How to train your self-supervised NLP model: Investigating pre-training objectives, data, and scale

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Abstract

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A robust language processing machine should be able to encode linguistic and factual knowledge across a wide variety of domains, languages, and even modalities. The paradigm of pre-training self-supervised models on large text corpora has driven much of recent progress towards this goal. In spite of this large scale pre-training, the best performing models have to be further fine-tuned on downstream tasks – often containing hundreds of thousands of examples – to achieve state of the art performance. The aim of this thesis is twofold: (a) to design efficient scalable pre-training methods which capture different kinds of linguistic and world knowledge, and (b) to enable better downstream performance with fewer human-labeled examples.

The first part of the thesis focuses on self-supervised objectives for reasoning about relationships between pairs of words. In NLI, for example, given the premise “golf is prohibitively expensive”, inferring that the hypothesis “golf is a cheap pastime” is a contradiction requires one to know that expensive and cheap are antonyms. We show that with the right kind of self-supervised objectives, such knowledge learned with word pair vectors (pair2vec) directly from text without using curated knowledge bases and ontologies.

The second part of the thesis seeks to build models which encode knowledge beyond word pair relations into model parameters. We present SpanBERT, a scalable pre-training method that is designed to better
represent and predict spans of text. Span-based pre-training objectives seek to efficiently encode a wider variety of knowledge, and improve the state of the art for a range of NLP tasks.

The third part of the thesis focuses integrating dynamically retrieved textual knowledge. Specifically, even large scale representations are not able to preserve all factual knowledge they have “read” during pre-training due to the long tail of entity and event-specific information. We show that training models to integrate background knowledge during pre-training is especially useful for downstream tasks which require reasoning over this long tail.

The last part of the thesis targets a major weakness of self-supervised models – while such models requires no explicit human supervision during pre-training, they still need lots of human-labeled downstream task data. We seek to remedy this by mining input-output pairs (and thus obtaining direct task-level supervision) from corpora using supervision from very few labeled examples.

Overall, this thesis presents a range of ideas required for effective pre-training and fine-tuning – (a) self-supervised objectives, (b) model scale, and (c) new types of data. As we will show in the following chapters, self-supervised objectives could have a large influence on the form of knowledge that is acquired during pre-training. Moreover, efficient objectives directly enable model scale both in terms of data and parameters. Finally, the training data and the kind of supervision derived from it itself dictates how well a model can learn different kinds of downstream tasks.
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I decided I was going to write this section first. It seemed like the right thing to do before I take up the task of summarizing my six-plus years of work at the University of Washington.

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DEDICATION

To my family
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Chapter 1

Introduction

1.1 Motivation

Reasoning about relationships between words, entities, sentences, and larger textual units is critical to understanding natural language. For example, consider this headline from the Sportstar magazine\footnote{https://sportstar.thehindu.com/cricket/icc-cricket-world-cup/news/world-cup-2019-england-vs-australia-arjun-tendulkar-nets-bowling-practice-lords-sachin-tendulkar/article28126936.ece} “With ball, Tendulkar junior helps England ahead of Australia clash” in Figure 1.1. Cricket fans, the intended readers of the article, might be able to assume that the phrase *Tendulkar junior* refers to *Arjun Tendulkar*, the son of famous cricketer Sachin Tendulkar. Likewise, the phrase *with ball* has a domain-specific meaning, and refers to bowling in cricket\footnote{https://en.wikipedia.org/wiki/Bowling_(cricket)} and that *clash* refers to an upcoming match between the English and Australian national cricket teams. In other words, understanding this piece of text requires a range of linguistic and factual knowledge. A robust language processing machine should therefore be able to encode such knowledge across a wide variety of domains, languages, and even modalities.

Much of research in natural language processing (NLP) seeks to build and evaluate models on their ability to encode, represent, and use this knowledge. For example, the task of coreference resolution could test whether the model is able to correctly predict that the phrases *Tendulkar junior* and *Arjun Tendulkar* are coreferent. Other such tasks could test for parts of speech, meaning of words or relation between them, syntactic parsing etc.

A complementary view of language processing would be to not just to test for factual and linguistic
With ball, Tendulkar junior helps England ahead of Australia clash

Aiming to live up to his illustrious surname, Arjun Tendulkar ran in fast and bowled at the England batsmen on the eve of their big-ticket clash against arch-rival Australia.

Tendulkar helped England ahead of its World Cup clash against Australia – not the man who owns almost all the batting records but the boy who aspires to shine with the ball.

Aiming to live up to his illustrious surname, Arjun Tendulkar ran in fast and bowled at the England batsmen on the eve of their big-ticket clash against arch-rival Australia.

The son of batting legend Sachin Tendulkar Monday marked his run-up at the Lord's nets during England's practice session, drawing, on expected lines, the attention of those present at the 'Mecca of Cricket'.

Figure 1.1: An article from Sportstar.

knowledge but test if machines can perform applied language tasks – for example, being able to ask and answer questions about a range of topics or being able to summarize articles. While such tasks could and often do require the kind of linguistic and factual knowledge we talked about, they could also require other cognitive skills closely aligned to core NLP. For example, news summarization might require the reader to pick out and articulate the most important parts of an article often in ways that are interesting to readers. In other words, apart from linguistic and factual background knowledge, performing these applied tasks could require task-specific knowledge.

1.1.1 Self-supervised Models: Pre-training and Fine-tuning

Self-supervised models use the natural supervision provided by unlabeled text for better initialization of parameters. Much of recent progress on both core and applied fronts has been enabled with the creation of large self-supervised models and downstream task datasets. The typical training pipeline works as follows:
self-supervised models are first “pre-trained” i.e. trained on unlabeled – and often downstream task-agnostic – text and then “fine-tuned” i.e. trained further on downstream task data.

Most pre-training objectives are denoising autoencoders that are trained to reconstruct text where a random subset of the words has been noised or hidden. For example, training left-to-right language models involve predicting a token from a given prefix and each time step. Likewise, masked language modeling involves predicting a small subset of tokens (replaced with special masked tokens) from the rest of the context. Recent work has shown that pre-trained models are able to encode a considerable amount of factual and linguistic knowledge ranging from word and entity relations to syntax Rogers et al. [2020].

What helps self-supervised models capture at least a part of world knowledge that is need for robust language processing? State of the art models contain millions of parameters and were pre-trained over large corpora using several thousand GPUs. For example, RoBERTa Liu et al. [2019c], with 350 million parameters was trained on 160 GB of text using 1024 GPUs. The scale of pre-trained models has continued to increase along with a pronounced increase performance over a wide variety of tasks.

In spite of this large scale pre-training, the best performing models have to be further fine-tuned on downstream tasks to achieve state of the art performance. For example, SQuAD Rajpurkar et al. [2016], one of the most popular NLP datasets for reading comprehension contains around 100,000 questions. Large scale training is effective but expensive. Pre-training itself is compute intensive while creating large high-quality datasets for downstream tasks requires considerable expertise and quality control. Both steps in turn translate into monetary cost.

The aim of this thesis is to provide training paradigms for efficient self-supervised models, and to minimize the cost of training these models. Specifically, we have the following goals:

1. Designing efficient pre-training methods to capture linguistic and world knowledge
2. Enabling better downstream performance with fewer human-labeled examples

1.2 Background

We categorize related work into three main groups: (i) general purpose language representations which encode world knowledge, (ii) integrating additional background knowledge for specific downstream tasks,
and (iii) data augmentation.

### 1.2.1 General Purpose Language Representations

Training general purpose language representations has a long history stretching as far back as matrix factorization methods like latent semantic analysis (LSA) [Deerwester et al. 1990]. Subsequent work used single-word embeddings such as Glove [Pennington et al. 2014] and Word2vec [Mikolov et al. 2013a], trained following the Distributional Hypothesis [Harris 1954]. Pre-trained contextualized word representations that can be trained from unlabeled text [Dai and Le 2015; Melamud et al. 2016; Peters et al. 2018] have had immense impact on NLP lately, particularly as methods for initializing a large model before fine-tuning it for a specific task [Howard and Ruder 2018; Radford et al. 2018; Devlin et al. 2018]. Beyond differences in model hyperparameters and corpora, these methods mainly differ in their pre-training tasks and loss functions, with a considerable amount of contemporary literature proposing augmentations of BERT’s masked language modeling (MLM) objective. We build upon this work in two ways: (1) in Chapter 3, we extend MLM-based methods for pre-training span representations consistently outperforming BERT, with the largest gains on span selection tasks such as question answering and coreference resolution, and (2) in Chapter 3, we re-use BERT-style representations for jointly encoding the input with dynamically-retrieved textual background knowledge.

### 1.2.2 Task-specific Background Knowledge

Earlier work [Ratinov and Roth 2009; Nakashole and Mitchell 2015] combined features over the given task data with hand-engineered features over knowledge repositories. Other forms of external knowledge include relational knowledge between word or entity pairs, typically integrated via embeddings from structured knowledge graphs (KGs) [Yang and Mitchell 2017; Bauer et al. 2018; Mihaylov and Frank 2018; Wang and Jiang 2019] or via word pair embeddings trained from text [Joshi et al. 2019a]. Weissenborn et al. [2017] used a specialized architecture to integrate background knowledge from ConceptNet and Wikipedia entity descriptions. For open-domain QA, recent works [Sun et al. 2019a; Xiong et al. 2019] jointly reasoned over text and KGs, via specialized graph-based architectures for defining the flow of information between them.
Most relevant to ours is work building upon these powerful pretrained representations, and further integrating external knowledge. Recent work focuses on refining pretrained contextualized representations using entity or triple embeddings from structured KGs [Peters et al., 2019; Yang et al., 2019a; Zhang et al., 2019b]. The KG embeddings are trained separately (often to predict links in the KG), and knowledge from KG is fused with deep Transformer representations via special-purpose architectures. Some of these prior works also pre-train the knowledge fusion layers from unlabeled text through self-supervised objectives [Zhang et al., 2019b; Peters et al., 2019]. Instead of separately encoding structured KBs, and then attending to their single-vector embeddings, we explore directly using wider-coverage textual encyclopedic background knowledge (Chapter 4). This enables direct application of a pretrained deep Transformer (RoBERTa) for jointly contextualizing input text and background knowledge. We showed background knowledge integration can be further improved by additional knowledge-augmented self-supervised pretraining.

In concurrent work, [Liu et al., 2019a] augment text with relevant triples from a structured KB. They process triples as word sequences using BERT with a special-purpose attention masking strategy. This allows the model to partially re-use BERT for encoding and integrating the structured knowledge. Our work uses wider-coverage textual sources instead and shows the power of additional knowledge-tailored self-supervised pretraining.

1.2.3 Data Augmentation

Data augmentation is a popular technique with a large body of work [Wang and Yang, 2015; Jia and Liang, 2016] among others. Recent work has explored model generated data augmentation for a range of tasks including text classification [Anaby-Tavor et al., 2020; Schick and Schütze, 2021a], question answering [Alberti et al., 2019], common-sense reasoning [Yang et al., 2020], and machine translation [Sennrich et al., 2016]. A common problem with model-generated data augmentation is the quality of the synthetic data. Attempts to remedy this have focused on variations of consistency [Xie et al., 2019] for a given task—such as round-trip consistency of question generation and answer prediction [Alberti et al., 2019; Puri et al., 2020] for QA or between source and targets in summarization [Fabbri et al., 2021]. Lee et al. (2021) focus on generating synthetic data for underrepresented or few-shot slices. Task augmentation [Vu et al., 2021] generates
data in the target domain by using a model trained on the auxiliary task of natural language inference. In contrast, in Chapter 5, we focus on a general framework for mining naturally occurring data for multiple tasks using supervision from a small labeled seed set.

1.3 Outline

This thesis presents solutions which can be divided into three broad paradigms – (a) self-supervised objectives, (b) model scale, and (c) new types of data. As we will show in the following chapters, self-supervised objectives could have a large influence on the form of knowledge that is acquired during pre-training. Moreover, efficient objectives directly enable model scale both in terms of data and parameters. Finally, the training data and the kind of supervision derived from it itself dictates how well a model can learn different kinds of downstream tasks, and could reduce the amount of human-labeling required for human performance.

1.3.1 Efficient pre-training methods to capture linguistic and world knowledge

One justification, particularly for large models, is that the kind of linguistic and factual knowledge we seek to encode is spread over millions of documents making large scale training arguably inevitable. While alternate paradigms (e.g. non-parametric methods) exist, large scale pre-training has driven much of empirical progress over the last few years. We argue that training paradigms for self-supervised models should aim to encode diverse kinds of knowledge across corpora of of varying domains. We seek to answer the following questions:

1. How can be design pre-training objectives to capture the kinds of knowledge we care about?

2. How can we scale up models in terms of data and parameters to maximize the coverage of training corpora?

Chapter 2 focuses on self-supervised objectives for relational knowledge i.e. reasoning about relationships between pairs of words. Such knowledge is crucial for several NLP tasks. In NLI, for example, given the premise “golf is prohibitively expensive”, inferring that the hypothesis “golf is a cheap pastime” is a contradiction requires one to know that expensive and cheap are antonyms. Our word-pair representations are learned by modeling the three-way co-occurrence between words \((x, y)\) and the context \(c\) that ties them
together. For example, it is easy to infer that the words “cheap” and “expensive” are antonyms based on co-occurring contexts such as “either $x$ or $y$” We show that they can be learned with word pair vectors (pair2vec), which significantly improve performance when added to existing cross-sentence attention mechanisms.

Chapter 3 focuses scalable efficient objectives which encode a wider variety of linguistic and world knowledge into model parameters. We present SpanBERT, a pre-training method that is designed to better represent and predict spans of text. Unlike token-based MLM, span based objectives focus on predicting longer spans. The intuition is target more efficient pre-training by preventing the model from making predictions based on immediate short-term context. We show that span-based pre-training improves the state of the art for a range of NLP tasks including those which do not require explicit span based reasoning.

Chapter 4 focuses integrating dynamically retrieved textual knowledge. Specifically, even large scale representations are not able to preserve all factual knowledge they have “read” during pre-training due to the long tail of entity and event-specific information. Training models to integrate background knowledge during pre-training is especially useful for downstream tasks which require reasoning over this long tail. Taken together, Chapters 3 and 4 focus on maximizing the coverage of knowledge in form and content.

1.3.2 Enabling better downstream performance with fewer human-labeled examples

As we discussed in Section 1.1, large scale pre-training, the best performing models have to be further fine-tuned on downstream tasks to achieve state of the art performance.

Chapter 5 focuses on reducing the amount of downstream data by mining input-output pairs (and thus obtaining direct task-level supervision) from corpora using supervision from very few labeled examples. We mine naturally-occurring examples from a large corpus using supervision from a small seed set of only 100 examples. Our method provides a way to collect more data using very few examples. Yet, unlike model generated data augmentation, we mine high-quality human-authored data which is less susceptible to the limitations synthetic data.
Chapter 2

pair2vec: Compositional Word-Pair Embeddings for Cross-Sentence Inference

This chapter discusses work originally published in [Joshi et al. 2019a].

Reasoning about relationships between pairs of words is crucial for cross sentence inference problems such as question answering (QA) and natural language inference (NLI). In NLI, for example, given the premise “golf is prohibitively expensive”, inferring that the hypothesis “golf is a cheap pastime” is a contradiction requires one to know that expensive and cheap are antonyms. Recent work [Glockner et al. 2018] has shown that current models, which rely heavily on unsupervised single-word embeddings, struggle to learn such relationships. In this chapter, we show that they can be learned with word pair vectors (pair2vec), which are trained unsupervised, and which significantly improve performance when added to existing cross-sentence attention mechanisms.

Unlike single-word representations, which typically model the co-occurrence of a target word $x$ with its context $c$, our word-pair representations are learned by modeling the three-way co-occurrence between words $(x, y)$ and the context $c$ that ties them together, as seen in Table 2.1. While similar training signals have been used to learn models for ontology construction [Hearst 1992; Snow et al. 2005; Turney 2005; Shwartz et al. 2016] and knowledge base completion [Riedel et al. 2013], this chapter shows, for the first time, that large scale learning of pairwise embeddings can be used to directly improve the performance of...

[https://github.com/mandarjoshi90/pair2vec]
neural cross-sentence inference models.

More specifically, we train a feedforward network $R(x, y)$ that learns representations for the individual words $x$ and $y$, as well as how to compose them into a single vector. Training is done by maximizing a generalized notion of the pointwise mutual information (PMI) among $x$, $y$, and their context $c$ using a variant of negative sampling [Mikolov et al. [2013a]]. Making $R(x, y)$ a compositional function on individual words alleviates the sparsity that necessarily comes with embedding pairs of words, even at a very large scale.

We show that our embeddings can be added to existing cross-sentence inference models, such as BiDAF++ [Seo et al. [2017]; Clark and Gardner [2018] for QA and ESIM [Chen et al. [2017]] for NLI. Instead of changing the word embeddings that are fed into the encoder, we add the pretrained pair representations to higher layers in the network where cross sentence attention mechanisms are used. This allows the model to use the background knowledge that the pair embeddings implicitly encode to reason about the likely relationships between the pairs of words it aligns.

Experiments show that simply adding our word-pair embeddings to existing high-performing models, which already use ELMo [Peters et al. [2018]], results in sizable gains. We show 2.72 F1 points over the BiDAF++ model [Clark and Gardner [2018] on SQuAD 2.0 [Rajpurkar et al. [2018]], as well as a 1.3 point gain over ESIM [Chen et al. [2017]] on MultiNLI [Williams et al. [2018a]]. Additionally, our approach generalizes well to adversarial examples, with a 6-7% F1 increase on adversarial SQuAD [Jia and Liang [2017] and a 8.8% gain on the Glockner et al. [2018] NLI benchmark. An analysis of pair2vec on word analogies

<table>
<thead>
<tr>
<th>X</th>
<th>Y</th>
<th>Contexts</th>
</tr>
</thead>
<tbody>
<tr>
<td>hot</td>
<td>cold</td>
<td>with X and Y baths</td>
</tr>
<tr>
<td></td>
<td></td>
<td>too X or too Y</td>
</tr>
<tr>
<td></td>
<td></td>
<td>neither X nor Y</td>
</tr>
<tr>
<td>Portland</td>
<td>Oregon</td>
<td>in X, Y</td>
</tr>
<tr>
<td></td>
<td></td>
<td>the X metropolitan area in Y</td>
</tr>
<tr>
<td></td>
<td></td>
<td>X International Airport in Y</td>
</tr>
<tr>
<td>crop</td>
<td>wheat</td>
<td>food X are maize, Y, etc</td>
</tr>
<tr>
<td></td>
<td></td>
<td>dry X, such as Y,</td>
</tr>
<tr>
<td></td>
<td></td>
<td>more X circles appeared in Y fields</td>
</tr>
<tr>
<td>Android</td>
<td>Google</td>
<td>X OS comes with Y play</td>
</tr>
<tr>
<td></td>
<td></td>
<td>the X team at Y</td>
</tr>
<tr>
<td></td>
<td></td>
<td>X is developed by Y</td>
</tr>
</tbody>
</table>

Table 2.1: Example word pairs with contexts.
suggests that it complements the information in single-word representations, especially for encyclopedic and lexicographic relations.

2.1 Self-supervised Pretraining

Extending the distributional hypothesis to word pairs, we posit that similar word pairs tend to occur in similar contexts, and that the contexts provide strong clues about the likely relationships that hold between the words (see Table 2.1). We assume a dataset of \((x, y, c)\) triplets, where each instance depicts a word pair \((x, y)\) and the context \(c\) in which they appeared. We learn two compositional representation functions, \(R(x, y)\) and \(C(c)\), to encode the pair and the context, respectively, as \(d\)-dimensional vectors (Section 2.1.1). The functions are trained using a variant of negative sampling, which tries to embed word pairs \((x, y)\) close to the contexts \(c\) with which they appeared (Section 2.1.2).

2.1.1 Representation

Our word-pair and context representations are both fixed-length vectors, composed from individual words. The word-pair representation function \(R(x, y)\) first embeds and normalizes the individual words with a shared lookup matrix \(E_a\):

\[
x = \frac{E_a(x)}{\|E_a(x)\|} \quad y = \frac{E_a(y)}{\|E_a(y)\|}
\]

These vectors, along with their element-wise product, are fed into a four-layer perceptron:

\[
R(x, y) = MLP^4(x, y, x \circ y)
\]

The context \(c = c_1...c_n\) is encoded as a \(d\)-dimensional vector using the function \(C(c)\). \(C(c)\) embeds each token \(c_i\) with a lookup matrix \(E_c\), contextualizes it with a single-layer Bi-LSTM, and then aggregates the
entire context with attentive pooling:

\[ c_i = E_c(c_i) \]
\[ h_1...h_n = \text{BiLSTM}(c_1...c_n) \]
\[ w = \text{softmax}_i(kh_i) \]
\[ C(c) = \sum_i w_i Wh_i \]

where \( W \in \mathbb{R}^{d \times d} \) and \( k \in \mathbb{R}^d \). All parameters, including the lookup tables \( E_a \) and \( E_c \), are trained.

Our representation is similar to two recently-proposed frameworks by Washio and Kato [2018a,b], but differs in that: (1) they use dependency paths as context, while we use surface form; (2) they encode the context as either a lookup table or the last state of a unidirectional LSTM. We also use a different objective, which we discuss next.

### 2.1.2 Objective

To optimize our representation functions, we consider two variants of negative sampling [Mikolov et al. 2013a]: bivariate and multivariate. The original bivariate objective models the two-way distribution of context and (monolithic) word pair co-occurrences, while our multivariate extension models the three-way distribution of word-word-context co-occurrences. We further augment the multivariate objective with typed sampling to upsample harder negative examples. We discuss the impact of the bivariate and multivariate objectives (and other components) in Section 2.3.3.

**Bivariate**

\[
J_{2NS} (x, y, c) = \log \sigma \left( R(x, y) \cdot C(c) \right) + \sum_{i=1}^{k_x} \log \sigma \left( -R(x, y) \cdot C(c_i^N) \right)
\]

**Multivariate**

\[
J_{3NS} (x, y, c) = J_{2NS} (x, y, c) + \sum_{i=1}^{k_x} \log \sigma \left( -R(x_i^N, y) \cdot C(c) \right) + \sum_{i=1}^{k_y} \log \sigma \left( -R(x, y_i^N) \cdot C(c) \right)
\]

**Table 2.2**: The bivariate and multivariate negative sampling objectives. The superscript \( N \) marks randomly sampled components, with \( k_x \) being the negative sample size per instance. The equations present per-instance objectives.

**Bivariate Negative Sampling** Our objective aspires to make \( R(x, y) \) and \( C(c) \) similar (have high inner products) for \((x, y, c)\) that were observed together in the data. At the same time, we wish to keep our pair
vectors dis-similar from random context vectors. In a straightforward application of the original (bivariate) negative sampling objective, we could generate a negative example from each observed \((x, y, c)\) instance by replacing the original context \(c\) with a randomly-sampled context \(c^N\) (Table 2.2, \(J_{2NS}\)).

Assuming that the negative contexts are sampled from the empirical distribution \(P(\cdot, \cdot, c)\) (with \(P(x, y, c)\) being the portion of \((x, y, c)\) instances in the dataset), we can follow Levy and Goldberg [2014] to show that this objective converges into the pointwise mutual information (PMI) between the word pair and the context.

\[
R(x, y) \cdot C(c) = \log \frac{P(x, y, c)}{k_c P(x, \cdot, \cdot) P(\cdot, \cdot, c)}
\]

This objective mainly captures co-occurrences of monolithic pairs and contexts, and is limited by the fact that the training data, by construction, only contains pairs occurring within a sentence. For better generalization to cross-sentence tasks, where the pair distribution differs from that of the training data, we need a multivariate objective that captures the full three-way \((x, y, c)\) interaction.

**Multivariate Negative Sampling** We introduce negative sampling of target words, \(x\) and \(y\), in addition to negative sampling of contexts \(c\) (Table 2.2, \(J_{3NS}\)). Our new objective also converges to a novel multivariate generalization of PMI, different from previous PMI extensions that were inspired by information theory \cite{Van_de_Cruys_2011} and heuristics \cite{Jameel_2018}.

Following Levy and Goldberg (2014), we can show that when replacing target words in addition to contexts, our objective will converge\(^3\) to the optimal value in Equation 2.1:

\[
R(x, y) \cdot C(c) = \log \frac{P(x, y, c)}{Z_{x,y,c}}
\]

where \(Z_{x,y,c}\), the denominator, is:

\[
Z_{x,y,c} = k_c P(\cdot, \cdot, c) P(x, y, \cdot) + k_x P(x, \cdot, \cdot) P(\cdot, y, c) + k_y P(\cdot, y, \cdot) P(x, \cdot, c)
\]

This optimal value deviates from previous generalizations of PMI by having a linear mixture of marginal

\(^2\)See supplementary material for their exact formulations.

\(^3\)A full proof is provided in the supplementary material.
Figure 2.1: A typical architecture of a cross-sentence inference model (left), and how pair2vec is added to it (right). Given two sequences, $a$ and $b$, existing models create $b$-aware representations of words in $a$. For any word $a_i$, this typically involves the BiLSTM representation of word $a_i$ ($\tilde{a}_i$), and an attention-weighted sum over $b$’s BiLSTM states with $a_i$ as the query ($\tilde{b}_i$). To these, we add the word-pair representation of $a_i$ and each word in $b$, weighted by attention ($r_i$). Thicker attention arrows indicate stronger word pair alignments (e.g. cheap, expensive).

probability products in its denominator. By introducing terms such as $P(x, \cdot, c)$ and $P(\cdot, y, c)$, the objective penalizes spurious correlations between words and contexts that disregard the other target word. For example, it would assign the pattern “$X$ is a $Y$” a high score with (banana, fruit), but a lower score with (cat, fruit).

Typed Sampling In multivariate negative sampling, we typically replace $x$ and $y$ by sampling from their unigram distributions. In addition to this, we also sample uniformly from the top 100 words according to cosine similarity using distributional word vectors. This is done to encourage the model to learn relations between specific instances as opposed to more general types. For example, using California as a negative sample for Oregon helps the model to learn that the pattern “$X$ is located in $Y$” fits the pair (Portland, Oregon), but not the pair (Portland, California). Similar adversarial constraints were used in knowledge base completion Toutanova et al. (2015) and word embeddings Li et al. (2017).
2.2 Integrating pair2vec into Models

We first present a general outline for incorporating pair2vec into attention-based architectures, and then discuss changes made to BiDAF++ and ESIM. The key idea is to inject our pairwise representations into the attention layer by reusing the cross-sentence attention weights. In addition to attentive pooling over single word representations, we also pool over cross-sentence word pair embeddings (Figure 2.1).

2.2.1 General Approach

Pair Representation  We assume that we are given two sequences \( a = a_1...a_n \) and \( b = b_1...b_m \). We represent the word-pair embeddings between \( a \) and \( b \) using the pretrained pair2vec model as:

\[
\begin{align*}
\mathbf{r}_{i,j} &= \frac{R(a_i, b_j)}{\|R(a_i, b_j)\|} ; \frac{R(b_j, a_i)}{\|R(b_j, a_i)\|} \quad (2.3)
\end{align*}
\]

We include embeddings in both directions, \( R(a_i, b_j) \) and \( R(b_j, a_i) \), because the many relations can be expressed in both directions; e.g., hypernymy can be expressed via “\( X \) is a type of \( Y \)” as well as “\( Y \) such as \( X \)”. We take the \( L_2 \) normalization of each direction’s pair embedding because the heavy-tailed distribution of word pairs results in significant variance of their norms.

Base Model  Let \( a_1...a_n \) and \( b_1...b_m \) be the vector representations of sequences \( a \) and \( b \), as produced by the input encoder (e.g. ELMo embeddings contextualized with model-specific BiLSTMs). Furthermore, we assume that the base model computes soft word alignments between \( a \) and \( b \) via co-attention (2.4, 2.5), which are then used to compute \( b \)-aware representations of \( a \):

\[
\begin{align*}
s_{i,j} &= f_{\text{att}}(a_i, b_j) \\
\alpha &= \text{softmax}_j(s_{i,j}) \quad (2.5) \\
\bar{b}_i &= \sum_{j=0}^m \alpha_{i,j} b_j \quad (2.6) \\
a_{i}^{\text{inf}} &= [a_i; \bar{b}_i] \quad (2.7)
\end{align*}
\]

\(^4\text{Applying typed sampling also changes the value to which our objective will converge, and will replace the unigram probabilities in Equation (2.2) to reflect the type-based distribution.}\)
The symmetric term $b_{j}^{inf}$ is defined analogously. We refer to $a_{i}^{inf}$ and $b_{j}^{inf}$ as the inputs to the inference layer, since this layer computes some function over aligned word pairs, typically via a feedforward network and LSTMs. The inference layer is followed by aggregation and output layers.

**Injecting pair2vec** We conjecture that the inference layer effectively learns word-pair relationships from training data, and it should, therefore, help to augment its input with pair2vec. We augment $a_{i}^{inf}$ (2.7) with the pair vectors $r_{i,j}$ (2.3) by concatenating a weighted average of the pair vectors $r_{i,j}$ involving $a_{i}$, where the weights are the same $\alpha_{i,j}$ computed via attention in (2.5):

$$r_{i} = \sum_{j} \alpha_{i,j} r_{i,j}$$

$$a_{i}^{inf} = [a_{i}; b_{i}; r_{i}]$$

The symmetric term $b_{j}^{inf}$ is defined analogously.

### 2.2.2 Question Answering

We augment the inference layer in the BiDAF++ model with pair2vec. BiDAF++ is an improved version of the BiDAFNoAnswer Seo et al. [2017]; Levy et al. [2017] which includes self-attention and ELMo embeddings from Peters et al. [2018]. We found this variant to be stronger than the baselines presented in Rajpurkar et al. [2018] by over 2.5 F1. We use BiDAF++ as a baseline since its architecture is typical for QA systems, and, until recently, was state-of-the-art on SQuAD 2.0 and other benchmarks.

**BiDAF++** Let $a$ and $b$ be the outputs of the passage and question encoders respectively (in place of the standard $p$ and $q$ notations). The inference layer’s inputs $a_{i}^{inf}$ are defined similarly to the generic model’s in (2.7), but also contain an aggregation of the elements in $a$, with better-aligned elements receiving larger
weights:

\[
\mu = \text{softmax}_i(\max_j s_{i,j}) \tag{2.10}
\]

\[
\hat{a}_i = \sum_i \mu_i a_i \tag{2.11}
\]

\[
a^{inf}_i = [a_i; \overline{b}_i; a_i \circ \overline{b}_i; \hat{a}] \tag{2.12}
\]

In the later layers, \(a^{inf}\) is recontextualized using a BiGRU and self attention. Finally a prediction layer predicts the start and end tokens.

**BiDAF++ with pair2vec** To add our pair vectors, we simply concatenate \(r_i\) to \(a^{inf}\):

\[
a^{inf}_i = [a_i; \overline{b}_i; a_i \circ \overline{b}_i; \hat{a}; r_i] \tag{2.13}
\]

### 2.2.3 Natural Language Inference

For NLI, we augment the ESIM model [Chen et al. 2017], which was previously state-of-the-art on both SNLI [Bowman et al. 2015] and MultiNLI [Williams et al. 2018a] benchmarks.

**ESIM** Let \(a\) and \(b\) be the outputs of the premise and hypothesis encoders respectively (in place of the standard \(p\) and \(h\) notations). The inference layer’s inputs \(a^{inf}_i\) (and \(b^{inf}_j\)) are defined similarly to the generic model’s in (2.7):

\[
a^{inf}_i = [a_i; \overline{b}_i; a_i \circ \overline{b}_i; a_i - \overline{b}_i] \tag{2.14}
\]

In the later layers, \(a^{inf}\) and \(b^{inf}\) are projected, recontextualized, and converted to a fixed-length vector for each sentence using multiple pooling schemes. These vectors are then passed on to an output layer, which predicts the class.
ESIM with \textit{pair2vec} To add our pair vectors, we simply concatenate $r_i$ (2.3) to $a_i^{inf}$ (2.14):

$$a_i^{inf} = [a_i; \overline{b}_i; a_i \odot \overline{b}_i; a_i - \overline{b}_i; r_i]$$

(2.15)

A similar augmentation of ESIM was recently proposed in KIM \cite{Chen2018}. However, their pair vectors are composed of WordNet features, while our pair embeddings are learned directly from text.

### 2.3 Experiments

For experiments on QA (Section 2.3.1) and NLI (Section 2.3.2), we use our full model which includes multivariate and typed negative sampling. We discuss ablations in Section 2.3.3.

**Data** We use the January 2018 dump of English Wikipedia, containing 96M sentences to train \textit{pair2vec}. We restrict the vocabulary to the 100K most frequent words. Preprocessing removes all out-of-vocabulary words in the corpus. We consider each word pair within a window of 5 in the preprocessed corpus, and subsample\footnote{Like in \textit{word2vec}, subsampling reduces the size of the dataset and speeds up training. For this, we define the word pair probability as the product of unigram probabilities.} instances based on pair probability with a threshold of $5 \cdot 10^{-7}$. We define the context as one word each to the left and right, and all the words in between each pair, replacing both target words with placeholders $X$ and $Y$ (see Table 2.1). More details can be found in the supplementary material.

#### 2.3.1 Question Answering

<table>
<thead>
<tr>
<th>Benchmark</th>
<th>BiDAF</th>
<th>+pair2vec</th>
<th>Δ</th>
</tr>
</thead>
<tbody>
<tr>
<td>SQuAD 2.0</td>
<td>EM 65.66</td>
<td>68.02</td>
<td>+2.36</td>
</tr>
<tr>
<td></td>
<td>F1 68.86</td>
<td>71.58</td>
<td>+2.72</td>
</tr>
<tr>
<td>AddSent</td>
<td>EM 37.50</td>
<td>44.20</td>
<td>+6.70</td>
</tr>
<tr>
<td></td>
<td>F1 42.55</td>
<td>49.69</td>
<td>+7.14</td>
</tr>
<tr>
<td>AddOneSent</td>
<td>EM 48.20</td>
<td>53.30</td>
<td>+5.10</td>
</tr>
<tr>
<td></td>
<td>F1 54.02</td>
<td>60.13</td>
<td>+6.11</td>
</tr>
</tbody>
</table>

Table 2.3: Performance on SQuAD 2.0 and adversarial SQuAD (AddSent and AddOneSent) benchmarks, with and without \textit{pair2vec}. All models have ELMo.
Benchmark | ESIM | + pair2vec | ∆
---|---|---|---
Matched  | 79.68 | 81.03 | +1.35
Mismatched | 78.80 | 80.12 | +1.32

**Table 2.4:** Performance on MultiNLI, with and without pair2vec. All models have ELMo.

<table>
<thead>
<tr>
<th>Model</th>
<th>Accuracy</th>
</tr>
</thead>
<tbody>
<tr>
<td>Rule-based Models</td>
<td>85.8</td>
</tr>
<tr>
<td>WordNet Baseline</td>
<td>85.8</td>
</tr>
<tr>
<td>Models with GloVe</td>
<td></td>
</tr>
<tr>
<td>ESIM [Chen et al., 2017]</td>
<td>77.0</td>
</tr>
<tr>
<td>KIM [Chen et al., 2018]</td>
<td>87.7</td>
</tr>
<tr>
<td>ESIM + pair2vec</td>
<td>92.9</td>
</tr>
<tr>
<td>Models with ELMo</td>
<td></td>
</tr>
<tr>
<td>ESIM [Peters et al., 2018]</td>
<td>84.6</td>
</tr>
<tr>
<td>ESIM + pair2vec</td>
<td>93.4</td>
</tr>
</tbody>
</table>

**Table 2.5:** Performance on the adversarial NLI test set of Glockner et al. [2018].

We experiment on the SQuAD 2.0 QA benchmark [Rajpurkar et al., 2018], as well as the adversarial datasets of SQuAD 1.1 [Rajpurkar et al., 2016; Jia and Liang, 2017]. Table 2.3 shows the performance of BiDAF++, with ELMo, before and after adding pair2vec. Experiments on SQuAD 2.0 show that our pair representations improve performance by 2.72 F1. Moreover, adding pair2vec also results in better generalization on the adversarial SQuAD datasets with gains of 7.14 and 6.11 F1.

### 2.3.2 Natural Language Inference

We report the performance of our model on MultiNLI and the adversarial test set from Glockner et al. [2018] in Table 2.5. We outperform the ESIM + ELMo baseline by 1.3% on the matched and mismatched portions of the dataset.

We also record a gain of 8.8% absolute over ESIM on the Glockner et al. [2018] dataset, setting a new state of the art. Following standard practice Glockner et al. [2018], we train all models on a combination of SNLI Bowman et al. [2015] and MultiNLI. Glockner et al. [2018] show that with the exception of KIM Chen et al. [2018], which uses WordNet features, several NLI models fail to generalize to this setting which involves lexical inference. For a fair comparison with KIM on the Glockner test set, we replace ELMo with GLoVE embeddings, and still outperform KIM by almost halving the error rate.
<table>
<thead>
<tr>
<th>Model</th>
<th>EM (Δ)</th>
<th>F1 (Δ)</th>
</tr>
</thead>
<tbody>
<tr>
<td><code>pair2vec (Full Model)</code></td>
<td>69.20</td>
<td>72.68</td>
</tr>
<tr>
<td>Composition: 2 Layers</td>
<td>68.35 (-0.85)</td>
<td>71.65 (-1.03)</td>
</tr>
<tr>
<td>Composition: Multiply</td>
<td>67.10 (-2.20)</td>
<td>70.20 (-2.48)</td>
</tr>
<tr>
<td>Objective: Bivariate NS</td>
<td>68.63 (-0.57)</td>
<td>71.98 (-0.70)</td>
</tr>
<tr>
<td>Unsupervised: Pair Dist</td>
<td>67.07 (-2.13)</td>
<td>70.24 (-2.44)</td>
</tr>
<tr>
<td><code>No pair2vec (BiDAF)</code></td>
<td>66.66 (-2.54)</td>
<td>69.90 (-2.78)</td>
</tr>
</tbody>
</table>

**Table 2.6:** Ablations on the SQuAD 2.0 development set show that argument sampling as well as using a deeper composition function are useful.

### 2.3.3 Ablations

Ablating parts of `pair2vec` shows that all components of the model (Section 2.1) are useful. We ablate each component and report the EM and F1 on the development set of SQuAD 2.0 (Table 2.6). The full model, which uses a 4-layer MLP for \( R(x, y) \) and trains with multivariate negative sampling, achieves the highest F1 of 72.68.

We experiment with two alternative composition functions, a 2-layer MLP (Composition: 2 Layers) and element-wise multiplication (Composition: Multiply), which yield significantly smaller gains over the baseline BiDAF++ model. This demonstrates the need for a deep composition function. Eliminating sampling of target words \((x, y)\) from the objective (Objective: Bivariate NS) results in a drop of 0.7 F1, accounting for about a quarter of the overall gain. This suggests that while the bulk of the signal is mined from the pair-context interactions, there is also valuable information in other interactions as well.

We also test whether specific pre-training of word pair representations is useful by replacing `pair2vec` embeddings with the vector offsets of pre-trained word embeddings (Unsupervised: Pair Dist). We follow the PairDistance method for word analogies [Mikolov et al., 2013b], and represent the pair \((x, y)\) as the L2 normalized difference of single-word vectors: \( (x - y) / \|x - y\| \). We use the same fastText Bojanowski et al. [2017] word vectors with which we initialized `pair2vec` before training. We observe a gain of only 0.34 F1 over the baseline.
Figure 2.2: Accuracy as a function of the interpolation parameter $\alpha$ (see Eq. (2.16)). The $\alpha=0$ configuration relies only on fastText [Bojanowski et al., 2017], while $\alpha=1$ reflects pair2vec.

Table 2.7: The top 10 analogy relations for which interpolating with pair2vec improves performance. $\alpha^*$ is the optimal interpolation parameter for each relation.

<table>
<thead>
<tr>
<th>Relation</th>
<th>3CosAdd</th>
<th>+pair2vec</th>
<th>$\alpha^*$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Country:Capital</td>
<td>1.2</td>
<td>86.1</td>
<td>0.9</td>
</tr>
<tr>
<td>Name:Occupation</td>
<td>1.8</td>
<td>44.6</td>
<td>0.8</td>
</tr>
<tr>
<td>Name:Nationality</td>
<td>0.1</td>
<td>42.0</td>
<td>0.9</td>
</tr>
<tr>
<td>UK City:County</td>
<td>0.7</td>
<td>31.7</td>
<td>1.0</td>
</tr>
<tr>
<td>Country:Language</td>
<td>4.0</td>
<td>28.4</td>
<td>0.8</td>
</tr>
<tr>
<td>Verb 3pSg:Ved</td>
<td>49.1</td>
<td>61.7</td>
<td>0.6</td>
</tr>
<tr>
<td>Verb Ving:Ved</td>
<td>61.1</td>
<td>73.3</td>
<td>0.5</td>
</tr>
<tr>
<td>Verb Inf:Ved</td>
<td>58.5</td>
<td>70.1</td>
<td>0.5</td>
</tr>
<tr>
<td>Noun+less</td>
<td>4.8</td>
<td>16.0</td>
<td>0.2</td>
</tr>
<tr>
<td>Substance Meronym</td>
<td>3.8</td>
<td>14.5</td>
<td>0.6</td>
</tr>
</tbody>
</table>

2.4 Analysis

In Section 2.3 we showed that pair2vec adds information complementary to single-word representations like ELMo. Here, we ask what this extra information is, and try to characterize which word relations are better captured by pair2vec. To that end, we evaluate performance on a word analogy dataset with over 40 different relation types (Section 2.4.1), and observe how pair2vec fills hand-crafted relation patterns (Section 2.4.2).

2.4.1 Quantitative Analysis: Word Analogies

Word Analogy Dataset Given a word pair $(a, b)$ and word $x$, the word analogy task involves predicting a word $y$ such that $a : b :: x : y$. We use the Bigger Analogy Test Set [BATS, Gladkova et al., 2016].
<table>
<thead>
<tr>
<th>Relation</th>
<th>Context</th>
<th>X</th>
<th>Y (Top 3)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Antonymy/Exclusion</td>
<td>either X or Y</td>
<td>accept, reject, refuse, recognise, soft, brittle, polished</td>
<td></td>
</tr>
<tr>
<td>Hypernymy</td>
<td>including X and other Y</td>
<td>copper google</td>
<td>ones, metals, mines, apps, browsers, searches</td>
</tr>
<tr>
<td>Hyponymy</td>
<td>X like Y</td>
<td>cities browsers</td>
<td>solaris, speyer, medina, chrome, firefox, netscape</td>
</tr>
<tr>
<td>Co-hyponymy</td>
<td>. X, Y</td>
<td>copper google</td>
<td>malachite, flint, ivory, microsoft, bing, yahoo</td>
</tr>
<tr>
<td>City-State</td>
<td>in X, Y</td>
<td>portland dallas</td>
<td>oregon, maine, dorset, tx, texas, va</td>
</tr>
<tr>
<td>City-City</td>
<td>from X to Y</td>
<td>portland dallas</td>
<td>salem, astoria, ogdensburg, denton, allatoona, addison</td>
</tr>
<tr>
<td>Profession</td>
<td>X, a famous Y</td>
<td>ronaldo monet</td>
<td>footballer, portuguese, player, painter, painting, butterfly</td>
</tr>
</tbody>
</table>

Table 2.8: Given a context \( c \) and a word \( x \), we select the top 3 words \( y \) from the entire vocabulary using our scoring function \( R(x,y) \cdot C(c) \). The analysis suggests that the model tends to rank correct matches (italics) over others.

which contains four groups of relations: encyclopedic semantics (e.g., person-profession as in *Einstein-physicist*), lexicographic semantics (e.g., antonymy as in *cheap-expensive*), derivational morphology (e.g., noun forms as in *oblige-obligation*), and inflectional morphology (e.g., noun-plural as in *bird-birds*). Each group contains 10 sub-relations.

**Method** We interpolate pair2vec and 3CosAdd \(^{Mikolov et al. \ 2013b; \ Levy et al. \ 2014} \) scores on fastText embeddings, as follows:

\[
\text{score}(y) = \alpha \cdot \cos(r_{a,b}, r_{x,y}) + (1 - \alpha) \cdot \cos(b - a + x, y)
\]  

(2.16)

where \( a, b, x, \) and \( y \) represent fastText embeddings \(^{6} \) and \( r_{a,b}, r_{x,y} \) represent the pair2vec embedding for the word pairs \( (a, b) \) and \( (x, y) \), respectively; \( \alpha \) is the linear interpolation parameter. Following prior work \(^{Mikolov et al. \ 2013b} \), we return the highest-scoring \( y \) in the entire vocabulary, excluding the given words \( a, b, \) and \( x \).

\(^{6}\) The fastText embeddings in the analysis were retrained using the same Wikipedia corpus used to train pair2vec to control for the corpus when comparing the two methods.
**Results**  
Figure 2.2 shows how the accuracy on each category of relations varies with $\alpha$. For all four groups, adding pair2vec to 3CosAdd results in significant gains. In particular, the biggest relative improvements are observed for encyclopedic (356%) and lexicographic (51%) relations.

Table 2.7 shows the specific relations in which pair2vec made the largest absolute impact. The gains are particularly significant for relations where fastText embeddings provide limited signal. For example, the accuracy for *substance meronyms* goes from 3.8% to 14.5%. In some cases, there is also a synergistic effect; for instance, in *noun+less*, pair2vec alone scored 0% accuracy, but mixing it with 3CosAdd, which got 4.8% on its own, yielded 16% accuracy.

These results, alongside our experiments in Section 2.3, strongly suggest that pair2vec encodes information complementary to that in single-word embedding methods such as fastText and ELMo.

### 2.4.2 Qualitative Analysis: Slot Filling

To further explore how pair2vec encodes such complementary information, we consider a setting similar to that of knowledge base completion: given a Hearst-like context pattern $c$ and a single word $x$, predict the other word $y$ from the entire vocabulary. We rank candidate words $y$ based on the scoring function in our training objective: $R(x, y) \cdot C(c)$. We use a fixed set of example relations and manually define their predictive context patterns and a small set of candidate words $x$.

Table 2.8 shows the top three $y$ words. The model embeds $(x, y)$ pairs close to contexts that reflect their relationship. For example, substituting *Portland* in the city-state pattern (“*in X, Y*”), the top two words are *Oregon* and *Maine*, both US states with cities named Portland. When used with the city-city pattern (“*from X to Y*”), the top two words are *Salem* and *Astoria*, both cities in Oregon. The word-context interaction often captures multiple relations; for example, *Monet* is used to refer to the painter (*profession*) as well as his paintings.

As intended, pair2vec captures the three-way word-word-context interaction, and not just the two-way word-context interaction (as in single-word embeddings). This profound difference allows pair2vec to complement single-word embeddings with additional information.
2.5 Related Work

Pretrained Word Embeddings  Many state-of-the-art models initialize their word representations using pretrained embeddings such as \textit{word2vec} \cite{Mikolov2013} or \textit{ELMo} \cite{Peters2018}. These representations are typically trained using an interpretation of the Distributional Hypothesis \cite{Harris1954} in which the bivariate distribution of target words and contexts is modeled. Our work deviates from the word embedding literature in two major aspects. First, our goal is to represent word \textit{pairs}, not individual words. Second, our new PMI formulation models the \textit{trivariate} word-word-context distribution. Experiments show that our pair embeddings can complement single-word embeddings.

Mining Textual Patterns  There is extensive literature on mining textual patterns to predict relations between words \cite{Hearst1992, Snow2005, Turney2005, Riedel2013, Van2014, Toutanova2015, Shwartz2016}. These approaches focus mostly on relations between pairs of nouns (perhaps with the exception of \textit{VerbOcean} \cite{Chkovski2004}). More recently, they have been expanded to predict relations between unrestricted pairs of words \cite{Jameel2018, Espinosa2018, Washio2018a}. Relax this assumption with a compositional model that can represent any pair, as long as each word appeared (individually) in the corpus.

These methods are evaluated on either intrinsic relation prediction tasks, such as BLESS \cite{Baroni2011} and CogALex \cite{Santus2016}, or knowledge-base population benchmarks, e.g. FB15 \cite{Bordes2013}. To the best of our knowledge, our work is the first to integrate pattern-based methods into modern high-performing semantic models and evaluate their impact on complex end-tasks like QA and NLI.

Integrating Knowledge in Complex Models  \cite{Ahn2016} integrate Freebase facts into a language model using a copying mechanism over fact attributes. \cite{Yang2017} modify the LSTM cell to incorporate WordNet and NELL knowledge for event and entity extraction. For cross-sentence inference tasks, \cite{Weissenborn2017, Bauer2018, Mihaylov2018} dynamically refine word representations by reading assertions from ConceptNet and Wikipedia abstracts. Our approach, on the
other hand, relies on a relatively simple extension of existing cross-sentence inference models. Furthermore, we do not need to dynamically retrieve and process knowledge base facts or Wikipedia texts, and just pretrain our pair vectors in advance.

KIM [Chen et al., 2017] integrates word-pair vectors into the ESIM model for NLI in a very similar way to ours. However, KIM’s word-pair vectors contain only hand-engineered word-relation indicators from WordNet, whereas our word-pair vectors are automatically learned from unlabeled text. Our vectors can therefore reflect relation types that do not exist in WordNet (such as profession) as well as word pairs that do not have a direct link in WordNet (e.g. bronze and statue); see Table 2.8 for additional examples.

2.6 Conclusion and Future Work

We presented new methods for training and using word pair embeddings that implicitly represent background knowledge. Our pair embeddings are computed as a compositional function of the individual word representations, which is learned by maximizing a variant of the PMI with the contexts in which the two words co-occur. Experiments on cross-sentence inference benchmarks demonstrated that adding these representations to existing models results in sizable improvements for both in-domain and adversarial settings.

Published concurrently, BERT [Devlin et al., 2018], which uses a masked language model objective, has reported dramatic gains on multiple semantic benchmarks including question-answering, natural language inference, and named entity recognition. Potential avenues for future work include multitasking BERT with pair2vec in order to more directly incorporate reasoning about word pair relations into the BERT objective.
Chapter 3

Improving Pre-training by Representing and Predicting Spans

This chapter discusses work originally published in Joshi et al. [2020a]

In this chapter, we focus on methods which encode knowledge beyond word pair relations into model parameters. Pre-training methods like BERT [Devlin et al. 2018] have shown strong performance gains using self-supervised training that masks individual words or subword units. However, many NLP tasks involve reasoning about relationships between two or more spans of text. For example, in extractive question answering [Rajpurkar et al. 2016], determining that the “Denver Broncos” is a type of “NFL team” is critical for answering the question “Which NFL team won Super Bowl 50?” Such spans provide a more challenging target for self supervision tasks, for example predicting “Denver Broncos” is much harder than predicting only “Denver” when you know the next word is “Broncos”. In this paper, we introduce a span-level pre-training approach that consistently outperforms BERT, with the largest gains on span selection tasks such as question answering and coreference resolution.

We present SpanBERT, a pre-training method that is designed to better represent and predict spans of text. Our method differs from BERT in both the masking scheme and the training objectives. First, we mask random contiguous spans, rather than random individual tokens. Second, we introduce a novel span-boundary objective (SBO) so the model learns to predict the entire masked span from the observed tokens at its boundary. Span-based masking forces the model to predict entire spans solely using the context in
\[ \mathcal{L}(\text{football}) = \mathcal{L}_{\text{MLM}}(\text{football}) + \mathcal{L}_{\text{SBO}}(\text{football}) \]
\[ = -\log P(\text{football} \mid x_7) - \log P(\text{football} \mid x_4, x_9, p_3) \]

Figure 3.1: An illustration of SpanBERT training. The span *an American football game* is masked. The span boundary objective (SBO) uses the output representations of the boundary tokens, \( x_4 \) and \( x_9 \) (in blue), to predict each token in the masked span. The equation shows the MLM and SBO loss terms for predicting the token, *football* (in pink), which as marked by the position embedding \( p_3 \), is the *third* token from \( x_4 \).

which they appear. Furthermore, the span-boundary objective encourages the model to store this span-level information at the boundary tokens, which can be easily accessed during the fine-tuning stage. Figure 3.1 illustrates our approach.

To implement SpanBERT, we build on a well-tuned replica of BERT, which itself substantially outperforms the original BERT. While building on our baseline, we find that pre-training on single segments, instead of two half-length segments with the next sentence prediction (NSP) objective, considerably improves performance on most downstream tasks. Therefore, we add our modifications on top of the tuned single-sequence BERT baseline.

Together, our pre-training process yields models that outperform all BERT baselines on a wide variety of tasks, and reach substantially better performance on span selection tasks in particular. Specifically, our method reaches 94.6% and 88.7% F1 on SQuAD 1.1 and 2.0 [Rajpurkar et al. 2016, 2018], respectively — reducing error by as much as 27% compared to our tuned BERT replica. We also observe similar gains on five additional extractive question answering benchmarks (NewsQA, TriviaQA, SearchQA, HotpotQA, and Natural Questions).

SpanBERT also arrives at a new state of the art on the challenging CoNLL-2012 (“OntoNotes”) shared task for document-level coreference resolution, where we reach 79.6% F1, exceeding the previous top model.

\[ ^1 \text{We use the modified MRQA version of these datasets. See more details in Section 3.3.1} \]
by 6.6% absolute. Finally, we demonstrate that SpanBERT also helps on tasks that do not explicitly involve span selection, and show that our approach even improves performance on TACRED [Zhang et al. 2017] and GLUE [Wang et al. 2019].

While others show the benefits of adding more data [Yang et al. 2019b] and increasing model size [Lample and Conneau 2019], this work demonstrates the importance of designing good pre-training tasks and objectives, which can also have a remarkable impact.

3.1 Model

Our approach is inspired by BERT [Devlin et al. 2018], but deviates from its bi-text classification framework in three ways. First, we use a different random process to mask spans of tokens, rather than individual ones. We also introduce a novel auxiliary objective – the span boundary objective (SBO) – which tries to predict the entire masked span using only the representations of the tokens at the span’s boundary. Finally, SpanBERT samples a single contiguous segment of text for each training example (instead of two), and thus does not use BERT’s next sentence prediction objective, which we omit.

3.1.1 Span Masking

Given a sequence of tokens $X = (x_1, x_2, \ldots, x_n)$, we select a subset of tokens $Y \subseteq X$ by iteratively sampling spans of text until the masking budget (e.g. 15% of $X$) has been spent. At each iteration, we first sample a span length (number of words) from a geometric distribution $\ell \sim \text{Geo}(p)$, which is skewed towards shorter spans. We then randomly (uniformly) select the starting point for the span to be masked. We always sample a sequence of complete words (instead of subword tokens) and the starting point must be the beginning of one word.

![Figure 3.2: We sample random span lengths from a geometric distribution $\ell \sim \text{Geo}(p = 0.2)$ clipped at $\ell_{max} = 10$.](image)
Following preliminary trials\(^2\), we set \( p = 0.2 \), and 
also clip \( \ell \) at \( \ell_{\text{max}} = 10 \). This yields a mean span length of \( \text{mean}(\ell) = 3.8 \). Figure 3.2 shows the distribution of span mask lengths.

As in BERT, we also mask 15% of the tokens in total: replacing 80% of the masked tokens with [MASK], 10% with random tokens and 10% with the original tokens. However, we perform this replacement at the span level and not for each token individually; i.e. all the tokens in a span are replaced with [MASK] or sampled tokens.

3.1.2 Span Boundary Objective (SBO)

Span selection models\(^\text{Lee et al. [2016, 2017]; He et al. [2018]}\) typically create a fixed-length representation of a span using its boundary tokens (start and end). To support such models, we would ideally like the representations for the end of the span to summarize as much of the internal span content as possible. We do so by introducing a span boundary objective that involves predicting each token of a masked span using only the representations of the observed tokens at the boundaries (Figure 3.1).

Formally, we denote the output of the transformer encoder for each token in the sequence by \( x_1, \ldots, x_n \). Given a masked span of tokens \((x_s, \ldots, x_e) \in Y\), where \((s, e)\) indicates its start and end positions, we represent each token \( x_i \) in the span using the output encodings of the \textit{external} boundary tokens \( x_{s-1} \) and \( x_{e+1} \), as well as the position embedding of the target token \( p_{i-s+1} \):

\[
y_i = f(x_{s-1}, x_{e+1}, p_{i-s+1})
\]

where position embeddings \( p_1, p_2, \ldots \) mark relative positions of the masked tokens with respect to the left boundary token \( x_{s-1} \). We implement the representation function \( f(\cdot) \) as a 2-layer feed-forward network with GeLU activations\(^\text{Hendrycks and Gimpel [2016]}\) and layer normalization\(^\text{Ba et al. [2016]}\):

\[
\begin{align*}
h_0 &= [x_{s-1}; x_{e+1}; p_{i-s+1}] \\
h_1 &= \text{LayerNorm} (\text{GeLU} (W_1 h_0)) \\
y_i &= \text{LayerNorm} (\text{GeLU} (W_2 h_1))
\end{align*}
\]

\(^2\)We experimented with \( p = \{0.1, 0.2, 0.4\} \) and found 0.2 to perform the best.
We then use the vector representation $y_i$ to predict the token $x_i$ and compute the cross-entropy loss exactly like the MLM objective.

SpanBERT sums the loss from both the span boundary and the regular masked language model objectives for each token $x_i$ in the masked span $(x_a, ..., x_e)$, while reusing the input embedding \cite{Press and Wolf [2017]} for the target tokens in both MLM and SBO:

$$L(x_i) = L_{\text{MLM}}(x_i) + L_{\text{SBO}}(x_i)$$

$$= - \log P(x_i | x_i) - \log P(x_i | y_i)$$

### 3.2 Single-Sequence Training

BERT’s examples contain two sequences of text $(X_A, X_B)$, and an objective that trains the model to predict whether they are connected (NSP). We find that this setting is almost always worse than simply using a single sequence without the NSP objective (see Section 3.4 for further details). We conjecture that single-sequence training is superior to bi-sequence training with NSP because (a) the model benefits from longer full-length contexts, or (b) conditioning on, often unrelated, context from another document adds noise to the masked language model. Therefore, in our approach, we remove both the NSP objective and the two-segment sampling procedure, and simply sample a single contiguous segment of up to $n = 512$ tokens, rather than two half-segments that sum up to $n$ tokens together.

In summary, SpanBERT pre-trains span representations by: (1) masking spans of full words using a geometric distribution based masking scheme (Section 3.1.1), (2) optimizing an auxiliary span-boundary objective (Section 3.1.2) in addition to MLM using a single-sequence data pipeline (Section 3.2).

### 3.3 Experimental Setup

#### 3.3.1 Tasks

We evaluate on a comprehensive suite of tasks, including seven question answering tasks, coreference resolution, nine tasks in the GLUE benchmark \cite{Wang et al. [2019]}, and relation extraction. We expect that the span selection tasks, question answering and coreference resolution, will particularly benefit from our
span-based pre-training.

**Extractive Question Answering**  Given a short passage of text and a question as input, the task of extractive question answering is to select a contiguous span of text in the passage as the answer.

We first evaluate on SQuAD 1.1 and 2.0 [Rajpurkar et al. 2016, 2018], which have served as major question answering benchmarks, particularly for pre-trained models [Peters et al. 2018; Devlin et al. 2018; Yang et al. 2019b]. We also evaluate on five more datasets from the MRQA shared task [Fisch et al. 2019]: NewsQA [Trischler et al. 2017], SearchQA [Dunn et al. 2017], TriviaQA [Joshi et al. 2017], HotpotQA [Yang et al. 2018] and Natural Questions [Kwiatkowski et al. 2019]. Because the MRQA shared task does not have a public test set, we split the development set in half to make new development and test sets. The datasets vary in both domain and collection methodology, making this collection a good testbed for evaluating whether our pre-trained models can generalize well across different data distributions.

Following BERT [Devlin et al. 2018], we use the same QA model architecture for all the datasets. We first convert the passage $P = (p_1, p_2, \ldots, p_l)$ and question $Q = (q_1, q_2, \ldots, q_{l'})$ into a single sequence $X = [\text{CLS}] p_1 p_2 \ldots p_l [\text{SEP}] q_1 q_2 \ldots q_{l'} [\text{SEP}]$, pass it to the pre-trained transformer encoder, and train two linear classifiers independently on top of it for predicting the answer span boundary (start and end). For the unanswerable questions in SQuAD 2.0, we simply set the answer span to be the special token [CLS] for both training and testing.

**Coreference Resolution**  Coreference resolution is the task of clustering mentions in text which refer to the same real-world entities. We evaluate on the CoNLL-2012 shared task [Pradhan et al. 2012] for document-level coreference resolution. We use the independent version of the [Joshi et al. 2019b] implementation of the higher-order coreference model [Lee et al. 2018]. The document is divided into non-overlapping segments of a pre-defined length[4] Each segment is encoded independently by the pre-trained transformer encoder, which replaces the original LSTM-based encoder. For each mention span $x$, the model learns a distribution $P(\cdot)$ over possible antecedent spans $Y$:

---

[3]https://github.com/mrqa/MRQA-Shared-Task-2019 MRQA changed the original datasets to unify them into the same format, e.g. all the contexts are truncated to a maximum of 800 tokens and only answerable questions are kept.

[4]The length was chosen from {128, 256, 384, 512}. 

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The span pair scoring function \( s(x, y) \) is a feedforward neural network over fixed-length span representations and hand-engineered features over \( x \) and \( y \):

\[
s(x, y) = s_m(x) + s_m(y) + s_c(x, y)
\]

\[
s_m(x) = \text{FFNN}_m(g_x)
\]

\[
s_c(x, y) = \text{FFNN}_c(g_x, g_y, \phi(x, y))
\]

Here \( g_x \) and \( g_y \) denote the span representations, which are a concatenation of the two transformer output states of the span endpoints and an attention vector computed over the output representations of the token in the span. \( \text{FFNN}_m \) and \( \text{FFNN}_c \) represent two feedforward neural networks with one hidden layer, and \( \phi(x, y) \) represents the hand-engineered features (e.g. speaker and genre information). A more detailed description of the model can be found in [Joshi et al., 2019b].

**Relation Extraction** TACRED [Zhang et al., 2017] is a challenging relation extraction dataset. Given one sentence and two spans within it – subject and object – the task is to predict the relation between the spans from 42 pre-defined relation types, including no_relation. We follow the entity masking schema from [Zhang et al., 2017] and replace the subject and object entities by their NER tags such as “[CLS][SUBJ-PER] was born in [OBJ-LOC] , Michigan, …”, and finally add a linear classifier on top of the [CLS] token to predict the relation type.

**GLUE** The General Language Understanding Evaluation (GLUE) benchmark [Wang et al., 2019] consists of 9 sentence-level classification tasks:

- Two sentence-level classification tasks including CoLA [Warstadt et al., 2018] for evaluating linguistic acceptability and SST-2 [Socher et al., 2013] for sentiment classification.

- Three sentence-pair similarity tasks including MRPC [Dolan and Brockett, 2005], a binary paraphrasing task sentence pairs from news sources, STS-B [Cer et al., 2017], a graded similarity task for news
headlines, and QQP® a binary paraphrasing tasking between Quora question pairs.


Unlike question answering, coreference resolution, and relation extraction, these sentence-level tasks do not require explicit modeling of span-level semantics. However, they might still benefit from implicit span-based reasoning (e.g., the Prime Minister is the head of the government). Following previous work [Devlin et al. 2018; Radford et al. 2018] we exclude WNLI from the results to enable a fair comparison. While recent work [Liu et al. 2019] has applied several task-specific strategies to increase performance on the individual GLUE tasks, we follow BERT’s single-task setting and only add a linear classifier on top of the [CLS] token for these classification tasks.

3.3.2 Implementation

We reimplemented BERT’s model and pre-training method in fairseq [Ott et al. 2019]. We used the model configuration of BERT_large as in 352018Devlin et al. and also pre-trained all our models on the same corpus: BooksCorpus and English Wikipedia using cased Wordpiece tokens.

Compared to the original BERT implementation, the main differences in our implementation include: (a) We use different masks at each epoch while BERT samples 10 different masks for each sequence during data processing. (b) We remove all the short-sequence strategies used before (they sampled shorter sequences with a small probability 0.1; they also first pre-trained with smaller sequence length of 128 for 90% of the steps). Instead, we always take sequences of up to 512 tokens until it reaches a document boundary. We refer readers to 912019c Liu et al. Liu, Ott, Goyal, Du, Joshi, Chen, Levy, Lewis, Zettlemoyer, and Stoyanov) for further discussion on these modifications and their effects.

As in BERT, the learning rate is warmed up over the first 10,000 steps to a peak value of 1e-4, and then linearly decayed. We retain β hyperparameters (β1 = 0.9, β2 = 0.999) and a decoupled weight decay [Loshchilov and Hutter 2019] of 0.1. We also keep a dropout of 0.1 on all layers and attention weights, and

5https://data.quora.com/First-Quora-Dataset-Release-Question-Pairs
6Previous work has excluded WNLI on account of construction issues outlined on the GLUE website – https://gluebenchmark.com/faq
a GeLU activation function [Hendrycks and Gimpel, 2016]. We deviate from the optimization by running for 2.4M steps and using an epsilon of 1e-8 for AdamW [Kingma and Ba, 2015], which converges to a better set of model parameters. Our implementation uses a batch size of 256 sequences with a maximum of 512 tokens. For the SBO, we use 200 dimension position embeddings \( p_1, p_2, \ldots \) to mark positions relative to the left boundary token. The pre-training was done on 32 Volta V100 GPUs and took 15 days to complete.

Fine-tuning is implemented based on HuggingFace’s codebase [Wolf et al., 2019]. We refer the reader to Joshi et al. [2020a] for further details.

### 3.3.3 Baselines

We compare SpanBERT to three baselines:

**Google BERT** The pre-trained models released by Devlin et al. [Devlin, Chang, Lee, and Toutanova, 2018].

**Our BERT** Our reimplementation of BERT with improved data preprocessing and optimization (subsection 3.3.2).

**Our BERT-1seq** Our reimplementation of BERT trained on single full-length sequences without NSP (subsection 3.2).

### 3.4 Results

We compare SpanBERT to the baselines per task, and draw conclusions based on the overall trends.

#### 3.4.1 Per-Task Results

**Extractive Question Answering** Table 3.1 shows the performance on both SQuAD 1.1 and 2.0. SpanBERT exceeds our BERT baseline by 2.0% and 2.8% F1 respectively (3.3% and 5.4% over Google BERT). In SQuAD 1.1, this result accounts for over 27% error reduction, reaching 3.4% F1 above human performance.

---

7On the average, this is approximately 390 sequences since some documents have fewer than 512 tokens

8https://github.com/google-research/bert
Table 3.1: Test results on SQuAD 1.1 and SQuAD 2.0.

<table>
<thead>
<tr>
<th></th>
<th>SQuAD 1.1</th>
<th></th>
<th>SQuAD 2.0</th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>EM</td>
<td>F1</td>
<td>EM</td>
<td>F1</td>
</tr>
<tr>
<td>Human Perf.</td>
<td>82.3</td>
<td>91.2</td>
<td>86.8</td>
<td>89.4</td>
</tr>
<tr>
<td>Google BERT</td>
<td>84.3</td>
<td>91.3</td>
<td>80.0</td>
<td>83.3</td>
</tr>
<tr>
<td>Our BERT</td>
<td>86.5</td>
<td>92.6</td>
<td>82.8</td>
<td>85.9</td>
</tr>
<tr>
<td>Our BERT-1seq</td>
<td>87.5</td>
<td>93.3</td>
<td>83.8</td>
<td>86.6</td>
</tr>
<tr>
<td>SpanBERT</td>
<td>88.8</td>
<td>94.6</td>
<td>85.7</td>
<td>88.7</td>
</tr>
</tbody>
</table>

Table 3.2: Performance (F1) on the five MRQA extractive question answering tasks.

<table>
<thead>
<tr>
<th></th>
<th>NewsQA</th>
<th>TriviaQA</th>
<th>SearchQA</th>
<th>HotpotQA</th>
<th>Natural Questions</th>
<th>Avg.</th>
</tr>
</thead>
<tbody>
<tr>
<td>Google BERT</td>
<td>68.8</td>
<td>77.5</td>
<td>81.7</td>
<td>78.3</td>
<td>79.9</td>
<td>77.3</td>
</tr>
<tr>
<td>Our BERT</td>
<td>71.0</td>
<td>79.0</td>
<td>81.8</td>
<td>80.5</td>
<td>80.5</td>
<td>78.6</td>
</tr>
<tr>
<td>Our BERT-1seq</td>
<td>71.9</td>
<td>80.4</td>
<td>84.0</td>
<td>80.3</td>
<td>81.8</td>
<td>79.7</td>
</tr>
<tr>
<td>SpanBERT</td>
<td>73.6</td>
<td>83.6</td>
<td>84.8</td>
<td>83.0</td>
<td>82.5</td>
<td>81.5</td>
</tr>
</tbody>
</table>

Table 3.3: Performance on the OntoNotes coreference resolution benchmark. The main evaluation is the average F1 of three metrics: MUC, B$^3$, and CEAF$^\phi_4$ on the test set.

<table>
<thead>
<tr>
<th></th>
<th>MUC</th>
<th>B$^3$</th>
<th>CEAF$^\phi_4$</th>
<th>Avg. F1</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>P</td>
<td>R</td>
<td>F1</td>
<td>P</td>
</tr>
<tr>
<td>Prev. SotA: Lee et al [<em>2018</em>]</td>
<td>81.4</td>
<td>79.5</td>
<td>80.4</td>
<td>72.2</td>
</tr>
<tr>
<td>Google BERT</td>
<td>84.9</td>
<td>82.5</td>
<td>83.7</td>
<td>76.7</td>
</tr>
<tr>
<td>Our BERT</td>
<td>85.1</td>
<td>83.5</td>
<td>84.3</td>
<td>77.3</td>
</tr>
<tr>
<td>Our BERT-1seq</td>
<td>85.5</td>
<td>84.1</td>
<td>84.8</td>
<td>77.8</td>
</tr>
<tr>
<td>SpanBERT</td>
<td>85.8</td>
<td>84.8</td>
<td>85.3</td>
<td>78.3</td>
</tr>
</tbody>
</table>

Coreference Resolution Table 3.3 shows the performance on the OntoNotes coreference resolution benchmark. Our BERT reimplementation improves the Google BERT model by 1.2% on the average F1 metric and single-sequence training brings another 0.5% gain. Finally, SpanBERT improves considerably on top of that, achieving a new state of the art of 79.6% F1 (previous best result is 73.0%).
<table>
<thead>
<tr>
<th>Model</th>
<th>CoLA</th>
<th>SST-2</th>
<th>MRPC</th>
<th>STS-B</th>
<th>QQP</th>
<th>MNLI</th>
<th>QNLI</th>
<th>RTE</th>
<th>Avg</th>
</tr>
</thead>
<tbody>
<tr>
<td>Google BERT</td>
<td>59.3</td>
<td>95.2</td>
<td>88.5/43</td>
<td>86.4/80</td>
<td>71.2/89</td>
<td>86.1/85</td>
<td>93.0</td>
<td>71.1</td>
<td>80.4</td>
</tr>
<tr>
<td>Our BERT</td>
<td>58.6</td>
<td>93.9</td>
<td>90.1/66</td>
<td>88.4/81</td>
<td>71.8/89</td>
<td>87.2/86</td>
<td>93.0</td>
<td>74.7</td>
<td>81.1</td>
</tr>
<tr>
<td>Our BERT-1seq</td>
<td>63.5</td>
<td>94.8</td>
<td>91.2/87</td>
<td>89.0/84</td>
<td>72.1/89</td>
<td>88.0/87</td>
<td>93.0</td>
<td>72.1</td>
<td>81.7</td>
</tr>
<tr>
<td>SpanBERT</td>
<td>64.3</td>
<td>94.8</td>
<td>90.9/79</td>
<td>89.9/81</td>
<td>71.9/89</td>
<td>88.1/87</td>
<td>94.3</td>
<td>79.0</td>
<td>82.8</td>
</tr>
</tbody>
</table>

**Table 3.4:** Test performance on the TACRED relation extraction benchmark.

**Table 3.5:** Test set performance on GLUE tasks. MRPC: F1/accuracy, STS-B: Pearson/Spearman correlation, QQP: F1/accuracy, MNLI: matched/mismatched accuracies and accuracy for all the other tasks. WNLI (not shown) is always set to majority class (65.1% accuracy) and included in the average.

**Relation Extraction** Table 3.4 shows the performance on TACRED. SpanBERT exceeds our reimplementation of BERT by 3.3% F1 and achieves close to the current state of the art [Soares et al., 2019] — Our model performs better than their $\text{BERT}_{\text{EM}}$ but is 0.7 point behind $\text{BERT}_{\text{EM}} + \text{MTB}$ which used entity-linked text for additional pre-training. Most of this gain (+2.6%) stems from single-sequence training although the contribution of span masking and the span boundary objective is still a considerable 0.7%, resulting largely from higher recall.

**GLUE** Table 3.5 shows the performance on GLUE. For most tasks, the different models appear to perform similarly. Moving to single-sequence training without the NSP objective substantially improves CoLA, and yields smaller (but considerable) improvements on MRPC and MNLI. The main gains from SpanBERT are in the SQuAD-based QNLI dataset (+1.3%) and in RTE (+6.9%), the latter accounting for most of the rise in SpanBERT’s GLUE average.

3.4.2 **Overall Trends**

We compared our approach to three BERT baselines on 17 benchmarks, and found that SpanBERT outperforms BERT on almost every task. In 14 tasks, SpanBERT performed better than all baselines. In 2
Table 3.6: The effect of replacing BERT’s original masking scheme (Subword Tokens) with different masking schemes. Results are F1 scores for QA tasks and accuracy for MNLI and QNLI on the development sets. All the models are based on bi-sequence training with NSP.

<table>
<thead>
<tr>
<th>Scheme</th>
<th>SQuAD 2.0</th>
<th>NewsQA</th>
<th>TriviaQA</th>
<th>Coreference</th>
<th>MNLI-m</th>
<th>QNLI</th>
<th>GLUE (Avg)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Subword Tokens</td>
<td>83.8</td>
<td>72.0</td>
<td>76.3</td>
<td><strong>77.7</strong></td>
<td>86.7</td>
<td>92.5</td>
<td>83.2</td>
</tr>
<tr>
<td>Whole Words</td>
<td>84.3</td>
<td>72.8</td>
<td>77.1</td>
<td>76.6</td>
<td>86.3</td>
<td>92.8</td>
<td>82.9</td>
</tr>
<tr>
<td>Named Entities</td>
<td>84.8</td>
<td>72.7</td>
<td>78.7</td>
<td>75.6</td>
<td>86.0</td>
<td>93.1</td>
<td>83.2</td>
</tr>
<tr>
<td>Noun Phrases</td>
<td>85.0</td>
<td>73.0</td>
<td>77.7</td>
<td>76.7</td>
<td>86.5</td>
<td>93.2</td>
<td><strong>83.5</strong></td>
</tr>
<tr>
<td>Geometric Spans</td>
<td><strong>85.4</strong></td>
<td><strong>73.0</strong></td>
<td><strong>78.8</strong></td>
<td>76.4</td>
<td><strong>87.0</strong></td>
<td><strong>93.3</strong></td>
<td>83.4</td>
</tr>
</tbody>
</table>

Table 3.7: The effects of different auxiliary objectives, given MLM over random spans as the primary objective.

<table>
<thead>
<tr>
<th>Scheme</th>
<th>SQuAD 2.0</th>
<th>NewsQA</th>
<th>TriviaQA</th>
<th>Coreference</th>
<th>MNLI-m</th>
<th>QNLI</th>
<th>GLUE (Avg)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Span Masking (2seq) + NSP</td>
<td>85.4</td>
<td>73.0</td>
<td>78.8</td>
<td>76.4</td>
<td>87.0</td>
<td>93.3</td>
<td>83.4</td>
</tr>
<tr>
<td>Span Masking (1seq)</td>
<td>86.7</td>
<td>73.4</td>
<td>80.0</td>
<td>76.3</td>
<td>87.3</td>
<td>93.8</td>
<td>83.8</td>
</tr>
<tr>
<td>Span Masking (1seq) + SBO</td>
<td><strong>86.8</strong></td>
<td><strong>74.1</strong></td>
<td><strong>80.3</strong></td>
<td><strong>79.0</strong></td>
<td><strong>87.6</strong></td>
<td><strong>93.9</strong></td>
<td><strong>84.0</strong></td>
</tr>
</tbody>
</table>

When considering the magnitude of the gains, it appears that **SpanBERT is especially better at extractive question answering**. In SQuAD 1.1, for example, we observe a solid gain of 2.0% F1 even though the baseline is already well above human performance. On MRQA, SpanBERT improves between 2.0% (Natural Questions) and 4.6% (TriviaQA) F1 on top of our BERT baseline.

Finally, we observe that **single-sequence training works considerably better than bi-sequence training with next sentence prediction (NSP)** with BERT’s choice of sequence lengths for a wide variety of tasks. This is surprising because BERT’s ablations showed gains from the NSP objective [Devlin et al. 2018]. However, the ablation studies still involved bi-sequence data processing, i.e. the pre-training stage only controlled for the NSP objective while still sampling two half-length sequences. We hypothesize that bi-sequence training, as it is implemented in BERT, impedes the model from learning longer-range features, and consequently hurts performance on many downstream tasks.
3.5 Ablation Studies

We compare our random span masking scheme with linguistically-informed masking schemes, and find that masking random spans is a competitive and often better approach. We then study the impact of the span boundary objective (SBO), and contrast it with BERT’s next sentence prediction (NSP) objective

3.5.1 Masking Schemes

Previous work Sun et al. [2019b] has shown improvements in downstream task performance by masking linguistically-informed spans during pre-training for Chinese data. We compare our random span masking scheme with masking of linguistically-informed spans. Specifically, we train the following five baseline models differing only in the way tokens are masked.

Subword Tokens   We sample random Wordpiece tokens, as in the original BERT.

Whole Words    We sample random words, and then mask all of the subword tokens in those words. The total number of masked subtokens is around 15%.

Named Entities    At 50% of the time, we sample from named entities in the text, and sample random whole words for the other 50%. The total number of masked subtokens is 15%. Specifically, we run spaCy’s named entity recognizer[^10] on the corpus and select all the non-numerical named entity mentions as candidates.

Noun Phrases   Similar as Named Entities, we sample from noun phrases at 50% of the time. The noun phrases are extracted by running spaCy’s constituency parser.

Geometric Spans   We sample random spans from a geometric distribution, as in our SpanBERT (see Section[3.1.1]).

[^9]: To save time and resources, we use the checkpoints at 1.2M steps for all the ablation experiments.
[^10]: [https://spacy.io/](https://spacy.io/)
evaluation. With the exception of coreference resolution, masking random spans is preferable to other strategies. Although linguistic masking schemes (named entities and noun phrases) are often competitive with random spans, their performance is not consistent; for instance, masking noun phrases achieves parity with random spans on NewsQA, but underperforms on TriviaQA (-1.1% F1).

On coreference resolution, we see that masking random subword tokens is preferable to any form of span masking. Nevertheless, we shall see in the following experiment that combining random span masking with the span boundary objective can improve upon this result considerably.

### 3.5.2 Auxiliary Objectives

In Section 3.4, we saw that bi-sequence training with the next sentence prediction (NSP) objective can hurt performance on downstream tasks, when compared to single-sequence training. We test whether this holds true for models pre-trained with span masking, and also evaluate the effect of replacing the NSP objective with the span boundary objective (SBO).

Table 3.7 confirms that single-sequence training typically improves performance. Adding SBO further improves performance, with a substantial gain on coreference resolution (+2.7% F1) over span masking alone. Unlike the NSP objective, SBO does not appear to have any adverse effects.

### 3.6 Related Work

Pre-trained contextualized word representations that can be trained from unlabeled text [Dai and Le 2015; Melamud et al. 2016; Peters et al. 2018] have had immense impact on NLP lately, particularly as methods for initializing a large model before fine-tuning it for a specific task [Howard and Ruder 2018; Radford et al. 2018; Devlin et al. 2018]. Beyond differences in model hyperparameters and corpora, these methods mainly differ in their pre-training tasks and loss functions, with a considerable amount of contemporary literature proposing augmentations of BERT’s masked language modeling (MLM) objective.

While previous and concurrent work has looked at masking [Sun et al. 2019b] or dropping [Song et al. 2019; Chan et al. 2019] multiple words from the input – particularly as pretraining for language generation tasks – SpanBERT pretrains span representations [Lee et al. 2016], which are widely used for question answering, coreference resolution and a variety of other tasks. ERNIE [Sun et al. 2019b]
shows improvements on Chinese NLP tasks using phrase and named entity masking. MASS [Song et al. 2019] focuses on language generation tasks, and adopts the encoder-decoder framework to reconstruct a sentence fragment given the remaining part of the sentence. We attempt to more explicitly model spans using the SBO objective, and show that (geometrically distributed) random span masking works as well, and sometimes better than, masking linguistically-coherent spans. We evaluate on English benchmarks for question answering, relation extraction, and coreference resolution in addition to GLUE.

A different ERNIE [Zhang et al. 2019b] focuses on integrating structured knowledge bases with contextualized representations with an eye on knowledge-driven tasks like entity typing and relation classification. UNILM [Dong et al. 2019] uses multiple language modeling objectives – unidirectional (both left-to-right and right-to-left), bidirectional, and sequence-to-sequence prediction – to aid generation tasks like summarization and question generation. XLM [Lample and Conneau 2019] explores cross-lingual pre-training for multilingual tasks such as translation and cross-lingual classification. Kermit [Chan et al. 2019], an insertion based approach, fills in missing tokens (instead of predicting masked ones) during pretraining; they show improvements on machine translation and zero-shot question answering.

Concurrent with our work, RoBERTa [Liu et al. 2019c] presents a replication study of BERT pre-training that measures the impact of many key hyperparameters and training data size. Also concurrent, XLNet [Yang et al. 2019b] combines an autoregressive loss and the Transformer-XL [Dai et al. 2019] architecture with a more than an eight-fold increase in data to achieve current state-of-the-art results on multiple benchmarks. XLNet also masks spans (of 1-5 tokens) during pre-training, but predicts them autoregressively. Our model focuses on incorporating span-based pre-training, and as a side effect, we present a stronger BERT baseline while controlling for the corpus, architecture, and the number of parameters.

Related to our SBO objective, pair2vec [Joshi et al. 2019a] encodes word-pair relations using a negative sampling-based multivariate objective during pre-training. Later, the word-pair representations are injected into the attention-layer of downstream tasks, and thus encode limited downstream context. Unlike pair2vec, our SBO objective yields “pair” (start and end tokens of spans) representations which more fully encode the context during both pre-training and finetuning, and are thus more appropriately viewed as span representations. Stern et al. [2018] focus on improving language generation speed using a block-wise parallel decoding scheme; they make predictions for multiple time steps in parallel and then back off to the longest
prefix validated by a scoring model. Also related are sentence representation methods Kiros et al. [2015]; Logeswaran and Lee [2018] which focus on predicting surrounding contexts from sentence embeddings.

### 3.7 Conclusion

We presented a new method for span-based pre-training which extends BERT by (1) masking contiguous random spans, rather than random tokens, and (2) training the span boundary representations to predict the entire content of the masked span, without relying on the individual token representations within it. Together, our pre-training process yields models that outperform all BERT baselines on a variety of tasks, and reach substantially better performance on span selection tasks in particular.
Chapter 4

Representations Using Dynamically Retrieved Textual Knowledge

This chapter discusses work originally published in Joshi et al. [2020b]

Current self-supervised representations, trained at large scale from document-level contexts, are known to encode linguistic [Tenney et al. [2019]] and factual [Petroni et al. [2019]] knowledge into their parameters. Yet, even large pretrained representations are unable to capture and preserve all factual knowledge they have “read” during pretraining due to the long tail of entity and event-specific information [Logan et al. [2019]].

On the other hand, when relevant text is provided as input, such as in reading comprehension tasks [Rajpurkar et al. [2016]], relation extraction, syntactic analysis, etc., which can be cast as tasks of labeling spans in the input text, prior work has not focused on drawing background information from external text sources. Instead, most research has

**Figure 4.1:** A TriviaQA example showing how background sentences from Wikipedia help define the meaning of phrases in the context and their relationship to phrases in the question. The answer *William Hickey* is connected to the question phrase *pen-name of the gossip columnist in the Daily Express* through the background sentence.
explored architectures to integrate background from structured knowledge bases to form input text representations [Bauer et al. 2018; Mihaylov and Frank 2018; Yang et al. 2019a; Zhang et al. 2019b; Peters et al. 2019].

We posit that representations should be able to directly integrate textual background knowledge since a wider scope of information is more readily available in textual form. Our method represents input texts by jointly encoding them with dynamically retrieved sentences from the Wikipedia pages of entities they mention. We term these representations TEK-enriched, for Textual Encyclopedic Knowledge (Figure 4.2 shows an illustration), and use them for reading comprehension (RC) by contextualizing questions and passages together with retrieved Wikipedia background sentences. Such background knowledge can help reason about the relationships between questions and passages. Figure 4.1 shows an example question from the TriviaQA dataset Joshi et al. 2017 asking for the pen-name of a gossip columnist. Encoding relevant background knowledge (pseudonymous byline of a gossip column published in the Daily Express) helps ground the vague reference to the William Hickey column in the given document context.

Using text as background knowledge allows us to directly reuse powerful pretrained BERT-style encoders Devlin et al. 2018. We show that an off-the-shelf RoBERTa Liu et al. 2019c model can be directly finetuned on minimally structured TEK-enriched inputs, which are formatted to allow the encoder to distinguish between the original passages and background sentences. This method considerably improves on current state-of-the-art methods which only consider context from a single input document (Section 3.4). The improvement comes without an increase in the length of the input window for the Transformer Vaswani et al. 2017.

Although existing pretrained models provide a good starting point for task-specific TEK-enriched representations, there is still a mismatch between the type of input seen during pretraining (single document segments) and the type of input the model is asked to represent for downstream tasks (document text with background Wikipedia sentences from multiple pages). We show that the Transformer model can be substantially improved by reducing this mismatch via self-supervised masked language model (MLM) Devlin et al. 2018 pretraining on TEK-augmented input texts.

Our approach records considerable improvements over state of the art base (12-layer) and large (24-
Figure 4.2: We contextualize the input text, in this case a question and a passage, together with textual encyclopedic knowledge (TEK) using a pretrained Transformer to create TEK-enriched representations.

layer) Transformer models for in-domain and out-of-domain document-level extractive question answering (QA), for tasks where factual knowledge about entities is important and well-covered by the background collection. On TriviaQA, we see improvements of 1.6 to 3.1 F1, respectively, over comparable RoBERTa models which do not integrate background information. On MRQA [Fisch et al., 2019], a large collection of diverse QA datasets, we see consistent gains in-domain along with large improvements out-of-domain on BioASQ (2.1 to 4.2 F1), TextbookQA (1.6 to 2.0 F1), and DuoRC (1.1 to 2.0 F1).

4.1 TEK-Enriched Representations

We follow recent work on pretraining bidirectional Transformer representations on unlabeled text, and fine-tuning them for downstream tasks [Devlin et al., 2018]. Subsequent approaches have shown significant improvements over BERT by improving the training example generation, the masking strategy, the pretraining objectives, and the optimization methods [Liu et al., 2019c; Joshi et al., 2020a]. We build on these improvements to train TEK-enriched representations and use them for extractive QA.

Our approach seeks to contextualize input text $X = (x_1, \ldots, x_n)$ jointly with relevant textual encyclopedic background knowledge $B$ retrieved dynamically from multiple documents. We define a retrieval function, $f_{ret}(X, \mathcal{D})$, which takes $X$ as input and retrieves a list of text spans $B = (B_1, \ldots, B_M)$ from the corpus $\mathcal{D}$. In our implementation, each of the text spans $B_i$ is a sentence. The encoder then represents $X$ by jointly encoding $X$ with $B$ using $f_{enc}(X, B)$ such that the output representations of $X$ are cognizant of the information present in $B$ (see Figure 4.2). We use a deep Transformer encoder operating over the input
sequence \([\text{CLS}] X [\text{SEP}] B [\text{SEP}]\) for \(f_{\text{enc}}(\cdot)\).

We refer to inputs \(X\) generically as contexts. These could be either contiguous word sequences from documents (passages), or, for the QA application, question-passage pairs, which we refer to as RC-contexts. For a fixed Transformer input length limit (which is necessary for computational efficiency), there is a trade-off between the length of the document context (the length of \(X\)) and the amount of background knowledge (the length of \(B\)). Subsection 4.4 explores this trade-off in detail with experiments showing that for an encoder input limit of 512, the values of \(N_C = 384\) for the length of \(X\) and \(N_B = 128\) for the length of \(B\) provide an effective compromise.

We use a simple implementation of the background retrieval function \(f_{\text{ret}}(X, D)\), using an entity linker for finetuning (subsection 4.1.1) and Wikipedia hyperlinks for pretraining (subsection 4.1.2), and a way to score the relevance of individual sentences using \(n\)-gram overlap.

### 4.1.1 TEK-Enriched Question Answering

The input \(X\) for the extractive QA task consists of the question \(Q\) and a candidate passage \(P\). We use the following retrieval function \(f_{\text{ret}}(X)\) to obtain relevant background \(B\).

**Background Knowledge Retrieval for QA** We detect entity mentions in \(X\) using a proprietary Wikipedia-based entity linker\(^2\) and form a candidate pool of background segments \(B_i\) as the union of the sentences in the Wikipedia pages of the detected entities. These sentences are then ranked based on their number of overlapping \(n\)-grams with the question (equally weighted unigrams, bigrams, and trigrams). To form the input for the Transformer encoder, each background sentence is minimally structured as \(B_i\) by prepending the name of the entity whose page it belongs to along with a separator ‘:’ token. Each sentence \(B_i\) is followed by \([\text{SEP}]\).

**QA Model** Following BERT, our QA model architecture consists of two independent linear classifiers for predicting the answer span boundary (start and end) on top of the output representations of \(X\). We assume that the answer, if present, is contained only in the given passage, \(P\), and do not consider potential mentions.

\(^2\)We also report results on publicly available linkers showing that our method is robust to the exact choice of the linker (subsection 4.4).
of the answer in the background $B$. For instances which do not contain the answer, we set the answer span to be the special token [CLS]. We use a fixed Transformer input window size of 512, and use a sliding window with a stride of 128 tokens to handle longer documents. Our TEK-enriched representations use document passages of length 384 while baselines use longer passages of length 512.

4.1.2 TEK-Enriched Pretraining

Standard pretraining uses contiguous document-level natural language inputs. Since TEK-augmented inputs are formatted as natural language sequences, off-the-shelf pretrained models can be used as a starting point for creating TEK-enriched representations. As one of our approaches, we use a standard single-document pretraining model.

While the input format is the same, there is a mismatch between contiguous document segments and TEK-augmented inputs sourced from multiple documents. We propose an additional pretraining stage—starting from the RoBERTa parameters, we resume pretraining using an MLM objective on TEK-augmented document text $X$, which encourages the model to integrate the knowledge from multiple background segments.

Background Knowledge Retrieval in Pretraining In pretraining, $X$ is a contiguous block of text from Wikipedia. The retrieval function $f_{ret}(X, D)$ returns $B = (B_1, \ldots, B_M)$ where each $B_i$ is a sentence from the Wikipedia page of some entity hyperlinked from a span in $X$. We use high-precision Wikipedia hyperlinks instead of an entity linker for pretraining. The background candidate sentences are ranked by their ngram overlap with $X$. The top ranking sentences in $B$ up to $N_B$ tokens are used. If no entities are found in $X$, $B$ is constructed from the context following $X$ from the same document.

Training Objective We continue pretraining a deep Transformer using the MLM objective [Devlin et al., 2018] after initializing the parameters with pretrained RoBERTa weights. Following improvements in SpanBERT [Joshi et al., 2020a], we mask spans with lengths sampled from a geometric distribution in the entire input ($X$ and $B$). We use a single segment ID, and remove the next sentence prediction objective which has been shown to not improve performance [Joshi et al., 2020a; Liu et al., 2019c] for multiple tasks including QA.
<table>
<thead>
<tr>
<th>Task</th>
<th>Train</th>
<th>Dev</th>
<th>Test</th>
</tr>
</thead>
<tbody>
<tr>
<td>TQA Wiki</td>
<td>61,888</td>
<td>7,993</td>
<td>7,701</td>
</tr>
<tr>
<td>TQA Web</td>
<td>528,979</td>
<td>68,621</td>
<td>65,059</td>
</tr>
<tr>
<td>MRQA</td>
<td>616,819</td>
<td>58,221</td>
<td>9,633</td>
</tr>
</tbody>
</table>

**Table 4.1:** Data statistics for TriviaQA and MRQA.

We evaluate two methods building textual-knowledge enriched representations for QA differing in the pretraining approach used:

**TEK\textsubscript{PF}**  Our full approach TEK\textsubscript{PF} consists of two stages: (a) 200K steps of TEK-pretraining on Wikipedia starting from the RoBERTa checkpoint, and (b) finetuning and doing inference on RC-contexts augmented with TEK background.

**TEK\textsubscript{F}**  TEK\textsubscript{F} replaces the first specialized pretraining stage in TEK\textsubscript{PF} with 200K steps for standard single-document-context pretraining for a fair comparison with TEK\textsubscript{PF}, but follows the same finetuning regimen.

The subscripts \textsubscript{P} and \textsubscript{F} stand for pretraining and finetuning, respectively.

### 4.2 Experimental Setup

We perform experiments on TriviaQA and MRQA, two large extractive question answering benchmarks (see Table 4.1 for dataset statistics).

**TriviaQA** TriviaQA [Joshi et al. 2017] contains trivia questions paired with evidence collected via entity linking and web search. The dataset is *distantly supervised* in that the answers are contained in the evidence but the context may not support answering the questions. We experiment with both the Wikipedia and Web tasks. For further details on dataset processing, we refer the reader to Joshi et al. [2020b]

**MRQA** The MRQA shared task [Fisch et al. 2019] consists of several widely used QA datasets unified into a common format aimed at evaluating out-of-domain generalization. The data consists of a training set, in-domain and out-of-domain dev sets, and a private out-of-domain test set. The training and the in-
domain dev sets consist of modified versions of corresponding sets from SQuAD [Rajpurkar et al. 2016], NewsQA [Trischler et al. 2017], SearchQA [Dunn et al. 2017], TriviaQA Web [Joshi et al. 2017], HotpotQA [Yang et al. 2018] and Natural Questions [Kwiatkowski et al. 2019]. The out-of-domain test evaluation, including access to questions and passages, is only available through Codalab. Due to the complexity of our system which involves entity linking and retrieval, we perform development and model selection on the in-domain dev set and treat the out-of-domain dev set as the test set. The out-of-domain set we evaluate on has examples from BioASQ [Tsatsaronis et al. 2015], DROP [Dua et al. 2019], DuoRC [Saha et al. 2018], RACE [Lai et al. 2017], RelationExtraction [Levy et al. 2017], and TextbookQA [Kembhavi et al. 2017].

4.2.1 Baselines

We compare TEK\(_{PF}\) and TEK\(_{F}\) with two baselines, RoBERTa and RoBERTa++. Both use the same architecture as our approach, but use only original RC-contexts for finetuning and inference, and use standard single-document-context RoBERTa pretraining. TEK\(_{PF}\) and TEK\(_{F}\) use \(N_C = 384\) and \(N_B = 128\), while both baselines use \(N_C = 512\) and \(N_B = 0\).

**RoBERTa** We finetune the model on QA data without knowledge augmentation starting from the same RoBERTa checkpoint that is used as an initializer for TEK-augmented pretraining.

**RoBERTa++** For a fair evaluation of the new TEK-augmented pretraining method while controlling for the number of pretraining steps and other hyperparameters, we extend RoBERTa’s pretraining for an additional 200K steps on single contiguous blocks of text (without background information). We use the same masking and other hyperparameters as in TEK-augmented pretraining. This pretrained checkpoint is also used to initialize parameters for our TEK\(_{F}\) approach.

4.3 Results

**TriviaQA** Table 4.2 compares our approaches with baselines and previous work. The 12-layer variant of our RoBERTa baseline outperforms or matches the performance of several previous systems including ELMo-based ones [Wang et al. 2018; Lewis 2018] which are specialized for this task. We also see that
<table>
<thead>
<tr>
<th></th>
<th>TQA Wiki EM</th>
<th>TQA Wiki F1</th>
<th>TQA Web EM</th>
<th>TQA Web F1</th>
</tr>
</thead>
<tbody>
<tr>
<td>Previous work</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Clark and Gardner</td>
<td>64.0</td>
<td>68.9</td>
<td>66.4</td>
<td>71.3</td>
</tr>
<tr>
<td>Weissenborn et al.</td>
<td>64.6</td>
<td>69.9</td>
<td>67.5</td>
<td>72.8</td>
</tr>
<tr>
<td>Wang et al.</td>
<td>66.6</td>
<td>71.4</td>
<td>68.6</td>
<td>73.1</td>
</tr>
<tr>
<td>Lewis</td>
<td>67.3</td>
<td>72.3</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>This work</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>RoBERTa (Base)</td>
<td>66.7</td>
<td>71.7</td>
<td>77.0</td>
<td>81.4</td>
</tr>
<tr>
<td>RoBERTa++ (Base)</td>
<td>68.0</td>
<td>72.9</td>
<td>76.8</td>
<td>81.4</td>
</tr>
<tr>
<td>TEK$_F$ (Base)</td>
<td>70.0</td>
<td>74.8</td>
<td>78.2</td>
<td>83.0</td>
</tr>
<tr>
<td>TEK$_PF$ (Base)</td>
<td>71.2</td>
<td>76.0</td>
<td>78.8</td>
<td>83.4</td>
</tr>
<tr>
<td>RoBERTa (Large)</td>
<td>72.3</td>
<td>76.9</td>
<td>80.6</td>
<td>85.1</td>
</tr>
<tr>
<td>RoBERTa++ (Large)</td>
<td>72.9</td>
<td>77.5</td>
<td>81.1</td>
<td>85.5</td>
</tr>
<tr>
<td>TEK$_F$ (Large)</td>
<td>74.1</td>
<td>78.6</td>
<td>82.2</td>
<td>86.5</td>
</tr>
<tr>
<td>TEK$_PF$ (Large)</td>
<td>74.6</td>
<td>79.1</td>
<td>83.0</td>
<td>87.2</td>
</tr>
</tbody>
</table>

Table 4.2: Test set performance on TriviaQA.

RoBERTa++ outperforms RoBERTa, indicating that despite large scale pretraining, there is still room for improvement by simply pretraining for more steps on task-domain relevant text.

Furthermore, the 12-layer and 24-layer variants of our TEK$_F$ approach considerably improve over a comparable RoBERTa++ baseline for both Wikipedia (1.9 and 1.1 F1 respectively) and Web (1.6 and 1.0 F1 respectively) indicating that TEK representations are useful even without additional TEK-pretraining. The base variant of our best model TEK$_PF$, which uses TEK-pretrained TEK-enriched representations records even bigger gains of 3.1 F1 and 2.0 F1 on Wikipedia and Web respectively over a comparable 12-layer RoBERTa++ baseline. The 24-layer models show similar trends with improvements of 1.6 F1 and 1.7 F1 over RoBERTa++.

MRQA Table 4.3 shows in-domain and out-of-domain evaluation on MRQA. As in the case of TriviaQA, the 12-layer variants of our RoBERTa baselines are competitive with previous work, which includes D-Net [Li et al. 2019] and Delphi [Longpre et al. 2019], the top two systems of the MRQA shared task, while the 24-layer variants considerably outperform the current state of the art across all datasets. RoBERTa++ again performs better than RoBERTa on all datasets except DROP and RACE. DROP is designed to test arithmetic reasoning, while RACE contains (often fictional and thus not groundable to
Table 4.3: In-domain and out-of-domain performance (F1) on MRQA. RE refers to the Relation Extraction dataset. MRQA-Out refers to the averaged out-of-domain F1.

Wikipedia) passages from English exams for middle and high school students in China. The performance drop after further pretraining on Wikipedia could be a result of multiple factors including the difference in style of required reasoning or content; we leave further investigation of this phenomenon for future work. The base variants of TEK\(_F\) and TEK\(_{PF}\) outperform both baselines on all other datasets. Comparing the base variant of our full TEK\(_{PF}\) approach to RoBERTa++, we observe an overall improvement of 1.6 F1 with strong gains on BioASQ (4.2 F1), DuoRC (2.0 F1), and TextbookQA (2.0 F1). The 24-layer variants of TEK\(_{PF}\) show similar trends with improvements of 2.1 F1 on BioASQ, 1.1 F1 on DuoRC, and 1.6 F1 on TextbookQA. Our large models see a reduction in the average gain mostly due to drop in performance on DROP. Like in the case of TriviaQA, TEK-pretraining generally improves performance even further where TEK-finetuning is useful (with the exception of DuoRC which sees a small loss of 0.24 F1 due to TEK-pretraining for the large model\(^3\)), with the biggest gains seen on BioASQ.

Takeaways Both TEK\(_{PF}\) and TEK\(_F\) record strong gains on benchmarks that focus on factual reasoning outperforming the RoBERTa-based baselines that use only RC-contexts. The success of TEK\(_F\) underscores the advantage of *textual* encyclopedic knowledge in that it improves current models even without additional TEK-pretraining. Finally, TEK-pretraining further improves the model’s ability to use the retrieved

\(^3\) According to the Wilcoxon signed rank test of statistical significance, the large TEK\(_{PF}\) is significantly better than TEK\(_F\) on BioASQ and TextbookQA p-value < .05, and is not significantly different from it for DuoRC.
### Table 4.4: Development set F1 on TriviaQA and MRQA for base models using different combinations of pretraining and finetuning. Metrics are average F1 over 3 random finetuning seeds.

<table>
<thead>
<tr>
<th>Pretraining</th>
<th>Finetuning</th>
<th>Wiki</th>
<th>Web</th>
<th>MRQA</th>
</tr>
</thead>
<tbody>
<tr>
<td>Context-O</td>
<td>Context-O</td>
<td>72.8</td>
<td>81.2</td>
<td>83.2</td>
</tr>
<tr>
<td>Context-O</td>
<td>TEK</td>
<td>74.2</td>
<td>82.4</td>
<td>83.4</td>
</tr>
<tr>
<td>TEK</td>
<td>Context-O</td>
<td>72.9</td>
<td>81.6</td>
<td>83.3</td>
</tr>
<tr>
<td>TEK</td>
<td>TEK</td>
<td>75.1</td>
<td>82.8</td>
<td>83.7</td>
</tr>
</tbody>
</table>

### Table 4.5: F1 on TriviaQA and MRQA dev sets for varying lengths of context ($N_C$) and background ($N_B$).

<table>
<thead>
<tr>
<th>$N_C$</th>
<th>$N_B$</th>
<th>Wiki</th>
<th>Web</th>
<th>MRQA</th>
</tr>
</thead>
<tbody>
<tr>
<td>384</td>
<td>0</td>
<td>72.4</td>
<td>80.4</td>
<td>83.0</td>
</tr>
<tr>
<td>512</td>
<td>0</td>
<td>72.8</td>
<td>81.2</td>
<td>83.2</td>
</tr>
<tr>
<td>384</td>
<td>128</td>
<td>74.2</td>
<td>82.4</td>
<td>83.4</td>
</tr>
<tr>
<td>256</td>
<td>256</td>
<td>73.6</td>
<td>82.2</td>
<td>83.3</td>
</tr>
<tr>
<td>128</td>
<td>384</td>
<td>68.1</td>
<td>79.5</td>
<td>81.7</td>
</tr>
</tbody>
</table>

4.4 Ablation Studies

**Comparing TEK Pretraining and Context-only Pretraining** We also compare the two pretraining setups for models which do not use background knowledge to form representations for the finetuning tasks. Table 4.4 shows results for all four combinations of the pretraining and finetuning method variables, using 12-layer base models on the development sets of TriviaQA and MRQA (in-domain). Comparing rows 1 and 3, we see marginal gains across all datasets for TEK pretraining indicating that pretraining with encyclopedic knowledge does not hurt QA performance even when such information is not available during finetuning and inference. While previous work [Liu et al., 2019c; Joshi et al., 2020a] has shown that pretraining with single contiguous chunks of text clearly outperforms BERT’s bi-sequence pipeline[^4] our results suggest that using background sentences from other documents during pretraining has no adverse effect on the downstream tasks we consider.

**Trade-off between Document Context and Knowledge** Our approach incorporates textual knowledge by using a part of the Transformer window for it, instead of additional context from the same document.

[^4]: BERT randomly samples the second sequence from a different document in the corpus with a probability of 0.5.
Having established the usefulness of the background knowledge even without tailored pretraining, we now consider the trade-off between neighboring context and retrieved knowledge (Table 4.5). We first compare using a shorter window of 384 tokens for RC-contexts with using 512 tokens for RC-contexts (the first two rows). Using longer document context results in consistent gains, some of which our TEK-enriched representations need to sacrifice. We then consider the trade-off for varying values of context length $N_C$ and background length $N_B$ (rows 2-5). The partitioning of 384 tokens for context and 128 for background outperforms other configurations. Moreover, adding up to 256 tokens of background knowledge improves performance over using only document context. This suggests that relevant encyclopedic knowledge from outside of the current document is more useful than long-distance neighboring text from the same document for these benchmarks.

**Choice of the Entity Linker**  Table 4.6 compares the performance of TEK$_{PF}$ when used with publicly available entity linkers, Google Cloud Natural Language API (abbreviated as GC$^5$ and TagMe Ferragina and Scaiella [2010]. Using TagMe results in a minor drop of around 0.3 F1 from TEK$_{PF}$ across benchmarks while still maintaining major gains over RoBERTa++. The results indicate that the choice of entity linker can make a difference but our method is robust and performs well with multiple linkers.

### 4.5 Discussion

When are TEK-enriched representations most useful for question answering? Across all evaluation benchmarks, the strongest gains are on TriviaQA, BioASQ, and TextbookQA. All three datasets involve questions targeting the long tail of factual information, which has sizable coverage in Wikipedia, the encyclopedic

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*Table 4.6: Performance (F1) of 12-layer TEK$_{PF}$ when used with publicly available entity linkers on TriviaQA test sets and MRQA in (In) and out-of-domain (Out).*

<table>
<thead>
<tr>
<th></th>
<th>Wiki</th>
<th>Web</th>
<th>In</th>
<th>Out</th>
</tr>
</thead>
<tbody>
<tr>
<td>RoBERTa++</td>
<td>71.7</td>
<td>81.4</td>
<td>83.2</td>
<td>68.4</td>
</tr>
<tr>
<td>TEK$_{PF}$</td>
<td>76.0</td>
<td>83.4</td>
<td>83.7</td>
<td>70.0</td>
</tr>
<tr>
<td>TEK$_{PF}$-GC</td>
<td>75.4</td>
<td>83.0</td>
<td>83.6</td>
<td>69.4</td>
</tr>
<tr>
<td>TEK$_{PF}$-TagMe</td>
<td>75.6</td>
<td>83.1</td>
<td>83.7</td>
<td>69.7</td>
</tr>
</tbody>
</table>

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*https://cloud.google.com/natural-language/docs/basics#entity analysis*
collection we use. We hypothesize that enriching representations with encyclopedic knowledge could be particularly useful when factual information that might be difficult to “memorize” during pretraining is important. Current pretraining methods are able to store a significant amount of world knowledge into model parameters [Petroni et al., 2019]; this might enable the model to make correct predictions even from contexts with complex phrasing or partial information. TEK-enriched representations complement this strength.

---

**Question:** Which river originates in the Taurus Mountains, and flows through Syria and Iraq?

**Our Answer:** Euphrates

**Baseline Answer:** Tigris

**Context:** The Southeastern Taurus mountains form the northern boundary... They are also the source of the Euphrates River and Tigris River.

**Background:** Originating in eastern Turkey, the Euphrates flows through Syria and Iraq to join the Tigris...

---

**Question:** What tyrosine kinase, involved in a Philadelphia- chromosome positive chronic myelogenous leukemia, is the target of Imatinib (Gleevec)?

**Our Answer:** BCR-ABL

**Baseline Answer:** imatinib

**Context:** Imatinib induces a durable response in most patients with Philadelphia chromosome-positive chronic myeloid leukemia...We show that the only hypothesis consistent with current data on ... gradual decrease in the BCR-ABL levels seen in most patients is that these patients exhibit a continual, gradual reduction of the LSCs. This observation may explain the ability to discontinue imatinib therapy without relapse in some cases.

**Background:** Chronic myelogenous leukemia : A 2006 follow up of 553 patients using imatinib (Gleevec) found an overall survival rate of 89% after five years. With improved understanding of the nature of the BCR-ABL protein and its action as a tyrosine kinase, targeted therapies (the first of which was imatinib) that specifically inhibit the activity of the BCR-ABL protein have been developed.

---

**Question:** Who did Germany defeat to win the 1990 FIFA World Cup?

**Our Answer:** Argentina

**Baseline Answer:** Italy

**Context:** At the 1990 World Cup in Italy, West Germany won their third World Cup title, defeating Yugoslavia (4-1), UAE on the way to a final rematch against Argentina.

**Background:** At international level, He is best known for scoring the winning goal for Germany in the 1990 FIFA World Cup Final against Argentina...

---

**Question:** The state in which matter takes on the shape but not the volume of its container is?

**Our Answer:** Liquid

**Baseline Answer:** gas

**Context:** Liquid takes the shape of its container. You could put the same volume of liquid in containers with different shapes. The shape of the liquid in the beaker is short and wide like the beaker, while the shape of the liquid in the graduated cylinder is tall and narrow like that container, but each container holds the same volume of liquid... How could you show that gas spreads out to take the volume as well as the shape of its container?

**Background:** Liquid : As such, it is one of the four fundamental states of matter is the only state with a definite volume but no fixed shape.

---

**Figure 4.3:** The first two examples (from TriviaQA and BioASQ) have background knowledge that provides information complementary to the context, while the last two (from TriviaQA and TextbookQA) provides a more direct, yet redundant, phrasing of the information need compared to the original context.
via dynamic retrieval of factual knowledge. Finally, improvements on the science-based datasets BioASQ and TextbookQA further suggest that Wikipedia can be used as a *bridge corpus* for more effective domain adaptation for QA.

For 75% of the examples in the TriviaQA Wikipedia development set where our approach outperforms the context-only baselines, the answer string is mentioned in the background text. A qualitative analysis of these examples indicates that the retrieved background information typically falls into two categories – (a) where the background helps disambiguate between multiple answer candidates by providing partial pieces of information missing from the original context, and (b) where the background sentences help by providing a redundant but more direct phrasing of the information need compared to the original context. Figure 4.3 provides examples of each category.

Even when the retrieved background contains the answer string, our model uses the background only to refine representations of the candidate answers in the original document context; possible answer positions in the background are not considered in our model formulation. This highlights the strength of an encoder with full cross-attention between RC-contexts and background knowledge. The encoder is able to build representations for, and consider possible answers in all document passages, while integrating knowledge from multiple pieces of external textual evidence.

The exact form of background knowledge is dependent on the retrieval function. Our results have shown that contextualizing the input with textual background knowledge, especially after suitable pretraining, improves state of the art methods even with simple entity linking and *ngram*-match retrieval functions. We hypothesize that more sophisticated retrieval methods could further significantly improve performance (for example, by prioritizing for more complementary information).

### 4.6 Related Work

**Background Knowledge Integration** Many NLP tasks require the use of multiple kinds of background knowledge [Fillmore 1976; Minsky 1986]. Earlier work [Ratinov and Roth 2009; Nakashole and Mitchell 2015] combined features over the given task data with hand-engineered features over knowledge repositories. Other forms of external knowledge include relational knowledge between word or entity pairs, typically integrated via embeddings from structured knowledge graphs (KGs) [Yang and Mitchell 2017; Bauer et al. 2015].
Wang and Jiang [2019] or via word pair embeddings trained from text Joshi et al. [2019a]. Weissenborn et al. [2017] used a specialized architecture to integrate background knowledge from ConceptNet and Wikipedia entity descriptions. For open-domain QA, recent works Sun et al. [2019a]; Xiong et al. [2019] jointly reasoned over text and KGs, via specialized graph-based architectures for defining the flow of information between them. These methods did not take advantage of large scale unlabeled text to pre-train deep contextualized representations which have the capacity to encode even more knowledge in their parameters.

Most relevant to ours is work building upon these powerful pretrained representations, and further integrating external knowledge. Recent work focuses on refining pretrained contextualized representations using entity or triple embeddings from structured KGs Peters et al. [2019]; Yang et al. [2019a]; Zhang et al. [2019b]. The KG embeddings are trained separately (often to predict links in the KG), and knowledge from KG is fused with deep Transformer representations via special-purpose architectures. Some of these prior works also pre-train the knowledge fusion layers from unlabeled text through self-supervised objectives Zhang et al. [2019b]; Peters et al. [2019]. Instead of separately encoding structured KBs, and then attending to their single-vector embeddings, we explore directly using wider-coverage textual encyclopedic background knowledge. This enables direct application of a pretrained deep Transformer (RoBERTa) for jointly contextualizing input text and background knowledge. We showed background knowledge integration can be further improved by additional knowledge-augmented self-supervised pretraining.

Liu et al. [2019a] augment text with relevant triples from a structured KB. They process triples as word sequences using BERT with a special-purpose attention masking strategy. This allows the model to partially re-use BERT for encoding and integrating the structured knowledge. Our work uses wider-coverage textual sources instead and shows the power of additional knowledge-tailored self-supervised pretraining.

**Question Answering** For open-domain QA, where documents known to answer the question are not given as input (e.g. OpenBookQA Mihaylov et al. [2018]), methods exploring retrieval of relevant textual knowledge are a necessity. Recent work in these areas has focused on improving the evidence retrieval components Lee et al. [2019]; Banerjee et al. [2019]; Guu et al. [2020], and has used Wikidata triples with textual descriptions of Wikipedia entities as a source of evidence Min et al. [2019]. Other approaches use pseudo-relevance feedback (PRF) Xu and Croft [1996] style multi-step retrieval of passages by query reformulation Buck et al.
[2018]; Nogueira and Cho [2017], entity linking Das et al. [2019b], and more complex reader-retriever interaction Das et al. [2019a]. When multiple candidate contexts are retrieved for open-domain QA, they are sometimes jointly contextualized using a specialized architecture Min et al. [2019]. We are the first to explore pretraining of representations which can integrate background from multiple documents, and hypothesize that these representations could be further improved by more sophisticated retrieval approaches.

4.7 Conclusion

We presented a method to build text representations by jointly contextualizing the input with dynamically retrieved textual encyclopedic knowledge. We showed consistent improvements, in- and out-of-domain, across multiple reading comprehension benchmarks that require factual reasoning and knowledge well represented in the background collection.
Gathering high-quality training data has been one of the most reliable ways of achieving empirical progress for a range of natural language processing tasks. However, creating natural language training data often involves significant human effort – in carefully designing the data collection tasks as well as getting contributors to perform them. The complexity of this process in turn drives up the cost of creating training data. In this paper, we mine naturally-occurring examples from large corpora using supervision from a small seed set of only 100 labeled examples.

Our method provides a way to collect more training data using very few labeled examples, and allows for more direct control over what the model learns compared to relatively brittle prompts [Lu et al. 2021]. Yet, unlike model generated data augmentation, we mine high-quality human-authored data which is less susceptible to the limitations of synthetic data. While similar unsupervised methods have been used for mining parallel data for machine translation [Tran et al. 2020], we show that they can be extended to other tasks using minimal human supervision.

One of the main challenges in mining high-quality data is the large search space which could be quadratic in the size of the corpora as inputs and outputs could be spread across multiple documents. Our approach consists of a two-stage pipeline which first mines data efficiently from large corpora and then filters out low-quality examples. More specifically, we use supervision from an initial seed set and train a dot-product...
Summary: The Scottish city of Edinburgh is looking to crack down on so-called "silent disco" walking tours as residents complain they make too much noise.

Passage: Silent disco tours in Edinburgh are 'too loud' and could face clampdown Silent discos in Edinburgh could be facing a clampdown - with locals upset that the crowds of boogying tourists are too loud. The "discos" involve people wearing their own headphones and dancing along as they follow a guided walking tour of the Scottish capital’s most famous spots. ...

Question: How long does it take for a crab to get full grown?

Passage: 10-13 moults the crab will reach maturity. This usually takes 3-4 years, but when food is limited it can take longer to reach maturity.

**Figure 5.1:** Examples of mined input output pairs for summarization and reading comprehension. Answer spans are indicated via italics.

similarity function over separately encoded fixed length dense representations of inputs and outputs (i.e. a dual-encoder or a biencoder). This function efficiently searches top-k candidate outputs (e.g. summary sentences) for each candidate input (e.g. news document) from the output corpus. We refer to this stage as coarse-grained search. It relies on maximal inner product search (MIPS) over dense encodings on inputs and outputs for efficiency. The initial list of paired inputs and outputs from this stage is geared towards recall and often contains examples with subtle errors. For example, it might link a document about World Cup 2006 with a summary sentence about World Cup 2010.

We further train a precision-oriented crossencoder-based filter which re-ranks the output of the first stage for better quality control. The crossencoder is trained using positive samples from the original seed set and negative examples from the coarse-grained stage. Jointly encoding inputs and outputs provides fine grained interaction between them. The crossencoder is able to filter out more subtle errors such as the one described earlier to give a high quality mined dataset set.

We apply our method to reading comprehension and summarization gathering high quality question-answer-passage and document-summary tuples respectively. The supervision from the small seed set helps embed relevant outputs closer to inputs across corpora for each task. This is in contrast to MT where cross-lingual cosine similarity functions are readily available without additional human supervision since self-supervised pre-training embeds sentences across languages in the same space.

Our method is able to add up to 5x as many examples as the seed set. On SQuAD [Rajpurkar et al. 2016], augmenting the seed set with the mined data results in an improvement of 13 F1 over a BART-large [Lewis et al. 2020b] baseline fine-tuned only on the seed set. Likewise, we see improvements of 1.46 ROUGE-L on XSum abstractive summarization [Narayan et al. 2018]. Our analysis shows that, compared
5.1 Mining

We describe our general pipeline for mining examples, and then describe how it is applied to reading comprehension and summarization. We assume access to a small labeled seed set of 100 examples which can be used to train components of the pipeline. The final output is a (ranked) list of input output pairs which can be augmented to the original seed set to train better-performing models.

The key idea consists of a two stage approach for mining input output pairs \((x, y)\) from their respective corpora \(C_x\) and \(C_y\) – (a) a coarse-grained but efficient similarity function which retrieves top-k similar candidates from \(C_y\) for every \(x \in C_x\) and (b) a fine-grained filtering stage which reranks top scoring candidate pairs mined in the first stage.

5.1.1 Coarse-grained Search

The coarse grained search relies on dense retrieval to construct a candidate list of input-output pairs. We first train a function \(f_c(\cdot, \cdot)\) to maximize similarity between input output pairs in the seed data, and then use the similarity function to mine the candidate input output pairs.
Training Coarse-grained Similarity

The aim is to create a vector space where the similarity between relevant input output pairs is higher than that between irrelevant pairs. Specifically, we use cosine similarity as our similarity function to enable efficient mining (Section 5.1.1).

**Objective**  Let \( D = \{(x_i, y_i^+, y_{i,1}^- \ldots y_{i,n}^-)\}_{i=1}^{m} \) be the training data that consists of \( m \) seed instances. Each instance contains one input \( x_i \) and one output \( y_i^+ \) along with \( n \) sampled negative outputs \( y_{i,*}^- \). Our biencoder first encodes inputs and outputs separately as \( x_* \) and \( y_* \). The training objective maximizes the negative log likelihood of the positive output.

\[
L(x_i, y_i^+; y_{i,1}^- \ldots y_{i,n}^-) = \frac{e^{x_i \cdot y_i^+}}{e^{x_i \cdot y_i^+} + \sum_{j=1}^{n} e^{x_i \cdot y_{i,j}^-}}
\]

We use in-batch negatives along with randomly sampled sentences from the output corpus to construct \( y_{i,*}^- \).

**Mining Candidate Pairs**

To mine input output pairs, we follow previous work on unsupervised machine translation and employ the margin function formulation Artetxe and Schwenk [2019]; Tran et al. [2020] based on K nearest neighbors (KNN). Let \( x \) and \( y \) be the vector representations of a candidate input output pair \((x, y)\). We score the “similarity” of \( x \) and \( y \) using a ratio margin function defined as the following.

\[
\text{score}(x, y) = \frac{\cos(x, y)}{\sum_{z \in N_x} \cos(x, z) + \sum_{z \in N_y} \cos(z, y)}
\]

where \( N_x \) is the KNN neighborhood of \( x \) in \( C_y \), the corpus of \( y \); and \( N_y \) is the KNN neighborhood of \( y \) in \( C_x \). The margin scoring function is interpreted as a cosine score normalized by average distances to the margin regions established by the KNN neighborhoods of the input and outputs. The KNN distance metrics are defined by \( \cos(x, y) \). The margin score is designed to take into account scale inconsistencies in cosine similarity, and has been shown to perform better than approaches which use a hard threshold over cosine similarity. We use the distributed dense vector similarity search library FAISS Johnson et al. [2019].
to search for all neighborhoods efficiently.

5.1.2 Fine-grained Filtering

We found the quality of the biencoder-mined data to be rather low for summarization and reading comprehension. Intuitively, separate encoding of inputs and outputs combined with cosine based scoring makes it much harder to control characteristics like abstraction for summarization. The fine grained filtering stage re-ranks the outputs of the previous stage using a crossencoder based ranking function to remove noisy input-output pairs. A crossencoder jointly encodes the input and output text enabling more fine grained interaction between them. Specifically, we encode a pair \((x, y)\) as sequence \([CLS]\ x [SEP]\ y [SEP]\) where \([CLS]\) and \([SEP]\) are special tokens indicating beginning and end of sequences. The same input is fed into the encoder and decoder. The pair is scored using a 2-layer MLP on top of the final hidden state of the final decoder token. A more detailed comparison of the data obtained from the two stages is presented in Section 5.5.

5.2 Application to Tasks

One of the main challenges in mining data is the scale of web corpora. In this section, we describe additional techniques which make our method scalable when applied to downstream tasks.

5.2.1 Reading Comprehension

Inputs and Outputs  For reading comprehension, the input sequence \(X\) consists of the question and the output sequence \(Y\) consists of a concatenation of the answer and the passage. Our input corpus consists of 20M random questions crawled from the popular community QA website answers.com. The output corpus consists of passages from Wikipedia with named entities\(^1\) as candidate answers resulting in 200M passage-answer pairs. Our input and output corpora were chosen to match the downstream evaluation data from SQuAD.

\(^1\)We use spaCy NER.
**Binary Classifier** To mitigate noise in the question corpus and to reduce the search space, we multitask a binary classifier with the biencoder to filter out questions which don’t look like those in SQuAD. The binary classifier is trained using questions from the seed set as positive examples with negatives sampled from the question corpus.

Furthermore, for faster processing, we filter out examples from the coarse grained stage, where the answer spans are found verbatim in the question. Finally, while fine-tuning using mined (and seed) data, we add a special token to the input document indicating the provenance of the example.

### 5.2.2 Summarization

**Inputs and Outputs** For summarization, the input sequence $X$ consists of the document and the output sequence $Y$ consists of the summary. The input corpus consists of documents from CC-News; we remove documents with less than four sentences to reduce noise. The output corpus consists of sentences from the same corpus. Following MARGE [Lewis et al.]\(^[2020a]\), we divide CC-News into shards based on document publishing dates, and restrict the space of candidate summaries for a given document to be from the same shard.

**Binary Classifier** Like reading comprehension, we multitask a binary classifier with the biencoder to remove sentences which don’t resemble XSum summaries. This allows us to filter out more than 80% of the sentences and makes the biencoder based mining a lot more scalable.

Finally, for faster processing, we filter out examples from the coarse grained stage, where the summary sentences are found verbatim in the document. Put together, this allows use to efficiently search over 40M documents and 550M sentences.

### 5.3 Experiments

#### 5.3.1 Benchmarks

We perform experiments on SQuAD v1.1 for reading comprehension and XSum for summarization – two competitive benchmarks which are used to evaluate state of the art pre-trained models. For each dataset, we randomly pick 100 examples from the training set as our seed set; we call this subset $X_{100}$. 

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<table>
<thead>
<tr>
<th>Method</th>
<th>EM</th>
<th>F1</th>
</tr>
</thead>
<tbody>
<tr>
<td>BART</td>
<td>35.27</td>
<td>49.43</td>
</tr>
<tr>
<td>Us</td>
<td>49.39</td>
<td>62.5</td>
</tr>
</tbody>
</table>

Table 5.1: Performance on the SQuAD dev set after training on 100 examples.

<table>
<thead>
<tr>
<th>Method</th>
<th>R-1</th>
<th>R-2</th>
<th>R-L</th>
</tr>
</thead>
<tbody>
<tr>
<td>BART</td>
<td>36.28</td>
<td>14.07</td>
<td>27.98</td>
</tr>
<tr>
<td>Us</td>
<td>37.67</td>
<td>14.86</td>
<td>29.44</td>
</tr>
<tr>
<td>BART*</td>
<td>35.17</td>
<td>13.29</td>
<td>27.20</td>
</tr>
<tr>
<td>WikiTransfer*</td>
<td>37.26</td>
<td>14.20</td>
<td>28.85</td>
</tr>
<tr>
<td>Pegasus*</td>
<td>39.07</td>
<td>16.44</td>
<td>31.27</td>
</tr>
</tbody>
</table>

Table 5.2: Performance on the XSum test set after training on 100 examples. Both BART and Us use the same training examples. * indicates that results have been taken from Fabbri et al. [2021]

SQuAD SQuAD Rajpurkar et al. [2016] is an extractive reading comprehension benchmark containing Wikipedia passages and crowdsourced questions.

Xsum Xsum Narayan et al. [2018] is an abstractive news summarization dataset collected by harvesting online articles from the British Broadcasting Corporation (BBC).

5.3.2 Baselines

BART Our main baseline for each dataset is a BART model fine-tuned on $X_{100}$ and is referred to as BART in the subsequent tables.

For summarization, we also compare our method to WikiTransfer Fabbri et al. [2021] and Pegasus Zhang et al. [2020] – both of which use data augmentation techniques tailored towards summarization.

WikiTransfer WikiTransfer uses an intermediate finetuning stage with 400K synthetic examples from Wikipedia along with additional auxiliary losses before finetuning on Xsum.

Pegasus Pegasus, a self-supervised pretraining method, simulates the summarization tasks during pretraining by masking (and then generating) important heuristically identified sentences from documents.
Figure 5.3: Performance (ROUGE-L) on the XSum dev set of various augmentation techniques with varying amounts of augmented data added to $X_{100}$.

5.3.3 Main Results

SQuAD Table 5.1 shows our performance on the SQuAD v1.1 dev set. The BART baseline reaches an F1 of 48.86; adding 500 mined examples gives us a boost of 13 F1 points.

XSum Table 5.2 shows our performance on the Xsum test set. Augmenting the 100 example training set with 500 mined examples increases the ROUGE-L score of the fine-tuned BART baseline from 27.98 (BART) to 29.44 (Us).

BART* refers to BART results taken from WikiTransfer\footnote{Our gains over the BART baseline are comparable to WikiTransfer despite using only 500 augmented examples indicating that our examples are high-quality. It is harder to make more direct controlled comparisons to Pegasus which uses a larger model and a tailored pre-training scheme compared to BART.}

Our approach is complementary to both WikiTransfer and Pegasus; in contrast to pre-training (or intermediate fine-tuning) on synthetic or heuristic-collected examples, we focus on mining fewer high quality examples aimed at mirroring the seed set so that they can be used directly during finetuning instead of pre-training.

\footnote{We posit that our numbers for BART are slightly higher due to a different seed set.}
Figure 5.4: Performance (F1) on the SQuAD dev set of various augmentation techniques with varying amounts of augmented data added to $X_{100}$.

5.4 Ablations

In this section, we investigate the impact of each part of our pipeline and compare it to model-generated data augmentation (Figures 5.3 and 5.4). All methods involve fine-tuning BART on the same seed set plus the exact same number of augmented examples, but differ on the source of the augmented data.

**Gold** The Gold method augments gold examples sampled uniformly at random from the full training set of each dataset.

**Full** Full refers to examples obtained by running our full pipeline including the fine-grained crossencoder stage.

**Biencoder** This refers to post-processed examples from the coarse-grained biencoder which are subsequently fed to the crossencoder (in our full model).

**Gen** Gen refers to self-training on model generated examples. Specifically, we take source documents (or answer passage pairs in case of reading comprehension) from the full/crossencoder stage and generate summaries (or questions) using the BART baseline trained on $X_{100}$. We then retrain the model by augmenting $X_{100}$ with the generated examples. This allows us to make a controlled comparison to the full model which uses naturally occurring mined examples.
5.4.1 Amount of Mined Data

For both SQuAD and XSum, we see an increase in performance for the Full model as we increase the number of mined examples up to 5x. There is still a considerable difference between our method and Gold indicating that there is still room for improvement in quality. We discuss these qualitative differences in Section 5.5.

5.4.2 Bi vs Crossencoder Differences

For SQuAD, input output pairs from the biencoder provide some improvement with 50 examples but performance quickly plateaus with more examples. For XSum, adding examples from the biencoder hurts performance. On the other hand, performance continues to improve until 5x examples from the crossencoder are added for both tasks. Section 5.5 contains a qualitative analysis of the bi and crossencoder examples.

5.4.3 Naturally Occurring vs. Model Generated Data

To show the value of mining naturally occurring data, we compare our method to the Gen baseline described in Section 5.4. For both XSum and SQuAD, adding model-generated examples provides some gains over BART, but performance quickly degrades with more examples. While model generated data augmentation has been shown to help for QA [Alberti et al. 2019], our results suggest that it isn’t particularly useful when training data is limited.

5.5 Discussion

We conducted a case study of the top ranking examples from the bi and cross encoders for both SQuAD and XSum (Table 5.3).

5.5.1 XSum

After examining outputs from the bi and crossencoder, we found that both stages were generally able to match documents to sentences from the same news story, but with the sentences taken from a parallel document. Exceptions to this included cases where similar events (e.g. World Cup games) occurring over different
Summary: BERLIN (AP) — A 44-pound minute hand has fallen off a clock on a Hamburg church tower, plunging 130 feet onto the sidewalk below.

Document: Minute hand plunges from Hamburg church tower; no one hurt BERLIN (AP) — A 20-kilogram (44-pound) minute hand has fallen off a clock on a Hamburg church tower, plunging 40 meters (130 feet) onto the sidewalk below...

Summary: Blackpool’s three historic piers have been put on an international preservation list amid fears their future could be under threat from climate change.

Document: ...The council is now completing an action plan to work with the World Monuments Fund which was launched in 1996 with founding partner American Express and issues a list every two years. Blackpool is unique in being the only UK seaside resort with three piers...

Summary: NEW LONDON, Conn. (AP) — The U.S. Coast Guard Academy is now offering an academic program in cyber systems, its first new major in a quarter century.

Document: Coast Guard Academy to offer new major in cyber systems NEW LONDON, Conn. (AP) — The U.S. Coast Guard Academy is offering a new major in cyber systems. It’s the first new academic program at the school in New London since the addition of mechanical engineering as a major in 1993...

Summary: Holidaymakers are being reminded to drink responsibly at Gatwick Airport as an annual campaign to tackle disruptive passengers is launched.

Document: The force, working closely with the airport, its pubs and bars, and airlines, will carry out increased patrols as part of Operation Disrupt..."You could be refused carriage or sent on the next plane home if you are considered to be drunk, disorderly or disruptive...

Question: What is most times one actor has been nominated?
Answer/Passage: The actress has also been nominated five times (most

Question: Where was Jesus baptised?
Answer/Passage: He was baptised at St Jude’s

Question: When was Regina Lobiondo born?
Answer/Passage: Other notable appearances include a recurring role in L.A. Law, a regular role in the 1993 The Untouchables television series, and starring in the 1996 film It’s My Party. Regina was born on October 25, 1956, in Brooklyn, New York.

Question: When was Gouverneur Morris born?
Answer/Passage: ...Gouverneur Morris Jr. Gouverneur Morris II (February 9, 1813 August 20, 1888) was an American railroad executive...

Table 5.3: Mined examples from the bi and crossencoders. Answer spans are indicated in italics.
time frames. However, we found three clear differences which could explain why data from the crossencoder is more helpful. First, summaries from the crossencoder were more abstractive than the biencoder. We measured abstractiveness using ROUGE precision scores with respect to the source; higher scores being indicative of higher extractiveness and lower abstractiveness. ROUGE-1/2/L precision scores for the crossencoder summaries (64.91 / 15.42 / 55.59) were closer to the XSum validation (66.85 / 17.94 / 59.82) compared to those from the biencoder (82.21 / 51.66 / 75.92). Second, the distribution of topics and locations from the top ranked crossencoder documents better matched XSum with most stories centered around UK politics and sports. On the other hand, top ranked pairs from the biencoder were more diverse topically. Lastly, the summaries mined by the biencoder rarely matched the style of XSum and often contained source markers (e.g. CNN or AP News). Our analysis suggests that the biencoder uses word overlap as its primary signal for scoring document summary pairs while the crossencoder is able to focus on finer details.

5.5.2 SQuAD

We found mining high-precision QA pairs to be a much harder problem in part due to the large search space of over 200M (answer, passage) tuples. Like summarization, biencoder outputs for QA focused on word overlap which resulted in the retrieval of very short passages (see Table 5.3). While the crossencoder was more successful in selecting longer passages, we still found pairs with subtle errors. For example, for the question, “When was Regina Lobiondo born?”, the retrieved passage actually refers to Paul Regina and not Regina Lobiondo. We hypothesize the negative impact of such noise is mitigated in the reading comprehension setting where the given evaluation passage always answer the question. Another limitation of data from both stages was the lack of diversity in question types with a significant proportion of questions seeking date or numerical answers.

5.6 Related Work

**Data augmentation** Data augmentation is a popular technique with a large body of work Wang and Yang [2015]; Jia and Liang [2016] among others. Recent work has explored model generated data augmentation for a range of tasks including text classification Anaby-Tavor et al. [2020]; Schick and Schütze [2021a], question answering Alberti et al. [2019], common-sense reasoning Yang et al. [2020], and machine transla-
A common problem with model-generated data augmentation is the quality of the synthetic data. Attempts to remedy this have focused on variations of consistency [Xie et al. 2019] for a given task—such as round-trip consistency of question generation and answer prediction [Alberti et al. 2019]; [Puri et al. 2020] for QA or between source and targets in summarization [Fabbri et al. 2021]. Lee et al. [2021] focus on generating synthetic data for underrepresented or few-shot slices. Task augmentation [Vu et al. 2021] generates data in the target domain by using a model trained on the auxiliary task of natural language inference. In contrast, we focus on a general framework for mining naturally occurring data for multiple tasks using supervision from a small labeled seed set.

**Improving fine-tuning** Work in this area has looked at improving finetuning particularly for small datasets either via better optimization or by using auxiliary tasks. Careful design and hyperparameter choices have a significant impact on performance and stability in limited data settings [Mosbach et al. 2021]; [Zhang et al. 2019a]. Likewise, regularization based approaches have also been shown to improve performance [Jiang et al. 2020]; [Aghajanyan et al. 2020]. While we use lessons about careful design choices, our basic models use standard fine-tuning for simplicity. Efforts on the data side have focused on intermediate fine-tuning either by using unlabeled target domain data [Karouzos et al. 2021]; [Gururangan et al. 2020] or via labeled data from other tasks [Phang et al. 2018]; [Aghajanyan et al. 2021]; [Vu et al. 2020].

**Few-shot learning** GPT-3 [Brown et al. 2020] is perhaps the most prominent recent work in this area which shows that massive language models can perform a variety of tasks if prompted with few input output pairs. Other work has shown that good few-shot performance can also be obtained by combining gradient based optimization with textual prompts [Schick and Schütze 2021b]; [Gao et al. 2021]; [Tam et al. 2021]; [Wang et al. 2021]. Other work on pre-training focuses on tailored masking schemes such as recurrent span masking [Ram et al. 2021] for question answering and salient sentence masking for summarization [Zhang et al. 2020]. Our approach is complementary to this line of work in that it is agnostic to pre-training schemes or textual prompts, and focuses instead on supervised automated collection of high-quality data.
5.7 Conclusion

We presented a method to mine input output pairs from large corpora from supervision from a small seed set of labeled examples. We showed consistent improvements on XSum and SQuAD, two popular NLP benchmarks, from adding up to 5x examples to the seed set. Our analysis shows that, compared to model generated data, mined data better matches several characteristics of the gold data (e.g. abstractiveness in summarization).
Chapter 6

Conclusion

This thesis presents training paradigms for efficient self-supervised models centered around pre-training objectives, model scale, and new types of data. In the previous chapters, we presented work with the following goals: (a) designing efficient pre-training methods to capture linguistic and world knowledge, and (b) enabling better downstream performance with fewer human-labeled examples.

In Chapter 2, we discussed how designing the right kind of objective function can help encode knowledge about word pairs into word pair vectors. Our pair embeddings are computed as a compositional function of the individual word representations, which is learned by maximizing a variant of the PMI with the contexts in which the two words co-occur. Bouraoui et al. [2020] have suggested that BERT based models do an even better job at capturing word pair relations but there is still room for improvement. Other methods Levine et al. [2021] have considered using PMI-based masking schemes for BERT for more efficient pre-training.

In Chapter 3, we present SpanBERT, a scalable pre-training method to encode more diverse kinds of knowledge into model parameters. Our approach extends BERT by (1) masking contiguous random spans, rather than random tokens, and (2) training the span boundary representations to predict the entire content of the masked span, without relying on the individual token representations within it. Subsequent work on self-supervised NLP models, T5 Raffel et al. [2020] and BART Lewis et al. [2020b] has used span-based masking as a part of their sequence-to-sequence pre-training. Other works have looked at improving span representations for coreference resolution Gandhi et al. [2021] and other tasks Toshniwal et al. [2020].
Chapter 4 focuses integrating dynamically retrieved textual knowledge. Our method represents input texts by contextualizing them jointly with dynamically retrieved textual encyclopedic background knowledge from multiple documents. We apply our method to reading comprehension tasks by encoding questions and passages together with background sentences about the entities they mention. [Borgeaud et al., 2022] present a specialized architecture for integrating background about a given text without using entity-focused retrieval.

6.1 Future Work

On a more speculative note, we expect ideas from this thesis to drive work in the following directions.

**Retrieval Augmented NLP** Retrieval Augmented NLP has received considerable attention from the point of view of learning retrieval [Guu et al., 2020] as well as integration of retrieved text [Joshi et al., 2020b]. Yet most applications of retrieval focus on question answering and language modeling. Subsequent research could look at a more general framework for using retrieval for arbitrary NLP tasks. For example, news summarization is typically viewed as a task which does not need context beyond the provided document(s). Yet abstractive headlines often contain facts which aren’t directly mentioned in the given documents. Using retrieval in the loop could help models generate summaries which require such additional world knowledge [An et al., 2021]. We posit that a single retrieval in the loop framework for multiple NLP tasks could significantly improve the performance and adoption.

**Multimodal Pre-training** Recent work has looked at combining text and image data for pre-training a single model [Aghajanyan et al., 2022]. An area for subsequent research could look into expanding this in terms of both scale and modalities. In particular, modalities like text and video could provide more direct evidence for several kinds of knowledge which are often more implicit in text, e.g. common sense.

**Massively Multitasked Pre-training** The advent of large scale pre-training has also resulted the use of a common encoder-decoder architectures for almost all NLP tasks. This, combined with common data mining techniques (Chapter 5), presents an opportunity for massively multitasked pre-training. The goal of this line
of research would be to move towards common representations with improved few-shot performance across multiple NLP tasks.
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