Abstract

Recent approaches to Open-domain Question Answering refer to an external knowledge base using a retriever model, optionally rerank passages with a separate reranker model and generate an answer using another reader model. Despite performing related tasks, the models have separate parameters and are weakly-coupled during training. We propose casting the retriever and the reranker as internal passage-wise attention mechanisms applied sequentially within the transformer architecture and feeding computed representations to the reader, with the hidden representations progressively refined at each stage. This allows us to use a single question answering model trained end-to-end, which is a more efficient use of model capacity and also leads to better gradient flow. We present a pre-training method to effectively train this architecture and evaluate our model on the Natural Questions and TriviaQA open datasets. For a fixed parameter budget, our model outperforms the previous state-of-the-art model by 1.0 and 0.7 exact match scores.

1 Introduction

Open-domain Question Answering (Open QA) is a knowledge-intensive task that finds the answer for the given question from a large-scale knowledge corpus that can easily surpass millions of documents. Thus, how to store and refer to the knowledge at such scales is important in terms of both performance and scalability for Open QA systems. Traditional systems rely on information retrieval engines such as Lucene. These score the relevance of knowledge to a given query by lexical overlaps between them in a sparse representation space based on TF-IDF or BM25 (Chen et al., 2017; Wang et al., 2018; Yang et al., 2019). However, recent advances in neural language modeling have enabled two new lines of approach: 1) referring to internal knowledge parameterized in the model (Brown et al., 2020; Petroni et al., 2019; Roberts et al., 2020), and 2) referring to external knowledge retrieved by matching query and knowledge in dense representation spaces (Karpukhin et al., 2020; Lee et al., 2019; Guu et al., 2020; Lewis et al., 2020; Izacard and Grave, 2021b).

Despite the simplicity of the approach, parametric models have limitations such as a large number of model parameters that require large compute for both training and inference and non-expandable knowledge without re-training. Their implicit knowledge reference also makes it hard to find supporting knowledge and often results in hallucinations (Shuster et al., 2021). The current dense retrieval models have advantages over parametric models on these issues (Karpukhin et al., 2020; Guu et al., 2020; Lewis et al., 2020). But most retrieval models only have a weak coupling between and separate parameters for the reader, reranker (if any), and retriever that limits these models from achieving optimal end-to-end training and efficient use of the total model capacity.

In this paper, we propose a single language model YONO (You Only Need One model) that can refer to external knowledge via its internal attention functions, which are trainable in a fully end-to-end manner. We achieve this by generalizing the retrieval and reranking as internal passage-wise attentions. At the lower retrieval layers, the query and passages are separately encoded allowing pre-computation of all the passage representations. Then passage-wise hard attention is applied to retrieve initial relevant passages from the entire knowledge base. While it would be optimal to retrieve passages based on cross-attention between the query and all the passages (Khattab and Zaharia, 2020), it is computationally intractable. Hence, we approximate this attention by a passage-wise hard-attention layer using decoupled query
and passage representations. The representations of the initial relevant passages are further encoded jointly with the query representation to compute more expressive coupled representations. These are used to select only the more relevant passages using another passage-wise hard-attention in the reranking layer. The representations of the final set of passages are then encoded by transformer encoders for deeper representations that are fused in the decoder to generate the answers.

We train this architecture fully end-to-end by self-supervised pre-training and weakly supervised fine-tuning without passage labels.

Our contributions are twofold:

• A single model that generalizes retrieval, reranking, and reading as internal attention functions. We show that this model trained end-to-end significantly improves the retrieval performance by leveraging a training signal from the answer generation decoder to allow better gradient flow across the whole model in Section 6.1. It also achieves better utilization of the model parameters, outperforming a stand-alone reader with the same number of parameters by 7.1% and 3.2% on NQ and TQA respectively as shown in Section 6.2.

• A method to train this architecture in a fully end-to-end manner. We show our pre-training method requires 51.5% fewer pre-training tokens compare to the previous state-of-the-art approach in Section 7.2.

2 YONO Architecture

As depicted in Figure 1, we propose a single encoder-decoder language model architecture consisting of 3 components: Retrieval Layer, Reranking Layer, and Reading Layer.

2.1 Retrieval Layer

This first layer retrieves the top-N relevant passages for a given query from the knowledge corpus using query and passage representations independently encoded with the first \( K \) transformer encoder layers. The query is encoded with ‘query:’ prefix while passages are encoded with ‘title:’ and ‘context:’ prefixes following previous approaches (Izacard and Grave, 2021b; Singh et al., 2021).

Passage-wise Disjoint Attention: Let \( q_0 \) and \( P_0 \) be the first tokens’ representations of the query and all the passages respectively encoded independently. The disjoint attention scores are calculated by the scaled dot-product attention scores (Vaswani et al., 2017) between \( q_0 \) and \( P_0 \) as:

\[
Q = \text{LayerNorm}(q_0 W_q)
\]
\[
K = \text{LayerNorm}(P_0 W_p)
\]
\[
\text{score}_{\text{disjoint}}(q, P) = \sigma(QK^T / \sqrt{d_k})
\]  

where \( W_q, W_p \in \mathbb{R}^{d \times d} \) are learned linear projections and \( 1/\sqrt{d_k} \) is the scaling factor following Vaswani et al. (2017).

The top-N relevant passages \( P^R \) with the highest \( \text{score}_{\text{disjoint}} \) for a given query are selected and passed to the next layer. In practice, we retrieve top-N passages by indexing the pre-computed passage representations \( P_0 \) using Maximum Inner Product Search tools (MIPS) such as FAISS (Johnson et al., 2021). During training, the index is iteratively refreshed by the most recent model’s representation following other neural retrieval approaches (Karpukhin et al., 2020; Lee et al., 2019; Guu et al., 2020; Izacard and Grave, 2021).

2.2 Reranking Layer

We further narrow down the retrieved passages by applying an additional passage-wise attention
based on more expressive representations from the joint encoding of query and passages.

**Passage-wise Joint Attention:** We concatenate query and retrieved passage representations and encode them with cross-attention for more expressive representations using the next $L$ transformer encoder layers. Let $h^n$ be the encoded representations of query and the $n^{th}$ passage and $H_0$ be the first token’s representations of all encoded representations. We apply the second passage-wise attention based on $score_{joint}(q, P^R)$, obtained from $H_0$:

$$h^n = Transformer(q \oplus p^n)$$  \hspace{1cm} (2)

$$H^0 = [h_0^0, h_0^1, h_0^2, ..., h_0^{N-1}]$$

$$score_{joint}(q, P^R) = \sigma(LayerNorm(H_0)W_{qp})$$

where $\oplus$ is the concatenation operation and $W_{qp} \in \mathbb{R}^{d \times 1}$ is a learnt vector.

### 2.3 Reading Layer

After the retrieval and reranking layers, the final representations are fed to the reading layer. These are further encoded using the remaining transformer encoder layers and fused in the decoder for multi-passage reading, following the approach of FiD (Izacard and Grave, 2021b).

### 3 Training YONO

#### 3.1 Training Objective

The whole model is always trained end-to-end by leveraging a training signal from the final answer generation. Due to non-differentiability of the passage-wise attentions, we combine additional losses $L_{\text{retrieval}}$ and $L_{\text{reranking}}$ to the answer generation $L_{\text{reading}}$ as below:

$$L = L_{\text{retrieval}} + L_{\text{reranking}} + L_{\text{reading}}$$  \hspace{1cm} (3)

**Retrieval and Reranking Loss:** The passage-wise attention scores $S_{\text{retrieval}}$ and $S_{\text{reranking}}$ for retrieval and reranking layers are calculated by Equation (1) and (2) using retrieved passages $P^R$ and in-batch negative passages $P^N$ as:

$$S_{\text{retrieval}} = score_{\text{disjoint}}(q, P^R \cup P^N)$$

$$S_{\text{reranking}} = score_{\text{joint}}(q, P^R)$$  \hspace{1cm} (4)

In-batch negative passages $P^N$ are used to expand $S_{\text{retrieval}}$ for more contrastive training signals. In-batch negatives not used for $S_{\text{reranking}}$ because the joint representation is only calculated for the retrieved passages, not the in-batch negatives.

These attention scores are not differentiable by the reader’s generation loss because they are only used to select top-$N$ passages at retrieval and reranking layers but not directly used in the answer generation. Instead, we train $score_{\text{retrieval}}$ and $score_{\text{reranking}}$ to approximate the target scores, which following previous work (Izacard and Grave, 2021a) are derived by accumulating the decoder’s attention scores across decoder layers and attention heads over all encoded passage tokens as:

$$score_{\text{decoder}}(P) = \sum_{l=0}^{N_1} \sum_{h=0}^{N_h} \sum_{t_p=0}^{N_T} SG(att_{\text{dec}}(0, l, h, t_p)) \mid p \in P$$

where $att_{\text{dec}}$ is decoder attention matrices toward encoded outputs, 0 is an output token index, $N_1$ is the number of layers, $N_h$ is the number of attention heads, $N_T^p$ is the number of tokens in a given passage, and $SG$ is a stop gradient function. The gradient flow back to the decoder’s attention scores is blocked by $SG$ to train the decoder by $L_{\text{reading}}$ only.

Using this scoring function, we get target scores $T_{\text{retrieval}}$ and $T_{\text{reranking}}$. The scores of in-batch negative passages $P^N$ are set to 0.

$$T_{\text{retrieval}} = score_{\text{decoder}}(P^R) \oplus (0 \mid p \in P^N)$$

$$T_{\text{reranking}} = score_{\text{decoder}}(P^R)$$  \hspace{1cm} (6)

Finally, the losses for training passage-wise attention scores are obtained by KL-Divergence between target scores $T$ and attention scores $S$ as:

$$L_{\text{retrieval}} = D_{KL}(T_{\text{retrieval}} \| S_{\text{retrieval}})$$

$$L_{\text{reranking}} = D_{KL}(T_{\text{reranking}} \| S_{\text{reranking}})$$  \hspace{1cm} (7)

In addition, we add a constant penalty $\gamma$ to $score_{\text{retrieval}}$ of in-batch negative passages $P^N$ before applying a softmax of Equation (1). This inductive bias enforces the model to further decrease scores of the random negative passages lower than the lowest score of the retrieved passages.

**Reading Loss:** We use a conventional autoregressive language modeling loss for generating an answer $a$ given a query $q$ and retrieved passages $P^R$:

$$L_{\text{reading}} = -\log \prod_{t=1}^{T_A} p(a_t \mid a_{<t}, q, P^R)$$  \hspace{1cm} (8)
3.2 Pre-training Corpus

We first pre-train our model to adapt the pre-trained encoder-decoder architecture to the YONO architecture and provide initial retrieval performance for fine-tuning without passage labels. Inverse Cloze Task (ICT) (Lee et al., 2019) and Masked Salient Span (MSS) (Roberts et al., 2020; Guu et al., 2020) are widely used tasks for pre-training. ICT uses ‘input-passage’ pairs that have explicit supervision for training passage-wise attention, but has no supervision for the answer generation. On the other hand, MSS trains the model by ‘input-output’ pairs that have strong supervision for the answer generation, but no supervision for the retriever, requiring additional warm-up training for retrieval such as ICT. Thus, these tasks are sequentially applied to pre-train the pipeline models to overcome their limitations (Guu et al., 2020; Singh et al., 2021). However, we train our single model architecture with retrieval, reranking, and reading layers at the same time using triples of ‘input-passage-output’ for pre-training. To provide such supervisions, we extend a masked salient span task with explicit passage labels.

Masked Salient Span with Passage Labels (MSS-P): We first pick one named entity and mask all instances of this entity from the sentence. We explicitly add a ground truth passage that contains the masked named entity from 2 previous and next passages except its original passage. We refine the data by simple heuristics (using only pairs of sentence and target passage that contain at least 1 common named entity other than the masked span, and selecting the target passage with the highest number of common named entities when there are multiple passages containing the masked span). In this way, we generate 53M triples from Wikipedia passages in total.

3.3 Training Procedure

The model is pre-trained and fine-tuned iteratively to refresh retrieved passages for a better approximation of the distribution over all the passages.

We start the first pre-training iteration using the initial pre-training data, extracted by the MSS-P method that has one ground-truth passage for each query sentence. Note that with one positive passage per query, $L_{\text{retrieval}}$ is equivalent to the negative log-likelihood loss of predicting the positive passage along with negative passages. However, $L_{\text{reranking}}$ is 0 at this pre-training iteration and does not yield any training signal because it can only learn from contrasting multiple retrieved passages.

From the second iteration, the model is trained with 100 passages fetched from the retrieval layer. We add the original ground truth passage to the retrieved passages to ensure that the model learns to refer to the knowledge instead of implicitly memorizing the answer in its internal parameters. We do not filter more passages at the reranking layer during training to compute $\text{score}_{\text{decoder}}$ of Equation (5) to allow the reader to learn from the maximum number of passages. We pre-train the model for several iterations until the performance of the retrieval converges based on the recall metric.

After the pre-training, the model is then fine-tuned following the same procedure as that after the first iteration. To prevent an over-fitting of the reader due to the limited size of the fine-tuning data, we simply re-initialize the model with the pre-trained YONO model after retrieval performance converges following Izacard and Grave (2021a). Note that the model is fine-tuned by only weak-supervision of question-answer pairs without gold passages.

4 Experiments

4.1 Model Configurations

We primarily compare our model with baselines that use 440M parameters in total. To get a single language model with 440M parameters, we initialize our model from the pre-trained T5-large (Raffel et al., 2020) discarding final 18 decoder layers. This results in our model with 24 encoder and 6 decoder layers. The retrieval layer uses the first 12 encoder layers that uses 25% fewer parameters than baselines’ bi-encoders retrievers (165M vs 220M). Since our reranking layer works on the representations of the retrieval layer, we only allocate 4 encoder layers for reranking. The total number of parameters used for retrieval and reranking is 220M. The remaining 220M parameters are allocated for the reading layer.

4.2 Training Details

At the first pre-training iteration, the model is trained with a batch of 800 question-passage-answer triplets for 100K steps. From the second iteration, we train the model for 1,250 steps per iteration using a batch with 64 question-passage-answer triplets, where each triplet is packed with
100 retrieved passages. In total, we run 42 additional iterations after the first iteration for pre-training.

After pre-training, the model is fine-tuned the same way as pre-training, except it is trained for 1 epoch at every iteration.

The model is optimized with the Adam optimizer (Kingma and Ba, 2015) with a learning rate $10^{-4}$. The first iteration takes 24 hours, and other iterations take around 5 hours each including MIPS indexing and passage refresh on 8 A100 GPUs. The penalty $\gamma$ for attention scores of the random in-batch negative passages is set to 5 in all our experiments.

We found that answer generation more easily over-fits compared to the retrieval during fine-tuning. To prevent this over-fitting, the model is once reinitialized from the pre-trained YONO model at the 6th iteration after the model achieves acceptable recall on the downstream task.

### 4.3 Datasets

We evaluate our model with two standard open-domain question answering datasets, Natural Questions (Kwiatkowski et al., 2019) and TriviaQA (Joshi et al., 2017) following short answer sub-sets processed by Lee et al. (2019). Our external knowledge base is built using the Wikipedia dump from Dec. 20, 2018, where articles are split into passages of 100 words without overlap which is the same as datasets used in Karpukhin et al. (2020); Izacard and Grave (2021b); Singh et al. (2021) for a fair comparison.

### 5 Evaluation

#### 5.1 Retrieval Performance

Table 1 and Table 2 show overall performance of our model and other baselines on Natural Questions and TriviaQA test sets. Our retrieval layer achieves the state-of-the-art recall@20/100 on Natural Questions regardless of model size even when compared with models with more than 4x model parameters. On TriviaQA, ours performs slightly worse than the state-of-the-art models, FiD-KD (Izacard and Grave, 2021a) and E2NR (Sachan et al., 2021), which use passage labels during training or 4x more parameters. Our approach achieves such performance without using passage labels making relevance for a larger range of applications that may not have these annotations. These results also do not use augmented data and as we show in Section 6.3 it only gives slight improvements on the end-to-end performance.

#### 5.2 Reranking Performance

As shown in Table 1, the reranking layer further improves the recall of our retrieved passages by 3.8 and 5.5 absolute recall@5 on NQ and TQA respectively when reranking 800 retrieved passages. This

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**Table 1:** Recall@N results on Natural Questions and TriviaQA test sets. The best retrieval and reranking scores except larger models are indicated in bold. Reranking200/800 refer to reranking the 200/800 retrieved passages. The GAR$^+$ model uses a further 406M params for augmenting the query.

| Model | Passage Aug. | Model # Params | Natural Questions | TriviaQA |
|-------|--------------|----------------|-------------------|----------|
|       | Label data  |                | $R@5$ | $R@20$ | $R@100$ | $R@5$ | $R@20$ | $R@100$ |
| BM25 (Mao et al., 2021a) | ✓ | 220M | 43.6 | 62.9 | 78.1 | 67.7 | 77.3 | 83.9 |
| DPR (Karpukhin et al., 2020) | ✓ | 220M | 68.1 | 80.0 | 85.9 | - | 79.4 | 85.0 |
| DPR$^{new}$ (Karpukhin et al., 2020) | ✓ | 220M | 72.2 | 81.3 | 87.3 | - | - | - |
| GARN (Mao et al., 2021a) | ✓ ✓ | 220M | 70.7 | 81.6 | 88.9 | 76.0 | 82.1 | 86.6 |
| DPR-PQA (Oguz et al., 2021) | ✓ | 220M | 75.8 | 84.3 | 89.0 | 76.8 | 83.2 | 87.3 |
| ANCE (Xiong et al., 2021a) | ✓ | 220M | - | 81.9 | 87.5 | - | 80.3 | 85.2 |
| E2NR (Sachan et al., 2021) | ✓ | 220M | 74.9 | 84.0 | 89.1 | - | - | - |
| R2-D2 (Ren et al., 2021) | ✓ ✓ | 230M | 70.7 | 81.6 | 88.9 | 76.0 | 82.1 | 86.6 |
| coCondenser (Gao and Callan, 2021) | ✓ | 220M | 74.2 | 84.0 | 89.2 | - | - | - |
| DPR-PAQ (Oguz et al., 2021) | ✓ | 220M | 72.2 | 81.3 | 87.3 | - | - | - |
| FiD-KD (Izacard and Grave, 2021a) | ✓ | 220M | 74.2 | 84.0 | 89.2 | 76.8 | 83.1 | 87.0 |
| Larger models | | | | |
| E2NR (Sachan et al., 2021) | ✓ | 460M | 76.2 | 84.8 | 89.8 | 78.7 | 84.1 | 87.8 |
| DPR-PQA (Oguz et al., 2021) | ✓ ✓ | 660M | 70.7 | 81.6 | 88.9 | 76.0 | 82.1 | 86.6 |
| YONO$^{Retrieval}$ | ✓ ✓ | 165M | 75.3 | 85.2 | 90.2 | 76.8 | 83.5 | 87.4 |
| Reranker models | | | | |
| GAR$^+$-BART (Mao et al., 2021b) | ✓ | 406M | 73.5 | 82.2 | - | - | - | - |
| GAR$^+$-RIDER (Mao et al., 2021b) | ✓ | 110M | 75.2 | 83.2 | 88.9 | 77.9 | 82.8 | 85.7 |
| R2-D2$^{Reranking200}$ (Fajcik et al., 2021) | ✓ | 110M | 76.8 | 84.5 | 88.0 | 78.9 | 83.5 | 86.0 |
| YONO$^{Reranking200}$ | ✓ | 55M | 79.1 | 86.7 | 90.7 | 82.1 | 86.0 | 88.1 |
| YONO$^{Reranking800}$ | ✓ | 55M | 79.1 | 86.6 | 91.1 | 82.3 | 86.4 | 88.7 |
Table 2: End-to-end Open QA Exact-Match results on Natural Questions and TriviaQA test sets. Our model uses top 100 retrieved or reranked passages to generate answers. The best EM scores except larger models are indicated in bold.

| Model               | # Params | NQ     | TQA     |
|---------------------|----------|--------|---------|
| **Discriminative models** |          |        |         |
| OrQA (Lee et al., 2019) | 330M     | 33.3   | 45.0    |
| REALM (Gu et al., 2020) | 330M     | 40.4   | -       |
| ANCE (Xiong et al., 2021a) | 330M     | 46.0   | 57.5    |
| **Generative models**   |          |        |         |
| RAG (Lewis et al., 2020) | 440M     | 44.5   | 56.8    |
| FiD (Izacard and Grave, 2021b) | 440M     | 49.6   | 68.8    |
| E2NR (Sachan et al., 2021) | 440M     | 45.9   | 56.3    |
| EMDR\(^2\) (Singh et al., 2021) | 440M     | 52.5   | 71.4    |
| **Larger models**      |          |        |         |
| E2NR (Sachan et al., 2021) | 1.4B     | 48.1   | 59.6    |
| FiD (Izacard and Grave, 2021b) | 990M     | 51.4   | 67.6    |
| FiD-KD (Izacard and Grave, 2021a) | 990M     | 53.7   | 72.1    |
| UnitedQA (Cheng et al., 2021) | 2.09B    | 54.7   | 70.5    |
| R2-D2 (Fajcik et al., 2021) | 1.29B    | 55.9   | 69.9    |
| YONO\(_{Retrieval}\) | 440M     | 53.2   | 71.3    |
| YONO\(_{Reranking200}\) | 440M     | 53.2   | 71.5    |
| YONO\(_{Reranking800}\) | 440M     | 53.2   | 72.1    |

Table 3: Effect of reader’s generation loss on zero shot retrieval performance after the first iteration of pre-training on Natural Questions development set.

| Loss                     | R@5  | R@20 | R@100 |
|--------------------------|------|------|-------|
| \(L_{\text{retrieval}}\) | 18.0 | 32.1 | 49.8  |
| \(L_{\text{reader}}\)   | 28.8 | 48.1 | 67.0  |
| \(\Delta\)               | +10.8| +16.0| +18.7 |

Table 4: Effect of sharing of retrieval and reranking representations on exact match scores of reader models that use 220M parameters on NQ and TQA development sets.

| Model               | Natural Questions | TriviaQA |
|---------------------|-------------------|----------|
| YONO Reader         | 51.4              | 70.0     |
| Stand-Alone Reader  | 48.0              | 67.8     |
| \(\Delta\)          | +3.4 (7.1%)       | +2.2 (3.2%) |

is 2.3 and 3.4 absolute point improvements over the previous state-of-the-art reranker model. Our model achieves these recall performances using only 55M parameters which is only half the size of the other reranker models. Similar to our retriever, our reranker does not require passage labels, unlike other rerankers. This improvement in recall when using the reranker persists even when reranking only 200 passages.

5.3 End-to-end Performance

Our model achieves the best end-to-end performance among the models of the same size on NQ and irrespective of the model size on TQA as shown in Table 2. Our best scores improve EM scores by 0.7 points on both NQ and TQA respectively over the previously best performing model of the same size, EMDR\(^2\) (Singh et al., 2021). Using data augmentation further boosts these improvements on NQ by 0.3 as shown in Table 5. Using reranking also improves the end-to-end scores on TQA by 0.8, a negligible improvement on NQ. We conjecture that this may be due to the higher recall of the retriever on NQ.

6 Ablation Studies

6.1 The Reader Loss on Retrieval Performance

The retrieval layer is trained by signals from both retrieval and reader losses. While the retrieval loss directly trains the retrieval scores, the reader loss is also a useful indirect training signal for the retriever. This signal is a key advantage of our approach over similar works such as Izacard and Grave (2021a); Singh et al. (2021). We evaluate the performance gain from the additional generation loss at the first pre-training iteration as shown in Table 3. The model trained with both losses shows significant improvement over the model trained with only the retrieval loss. These relative gains are larger the fewer the number of retrieved passages. This result shows that reader’s generation loss is very effective for training the retriever. We evaluate after the first iteration because the reader loss is necessary for training with multiple retrieved passages in the following iterations.

6.2 Shared Representations on Reader Performance

Our reading layer uses 220M parameters but shares representations encoded by its preceding retrieval and reranking layers which use another 220M parameters. To measure gains of the shared representations, we compare our reader performance with that of a stand-alone reader model that uses 220M parameters that is the same as our reading layers. For a fair comparison, the stand-alone reader model is pre-trained and fine-tuned for the same amount of training tokens using the data retrieved by our YONO retriever. Table 4 shows that the reader model sharing representations outperforms the stand-alone reader by 7.1% and 3.2% on NQ and TQA respectively.
### 6.3 Effectiveness of MSS-P pre-training

To show the effectiveness of our MSS-P pre-training method, we evaluate this by fine-tuning our architecture without any pre-training using initial retrievals from DPR (Karpukhin et al., 2020) and fine-tuning after the first pre-training iteration. We also compare our pre-training to that of the additional data augmentation (Mao et al., 2021a; Ren et al., 2021; Oguz et al., 2021). We generate ‘question-answer’ pairs from a Wikipedia dump using a question and answer generation model trained on the NQ dataset using the ASGen approach (Back et al., 2021). The model is further trained after the pre-training by this augmented data for 12 more iterations before fine-tuning.

Table 5 shows retrieval, reranking, and reading performance on Natural Questions and TriviaQA test sets. Our MSS-P pre-training dramatically boosts the performance of our architecture by 4.8 and 13.3 EM points on NQ and TQA even with only the first pre-training iteration. Further iterations of our pre-training improve EM by 1.7 and 2.9 EM points. The further data augmentation pre-training improves performance on NQ consistently but only slightly, while the improvements on TQA are inconsistent, as the data was generated by the model trained on NQ dataset. These results clearly demonstrate that our simple self-supervised MSS-P pre-training is strong enough to compete favorably against sophisticated data augmentation approaches.

### 7 Analysis

#### 7.1 Computational Efficiency of Reranking

In many dense retrieval systems, a reranker is often omitted due to functional overlaps with the reader and computational overhead (Guu et al., 2020; Lewis et al., 2020; Singh et al., 2021). Thanks to the shared representations across the reader and reranker, our model can incorporate a reranking function without significantly more parameters or computation. By dropping irrelevant passages early at the reranking layer, we can achieve better computational efficiency. Figure 2 shows exact match scores for given N retrieved or reranked passages on NQ development set. Rerank EM scores are from reranking only 100 retrieved passages.

![Figure 2: Exact Match scores for given N retrieved or reranked passages on NQ development set. Rerank EM scores are from reranking only 100 retrieved passages.](image)

### Table 6: Total pre-training tokens. The first and second stages of REALM and EMDR\(^2\) are ICT and MSS pre-training respectively.

| Input Len. | First Stage Passages Steps | Second Stage Passages Steps | Total Tokens |
|------------|----------------------------|----------------------------|--------------|
| REALM      | 288                        | 4096                       | 100K         | 4096          | 200K         | 352B         |
| EMDR\(^2\) | 256                        | 4096                       | 100K         | 3200          | 82K          | 171B         |
| YONO       | 200                        | 800                        | 100K         | 6400          | 52.5K        | 83B          |

#### 7.2 Pre-training Efficiency

The number of pre-training tokens is an important metric to measure the efficiency of the pre-training objective. As shown in Table 6, REALM (Guu et al., 2020) and EMDR\(^2\) (Singh et al., 2021) use 352B and 171B tokens in total respectively. In contrast, our method uses only 83B tokens, which is 76.4% and 51.5% less than the training tokens used to train REALM and EMDR\(^2\) respectively. Furthermore, the retrieval index is updated only 43 times during our pre-training, while EMDR\(^2\) updates the index 164 times. This is a significant reduction of...
the computation overhead for pre-training.

8 Related Works

Neural Retriever Augmented Language Modeling (NRALM): Augmenting language models with neural retrieval has been shown to be very effective, such as by retrieving nearest neighbor words for LM tasks (Khandelwal et al., 2020; Yogatama et al., 2021) or Machine Translation (Khandelwal et al., 2021). Dinan et al. (2019) proposed a decomposed transformer for conversation tasks, which enabled pre-computation of the external knowledge embeddings.

ORQA (Lee et al., 2019) proposed the ICT task to pre-train a decomposed retriever, and DPR (Karpukhin et al., 2020) enhanced this approach with in-batch negatives and hard negatives to eliminate the pre-training. Synthetic Data Augmentation is also commonly used, such as in DPR-PAQ (Oguz et al., 2021), PAIR (Ren et al., 2021), Hu et al. (2021). Per-token embeddings or multiple embeddings were used in ColBERT (Khattab et al., 2020), ME-BERT (Luan et al., 2021), Lin et al. (2021), Lee et al. (2021).

Similar to our approach of re-ranker on top of a shared retriever, PreTTR (MacAvaney et al., 2020) pre-computed term representations for all documents, and used these to run only the upper layers of a transformer reranker model. Decoupled Transformer (Elfdaeel and Peshterliev, 2021) also shares the lower layers of a transformer encoder to serve as a reranker, using the upper layers as a reader and focuses on computationally efficient reranking. Our approach extends these approaches by also incorporating a retriever and a decoder in the model.

E2E Optimization of NRALM: It is intractable to re-compute the embeddings of the knowledge for every weight update. REALM (Guu et al., 2020) and ANCE (Xiong et al., 2021a) proposed async index refresh to propagate updates to the index to yield better negatives. TAS (Hofstätter et al., 2021) and Xiong et al. (2021b) used clustering of embeddings for the same. RAG (Lewis et al., 2020) used DPR with BART generator to marginalize over generated tokens, which is back-propagated to the retriever. REALM++ (Balachandran et al., 2021) added a re-ranker to REALM.

Similar to our work, Bruyn et al. (2020) and TREAD (Shuster et al., 2021) utilize BART and T5 reader’s encoders as a retriever. In contrast to these methods, our work has a unified pre-training method to train all the components of the model. Furthermore, our model also has an integrated re-ranker, and the query and passage are cross-encoded for more expressive representations.

Multi-passage Readers: Reading multiple passages at the same time is difficult, as concatenating multiple passages increases computation quadratically for transformers. Zhao et al. (2020) reduced multiple passages and sentences to few via a knowledge selector, which were then concatenated and passed on to GPT (Radford et al., 2019). FiD (Izacard and Grave, 2021b) concatenated the encoded representations of documents, which can then be attended by the decoder, achieving large performance gains. This approach was also applied in RocketQA (Qu et al., 2021). UnitedQA (Cheng et al., 2021) and R2D2 (Fajcik et al., 2021) combine results from an ensemble of extractive and generative readers, whereas PAQ (Lewis et al., 2021) directly retrieves answers with an FiD fallback.

Similar to our work, both REALM (Izacard and Grave, 2021a) and EMDR$^2$ (Singh et al., 2021) train the retriever with a signal from the reader. Unlike these approaches, our model has shared lower layers for more effective utilization of model parameters and better end-to-end gradient flow across the whole model. Furthermore, our training methodology results in propagating the answer generation loss of the retriever, which has a large effect on performance as we show in Table 3.

9 Conclusion

In this paper, we propose a novel language model architecture that embeds the retriever and the reranker as internal passage-wise attention mechanisms and a training method to effectively train this model. This singular model architecture efficiently uses model capacity by cascading and sharing the representations from retriever to reranker to the reader leading to better gradient flow for end-to-end training. We evaluate our model on Natural Questions and TriviaQA open datasets and for a fixed parameter budget, our model outperforms the previous state-of-the-art model by 1.0 and 0.7 exact match scores. We show detailed ablations and analyses of each component of our approach. Our future work is to conduct more experiments on various knowledge-intensive tasks and extend this model to match query and passage in multiple or hierarchical representation spaces.
Limitations

One caveat of sharing representation for multiple tasks like retrieval, reranking, and reading is that these show different over-fitting tendencies during fine-tuning where the training data is limited. We found that answer generation over-fits more easily compared to the retrieval. Answer generation relies on more expressive representation via cross attention, which may make it easier to memorize the output and hence make it more vulnerable to over-fitting. Furthermore, at the first fine-tuning iteration, the model is trained by zero-shot retrieval results from the pre-trained model that has a relatively low recall rate and can harm the answer generation training. To refresh the over-fitted answer generation parameters, and to start from training data with a high recall rate, we simply re-initialize the model with the pre-trained YONO model after a few fine-tuning iterations. However, we believe that this issue should be addressed carefully using a more sophisticated solution. We further discuss the over-fitting issue and effect of re-initialization in Appendix A.

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Appendix

A Model Re-initialization during Fine-tuning

To overcome over-fitted reader parameters, we refresh the model parameter using the pre-trained YONO model at the fine-tuning iteration where the EM score starts to drop.

Figure 3 shows retrieval and end-to-end performance at each fine-tuning iteration. The Exact Match score drops at the 5th iteration while the retrieval score keeps increasing. After re-initializing the model before the 6th iteration, the model restarts with a higher recall and EM score. However, the EM score drops again from the 10th iteration after achieving the best end-to-end performance, while the retrieval performance continues to improve. We leave further approaches for preventing over-fitting of our model such as freezing the model partially as future work.

B Effect of Pre-training Iterations on Retrieval Performance

Figure 4 shows recall@N at each training stage across the pre-training and fine-tuning using Natural Question development set. The first iteration of the pre-training results in zero-shot recall@100 of 67.0%, which is further improved by additional pre-training iterations to 71.8% recall@100. These zero-shot recall scores enable us to fine-tune our model without passage labels resulting in state-of-the-art retrieval and reranking performance.

C Experiment Details

On Table 7, 8, and 9, we provide all training details and parameters used to conduct experiments on this paper.

D Raw Values for Plots in Figures

In Table 10 and 11, we provide raw values for plots in Figure 2 and 4.
Table 7: Model Parameters.

| Parameters            | Values |
|-----------------------|--------|
| Initial model         | T5-Large |
| Dimensions            |        |
| - Model               | 1,024  |
| - Feed Forward        | 4,096  |
| - Attention head      | 64     |
| Attention head count  | 16     |
| # of layers and parameters |      |
| - Total               | 24 enc + 6 dec | 440M |
| - Retrieval layer     | 12 enc  | 165M |
| - Reranking layer     | 4 enc   | 55M  |
| - Reading layer       | 8 enc + 6 dec | 220M |

Table 8: Training Parameters.

| Parameters              | Values |
|-------------------------|--------|
| Pre-training            |        |
| Total iterations        | 43     |
| Training tokens         |        |
| - Total                 | 83B    |
| - The 1st iteration     | 16B    |
| - One iteration from 2nd | 1.6B   |
| - One batch             | 160K   |
| Fine-tuning             |        |
| Best scoring iteration  | NQ 10 / TQA 11 |
| Training tokens         |        |
| - Total to the best iteration | NQ 15.88B / TQA 17.3B |
| - One iteration         | NQ 1.58B / TQA 1.58B |
| - One batch             | 160K   |
| Optimization            |        |
| Learning rate           | \(10^{-4}\) (fixed) |
| Drop-out                | 0.1    |
| Precision               | float32|
| Gradient clipping       | 1.0    |
| Gradient accumulation   |        |
| - The 1st pretraining iteration | None |
| - otherwise             | 8 batches |

Table 10: Raw Values for EM for Figure 2

| Passages | Retrived EM | Reranked EM |
|----------|-------------|-------------|
| 1        | 36.7        | 41.7        |
| 5        | 46.1        | 48.5        |
| 10       | 48.3        | 50.7        |
| 20       | 49.5        | 51.0        |
| 50       | 50.5        | 51.1        |
| 100      | 51.1        | 51.1        |

Table 11: Raw Values for Recall@N for Figure 4

| Passages | FT Rerank@N | FT Retrieval | PT | PT Iter. |
|----------|-------------|--------------|----|---------|
| 1        | 58.8        | 52.5         | 16.1 | 10.9    |
| 5        | 80.0        | 75.4         | 36.4 | 28.8    |
| 10       | 84.1        | 81.0         | 46.1 | 38.6    |
| 20       | 86.8        | 84.7         | 55.5 | 48.1    |
| 50       | 89.0        | 87.7         | 65.6 | 60.0    |
| 100      | 90.2        | 89.3         | 71.8 | 67.0    |

Table 12: Raw values for Central Tendency and Standard Error on NQ development set for 3 finetuning runs of our model, as shown in Figure 3

| Finetuning Iter. | Exact Match@100 | Recall@100 |
|------------------|-----------------|------------|
| 1                | 45.3 ± 0.1      | 86.0 ± 0.1 |
| 2                | 48.7 ± 0.1      | 87.9 ± 0.0 |
| 3                | 50.2 ± 0.3      | 88.5 ± 0.1 |
| 4                | 50.9 ± 0.2      | 88.8 ± 0.1 |
| 5                | 50.6 ± 0.2      | 89.9 ± 0.1 |
| 6                | 47.2 ± 0.1      | 87.9 ± 0.1 |
| 7                | 49.6 ± 0.1      | 88.3 ± 0.1 |
| 8                | 50.4 ± 0.1      | 88.7 ± 0.1 |
| 9                | 50.4 ± 0.2      | 88.9 ± 0.1 |
| 10               | 51.0 ± 0.2      | 88.9 ± 0.1 |
| 11               | 50.8 ± 0.2      | 89.0 ± 0.1 |
| 12               | 50.8 ± 0.3      | 89.1 ± 0.1 |
| 13               | 50.9 ± 0.3      | 89.1 ± 0.1 |
| 14               | 50.9 ± 0.2      | 89.1 ± 0.1 |
| 15               | 50.5 ± 0.2      | 89.2 ± 0.1 |

Table 9: Other Parameters.

Table 13: Other Parameters.

F Links to Source Code and Datasets

The source code is based on the original implementation of FiD (Izacard and Grave, 2021b), which can be found at their Github.

Data for the Wikipedia dump, Natural Questions, and TriviaQA can also be downloaded from FiD’s github using this script.

G Evaluation Metrics and Scripts

The evaluation script is based on the original FiD script.

Exact Match - This is the average across all examples of the per-example exact match score, which is 0 or 1 if all the words in the generated answer exactly match the annotated answer after unicode normalization by lower-casing, removing punctuation and spaces.

Recall@N - Recall@N measures the percentage of examples for which at least one of the top-N pas-
sages contains a span that matches the annotated answer as in Exact Match above.

H Dataset Statistics

Table 13 provides the statistics of our evaluation datasets.

| Dataset        | # Train | # Dev | # Test |
|----------------|---------|-------|--------|
| Natural Questions | 79K     | 8.8K  | 3.6K   |
| TriviaQA        | 79K     | 8.8K  | 11K    |

Table 13: Dataset Statistics

I Computing Infrastructure

GPU model - 8x Nvidia A100 80 GB. CPU Model - 2x AMD EPYC 7543 32-Core Processor. RAM - 1000GB. PyTorch version - 1.8.0+cu111. Hugging-face Transformers version - 3.0.2.