFQ rule set lattice – specifically one of half-l-CFQ, l-CFQ, half-x-CFQ or x-CFQ – with examples generatable by the B-CFQ rule set filtered out. We omit experiments involving half-n-CFQ or N-CFQ, which do not lend themselves well to this experiment setup, due to the high overlap between their domains and B-CFQ. (See Appendix E for details.)

For all the experiments we use an approach similar to the one in Keysers et al., 2020:

- We use a Transformer architecture with hyperparameters described in Appendix E.
- For each split we train 5 replicas and average the results.

Details of how the train sets $W^{TRAIN}$ and $V^{TRAIN}$ are blended are described in Appendix F.

In all experiments we used a fixed test set of 95,742 examples sampled randomly from B-CFQ.

### 6.1 Equal Weighting of Examples from Target and Related Domains

Transformers are sensitive to the training distribution, not just the information contained in the training data. When highly data-starved, adding training examples from a related domain can improve performance. As training size increases, however, the skew in train vs. test distribution resulting from expansion of the train set quickly outweighs any benefits from the additional training examples.

In this experiment, we weight examples from $W^{TRAIN}$ and $V^{TRAIN}$ equally, so that as the number of examples in $V^{TRAIN}$ increases, we can observe the same dynamics we would see when scaling to increasing scopes of language, where expanding the scope of the train set simultaneously increases the amount of total information in the train set while also diluting the fraction of the train set that is directly relevant to any given slice of test examples.

Figure 3(a) summarizes the results when $n_{in}$ is fixed at 10k examples and $n_{sup}$ varies between 10k and 8M. As in Figure 1, error rate varies with training size in a clear power law relation for training sizes up to around 100k-300k (depending on the dataset), after which performance plateaus. However, the more distant the related domain is from the target domain in terms of number of leaf or non-leaf rules added, the more slowly the error rates drop, and the higher the asymptotic value at which they plateau. This reinforces that the increased error rates observed in Section 5 for increased rule scope are indeed driven largely by the changing composition of the train set, rather than purely by test set effects.

For easier comparison with Figure 1 we mark on each curve the point at which the relative size of $n_{sup}$ vs. $n_{in}$ matches the ratio that would be expected based on the relative sizes of the domains of $V$ vs. $W$, if the train set were sampled from $V$ as a whole, while the test set were simply fixed to observe the performance on the subset of $V$ generated by the narrower rule set $W$. It can be seen that the error rates at the marked points in Figure 3 are slightly higher than at similar training sizes in Figure 1, suggesting that a small degree of test set effect is also at play.

Figure 3(b) summarizes the results when $n_{in}$ is fixed at the larger value of 100k examples, while $n_{sup}$ varies as before between 10k and 8M. Here, unlike in the data-starved scenario of Figure 3(a), the benefit from the additional training data is more limited, with error rates actually increasing when $n_{sup}$ is significantly larger than $n_{in}$. This suggests that as training size increases, the skew in train vs. test distribution resulting from expansion of the train set quickly outweighs any benefits from the additional training examples. Notably, by the time that $n_{sup}$ approaches 100x the value of $n_{in}$, error rates have already increased to levels comparable to those at which they are seen to plateau in Figure 3(a) for the same choice of $V$, despite the order of magnitude difference in the amount of in-domain training data.

Results for other choices of $n_{in}$ ranging from 10k up through 500k examples are presented in Appendix I.

### 6.2 Over-weighting of Examples from Target Domain

If sample weighting is controlled, then additional data from a related domain can be made to yield a strictly positive effect. However, the performance benefits achievable through this method are limited.

If we had the luxury of being able to train a separate model for each domain, we could consider mitigating the
Figure 3: Error rate vs train set size, log-log scale, equal weighting of examples from target and related domains: \(10\text{k}\) examples (a) and \(100\text{k}\) examples (b), B-CFQ test set, B-CFQ + others train set.

7 Related Work

The relationship between training size and error rates or generalization loss has been studied in a variety of settings. Early research observed that accuracy varies roughly with the log of the training size, both in shallow ML approaches on a natural language disambiguation task (Banko and Brill 2001) and in convolutional neural networks on an object detection task (Sun et al. 2017). Others, noting the connection with learning curves observed during training on a large train set, have tried fitting a power law learning curve to the relationship between training size and error rate (Figueroa et al. 2012). More recent research has observed consistent power law relationships between training size and cross-entropy error across a range of deep learning architectures, including LSTMs on language modeling and machine translation tasks (Hestness et al. 2017) and LSTMs or Transformers on language modeling tasks (Rosenfeld et al. 2019; Kaplan et al. 2020; Brown et al. 2020), provided that training size and model size are increased in tandem. In particular, Kaplan et al. (2020) observe that a highly consistent power law relationship between cross-entropy loss and either of training size or model size persists across many orders of magnitude when not bottlenecked by the other of the two. Our approach differs from this previous research by specifically investigating the effect of the compositional structure of a task on the training size to error rate relationship.

The degree to which additional training data from a related domain can help or hurt performance has been investigated also in the context of multi-domain learning (Yang and Hospedales 2014; Herzig and Berant 2017; Britz, Le, and Pryzant 2017; Tars and Fishel 2018; Mghabbar and Ratinamogan 2020; Wang et al. 2020) and domain adaptation (Wang et al. 2017; Chu and Wang 2018; Zhang et al. 2019; Wilson and Cook 2020).

Our experiments in Section 6.1 resemble the scenario of multi-domain learning (MDL) in that we aim to train a single model that can apply to multiple domains, not just the single domain from which our test set is drawn. Multi-domain learning seeks, however, to improve performance on individual domains by explicitly distinguishing the domain of each example at train and test time, which is not our focus here. We expect that explicitly distinguishing domains would be less beneficial in the *-CFQ tasks than in scenarios where
our approach differs from this previous research again by using knowledge of the compositional structure of the task to characterize the relationship between the target domain and related domains, and illustrating the effect of these factors on the slope and limit value of the performance curves.

8 Conclusion and Outlook

In this paper we present *-CFQ, a suite of large-scale datasets designed for principled investigation into the scalability of ML systems on a compositional NLU task. To the best of our knowledge, *-CFQ is uniquely suited for this investigation, because it is the first dataset to achieve this scale while providing full details on the compositional structure of each example. We use this dataset to perform experiments illustrating that scalability is indeed a concern even at a scope that is only a tiny fraction of full natural language.

The experiments presented in this paper, however, only scratch the surface of the types of controlled investigations of ML scaling behavior possible using *-CFQ. We hope that this dataset suite will aid the deep learning and NLU communities in the development of more robust and scalable solutions to language understanding.

In particular, we hope to re-use *-CFQ to evaluate the degree to which language model pre-training and increase of model size affect the scalability curves in the compositional setting. We are interested in exploring the combined effects of compound divergence and rule scope. Further, we are interested to estimate the necessary data sizes and computational power that would be required by current ML approaches to achieve robust levels of language understanding across arbitrary domains and syntax, based on the above results together with an estimate of the effective number of language features in full natural language compared to X-CFQ.
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Ethics Statement

The purpose of this paper is well aligned with sustainability and efficient use of resources. More scalable models need fewer training examples and thus fewer resources to reach the same accuracy than less scalable ones.

Since the *-CFQ datasets are generated and ungrounded (except for o-CFQ), they do not contain any personal data. o-CFQ does not contain private data as it is grounded on Freebase which is publicly available.

In general, when preparing datasets for use in training language models, care should be taken to avoid inclusion of potentially harmful biases which may be propagated to the language models. Due to their systematic, rule-based generation method, the risk of unintended bias in *-CFQ, as in CFQ, is low compared to datasets mined from large corpora of text in the wild. The main source of potential bias would be in the distribution of entities in the Freebase dataset itself, which may be propagated to the resulting generated questions, particularly during the grounding step. The risk of such bias is reduced in *-CFQ through the use of ungrounded questions in most of its datasets. In the choice of adjectives modeled in the dataset, some bias (or loss of comprehensiveness) is also introduced due to our choice of only those adjectives whose corresponding entities are relatively frequently used in Freebase.

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Appendix

A Contributions

Dmitry designed most of the experiments and the dataset lattice, generated dataset pools, conducted divergence-related experiments, wrote initial paper draft, contributed to the final paper writing, and made all figures for the paper.

Tibor extended the CFQ dataset with new leaf rules; wrote the infrastructure for dataset blending and generating reproducible random splits; conducted all experiments involving random splits and to find an optimal number of training steps; contributed to writing several sections in the Appendix and the Ethics statement; analyzed the similarity of domains; did the data quality analysis of X-CFQ; and populated most of the tables used in the paper.

Nathan proposed the paper messaging, researched related work, and wrote the bulk of the main body text.

Nikola supervised the work on extending the CFQ dataset, provided overall technical guidance and contributed to writing Appendix B.

Danila extended the CFQ dataset with the new grammar features, improved scalability of the dataset generation pipeline, did the data quality analysis of U-CFQ, wrote the corresponding section in the Appendix.

Nathanael provided high-level project direction, wrote the CFQ benchmark section, and provided suggestions while iterating on the messaging.

B Grounded vs. Ungrounded Datasets

The CFQ dataset was generated using grounding into Freebase. The process of grounding has a couple of effects on the CFQ dataset: 1.) It replaces entity placeholders with concrete entities and 2.) it filters out questions which can not be grounded as they are deemed "unnatural". Unfortunately the grounding process poses a significant challenge in scaling the dataset to a larger number of questions. Grounding is one of the main performance bottlenecks of the CFQ generation algorithm due to the limited throughput of the Freebase SPARQL server. In addition, the requirement that every question needs to be grounded in Freebase results in filtering out a large number of natural questions which describe scenarios not present in Freebase. E.g. the question “What Dutch film editor influenced a person.” would be filtered out during grounding as Freebase does not contain a set of entities that satisfy it.

In this work we overcome this problem by skipping the grounding step and hence removing the dependency on the SPARQL server. This allows us to scale the dataset to significantly larger size but it introduces a couple of potentially undesirable effects:

• Over-generation: it increases the fraction of unnatural questions, many of which could be filtered out based on missing Freebase mappings.

• Skew in the sample distribution: Grounding in Freebase implicitly applies a semantic filtering of the sentences. Removing the semantic filtering could result in a significant distribution skew on the set of examples which could affect the behavior of Transformers on tasks built on top of this dataset.

Given our focus on investigating the scalability of ML systems on the realistic language understanding task represented by the original CFQ dataset, our primary concern here is whether the above two effects could lead to materially different scaling behaviors of ML systems on the ungrounded datasets compared to the original grounded one.

In order to address this concern we perform a series of experiments aimed at determining the effect of grounding on the performance of Transformers. Based on the results of those experiments we conclude that the scalability experiments performed in this paper over the ungrounded *-CFQ dataset suite should be indicative for the behavior of Transformers on grounded datasets.

In section Appendices [B.1] and [B.2] we describe the pair of datasets used to perform the aforementioned experiments and in Appendices [B.3] and [B.4] we describe the experiments in detail.

B.1 o-CFQ and u-CFQ

In order to facilitate a set of experiments which evaluate the effect of grounding we generated a pair of datasets (o-CFQ and u-CFQ) which only differ by the fact that o-CFQ is grounded, while u-CFQ is not.

o-CFQ and u-CFQ are generated from the same set of rules, which we call the u-CFQ rule set. The u-CFQ rule set is very close to the set of rules used in the original CFQ dataset (see Appendix D.1 for minor differences). This set of rules was used in two different ways in order to generate the two datasets:

• o-CFQ: The initial set of examples were generated by using the u-CFQ rules to parse the questions from the CFQ dataset, yielding the same questions as in CFQ, but instrumented with atoms and compounds based on the u-CFQ grammar, and with potentially different SPARQL output due to slightly adjusted property mappings (see Appendix [D.1]). Due to the minor differences between the CFQ and u-CFQ grammars, a small fraction (4.4%) of the CFQ questions were not parsable by the u-CFQ grammar. These questions were discarded.

• u-CFQ: u-CFQ was produced using the randomised generation procedure described in [Keysers et al., 2020], except that the grounding step was skipped.

For more details on the u-CFQ rule set, see Appendix [D.1].

B.2 Data Quality Analysis of u-CFQ

During the development of our data generation pipeline, we manually checked the generated examples for quality. Below is a random selection of 50 examples of the final u-CFQ dataset (no cherry-picking was used).

1. What did a costume designer that M1 played and M2 played found?

2. What male actor was a cinematographer and editor of M2?
3. Was M5 a Japanese Dutch male Spanish screenwriter’s country of nationality?
4. What was directed and executive produced by a Swedish male costume designer that an actor played?
5. What was edited and directed by a German Japanese French male art director’s parent’s sibling?
6. What Chinese employee and founder of M1 influenced M0?
7. Was M2 played by a male cinematographer and star of M0 and played by M3?
8. Which female writer and executive producer of M0 and M1 was a Canadian Swedish Chinese editor of M6?
9. Who was played by a film editor’s parent’s parent and spouse?
10. Was M1’s cinematographer and producer a Dutch female art director’s country of nationality’s Swedish male art director?
11. Was M3 founded by M1’s female Japanese parent?
12. Was M4’s child a Canadian female Spanish Italian costume designer of M0?
13. Was M2’s star M1’s Spanish male child?
14. Who was a male child of a Japanese film editor?
15. Was M1 written by M0’s director, writer, editor, and art director?
16. Which French parent of a costume designer did a male costume designer marry?
17. What film was written by, edited by, directed by, and executive produced by a character’s Italian spouse?
18. Was M1’s Mexican spouse a female German screenwriter’s parent, sibling, spouse, and child?
19. Did M1 marry and influence a art director’s sibling, child, and spouse?
20. What was produced and distributed by a costume designer’s female Chinese Swedish Japanese parent?
21. Who married M3’s Italian female Chinese parent?
22. Was a male Spanish child of a Japanese art director’s child M2’s Chinese star?
23. Did M1 direct M2 and write a prequel of M0?
24. What did a Italian male writer of M0, M1, M2, and M3 produce?
25. Who was employed by M2’s parent, was influenced by a film producer, and was employed by M1?
26. Did a Japanese executive producer, art director, producer, and star of M0, M1, and M2 executive produce M3?
27. Was M1’s Mexican spouse a female German screenwriter’s parent, sibling, spouse, and child?
28. Did M1 influence a art director, costume designer, and cinematographer of M0, write M2, and marry M3?
29. Was a film editor a male art director that married M3?
30. Was M5 executive produced by a female Spanish American Swedish art director’s parent and child?
31. Who was a Dutch Swedish costume designer’s Swedish Mexican sibling?
32. Which male spouse of M2’s child was played by M0?
33. Which writer, cinematographer, director, producer, executive producer, star, and costume designer of M0 produced M1’s sequel?
34. Was M0 a producer, writer, executive producer, cinematographer, costume designer, and star of M1, M2, M3, M4, and M5?
35. Who influenced M2’s female editor?
36. Was M1’s cinematographer and producer a Dutch female art director’s country of nationality’s Swedish male art director?
37. Was a film’s star M0’s producer, costume designer, cinematographer, director, executive producer, writer, art director, and editor?
38. Was a parent, child, sibling, and spouse of a art director a female child of M0?
39. What film was executive produced by a cinematographer and starred M1?
40. Who was a male actor that married and influenced a female costume designer’s male child?
41. Did a female Swedish British film director’s child acquire M0?
42. Which Chinese Mexican founder of M0 produced M3?
43. Which Spanish Italian film director was played by M1?
44. What did a French employee of a film producer write?
45. Was a person M1’s art director’s parent’s parent?
46. Were M2, M3, M4, M5, M6, M7, and M8 edited by M1’s male editor?
47. Who was a American child of a male American German French actor’s American parent?
48. Was a child and parent of a company M0’s star and executive producer?
49. Was M4’s female Canadian Italian French Chinese child’s gender M6?
50. Did a male Canadian person whose spouse founded M4 edit M1?

Manual checking showed that all SPARQL queries associated with these questions are semantically correct, but several examples sound unnatural. These examples can be divided in two groups:

1. Questions that require an entity to fill multiple roles of another entity which for some pairs of roles is impossible in reality (e.g. someone’s parent and child cannot be the same person). The 3 examples in this group are

2. Questions, where an entity is used with a property that does not match the type of that entity (e.g. “country of nationality’s art director”). There are 3 such questions in our sample:
Figure 5: Effect of grounding on scalability curve. Accuracy vs train set size for random splits of CFQ, o-CFQ, and u-CFQ. Note that the curves for CFQ and o-CFQ are virtually identical and largely overlap.

Comparing these results with quality analysis of the CFQ dataset described in Keysers et al. (2020), we see that the unnatural-sounding questions are approximately two times more frequent in u-CFQ that can be attributed to the fact that grounding in Freebase performed for CFQ allowed to eliminate at least some questions with incompatible roles and/or properties.

The presence of these questions in the u-CFQ dataset doesn’t materially affect any of our findings, because every such question can still be unambiguously represented as a SPARQL query.

B.3 Effect of Testing on Ungrounded vs. Grounded Data

To explore the degree to which ML systems’ scalability behaviors differ between u-CFQ and o-CFQ, we generate random train/test splits with varying train set sizes from each of these datasets and compare the accuracy trajectories of the trained models.

The training sizes for u-CFQ range from 9.5k up to 8.7M examples. The training sizes for o-CFQ range from 9.5k up to 640k examples (larger sizes omitted for o-CFQ due to the limited size of the grounded dataset).

The results are presented in Figure 5.

We observe that while error rates on u-CFQ are somewhat higher than on o-CFQ, error rates follow qualitatively similar trajectories on both sets.

Based on this, we conclude that performing experiments on ungrounded data should be a reasonable proxy for experimenting on grounded data and that we can expect findings from experiments on ungrounded CFQ-like datasets to carry over to the case of grounded datasets as well. For the bulk of this paper, we thus focus primarily on experiments on ungrounded data due to the increased feasibility of generating large quantities of ungrounded data.

B.4 Effect of Training on Ungrounded vs. Grounded Data

While the CFQ and *-CFQ datasets use rule-based data generation primarily as a means of constructing a controlled testing environment for understanding the behavior of ML systems, a similar auto-generation approach, if applied across a broader range of domains, could conceivably be used as a means to provide or augment training data for a system intended to be applied in real-life scenarios. One question that arises in such a scenario is how effective it would be to apply the cheaper process of generating (potentially large numbers of) ungrounded training examples, compared to generating a smaller number of more realistic training examples via the more expensive grounding process.

To explore this trade-off between data size and data purity, we conduct an experiment in which the test set consists of “realistic” grounded examples from o-CFQ, while the train set consists of ungrounded examples from u-CFQ, with the train size ranging from 9.5k up to 8.7M examples. The resulting accuracies are compared with a baseline of a pure random split on o-CFQ.

The results are presented in Figure 6.

As expected, at any given train size, training on ungrounded data leads to lower accuracies than when training on grounded data from the same distribution as the test set, if significantly larger amounts of ungrounded data are available, then the larger training size can compensate for this accuracy loss.
amount of ungrounded training data increases, suggesting that if an auto-generation process were able to generate significantly larger amounts of ungrounded training data than could be acquired for grounded examples, the larger training size can compensate for the nominal accuracy loss that results from the inclusion of “unrealistic” examples in the train set.

C Dataset Stats

Table 4 shows a complete list of the datasets included in *-CFQ, with characteristics including their size and complexity in comparison with the original CFQ dataset.

D Rule Sets

D.1 CFQ / U-CFQ Rule Set

The examples from CFQ that are not included in U-CFQ can be split to the following groups:

1. 9037 questions mentioning actor as a role, for example “Did M1 influence M0’s actor?”. This includes unnatural questions such as “Was M1 a company’s actor?”, and moreover, it was always assumed that it referred to an actor of a character (not an actor of a movie) which sometimes resulted in non-obvious SPARQL queries. In lieu of a better solution, all questions containing actor as a role have been removed.

2. 1306 unnatural questions that treat countries of nationalities as organizations, for example “Who did M1’s country of nationality employ?”. 

3. 930 questions that require a non-person writer, for example “Was a company M1’s writer?”. 

4. 34 questions containing the unnatural phrase “playing a film”, for example “Who played a film?”. 

The generated SPARQL can also be different for the same question in CFQ and O-CFQ, due to the following differences in the U-CFQ rule set:

1. Directing, producing and writing were mapped in CFQ solely to movie-related Freebase properties. The U-CFQ rule set covers also TV programs so these actions are mapped to the disjunction of the movie and TV program related Freebase properties. For example, U-CFQ maps “Who directed M0?” to a SPARQL query representing a person directing a movie or a TV program. In the *-CFQ datasets, this is important to ensure that the SPARQL is independent of the type of M0. In the case of O-CFQ and U-CFQ, this is just a technicality that makes these datasets compatible with the *-CFQ datasets.

2. Knowledge rules in the CFQ rule set map genders only to the Freebase property representing the gender of a real person. The U-CFQ rule set maps genders to a disjunction of Freebase properties corresponding to the gender of a real person and the gender of a fictional character. This seems like an oversight in CFQ since it already covered fictional characters in other cases.

D.2 B-CFQ

A natural choice for the bottom of the rule set lattice would be the U-CFQ rule set, as it was the starting point of our rule set extension that lead to generation of X-CFQ. This choice, however, would be sub-optimal with respect to one of the desired criteria for the experiments we plan to run.

Specifically, one of the goals of this research is to compare the effect of rule scope increase from addition of leaf rules vs. addition of non-leaf rules. In order to do this, we would ideally like to separate the new rules into two disjoint sets: one consisting of only new leaf rules (for inclusion in L-CFQ) and one consisting of only new non-leaf rules (for inclusion in N-CFQ).

A clean separation is difficult, however, due to certain interdependencies between the leaf and non-leaf rules. For example, one of the additions we make for X-CFQ is to introduce film genres. While it naturally counts as a leaf change (29 added leaf rules), its support requires the implementation of a number of non-leaf rules as well. If U-CFQ is the bottom of the lattice, this would prevent us from having a clear separation between leaf and non-leaf rules.

In order to mitigate this problem, we define a new rule set B-CFQ to service as the lattice’s bottom. We design it to be as close as possible to U-CFQ (in terms of size and complexity), but allowing clear separation of leaf and non-leaf rule additions. B-CFQ differs from U-CFQ in the following ways:

• Adds 2 non-leaf and 2 leaf grammar rules related to genres.

• Removes all rules related to genre.

• Removes a leaf rule corresponding to “what” in certain places.

• Removes 10 leaf rules corresponding to nationalities (keeping the other 2 rules).

These changes aim to maintain a balance between added/removed rules while maintaining the additivity property of the rule set lattice.

D.3 Rule Set Lattice

Rule set lattice, corresponding to *-CFQ, is illustrated in Figure [7] in which each rule set is a superset of its child rule set(s).

The description of rule sets L-CFQ, N-CFQ follows directly from the rule sets X-CFQ and B-CFQ, taking into account the additivity principle described in Appendix D.2. There are more choices for the half datasets available. Below we describe the reasons behind the particular rule set’s content.

half-L-CFQ. For this rule set we go through all newly supported Freebase types and properties (see Table 6 for details and examples) and pick half of the leaves in each category, rounded down. We also include all the surface forms in this rule set.

half-N-CFQ. It is harder to choose the rules for this set, as individual rules are not independent: some of them are required for the others to be able to trigger. In the end
Table 4: A list of all datasets included in *-CFQ, with their characteristics. The first row is the original CFQ from Keysers et al. (2020), for comparison. The second section are newly introduced datasets based on roughly the same rule set as CFQ. The third section are the datasets corresponding to the nodes of the rule set lattice described in Section 3.3.

| Dataset   | Description                                      | Questions | Queries | Question patterns | Query patterns |
|-----------|--------------------------------------------------|-----------|---------|------------------|----------------|
| CFQ       | From Keysers et al. (2020)                       | 239,357   | 228,149 | 49,320           | 34,921         |
| o-CFQ     | Slightly filtered and re-instrumented            | 228,901   | 165,736 | 44,465           | 34,278         |
| u-CFQ     | Larger ungrounded version                        | 9,925,221 | 6,551,678| 319,407          | 762,680        |
| b-CFQ     | Base of rule set lattice                         | 8,663,352 | 4,617,765| 419,611          | 696,840        |
| n-CFQ     | Base + additional non-leaf rules                 | 8,716,725 | 4,580,018| 608,651          | 841,749        |
| half-n-CFQ| Base + half the additional non-leaf rules        | 8,699,762 | 4,385,655| 425,815          | 700,452        |
| l-CFQ     | Base + additional leaf rules                     | 9,874,258 | 7,266,600| 618,079          | 1,630,225      |
| half-l-CFQ| Base + half the additional leaf rules            | 9,297,045 | 6,656,162| 558,990          | 1,484,723      |
| x-CFQ     | Base + both types of additional rules            | 9,879,894 | 7,249,705| 713,137          | 1,847,555      |
| half-x-CFQ| Base + half of both types of rules               | 9,294,958 | 6,469,571| 530,405          | 1,535,828      |

D.4 Data Quality Analysis of X-CFQ

We also analysed the data quality of X-CFQ. Below is a random selection of 50 examples of the final X-CFQ dataset (again, no cherrypicking was used).

1. What executive producer and producer of M0 was M1’s editor, art director, star, costume designer, and executive producer?
2. Was M5 a art director whose Mormon spouse, father, husband, and wife produced M0 and M1?
3. Was a Hindu Jewish Chinese Irish American brother of a drama film’s producer’s child M2?
4. Was M2 a daughter, spouse, and sibling of the thriller movie’s executive producer, costume designer, director, cinematographer, and star?
5. Was M2’s child’s friend, offspring, parent, and sibling M0’s child and parent?
6. Who was M2’s Hindu costume designer’s husband, sibling, friend, and parent?
7. Was a movie whose art director and executive producer influenced and was influenced by a film distributor’s employee and founder M1?
8. Who was the Dutch sibling and husband of M0?
9. Which Buddhist Mormon male Muslim parent of M6’s star was M1’s Hindu spouse?
10. Who was a parent of a company’s white Catholic Canadian founder?
11. What female Irish American Indian child of a cinematographer did M2 and M3 employ?
12. Was a Hindu costume designer’s parent, spouse, and son a Mexican child of the creator and producer of M2?
13. Was M3 a actor whose parent and wife distributed and produced M0 and M1?
14. Was M2’s Hindu spouse a English wife of M3?
15. Was M2’s producer’s Buddhist sibling a Jewish TV director’s daughter?
16. Was the woman’s spouse, sibling, father, and child M2?
17. Who was the child, sibling, parent, and husband of M2’s friend and sister?
18. Was M0’s art director, costume designer, executive producer, producer, writer, editor, and star M2’s mother?
19. Was the man the executive producer of M1, M2, M3, M4, and M5?
Table 5: Statistics for newly supported surface forms, Freebase types, properties and entities.

| New language feature                        | # affected grammar rules | # affected tokens | # added Freebase properties | # added Freebase types | # added Freebase entities |
|---------------------------------------------|--------------------------|-------------------|-----------------------------|------------------------|--------------------------|
| TV program and contributions                | 32                       | 20                | 10                          | 5                      | 0                        |
| Film genre                                  | 30                       | 16                | 2                           | 0                      | 13                       |
| Religion                                    | 27                       | 12                | 2                           | 1                      | 8                        |
| Ethnicity                                   | 18                       | 9                 | 2                           | 1                      | 6                        |
| Movie language                              | 16                       | 11                | 2                           | 1                      | 9                        |
| Additional family relations                  | 16                       | 8                 | 0                           | 0                      | 0                        |
| Additional film related verbs               | 9                        | 8                 | 8                           | 1                      | 0                        |
| Generic notion of “contributing to” a film  | 4                        | 2                 | 2                           | 0                      | 0                        |
| Woman/Man                                   | 4                        | 2                 | 0                           | 0                      | 0                        |
| Celebrity                                   | 2                        | 1                 | 0                           | 1                      | 0                        |
| Friend                                      | 1                        | 1                 | 2                           | 0                      | 0                        |
| 'Script(-)writer' (meaning 'Screenwriter')  | 2                        | 2                 | 0                           | 0                      | 0                        |
| ‘Offspring’ (meaning ‘Child’ of a person)   | 2                        | 1                 | 2                           | 0                      | 0                        |
| ‘Subsidiary’ (meaning ‘Child’ of a company) | 2                        | 1                 | 2                           | 0                      | 0                        |
| ‘Movie’ (meaning ‘Film’)                    | 1                        | 1                 | 0                           | 0                      | 0                        |
| ‘Which’ (synonym for ‘That’)                | 1                        | 1                 | 0                           | 0                      | 0                        |
| Definite article                            | 1                        | 1                 | 0                           | 0                      | 0                        |

20. Was M2 a drama sequel and prequel of the German speaking film?
21. Which husband of the person and atheist art director of M1 and M2 were M4, M5, and M6 directed by?
22. Was the TV show’s art director M1’s mother?
23. What did the production company’s Canadian white child’s French mother’s friend distribute?
24. What was M0’s Buddhist Anglican producer’s employer’s parent and subsidiary?
25. What was a country of nationality of M5’s American female Italian Irish American Japanese spouse?
26. Was a screenwriter M1’s friend, offspring, and mother?
27. Was M1’s Dutch producer the art director’s child, wife, and friend?
28. Was the religion’s Catholic white costume designer M4’s Muslim executive producer’s spouse, mother, and friend?
29. Was a German parent of M1 a father and spouse of M3’s adherent?
30. Was M1 a costume designer’s Mormon English Buddhist Indian white wife?
31. Who was a African-American son of M3’s sibling?
32. Did a Hindu Irish American person’s Hindu Muslim mother write M0?
33. Were M2, M3, M4, M5, M6, M7, M8, and M9 created by M1’s cinematographer and M0’s child?
34. Was a costume designer’s husband’s daughter’s husband’s race M3?
35. Was M2 M1’s female producer’s sister’s sibling and mother?
36. Who was a religion’s costume designer’s English Chinese Jewish son’s brother and child?
37. Was M3 the child of the Swedish speaking animation film’s sequel’s producer, art director, and editor?
38. Who was the Dutch speaking action movie’s star’s child, spouse, father, and sibling?
39. Who was the parent of a film director’s white female Buddhist Jewish French Anglican spouse?
40. What was produced by a character’s parent’s founder?
41. Who was a Muslim mother of the Muslim woman?
42. Who was a screenwriter’s spouse, brother, child, and parent?
43. Was M1 the costume designer’s Muslim wife?
44. What did a Indian Mexican TV producer whose employer wrote M3 create?
45. Did the science fiction movie’s Hindu English white director write M0 and M1?
46. Did a brother of a person distribute M0 and M1?
47. Who was a Canadian male TV program creator whose child was acquired by and acquired the TV writer’s child?
48. Was a TV programme’s executive producer’s mother, friend, and offspring M1?
49. What did a TV director’s religion’s TV program star?
50. Who was M3’s Anglican Catholic African American husband?

Manual checking also indicated that all questions are associated with the semantically correct SPARQL queries, but similarly to U-CFQ, several examples sound unnatural. These examples can again be divided in two groups:
New language feature | Example question
--- | ---
Verb + preposition (with object) | Who played M3 in M2
Verb + preposition (without object) | In which TV program did M1 play
AND of prepositional phrases | Who played in M1 and in M2
AND of determined noun phrases | Did M1’s father marry M2 and a TV program creator
AND of possessives | Which Mexican German adherent of M5 and sister of M0 created M3
AND of verb phrases (with object) | Did M0 direct M2 and marry M1
Additional passive sentence types | Which company was M1 employed by
TV programs (and related properties) | Was a creator of M1’s TV program executive produce
Film genre | Was a crime fiction film’s Indian writer
Religion | Was a religion’s Mexican adherent found
Ethnicity | Was M1’s Anglican art director’s ethnicity
Movie language | Did M2 distribute a French speaking film
Additional family relations | Was the daughter of the brother of M0 M2
Additional film-related verbs | Did a scriptwriter’s mother art direct M1
Generic notion of “contributing to” a film | Did M2’s husband contribute to M0
Woman/Man | Did M1’s husband play a woman
Celebrity | Was the art director of M1 a celebrity’s father
Friend | Who was a friend of a TV producer’s child
'Script(-)writer’ (meaning ‘Screenwriter’) | Was a script-writer M1’s Canadian employee
‘Offspring’ (meaning ‘Child’ of a person) | Who was M3’s offspring’s African-American son
‘Subsidiary’ (meaning ‘Child’ of a company) | What was M0’s distributor’s parent’s subsidiary
‘Movie’ (meaning ‘Film’) | Was M0 a German speaking family movie
‘Which’ (synonym for ‘That’) | Was M0 a film director which M2 married
Definite article | Did the spouse of a film editor create M0

| Hyperparameter | Value |
| --- | --- |
| train steps | 500,000 |
| batch size | 4,096 |
| hidden size | 128 |
| num hidden layers | 2 |
| num heads | 16 |
| learning rate schedule | 0.08*linear_warmup*rsqrt_decay |
| learning rate warmup steps | 4,000 |

Table 6: Examples of questions enabled via newly added grammar rules. The first section represent newly supported grammatical constructs. The middle section represent newly supported Freebase types and properties. The last section represent addition of new surface forms that are treated as synonyms for an existing one.

1. Questions that require an entity to fill multiple roles of another entity which for some pairs of roles is impossible in reality (e.g. someone’s parent and child cannot be the same person). The 18 examples in this group are 4, 5, 6, 8, 12, 16, 17, 20, 24, 26, 27, 28, 29, 35, 38, 42, 47, and 48.

2. Questions, where an entity is used with a property that does not match the type of that entity (e.g. “religion’s costume designer”). There are 8 such questions in our sample: 23, 28, 36, 40, 44, 46, 47, and 49.

The presence of these questions in the X-CFQ dataset doesn’t materially affect any of our findings either, because every such question can still be unambiguously represented as a SPARQL query.

E Hyperparameters and Hardware

Unless explicitly stated otherwise, for all experiments in this paper, we use a Transformer architecture with hyperparameters identical to those used in Keysers et al. (2020), with the exception of the training steps, which we increase to 500,000, instead of the original 35,000.

We measured the impact of changing this metric and found 500,000 to be the best trade-off between computational cost and usefulness, given our choice of model size for the experiments (see Figure 8).

The hyperparameters used are summarized in Table 7.

The experiments are run on a variety of hardware depending on the resource requirements of particular experiment stages. All stages that could benefit from ML acceleration (namely, training and evaluation) are run using NVidia P100 GPUs. The most memory-intensive parts of the experiments (namely, preprocessing of splits) are run on a cluster of CascadeLake 2200MHz servers with 767Gb of memory.

F Domain Size Estimate

We use the term domain in a sense compatible with that used, for example, by Gururangan et al. (2020), who defines this as “a distribution over language characterizing a
played are defined as follows: the binary distinction of whether a given sentence is “in domain” or “out of domain”, rather than the precise probability of the sentence’s occurrence. From this perspective, for the purposes of this paper, we can consider domain to refer more simply to the set of all possible sentences generated by a given set of grammar rules – also referred to in grammar research as the language generated by the given grammar (Chomsky 1956).

Table 8 summarizes the estimated size of each of the domains in the *-CFQ rule set lattice relative to relevant baseline domains, along with several other metrics that can be considered indicators of domain proximity. The metrics displayed are defined as follows:

- **Relative size** is calculated based on the ratio of examples in the dataset associated with the given domain that are also in the baseline domain. The underlying assumption is that the datasets have a roughly even distribution of examples in the domain that they cover. The step in the generation pipeline that subsamples the original, larger pools to maximize rule divergence helps to achieve this.

- **Vocabulary overlap** indicates the fraction of tokens used in the given rule set that are also in the rule set of the baseline domain. This is comparable to the “vocabulary overlap” used by Gururangan et al. (2020) as a rough indicator of domain proximity. While Gururangan et al. (2020) calculate this based on the top 10k most frequent words from each domain, in our case we consider all tokens from the domain, given the relatively small number of tokens used.

- **Rule overlap** indicates the fraction of rules in the given rule set that are also in the rule set of the baseline domain.

- **Rule occurrence overlap** indicates the fraction of occurrences of rules across all examples in the dataset associated with the given domain that correspond to rules that are in the rule set of the baseline domain.

We use B-CFQ as baseline as all of the rule sets are supersets of it. We also compare each half-*-CFQ dataset to the corresponding *-CFQ dataset. As L-CFQ and X-CFQ are also supersets of O-CFQ, we additionally include the relative sizes of these datasets compared to O-CFQ.

### Table 8: Metrics estimating the relative size and proximity of the domains of the *-CFQ rule sets.

| Domain (rule set) | Baseline | Relative size | Vocabulary overlap | Rule overlap | Rule occurrence overlap |
|-------------------|----------|---------------|--------------------|--------------|-------------------------|
| N-CFQ             | B-CFQ    | 1.28x         | 98.88%             | 90.53%       | 98.02%                  |
| half-N-CFQ        | B-CFQ    | 1.07x         | 98.88%             | 92.15%       | 98.70%                  |
| N-CFQ             | half-N-CFQ | 1.21x       | 100.00%            | 98.24%       | 99.31%                  |
| L-CFQ             | B-CFQ    | 26.14x        | 54.32%             | 55.84%       | 79.97%                  |
| half-L-CFQ        | B-CFQ    | 9.24x         | 66.67%             | 68.84%       | 83.28%                  |
| L-CFQ             | half-L-CFQ | 6.08x       | 81.37%             | 80.89%       | 94.02%                  |
| X-CFQ             | B-CFQ    | 32.40x        | 52.73%             | 51.44%       | 77.41%                  |
| half-X-CFQ        | B-CFQ    | 10.14x        | 66.17%             | 65.03%       | 81.73%                  |
| X-CFQ             | half-X-CFQ | 7.57x       | 80.12%             | 79.10%       | 92.97%                  |
| L-CFQ             | O-CFQ    | 21.50x        | 50.17%             | 60.03%       | 83.07%                  |
| X-CFQ             | O-CFQ    | 26.07x        | 55.15%             | 55.32%       | 81.20%                  |

Figure 8: Error rate vs number of training steps on a U-CFQ random split. Training for more steps reduces error rate consistently, particularly at large training sizes, but with diminishing returns after 500,000 steps.

**G Effect of Compound Divergence**

Table 2 shows mean error rates observed for each train set size for compound divergence splits at various levels of compound divergence from our experiments performed on U-CFQ. This is the same information as in Figure 2, but in tabular form. Figure 9 also shows the same information as in Figure 2, but plotting accuracy instead of the error rate, for easier comparison with the results obtained by Keysers et al. (2020) in smaller scale experiments using CFQ. Overall, our experiments show a similar trend to that seen in Keysers et al. (2020), but in a clearer form due to averaging over
The complete results for experiments summarized in Section 6.1 are presented in Figures 10 and 11. Here the exper-
iments are done with size of target domain data \( n_{in} \) being 10k, 20k, 30k, 50k, 100k, 200k, 300k, and 500k. A curve with \( n_{in} = 0 \) (i.e., no target domain data) is also shown for comparison.

From Figure 10 we can observe that in all cases a nearly identical plateau is reached as the distribution of the training set gets closer and closer to that of the supplementary domain \( V \), regardless of the number of in-domain examples provided. Specifically, the half-L-CFQ error rate stabilizes at roughly 0.03, while for L-CFQ the plateau is at value 0.02. Note that these accuracies could be achieved equivalently by training with just 30k (resp. 50k) training examples from \( B \)-CFQ alone, without the benefit of any supplementary data. Also note that starting from \( n_{in} = 200k \) adding related data does not improve error rate.

Figure 11, which represents data for half-X-CFQ and X-CFQ, demonstrates similar behaviour. On the graphs with smaller values of \( n_{in} \) the error rate stabilizes at roughly 0.04 (for half-X-CFQ) and 0.03 (for X-CFQ).

### J Augmenting with Examples from N-CFQ or half-N-CFQ

Figure 12 shows for completeness the results of experiments in mixing examples from a related domain, where the related domain is one that differs from the target domain only by the addition of non-leaf rules – i.e., either N-CFQ or half-N-CFQ. The results from these experiments are unusual in that error rates when augmenting with half-N-CFQ are even higher than when augmenting with N-CFQ, contrary to the trend observed elsewhere that error rates drop more slowly the more distant the related domain is from the target domain.

We do not consider N-CFQ or half-N-CFQ to be well-suited to this particular experiment setup, however, due to the large overlap between these domains and the target domain \( B \)-CFQ, and have accordingly omitted these results from the discussion in the main body. Specifically, as the N-CFQ domain is only 1.28x the size of that of \( B \)-CFQ (see Appendix F), this means that the space of related domain examples excluding those that are part of the target domain is only 0.28x the size of the target domain. This effect is even more pronounced for half-N-CFQ, whose domain is only 1.07x the size of that of \( B \)-CFQ. This makes the results difficult to interpret, as the large fraction of N-CFQ or half-N-CFQ examples that are filtered out due to overlap with the \( B \)-CFQ domain would magnify any potential side effects on the question distribution that might result from this filtering process, potentially to the point that this factor may dominate any observed changes in the error rate. We suspect this to be the primary reason for the observed higher error rates when augmenting with half-N-CFQ, but would require deeper investigation to confirm.

Figure 13 is similar to Figure 4 but demonstrates the effect of blending with N-CFQ and half-N-CFQ.
Figure 10: Error rate vs train set size, log-log scale, leaf changes (B-CFQ test set, B-CFQ + L-CFQ train set), all initial sizes.
Figure 11: Error rate vs train set size, log-log scale, leaf and non-leaf changes (B-CFQ test set, B-CFQ + X-CFQ train set), all initial sizes.
Figure 12: Error rate vs train set size, log-log scale, **non-leaf** changes (B-CFQ test set, B-CFQ + N-CFQ train set), all initial sizes.
Figure 13: Error rate vs train set size, log-log scale, fixed ratio: 10k b-CFQ examples (a) and 100k b-CFQ examples (b), b-CFQ test set, b-CFQ + (N-CFQ or half-N-CFQ) train set.