Refining Query Representations for Dense Retrieval at Test Time

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Abstract

Dense retrieval uses a contrastive learning framework to learn dense representations of queries and contexts.\textsuperscript{1} Trained encoders are directly used for each test query, but they often fail to accurately represent out-of-domain queries. In this paper, we introduce a framework that refines instance-level query representations at test time, with only the signals coming from the intermediate retrieval results. We optimize the query representation based on the retrieval result similar to pseudo relevance feedback (PRF) in information retrieval. Specifically, we adopt a cross-encoder labeler to provide pseudo labels over the retrieval result and iteratively refine the query representation with a gradient descent method, treating each test query as a single data point to train on. Our theoretical analysis reveals that our framework can be viewed as a generalization of the classical Rocchio’s algorithm for PRF, which leads us to propose interesting variants of our method. We show that our test-time query refinement strategy improves the performance of phrase retrieval (+8.1\% Acc@1) and passage retrieval (+3.7\% Acc@20) for open-domain QA with large improvements on out-of-domain queries.

1 Introduction

Recent progress in neural network gave birth to dense retrieval that uses a contrastive learning framework to learn dense representations of queries and passages (Lee et al., 2019b; Karpukhin et al., 2020). By overcoming the term mismatch problem, dense retrieval has been shown to be more effective than sparse retrieval on passage/phrase retrieval for open-domain question answering (QA) (Lee et al., 2019b; Karpukhin et al., 2020; Lee et al., 2021a) and information retrieval (Khattab and Zaharia, 2020; Xiong et al., 2020).

\textsuperscript{\ast}Work partly done while visiting Princeton University.

\textsuperscript{1}We define context as a generalized unit of retrieval including phrases, passages, and documents.

Dense retrieval often uses a dual encoder architecture to support the pre-computation of context representations while the query representations are often directly computed from the trained encoder at inference. However, directly using the dense representations of queries from trained encoders often fails to retrieve relevant contexts, especially with out-of-domain queries (Thakur et al., 2021; Sciavolino et al., 2021). In particular, dense retrieval seems to fall short of traditional sparse retrieval in an out-of-domain setting where the distribution of test queries differs from the one that the retrievers were trained on.

In this paper, we introduce a new framework that refines instance-level query representations at test time for dense retrieval. Specifically, we treat each test query as a single data point to train on and iteratively refine the query representation initially obtained from the query encoder. This resembles the query-side fine-tuning for phrase retrieval (Lee et al., 2021a), which fine-tunes the query encoder over training queries in a new domain. Instead, we refine instance-level query representations at test time. Since we do not have target labels to train on for test queries, we leverage a cross-encoder labeler (Nogueira and Cho, 2019) to provide pseudo labels on the retrieval result of each test query. We then iteratively refine the query representation at test-time using a stochastic gradient descent method. We theoretically show that our framework can be viewed as a generalized version of the Rocchio’s algorithm for pseudo relevance feedback (Rocchio, 1971), which is a common technique in information retrieval for improving query representations with retrieval results.

We apply our test-time query refinement (TQR) on dense phrase retrieval (Lee et al., 2021a) and dense passage retrieval (Karpukhin et al., 2020) for open-domain question QA. Since phrase retrieval formulates open-domain QA with a single-stage retriever (Seo et al., 2019; Lee et al., 2019a), apply-
ing test-time query refinement could directly lead to the improvement of end-to-end performance on open-domain QA. While we use an off-the-shelf cross-encode re-ranker (Fajcik et al., 2021) as our pseudo labeler for passage retrieval, we also develop a phrase re-ranker for phrase retrieval, which hasn’t been studied in previous work.

Experiments on five open-domain QA benchmarks show that our test-time query refinement improves the accuracy of dense phrase retrieval by 8.1% (Acc@1) and dense passage retrieval by 3.7% (Acc@20) on average. For the out-of-domain evaluation of end-to-end open-domain QA, we train models on a single open-domain QA dataset (Natural Questions; Kwiatkowski et al., 2019) and evaluate on the rest. While existing models show poor zero-shot generalization performance, TQR consistently improves the performance of dense retrievers. On the out-of-domain evaluation for passage retrieval, we use Entity Questions (Sciavolino et al., 2021) and show that the top-k accuracy can be improved with TQR, which is not possible when re-ranking the top-k results.

2 Background

2.1 Dense Retrieval

Dense retrieval typically uses query and context encoders—\( E_q(\cdot) \) and \( E_c(\cdot) \)—for representing queries and contexts, respectively (Lee et al., 2019b; Karpukhin et al., 2020). In this work, we focus on improving phrase or passage retrievers for open-domain QA. The similarity of a query \( q \) and a context \( c \) is computed based on their dense representations:

\[
sim(q, c) = f(E_q(q), E_c(c)) = f(q, c),
\]

where \( f \) is a similarity measure. Following previous work, we use the inner product as our similarity measure, namely, \( f(q, c) = q^T c \).

Dense retrievers often use the contrastive learning framework to train the encoders \( E_q \) and \( E_c \). After training the encoders, top-k results are retrieved from a set of contexts \( C \):

\[
C_{1:k}^q = [c_1, \ldots, c_k] = \text{top-}k_{c \in C} f(q, c),
\]

where the top-k operator returns a sorted list of contexts by their similarity score \( f(q, c) \) in a descending order (i.e., \( f(q, c_1) \geq \cdots \geq f(q, c_k) \)). Dense retrievers aim to maximize the probability that a relevant context \( c^* \) exists (or is highly ranked) in the top results.

2.2 Query-side Fine-tuning

After training the query and context encoders, the context representations \( \{c \mid c \in C\} \) are typically pre-computed for efficient retrieval while the query representations \( q \) are directly computed from the query encoder during inference. However, using the dense representations of queries as is often fails to retrieve relevant contexts especially given out-of-domain queries.

To mitigate the problem, Lee et al. (2021a) propose to fine-tune the query encoder over the retrieval results of training queries \( \{q \mid q \in Q_{\text{train}}\} \) over the entire corpus \( C \). For phrase retrieval (i.e., \( c \) denotes a phrase), they maximize the marginal likelihood of relevant phrases in the top-k results:

\[
\begin{align*}
L_{\text{query}}(q, C_{1:k}^q) &= -\log \sum_{c \in C_{1:k}^q} \frac{P_k(c|q)}{L_c}, \\
E_q^* &= \arg\min_{q \in Q_{\text{train}}} \sum_{q \in Q_{\text{train}}} L_{\text{query}}(q, C_{1:k}^q).
\end{align*}
\]

where \( P_k(c|q) = \frac{\exp f(q^T c)}{\sum_{c' \in C} \exp f(q^T c')} \) and \( c = c^* \) checks whether each context matches the gold context \( c^* \) or not. Note that \( c^* \) is always given for training queries. It has been shown that the query-side fine-tuning largely improves performance of in-domain queries and provides a means of efficient transfer learning for out-of-domain queries. In this work, compared to training on the entire training queries (possibly in a new domain) as in Eq. (3), we treat each test query \( q \in Q_{\text{test}} \) as a single data point to train on and refine instance-level query representations at test time.

2.3 Pseudo Relevance Feedback

In fact, pseudo relevance feedback (PRF) techniques in information retrieval (Rocchio, 1971; Lavrenko and Croft, 2001) share a similar motivation with ours in that they refine query representations for single testing query. While most previous work utilized PRF for sparse retrieval (Zamani et al., 2018; Croft et al., 2010), recent work also started to apply PRF on dense retrieval (Yu et al., 2021; Wang et al., 2021; Li et al., 2021). However, they simply consider the top-k results as pseudo-relevant, while we use a cross-encoder labeler to provide richer and more fine-grained pseudo labels.

PRF aims to improve the quality of the retrieval by updating the initial query representation from the query encoder (i.e., \( E_q(q) = q_0 \)):

\[
q_{t+1} \leftarrow g(q_t, C_{1:k}^q),
\]
where $g$ is an update function and $q_t$ denotes the query representation after $t$-th updates over $q_0$.

The classical Rocchio’s algorithm for PRF (Rocchio, 1971) updates the query representation as:

$$g(q_t, C_{i:k}) = \alpha q_t + \beta \frac{1}{|C_r|} \sum_{c_r \in C_r} c_r - \gamma \frac{1}{|C_{nr}|} \sum_{c_{nr} \in C_{nr}} c_{nr},$$

where $C_r$ and $C_{nr}$ denote relevant and non-relevant sets of contexts, respectively. $\alpha$, $\beta$, and $\gamma$ determines the relative contribution of the current query representation $q_t$, relevant context representations $c_r$, and non-relevant context representations $c_{nr}$, respectively, when updating to $q_{t+1}$. A common practice is to choose top-$k'$ contexts as pseudo-relevant among top-$k$ ($k' < k$), i.e., $C_r = C_{1:k'}$.

$$g(q_t, C_{1:k}) = \alpha q_t + \beta \frac{1}{k'} \sum_{i=1}^{k'} c_i - \gamma \frac{1}{k-k'} \sum_{i=k'+1}^{k} c_i.$$  

In this work, we theoretically show that our test-time query refinement is a generalization of the Rocchio’s algorithm. While Eq. (6) treats the positive (or negative) contexts equally, we use cross-encoder re-rankers (Nogueira and Cho, 2019) as our labeler to provide fine-grained pseudo labels and refine the query representations with a gradient descent method.

### 3.1 Test-time Query Refinement

Figure 1: An overview of test-time query refinement (TQR) for dense retrieval. During inference, the query and context encoders ($E_q$ and $E_c$) are often used by freezing their parameters. In this setting, TQR iteratively refines the representation of a test query $q_{test}$. Given the top-$k$ retrieval results for $q_{test}$, our cross-encoder labeler $\phi(\cdot)$ provides a pseudo label for each top retrieval result. Here, we show top 5 contexts with their representations $c_1$, $c_2$, $c_3$, $c_4$, and $c_5$, and the darker colors of $c_i$ denote that they are more relevant as judged by $\phi(\cdot)$. Then, TQR iteratively updates $q_t$ with gradients by considering the relevance judgement. $\mathcal{C}$: a corpus used to build the index.

### 3. Methodology

#### 3.1 Test-time Query Refinement

We propose Test-time Query Refinement (TQR), which refines query representation at instance level. In our setting, the query and context encoders are fixed after training and we refine the query representations solely based on its retrieval results. Figure 1 illustrates an overview of TQR.

First, given a single test query $q \in Q_{test}$, we use a cross-encoder labeler $\phi(\cdot)$ to pseudo-label each top-$k$ result $c \in C_{1:k}^q$. Unlike dual-encoders for dense retrieval, which encode queries and contexts with separate encoders, cross-encoders concatenate a question and a context and process them with a single encoder that uses self-attention layers (Devlin et al., 2019). Since cross-encoders allow rich token-level interaction between queries and contexts, it has been shown to be stronger than the dual-encoders (Humeau et al., 2019). However, since it has higher computational cost and does not allow the pre-computation of context representations, it can only be used in a re-ranker or reading comprehension setting (Nogueira and Cho, 2019).

In our case, we use the cross-encoder to provide a score of how relevant each of the top-$k$ contexts is with respect to a query:

$$s = \phi(q, c),$$

where $\phi(\cdot)$ is often parameterized with a pre-trained language model (Devlin et al., 2019), which we detail in §3.3. Compared to simply setting top-$k'$ results as pseudo positive in PRF, using cross-encoders enables more fine-grained judgement of
relevance over the top results. Also, it allows us to label results for test queries as well without an access to the gold label $c^*$. Using the scores from the cross-encoder labeler $\phi$, we select a set of pseudo-positive contexts $C_p^q \subset C_{1:k}^q$ defined as the smallest set such that:

$$P_k(\tilde{c} = c^* | q, \phi) = \frac{\exp(\phi(q, \tilde{c}) / \tau)}{\sum_{i=1}^k \exp(\phi(q, \tilde{c}_i) / \tau)}$$

$$\sum_{\tilde{c} \in C_p^q} P_k(\tilde{c} = c^* | q, \phi) \geq p,$$

(8)

where $\tau$ is a temperature parameter and $\tilde{c} \in C_p^q$ denotes a pseudo-positive context selected by $\phi$. Intuitively, we choose the smallest set of contexts as $C_p^q$ whose marginal relevance with respect to a query under $\phi$ is larger than the threshold $p$. This is similar to Nucleus Sampling for stochastic decoding (Holtzman et al., 2020).

Then, TQR refines the query representation with a gradient descent algorithm based on the relevance judgement $C_p^q$ made by $\phi$:

$$L(q, C_{1:k}^q) = -\log \sum_{\tilde{c} \in C_p^q} P_k(\tilde{c} \mid q)$$

$$q^* = \arg\min_q L(q, C_{1:k}^q)$$

(9)

where $P_k(\tilde{c} \mid q) = \frac{\exp(f(q, \tilde{c}))}{\sum_{i=1}^k \exp(f(q, \tilde{c}_i))}$. Similar to the query-side fine-tuning in Eq. (3), TQR maximizes the marginal likelihood of (pseudo) positive contexts $C_p^q$. We also test other objectives in §3.2.

Unlike the query-side fine-tuning that updates the model parameters of $E_q(\cdot)$, we directly refine the representation $q$ itself. Also, TQR is an instance-level optimization over a single test query $q \in \mathcal{Q}_{test}$ without having an access to the gold label $c^*$.

For the optimization, we use a gradient descent method.

$$q_{t+1} \leftarrow q_t - \eta \frac{\partial L(q_t, C_{1:k}^q)}{\partial q_t},$$

(10)

where $\eta$ denotes the learning rate for the gradient descent and the initial query representation is used as $q_0$. Applying the gradient descent over the test queries shares the motivation with dynamic evaluation for language modeling (Krause et al., 2019), but we treat each test query independently unlike the series of tokens for the evaluation corpus of language modeling. For every iteration, we perform a single step of gradient descent followed by another retrieval with $q_{t+1}$ to update $C_{1:k}^q$ into $C_{1:k}^{q_{t+1}}$.

### Relation to the Rocchio’s algorithm

Eq. (10) could be viewed as performing PRF by setting the update function $g(q_t, C_{1:k}^q) = q_t - \eta \frac{\partial L(q_t, C_{1:k}^q)}{\partial q_t}$.

In fact, our update rule Eq. (10) is a generalized version of Rocchio’s algorithm (proof in Appendix A) as shown below:

$$g(q_t, C_{1:k}^q) = q_t + \eta \sum_{\tilde{c}} P(\tilde{c} | q_t)(1 - P_k(\tilde{c} | q_t))\tilde{c}$$

$$- \eta \sum_{\tilde{c} \in C_{1:k}^q, \tilde{c} \neq \tilde{c}} P(\tilde{c} | q_t) P_k(\tilde{c} | q_t)\tilde{c}.$$  

(11)

where $\tilde{c} \in C_p^q$ and $P(\tilde{c} | q_t) = \frac{\exp(f(q_t, \tilde{c}))}{\sum_{\tilde{c}} \exp(f(q_t, \tilde{c}))}$.

While our update rule seems to fix $\alpha$ in Rocchio’s to 1, it can be dynamically changed by applying weight decay during the gradient descent, which sets $\alpha = 1 - \eta \lambda_{\text{decay}}$ multiplied to $q_t$. Then, the equality between Eq. (6) and Eq. (11) holds when $C_{1:k}^q = C_{1:k}$, with $P_k(\tilde{c} | q_t)$ being equal for all $\tilde{c} \in C_q^{C_{1:k}}$, namely $P_k(\tilde{c} | q_t) = 1/k$. This reflects that the Rocchio’s algorithm treats all top-$k$ results equally positive (i.e., $P(\tilde{c} | q_t) = 1$). Then, $\beta = \frac{k-1}{k} \eta$ and $\gamma = \frac{(k-1)(k-k')}{kk'} \eta$ hold.

In practice, $C_{1:k}^q$ would be different from $C_q^{C_{1:k}}$ if some re-ranking happens by $\phi$. Also each pseudo-positive context vector $\tilde{c}$ in the second term of RHS of Eq. (11) has a different weight. The contribution of $\tilde{c}$ is maximized when it has a larger probability mass $P(\tilde{c} | q_t)$ among the pseudo-positive contexts, but a smaller probability mass $P_k(\tilde{c} | q_t)$ among the top-$k$ contexts; this is desirable since we want to update $q_t$ a lot when the initial ranking of pseudo positive context in top-$k$ is low. For instance, if there is a single pseudo-positive context $\tilde{c}$ (i.e., $P(\tilde{c} | q_t) = 1$) ranked at the bottom of top-$k$ with a large margin with top-1 (i.e., $P_k(\tilde{c} | q_t) = 0$), then $P(\tilde{c} | q_t)(1 - P_k(\tilde{c} | q_t)) = 1$ is maximized.

### 3.2 A Variant of TQR

From Eq. (11), we observe that it uses pseudo-positive contexts $C_{1:k}^q$ sampled by the cross-encoder labeler $\phi$, but the contribution of $\tilde{c}$ (the second term in RHS) does not directly depend on the scores from $\phi$. The scores are only used to make a hard decision of pseudo-positive contexts. We can simply change the maximum marginal likelihood objective in Eq. (9) to reflect the scores from $\phi$ in $g$. Specifically, we change Eq. (9) to minimize Kullback-
Also for each context, we prepend a title of its

where \( P(c_i|q_t, \phi) = P(c_i = c^+|q_t, \phi) \) defined in

Eq. (8). Then the update rule \( q \) for TQR changes as follows (proof in Appendix B):

\[
\begin{align*}
q_{t+1} &= q_t + \eta \sum_{i=1}^{k} P(c_i|q_t, \phi) c_i - \eta \sum_{i=1}^{k} P_k(c_i|q_t) c_i. \\
&= q_t + \eta \sum_{i=1}^{k} P(c_i|q_t, \phi) c_i - \eta \sum_{i=1}^{k} P_k(c_i|q_t) c_i.
\end{align*}
\]  

Eq. (13) shows that \( q_{t+1} \) will reflect \( c_i \) weight-averaged by the cross-encoder (i.e., \( P(c_i|q_t, \phi) \)) while removing \( c_i \) weight-averaged by the current retrieval result (i.e., \( P_k(c_i|q_t) \)). This is a soft version of Eq. (11) since it leverages all top-\( k \) results and their probabilities while Eq. (11) makes a hard decision for choosing \( c^+_{qi} \).

3.3 Relevance Labeler

As described in the previous section, we use the cross-encoder \( \phi \) to provide a confidence score \( s_i \) over a pair of a query \( q \) and a context \( c \). While we test some off-the-shelf re-rankers for TQR in our experiments (Fajcik et al., 2021), we also introduce a simple baseline labeler for dense retrievers in case there are not any off-the-shelf re-rankers. For instance, for phrase retrieval (Lee et al., 2021b), no prior work has studied applying a cross-encoder re-ranker.

**Inputs for re-rankers** To train our re-ranker, we first construct a training set from the retrieval results of a dense retriever given a set of training queries \( Q_{\text{train}} \). Specifically, from the top retrieved contexts \( C_{1:k} \) for every \( q \in \mathcal{Q}_{\text{train}} \), we sample one positive context \( c^+_{qi} \) and one negative context \( c^-_{qi} \). In open-domain question answering, a context that contains a correct answer to each \( q \) is assumed to be relevant (positive). For phrase retrieval, we use sentences containing each retrieved phrase as our context following Lee et al. (2021b). Also for each context, we prepend a title of its document. Our re-ranker is trained on a dataset \( \mathcal{D}_{\text{train}} = \{(q, c^+_{qi}, c^-_{qi})|q \in \mathcal{Q}_{\text{train}}\} \).

**Architecture** We use RoBERTa-large model (Liu et al., 2019) as the base model for our re-ranker. Given a pre-trained LM \( \mathcal{M} \), the cross-encoder re-ranker \( \phi \) outputs a score of a context being relevant:

\[
s = \phi(q, c) = w^\top \mathcal{M}(q \oplus c)[\text{CLS}]
\]  

where \( \{\mathcal{M}, w\} \) are the trainable parameters and \( \oplus \) denotes a concatenation of \( q \) and \( c \) using a [SEP] token. Since phrase retrievers return both phrases and their contexts, we use special tokens [S] and [E] to mark the retrieved phrases within the contexts.

Re-rankers are trained to maximize the probability of a positive context \( c^+_{qi} \) for every \( (q, c^+_{qi}, c^-_{qi}) \in \mathcal{D}_{\text{train}} \). We use the cross entropy loss defined over the probability \( P^+ = \frac{\exp(h^+)}{\exp(h^+)+\exp(h^-)} \) where \( h^+ = \phi(q, c^+_{qi}) \) and \( h^- = \phi(q, c^-_{qi}) \). We found pre-training \( \phi \) with reading comprehension datasets (Kwiatkowski et al., 2019; Rajpurkar et al., 2016) is helpful.

**Score aggregation** While the re-ranker is used to provide pseudo relevance labels for TQR, it also serves as a strong baseline for dense retrieval. We found that adding a final re-ranking step at the end of TQR provides consistent improvement. We linearly interpolate the retrieval score \( f(q, c_i) \) with \( s_i \) for the final re-ranking: \( \lambda s_i + (1 - \lambda) f(q, c_i) \).

3.4 Efficient Inference

The main computational bottleneck of using TQR comes from labeling top-\( k \) retrieval results with a cross-encoder and performing additional retrieval with \( q_i \). To minimize the additional time complexity TQR, we perform up to 3 iterations of TQR with a stop condition of the top-1 retrieval result being pseudo-positive, i.e., \( c_1 \in c^+_{qi} \). When using \( \mathcal{L}_{\text{KL}} \), we only perform a single iteration of TQR since there is no hard decision for pseudo-positive contexts. We also cache \( \phi(q, c_i) \) for each query to skip redundant computation. We compare the time complexity of different settings in §5.3.

| Dataset                  | Train | Dev  | Test  |
|--------------------------|-------|------|-------|
| Natural Questions        | 79,168| 8,757| 3,610 |
| TriviaQA                 | 78,785| 8,837| 11,313|
| WebQuestions             | 3,417 | 361  | 2,032 |
| CuratedTrec              | 1,353 | 133  | 694   |
| SQuAD                    | 78,713| 8,886| 10,570|
| Entity Questions         | -     | -    | 22,075|

Table 1: Statistics of open-domain QA datasets. For EntityQuestions, we only use its test set for the out-of-domain evaluation.
Table 2: Open-domain QA results. We report Acc@1 (%) on each test set. DensePhrases and DPR are trained on all five open-domain QA datasets except DPR excluding SQuAD.

4 Experiments

We test TQR on multiple open-domain QA datasets. Specifically, we evaluate its performance on phrase retrieval and passage retrieval.

4.1 Datasets

We mainly use five open-domain QA datasets: Natural Questions (Kwiatkowski et al., 2019), TriviaQA (Joshi et al., 2017), WebQuestions (Berant et al., 2013), CuratedTrec (Baudiš and Šedivý, 2015), and SQuAD (Rajpurkar et al., 2016). For end-to-end open-domain QA, we use all the five datasets for the in-domain evaluation while performing the out-of-domain evaluation by training models only on Natural Questions and evaluating them on the rest. For passage retrieval for open-domain QA, we use Natural Questions and TriviaQA for the in-domain evaluation and evaluate on EntityQuestions (Sciavolino et al., 2021) for the out-of-domain evaluation. Table 1 summarizes the statistics of the datasets.

4.2 Open-domain Question Answering

For end-to-end open-domain QA, we use phrase retrieval (Seo et al., 2019; Lee et al., 2021a) for TQR, which directly retrieves phrases from entire Wikipedia using a phrase index. Since a single-stage retrieval is the only component in phrase retrieval, it is easy to show how its open-domain QA performance can be directly improved with TQR. We use DensePhrases (Lee et al., 2021a,b) for our base phrase retrieval model and train a cross-encoder labeler as described in §3.3. We report the top-1 retrieval accuracy (Acc@1) of phrase retrieval, which corresponds to the exact match score in open-domain QA. For the implementation details of TQR including its hyperparameters, see Appendix C.

Baselines Many open-domain QA models take the retriever-reader approach (Chen et al., 2017; Lee et al., 2019b). As our baselines, we mainly use state-of-the-art retriever-reader models that use extractive reader models, which is a fair comparison with retriever-only (+ re-ranker) models whose answers are always extractive. For re-ranking baselines of retriever-reader models, we report ReConsider (Iyer et al., 2021), which re-ranks the outputs of DPR + BERT. We also include RePAQ (Lewis et al., 2021) for a retriever-only model.

Results Table 2 shows the results on the five open-domain QA datasets in the in-domain evaluation setting where all models utilize the training sets of each dataset they are evaluated on. First, we observe that using our cross-encoder labeler φ as a re-ranker largely improves the performance of DensePhrases. Compared to adding a re-ranker on the retriever-reader model (DPR +
Table 3: Out-of-domain open-domain QA results. All models are trained only on Natural Questions. We report Acc@1 (%) on each test set. †: results obtained from evaluating the model provided by the authors. The publicly available implementation of DPR does not support running end-to-end QA on WebQuestions and CuratedTREC.

| Model                                | In-domain | Out-of-domain |
|--------------------------------------|-----------|---------------|
|                                      | NQ        | TRIVIAQA      | QW    | TREC | SQUAD |
| DPRNQ† (Karpukhin et al., 2020)      | 39.4      | 29.4          | -     | -    | 0.1   |
| DensePhrasesNQ (Lee et al., 2021a)   | 40.8      | 33.4          | 23.8  | 33.6  | 15.4  |
| + Re-ranker                          | **46.6**  | 41.7          | 25.0  | 39.0  | 20.4  |
| + TQR                                | 46.5      | 42.6          | 26.4  | **39.6** | **21.4** |
| + TQR + Re-ranker                    | **46.6**  | **42.7**      | **27.3** | **39.6** | **21.4** |
| DensePhrasesmulti                    | 41.6      | 56.3          | 41.5  | 53.9  | 34.5  |

Table 4: Passage retrieval results. We report Acc@5 / Acc@20 / Acc@100 (%) on each test set. Each retriever (and re-ranker) is trained on multiple open-domain QA datasets described in §4.1, which makes Natural Questions and TriviaQA in-domain evaluation while leaving EntityQuestions as out-of-domain evaluation.

| Model                                | In-domain | Out-of-domain |
|--------------------------------------|-----------|---------------|
|                                      | NQ        | TRIVIAQA      | ENTITYQ |
| DensePhrasesmulti                    | 69.6 / 79.8 / 86.0 | 75.0 / 81.6 / 85.8 | 51.4 / 61.0 / 71.2 |
| + Re-ranker (Fajcik et al., 2021)   | 76.3 / 83.2 / 86.0 | **78.2** / 83.0 / 85.8 | 58.8 / 65.3 / 71.2 |
| + TQR                                | 74.4 / 81.9 / **86.9** | 77.1 / 82.4 / **86.1** | 57.3 / 64.4 / **72.4** |
| + TQR+ Re-ranker                     | **77.1** / **84.0** / **86.9** | **78.0** / **83.2** / **86.1** | **59.9** / **66.2** / **72.4** |
| DPRmulti                             | 67.8 / 79.4 / 86.5 | 70.3 / 79.0 / 84.8 | 44.7 / 57.9 / 70.8 |
| + Re-ranker (Fajcik et al., 2021)   | **76.4** / **83.6** / **86.5** | **76.5** / **81.6** / **84.8** | 57.6 / 64.4 / 70.8 |
| + TQRKL                              | 73.1 / 81.7 / **87.2** | 74.5 / 80.5 / **85.1** | 56.2 / 63.8 / **72.5** |
| + TQRKL+ Re-ranker                   | **76.4** / **84.2** / **87.2** | 76.4 / **81.6** / **85.1** | **59.3** / **66.2** / **72.5** |

Re-ranker by Iyer et al., 2021), the gain is much larger possibly due to its high top-k accuracy (k > 1) that we observed. Unlike using the simple Rocchio’s algorithm, using TQR on DensePhrase$\text{multi}$ improves the performance drastically, even beating the strong re-ranker. It advances the dense phrase retriever by 8.1% on average when combined with the re-ranker.

Out-of-domain evaluation In Table 3, we show results on the out-of-domain evaluation of two open-domain QA models trained on Natural Questions: DPRNQ and DensePhrasesNQ. All hyperparameters of TQR were tuned using the in-domain development set. As a reference, we show the result by DensePhrase$\text{multi}$ (last row), which was trained on all five datasets. While the in-domain accuracy of DPRNQ and DensePhrasesNQ is comparable to DensePhrase$\text{multi}$, we observe a huge performance drop on out-of-domain datasets for both models. In particular, DPR seems to suffer more (e.g., 0.1 on SQuAD) since both of its retriever and reader models were trained on NQ, which exacerbate the problem when combined.

On the other hand, using TQR with or without a re-ranker largely improves the performance of DensePhrase$\text{NQ}$ in the out-of-domain setting. When using TQR + Re-ranker, we observe 6.2% improvement on average for out-of-domain datasets. Interestingly, we find that applying a re-ranker, which was also trained on Natural Questions, is a strong baseline for the out-of-domain evaluation.

4.3 Passage Retrieval

We test TQR with passage and phrase retrievers on the passage retrieval task for open-domain QA. We use DPR as a passage retriever and DensePhrases as a phrase retriever. For both DPR and DensePhrases, we use off-the-shelf passage re-ranker (Fajcik et al., 2021) to show how existing re-rankers can serve as a pseudo labeler for TQR. For DPR, we use the KL-divergence variant of TQR introduced in §3.2 (denoted as TQR$\text{KL}$), which consistently performed better than TQR on this task. We report top-k retrieval accuracy, which is 1 when the answers exist in top-k retrieval results.

2We follow Lee et al. (2021b) to run phrase retrieval for passage retrieval.
Query: which type of wave requires a medium for transmission?
Answers: [sound, heat energy, mechanical waves]

![Diagram of TQR predictions from Natural Questions](image)

Table 2: A sample prediction of TQR from Natural Questions. For every \( t \)-th iteration of TQR, we show top 5 phrases (denoted in bold) retrieved from DensePhrases along with their passages. The score \( s_t \) from the cross-encoder labeler \( \phi \) is shown in each parenthesis. \( t = 0 \) denotes initial retrieval results. When \( t = 1 \), TQR obtains three new results and the correct answer “Sound” becomes the top-1 prediction at \( t = 3 \).

| NQ   | WQ   |
|------|------|
| DensePhrases\( \alpha \) | 42.4 | 20.5 |
| Rocchio’s (\( \alpha = 1, \beta = 0.3, \gamma = 0 \)) | 42.5 | 21.1 |

| DensePhrases\( \alpha \) + TQR | 48.1 | 24.4 |
| \( C_p^0 \Rightarrow C_{1,k'} \) (\( k' = 3 \)) | 42.0 | 20.5 |
| SGD \( \Rightarrow \) interpolation (\( \beta = 0.3 \)) | 47.1 | 24.9 |
| \( \mathcal{L} \Rightarrow \mathcal{L}_{\text{KL}} \) | 44.1 | 22.7 |
| No weight decay (\( \lambda_{\text{decay}} = 0 \)) | 48.0 | 24.4 |

| DensePhrases\( \alpha \) + TQR + Re-ranker | **48.2** | **25.2** |
| \( \lambda = 0.1 \Rightarrow \lambda = 1 \) | 47.9 | **25.2** |

Table 3: Ablation study of TQR on two open-domain QA development sets. We report top-1 accuracy of phrase retrieval. Since DensePhrases\( \alpha \) is trained on Natural Questions (NQ), WebQuestions (WQ) serves as an out-of-domain dataset. See §5.1 for description.

**Results** Table 3 shows results of passage retrieval for open-domain QA. We find that using TQR with off-the-shelf re-rankers can improve the passage retrieval performance on both in-domain and out-of-domain settings although it does not outperform the re-ranking method on Acc@5 and Acc@20 when used alone. However, when combining TQR (or TQR\( \text{KL} \)) with the re-ranker, we observe more consistent gains on all settings and metrics. Gains on the out-of-domain dataset (EntityQuestions by Sciavolino et al., 2021) stand out even for Acc@5. Notably, Acc@100 always improves whenever we use TQR, which is not possible for re-rankers since they do not update the top retrieval results.

**5 Analysis**

### 5.1 Ablation Study

Table 5 shows an ablation study of TQR on two open-domain QA datasets. With the Rocchio’s algorithm, the best configuration of \( \alpha, \beta, \gamma \) is shown in each parenthesis. When \( t = 1 \), TQR obtains three new results and the correct answer “Sound” becomes the top-1 prediction at \( t = 3 \).
domain setting. This shows that there could be a better setting of TQR for the out-of-domain setting since we chose our hyperparameters using the in-domain datasets. Other settings including the weight decay $\lambda_{\text{decay}}$ and the interpolation parameter $\lambda$ seem to have smaller effect while $\mathcal{L}$ is clearly a better choice for DensePhrases than $\mathcal{L}_{\text{KL}}$.

5.2 Effect of Iterations in TQR

Figure 3 shows the effect of iterative TQR compared to the Rocchio’s algorithm. Note that when $t = 0$ (i.e., # of iterations = 0), TQR and Rocchio’s denote the initial retrieval accuracy while TQR + Re-ranker denotes the accuracy of applying a re-ranker on DensePhrases. The performance of the Rocchio’s algorithm marginally improves or even degrades with a larger number of iterations. On the other hand, the performance of TQR largely improves especially when $t = 1$. Adding a final re-ranking step gives additional gains for TQR.

Sample prediction Figure 2 shows a sample prediction from TQR. We use DensePhrases + TQR with $k = 10$, from which top-5 results are shown. While the initial result at $t = 0$ failed to retrieve correct answers in the top-10, the next round of TQR gives new results including the correct answer, which were not retrieved before.

5.3 Run-time Analysis

Figure 4 summarizes the run-time analysis of TQR. With multiple iterations of TQR, the run-time of TQR increases linearly. By adding the caching mechanism for $\phi$ and the stop condition of $c_1 \in C^P$, the run-time is reduced drastically.

6 Conclusion

In this paper, we propose a novel framework that iteratively refines the representation of a test query for dense retrieval. Specifically, we refine instance-level query representations at test time using gradient-based optimization method over the top retrieval results. Our cross-encoder labeler provides pseudo labels for the optimization. We theoretically show that the gradient-based optimization provides a generalized form of the classical Rocchio’s algorithm for pseudo relevance feedback. Experiments show that our test-time query refinement combined with dense phrase (or passage) retrievers largely improves the retrieval accuracy on multiple open-domain QA datasets in both in-domain and out-of-domain settings.

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A Derivation of the Gradient for Test-time Query Learning

Proof. We compute the gradient of $L(q_t, C_{1:k}^{g})$ in Eq. (10) with respect to $q_t$. Denoting $\sum_{c} P_k(c|q_t)$ as $Z$, the gradient is:

$$
\frac{\partial L(q_t, C_{1:k}^{g})}{\partial q_t} = \frac{\partial L(q_t, C_{1:k}^{g})}{\partial Z} \frac{\partial Z}{\partial q_t}
$$

$$
= \frac{1}{Z} \sum_{c} \frac{\partial P_k(c|q_t)}{\partial q_t} c
$$

$$
= -\frac{1}{Z} \sum_{c} \sum_{i=1}^{k} \frac{\partial P_k(c|q_t)}{\partial q_t^i} \partial q_t^i c
$$

$$
= -\frac{1}{Z} \sum_{\tilde{c}} \sum_{i=1}^{k} (\delta[c_i = \tilde{c}] - P_k(c_i|q_t)) P_k(\tilde{c}|q_t^i) c_i
$$

$$
= -\sum_{\tilde{c}} P(\tilde{c}|q_t) \sum_{i=1}^{k} (\delta[c_i = \tilde{c}] - P_k(c_i|q_t)) c_i
$$

$$
= -\sum_{\tilde{c}} P(\tilde{c}|q_t) \sum_{i=1}^{k} P_k(\tilde{c}|q_t^i) c_i
$$

$$
+ \sum_{\tilde{c}} P(\tilde{c}|q_t) \sum_{c \in C_{1:k}^{g}, c \neq \tilde{c}} P_k(c|q_t) c
$$

where for $f(q, c)$, we used $q^\top c$. Then, we have:

$$
g(q_t, C_{1:k}^{g}) = q_t - \eta \frac{\partial L(q_t, C_{1:k}^{g})}{\partial q_t}
$$

$$
= q_t + \eta \sum_{\tilde{c}} P(\tilde{c}|q_t) (1 - P_k(\tilde{c}|q_t)) \tilde{c}
$$

$$
- \eta \sum_{\tilde{c}} P(\tilde{c}|q_t) \sum_{c \in C_{1:k}^{g}, c \neq \tilde{c}} P_k(c|q_t) c.
$$

B Derivation of the Gradient for Test-time Query Learning (KL)

Proof. We compute the gradient of $L_{KL}(q_t, C_{1:k}^{g})$ in Eq. (12) with respect to $q_t$. Denoting $P(c_i = c^*|q_t, \phi)$ as $P_t$, we expand the loss term as:

$$
L_{KL}(q_t, C_{1:k}^{g}) = -\sum_{i=1}^{k} P_t \log \frac{P_k(c_i|q_t)}{P_t}
$$

$$
= -\sum_{i=1}^{k} P_t(q_t^i c_i - \log \sum_{j=1}^{k} \exp(q_t^i c_j) - \log P_t).
$$

Then, the gradient is:

$$
\frac{\partial L_{KL}(q_t, C_{1:k}^{g})}{\partial q_t^i}
$$

$$
= -\sum_{i=1}^{k} P_t \frac{\partial}{\partial q_t^i} (q_t^i c_i - \log \sum_{j=1}^{k} \exp(q_t^i c_j) - \log P_t).
$$
Putting it all together:

\[
g(\mathbf{q}_t, C_{1:k}) = \mathbf{q}_t - \eta \frac{\partial L_{KL}(\mathbf{q}_t, C_{1:k})}{\partial \mathbf{q}_t}
\]

\[
= \mathbf{q}_t + \eta \sum_{i=1}^{k} P_i(c_i | q_t, \phi) c_i - \eta \sum_{i=1}^{k} P_k(c_i | q_t) c_i.
\]

\[\Box\]

### C Implementation Details

**Re-ranker** To train a cross-encoder re-ranker described in §3.3, we first annotate the top 100 retrieved results from DensePhrases. We use three sentences as our context, one that contains a retrieved phrase and the other two that surround it. This leads to faster inference than using the whole paragraph as an input while preserving the performance. During the 20 epochs of training, we sample positive and negative contexts for every epoch while selecting the best re-ranker based on the validation accuracy of the re-ranker. We modified the code provided by the Transformers library\(^3\) (Wolf et al., 2020) and used the same hyperparameters as specified in their documentation except the number of training epochs.

**Dense retriever** We modified the official code of DensePhrases\(^4\) (Lee et al., 2021a) and DPR\(^5\) (Karpukhin et al., 2020) to implement TQR on dense retrievers. While pre-trained models and indexes of DensePhrases\(_{multi}\) and DPR\(_{NQ}\) are publicly available, the indexes of DensePhrases\(_{NQ}\) and DPR\(_{multi}\) have not been released as of May 25th, 2022. We reimplemented them to experiment with out-of-domain open-domain QA and passage retrieval, respectively.

\(^3\)https://github.com/huggingface/transformers/blob/v4.13.0/examples/pytorch/text-classification/run_glue.py
\(^4\)https://github.com/princeton-nlp/DensePhrases
\(^5\)https://github.com/facebookresearch/DPR

### Table 6: Hyperparameters of TQR for open-domain QA and passage retrieval.

| Hyperparameter | Open-domain QA | Passage Retrieval |
|----------------|----------------|-------------------|
| Loss function  | \(L\)           | \(L\)             |
| \(L_{KL}\)     | \(L_{KL}\)     |                   |
| Learning rate \(\eta\) | 1.2 | 1.2 | 0.2 |
| Max iterations | 3              | 1                 | 1   |
| Retrieval top-\(k\) | 10            | 100               | 100 |
| Re-ranker top-\(k\) | 10            | 100               | 100 |
| Re-ranker \(\lambda\) | 0.1 (0.4 for TQA) | 1 | 1 |

**Hyperparameter** When running TQR, we use the gradient descent with momentum set to 0.99 and use weight decay \(\lambda_{\text{decay}} = 0.01\). We also perform a linear learning rate scheduling per iteration. Both the threshold \(\rho\) and temperature \(\tau\) for pseudo labels are set to 0.5. Table 6 lists the hyperparameters that are used differently for each task.