Rethinking the Evaluation of Neural Machine Translation

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Abstract

The evaluation of neural machine translation systems is usually built upon generated translation of a certain decoding method (e.g., beam search) with evaluation metrics over the generated translation (e.g., BLEU). However, this evaluation framework suffers from high search errors brought by heuristic search algorithms and is limited by its nature of evaluation over one best candidate. In this paper, we propose a novel evaluation protocol, which not only avoids the effect of search errors but provides a system-level evaluation in the perspective of model ranking. In particular, our method is based on our newly proposed exact top-$k$ decoding instead of beam search. Our approach evaluates model errors by the distance between the candidate spaces scored by the references and the model respectively. Extensive experiments on WMT’14 English-German demonstrate that bad ranking ability is connected to the well-known beam search curse, and state-of-the-art Transformer models are facing serious ranking errors. By evaluating various model architectures and techniques, we provide several interesting findings. Finally, to effectively approximate the exact search algorithm with same time cost as original beam search, we present a minimum heap augmented beam search algorithm.

1 Introduction

Recent sequence-to-sequence (Seq2Seq) models have shown promising results in neural machine translation (NMT), where methods typically frame a conditional probability distribution from a source sentence to a target sentence. Generally, an NMT system aims to find the target translation with the highest conditional probability, i.e., maximum-a-posterior (MAP). Unfortunately, the framework of Seq2Seq models makes the search space of an NMT system intractable. For instance, Transformer models for the WMT’14 English-German task usually have a vocabulary with the size of tens of thousands. Then the search space of a source sentence becomes target length powers of vocabulary size, which is difficult to tackle by modern computer architectures. As a result, most state-of-the-art NMT benchmarks are attained using beam search as the common surrogate for MAP decoding and achieve remarkable results evaluated by BLEU.

Despite its success in applications and benchmarking, beam search decoding is pruned to various biases (such as label bias, length bias [5]) and brings in huge search errors [22], which is entangled with the NMT model errors in the evaluation process. This coupling feature makes beam search an imperfect option for evaluating NMT models and may hinder progress in NMT. For example,
suppose we observe model improvement over the commonly used beam search+BLEU evaluation protocol. In that case, there is nowhere to discover whether the model errors are reducing due to the existence of beam search blessing \cite{15}. One promising direction is using exact search \cite{22} to evaluate model errors, which is able to find the highest probability candidate (mode) in all possible candidates (candidate space). However, decoding with mode lacks the sense of all other possible candidates, possibly with high probabilities, and limits its usefulness.

Furthermore, conventional evaluation metrics \cite{19, 3, 4, 7} for machine translation systems focus on evaluating similarities of one best translation versus the reference. However, the evaluation of the one best candidate neglects the system-wise ranking over the candidate space. Intuitively, a candidate $y_i$ with higher BLEU should have a larger probability than $y_j$ with lower BLEU. Such ranking capability cannot be evaluated using the one best candidate metrics. Therefore, a new system-level evaluation protocol to assess model errors in terms of ranking capability is essential.

This paper argues that the better evaluation protocol should consist of 1) an exact search algorithm that has access to candidate space, and 2) an evaluation metric capable of evaluating rankings over the candidate space. To this end, we take a first step and propose a new evaluation protocol for NMT model errors instead of the beam search with BLEU protocol. Particularly, to evaluate candidate-level ranking, we provide formal definitions of model errors, based on our newly proposed exact top-$k$ decoding. Experiments show that the state-of-the-art Transformer models perform poorly on ranking capability. In addition, we show that regularization terms like length normalization \cite{2, 27} and uniform information density (UID) regularization \cite{15} decrease model errors. Finally, to effectively approximate the exact search algorithm with the same time cost as original beam search, we present a minimum heap augmented beam search algorithm. \footnote{Codes will be released to public soon.}

2 Related Work

Decoding Methods. The most popular decoding of NMT systems aims to find the candidate with the highest conditional probability. This is called the maximum-a-posterior (MAP) decoding algorithm. Among all MAP decoding methods, beam search is the most widely applied method in the modern NMT systems for evaluation, which utilizes a fixed size of beam for each decoding step. Naive beam search with log-probabilities has several known drawbacks, for example, favoring short translations and its monotonic constraint. Hence, many regularization/rescoring methods \cite{2, 27, 8, 28, 16} or beam search variants \cite{6, 21} are proposed to improve the performance of beam search. Other than beam search, one promising MAP decoding technique for evaluation is the DFS-based exact search \cite{22}, which is designed to find the mode of model distributions. Despite its high computational cost, it reveals important information about model distributions. We follow this approach and present a top-$k$ exact search method, which can evaluate model errors from the perspective of ranking candidates.

In addition, there are some proposed non-MAP decoding algorithms. One typical case is the stochastic sampling-based decoding methods \cite{1, 10}, which randomly choose candidates from each step’s output distribution. Eikema and Aziz \cite{5} introduces a Minimum Bayesian Risk decoding method based on sampling. Leblond et al. \cite{13} propose a metric-driven search approach via Monte-Carlo Tree Search (MCTS).

Error Evaluation. Evaluation of NMT errors focuses on studying the gap between machine-translated results and human-translated references. Statistical matching metrics, such as BLEU, METEOR \cite{19, 3, 12, 4, 7}, are dominant in evaluating errors. Their work proves that linguistic similarity between references and machine translations correlates the human evaluation well. However, to the best of our knowledge, these statistical metrics only evaluate one best candidate (i.e., sentence or document). None of them evaluate the system-level ranking of generated candidates. In contrast, we take the system-level ranking into account, which takes the first step from fixed candidate evaluation to system-level ranking evaluation.

Recently, some efforts \cite{17, 23, 22} are devoted to evaluate model errors without search errors. Interesting results are provided by Stahlberg and Byrne \cite{22}, where they find a phenomenon that about half of the modes of model distribution are empty. However, using the percentage of empty modes is easy to evaluate model errors and sometimes fails when models are trained with pseudo-parallel data. Meister et al. \cite{15} points out high search errors in beam search provide a lucky bias...
for NMT systems. Eikema and Aziz [5] shows that mode only accumulates little probability mass and utilizes non-MAP sampling-based methods to evaluate model errors. Our work follows the exact search algorithm but differs from Stahlberg and Byrne [22]. We provide a more comprehensive definition of model errors from the perspective of candidate-level ranking and show the mode analysis only offers a special case for ranking-based model errors evaluation.

3 Exact Top-k Decoding

Obtaining the whole candidate space is intractable because of the unlimited search space. One reasonable approximation is to focus more on top-ranking candidates. Here we take a step forward and propose a top-k DFS-based exact search method. Our decoding method is guaranteed to find the exact top-k candidates from the model’s output distribution. Specifically, a min-heap is equipped and used to maintain current top-k candidates during the search procedure. We use beam search results as our initial lower bound to reduce the search space, and the candidate with the lowest score in the minimum heap serves as our lower bound during searching. Once we find a newly finished candidate (i.e., end with <EOS>), we push the candidate into the heap and make adjustments to retain the heap size equals k. It is no easy to make top-k exact search tractable. Many efforts have been devoted to implementation to make the search time under the acceptable line, and sometimes our method is even faster than the DFS algorithm provided by [22]. Implementation details and algorithm can be found in Appendix.

The proposed top-k exact search algorithm has two keys advantages compared with the top-1 counterpart. Firstly, it enables further analysis over the model’s candidate list and beam search curse (Section 4). Secondly, the theoretical runtime of our top-k method is at the same scale as the top-1 search algorithm, and decoding outputs are much more informative (See Appendix).

3.1 Comparison with Beam Search Decoding

The proposed exact top-k decoding method enables us to investigate the relationship between the beam search outputs and the exact top-k results. Specifically, we first run the algorithm of exact top-100 decoding and beam search with beam sizes of 5, 10, 20, 50, 100 on WMT’ 14 English-German testset respectively[3]. The differences between the two results can help us understand to what extent they disagree. Then, we plot the ranked positions of the beam search results over the exact outputs in Figure 1a. This figure clearly shows that a larger beam size leads to fewer search errors since the ranked positions of those candidates get higher. As normally would do, we compute the BLEU of those candidates. The results demonstrate that the higher ranked candidates exhibit worse BLEU scores (see Figure 1b), which depicts that the NMT system has defects on ranking, i.e., it tends to place a poor candidate at a relatively high position. Previous works call this phenomena beam search curse [28] - translation quality degrades as beam sizes increases.

3The experimental details can be found in Appendix.
Besides, we generate translations of each source sentence with different beam sizes. Then, we compute and compare the sentence-level BLEU scores of those translations. Based on the results shown in Figure 1a, one may guess the BLEU changes on sentence-level are consistently along with the increments of the beam size, as previous experiments show. In contrast, the changes are random (see Figure 1c), which means a source sentence might be translated to a better target sentence or a worse target sentence randomly when the beam size gets larger. This reveals that the NMT model also have a large number of ranking errors, i.e., two very close candidates may be ordered falsely by the model.

Based on the above experimental results, we discover that beam search curse is closely related to the ranking capability of an NMT model. This interesting finding motivates us to study how to evaluate the ranking capability of an NMT system. Because if an NMT model can successfully order all candidates by a certain scoring function, the beam search curse will disappear.

### 4 Evaluation Metrics for Model Errors

#### 4.1 Definition of Model Errors

This section provides a new evaluation protocol with the aid of both exact top-k decoding and newly proposed ranking-based metrics.

First of all, let us briefly introduce NMT models. Most of the NMT models are autogressive models, which are trained using Cross-Entropy objective guided by target reference $\hat{y}$,

$$\mathcal{L}_{CE} = \sum_{t \in (1,T)} \hat{y}^t \log P(\hat{y}^t|x; \hat{y}^{1:t-1})$$

where $t$ represents the time step for target side and $T$ is total length for the target sentence. Then, a NMT model defines a conditional distribution for each target candidate $y_i$ as:

$$\log P(y_i|x) = \sum_{t \in (1,T)} \log P(y_i^t|x; y_i^{1:t-1}), y_i \in Y,$$

over all $n$ possible candidates $Y = \{y_1, y_2, \cdots, y_n\}$.

Next, we can discuss how the ideal ranking over candidate space works. Since we find that the candidate-level ranking is closely related to model errors, the candidate space scored by model log-probabilities should align with the candidate space scored by translation quality metrics. Specifically, if the translation quality of specific candidate translation $y_i$ is better than that of $y_j$, the model’s probabilities over $y_i$ should also be higher than that over $y_j$. Hence, by extending such ability to all candidates for a source sentence $x$, we have a perfectly ordered candidate list with the index sorted by translation quality. We refer to such ability as candidate-level ranking (CR). Formally,

$$Y_{CR} = [y_{I_{CR}}^1, y_{I_{CR}}^2, \cdots, y_{I_{CR}}^n]; I_{CR} = \text{argsort}([Q(y_1), \cdots, Q(y_n)]),$$

$$Y_{M} = [y_{I_{M}}^1, y_{I_{M}}^2, \cdots, y_{I_{M}}^n]; I_{M} = \text{argsort}([\log P(y_1|x), \cdots, \log P(y_n|x)]),$$

where $Q(y)$ is the translation quality function that simplifies $Q(y, \hat{y}, x)$, e.g., BLEU. $Y_{CR}$ and $Y_{M}$ are candidate lists sorted by $Q$ and $P$, respectively.

Thus, we can now define the ranking-based model errors be the gap between these two sorted list,

$$\text{ME} = D(Y_{CR}, Y_{M}),$$

where $D$ is a distance function over two lists.

#### 4.2 Evaluate Ranking Capability

4.2.1 Mode and Empty Sentences.

First, let us take a look at the metrics proposed by previous work [22]. Powered by the exact decoding method, we can find the candidate $y_m$ that has the highest score in the model distribution. Then, we define the ratio for empty mode by checking $y_m = y_{emp}$, where $y_{emp} = "<\text{EOS}>"$. 

4
Now, we show the empty ratio is a special case of the definition of our CR-based model errors. On the one hand, given any matching-based translation quality function $Q$, the empty output should always rank to the last of $Y_{CR}$. On the other hand, $y_m$ is the mode of model distribution and should rank the first in $Y_M$.

$$y_m = Y_M[0]; \quad y_{emp} = Y_{CR}[n-1].$$  \hfill (6)

The corresponding distance function is:

$$D_{empty} = \begin{cases} 1 & \text{if } Y_M[0] = Y_{CR}[n-1] \\ 0 & \text{else} \end{cases},$$  \hfill (7)

As shown, the ratio of empty mode is a special case of our CR modeling. In the following context, we discuss about how to define our metrics which fully evaluate ranking capability.

### 4.2.2 CR-based Model Errors.

Here, we present our CR-based model error metrics, which are defined over the CR ranked list $Y_{CR}$ and model ranked list $Y_M$. It is worth noting that getting the complete model and CR ranked list are both non-trivial. Our metrics have to rely on approximations. Luckily, in real-world NMT systems, we prioritize top-ranking candidates. Thus we propose to use the top-$k$ exact search (Section 3) and define our metrics on these top-ranking candidates. Formally, we define a truncated ranked list:

$$\tilde{Y}_M = Y_M[0:k]; \quad \tilde{I}_M = I_M[0:k],$$  \hfill (8)

where $k$ denotes how many top-ranking candidates we use. Then, the model error formulation becomes

$$ME = D(Y_{CR}, \tilde{Y}_M),$$  \hfill (9)

**Edit-Distance Based Ranking.** Question left unsolved is how to find $Y_{CR}$. The main challenge of getting $Y_{CR}$ is to enumerate the unlimited space of translation candidates. To this end, we use the top-candidates found before to query $Y_{CR}$.

Inspired by [18], we propose to model $Y_{CR}$ with a edit-distance based ranked list, where each candidate is ranked by its edit-distance to the references,

$$Q(y, \hat{y}, x) = \text{Edit\_Distance}(y, \hat{y}).$$  \hfill (10)

Then, given a candidate $y_i$ with $e$ edits to reference, we can estimate the number of candidates with $e$ edits by,

$$c(e, T) = \sum_{s=0}^{T} \binom{T}{s} \cdot \binom{T + e - 2s}{e - s} |V|^e,$$  \hfill (11)

where $s$ represents the number of substitution operations and $|V|$ is the vocabulary size. For more details, we refer our readers to [18]. Then we can estimate the rank of candidate $y_i$ with the sum of numbers of candidates with edit distance lower than $e$,

$$\text{Rank}(y) = \sum_{e' \in [0,e)} c(e', T).$$  \hfill (12)

The visualization of edit-distance rankings is shown in Figure 2 to illustrate how the model error changes when using different model architectures and techniques.

Note that we are using exact top-100 candidates of model distribution for this visualization. We would expect the candidates are located among the top $0 \sim 10\%$ of edit-distance rankings. Interestingly, across all models, the probability mass of these top-ranking candidates lies either in the top $10\%$ or the last $10\%$ of edit-distance ranks. About $70\%$ of the candidate sentences are located in the last $10\%$. It indicates very severe model errors, where the model prefers both good candidates (ranked $0 \sim 10\%$) and bad candidates (ranked $90\% \sim 100\%$). In addition, we have several observations:

- Model without label smoothing strongly decreases the number of top candidates located in the last $10\%$ of ranks.
• Pseudo generated techniques decrease the model error. The model with forward-translated data significantly decreases model errors.
• Increasing the dropout does not necessarily improve model errors.
• Increasing model capacity, like deepening or widening model architectures, generally reduces model errors monotonically.

Even though the edit-distance ranking analysis looks interesting, edit-distance is not a conventional evaluation metric used in NMT.

**Our Proposed Evaluation Metrics.** To solve above issue, we propose another approach heading for CR-based ME metrics. Since $Y_{CR}$ is hard to get, we select candidates appeared in $Y_M$ to form a locally CR ranked list $Y_{CR}$. Formally,

$$Y^C_R = \{y_{f_{CR}}^0, y_{f_{CR}}^1, \cdots, y_{f_{CR}}^k\}; \hat{I}_{CR} = \text{argsort}([Q(y_{f_{CR}}^0), \cdots, Q(y_{f_{CR}}^k)]).$$

(13)

Then, we have our new local ME metrics as,

$$\text{ME} = D(Y_{CR}, Y_M)$$

(14)

For ranking distance $D$, we provide two distance metrics here. Firstly, we propose an extended version of nDCG $^1$, $\text{ME}_{\text{RANK}}$:

$$\text{ME}_{\text{RANK}} = 1 - \frac{\text{DCG}(Y_M)}{\text{DCG}(Y_{CR})},$$

(15)

$$\text{DCG}_k(Y) = \sum_{y_j \in Y^{[0:k]}} 2^{f(y_j)} D(j); f(y_j) = k - \text{Rank}(y_j, Y),$$

(16)

where $D(r)$ is an exponential discount function. The $\text{ME}_{\text{RANK}}$ directly measures the ranking ability of a model’s outputs, where 1 means completely wrong ranking and 0 means perfect ranking.

Next, in the concern of both translation quality and global ranking ability, we further propose $\text{ME}_{\text{GRANK}}$ over globally ranked list $Y_{CR}$:

$$\text{ME}_{\text{GRANK}} = 1 - \frac{\text{DCG}_{bk}(Y_M)}{\text{DCG}_{bk}(Y_{CR})}; \text{DCG}_{bk}(Y) = \sum_{y_j \in Y^{[0:k]}} 2^{Q(y_j)} D(j),$$

(17)

and we approximate $\text{DCG}_{bk}(Y_{CR})$ with its upper-bounds:

$$\text{DCG}_{bk}(Y_{CR}) = \sum_{y_j \in Y_{CR}^{[0:k]}} 2^{Q(y_j)} D(j) <= \sum_{j \in [0:k]} 2^{1.0} D(j),$$

(18)

where in practice we use BLEU scores for $Q$.

The $\text{ME}_{\text{RANK}}$ accounts for how translated candidates are ranked, while $\text{ME}_{\text{GRANK}}$ accounts for how translated outputs performs globally in terms of translation quality. Table I demonstrates the results of different model error metrics for different Transformer-based models in WMT’14 English-German task. We make the following observations.

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Figure 2: The edit-distance ranking visualization of Transformer models with different techniques. Here, we use top-10 candidates of exact search, **para ft** and **para bt** denote the model trained with both golden dataset and forward/backward generated pseudo dataset.
Table 1: Model errors of different models in WMT’14 En-De task. All numbers range in [0, 100%].

| Method                      | Beam Search | Mode | CR-Based       |
|-----------------------------|-------------|------|----------------|
|                             | BLEU(↑)     | ↑    | ME_RANK(↓)     |
|                             | # Empty(↓)  | ↓    | ME_RANK(↓)     |
| Transformer(base)           | 27.22       | 64.70| 49.67 (ref)    |
| - label smoothing           | 26.76       | 34.85| 48.38 (-1.29)  |
| + para bt                  | 27.36       | 27.26| 48.30 (-1.40)  |
| + para ft                  | 28.06       | 0.93 | 46.24 (-3.43)  |
|                            |             |      | 81.30 (-8.20)  |
| Transformer(12-layer Encoder)| 27.75       | 58.11| 49.16 (-0.51)  |
| Transformer(18-layer Encoder)| 28.03       | 53.58| 48.45 (-1.22)  |
| Transformer(Dim 768)        | 28.00       | 50.18| 48.44 (-1.23)  |
| Transformer(Dim 1024)       | 28.49       | 44.72| 48.42 (-1.25)  |

Firstly, let us take a look at the empty ratios. We find that removing label smoothing, adding pseudo-parallel data will drastically decrease the number of empty ratios, even close to 0 (para ft), indicating relatively small model errors. However, it is not the case. Therefore, empty ratios evaluation may collapse when evaluating specific models. In contrast, our metrics are more steady for various models, showing the superiority of our model error metrics.

Secondly, we find that the current SOTA Transformer models are far from perfection. Regarding our ME_RANK results, the results range from about 46% ~ 50%, indicating that our Transformer models face serious ranking problems.

Thirdly, when including the translation quality into accounts, i.e., ME_RANK, we find the system-level errors range from 80% ~ 90%. It proves that our models include too many low-quality translations into top-ranking candidates.

Fourthly, increasing model capacity gives minor improvements over baseline models. Various dropout settings provide minor impacts on model errors. These findings are consistent with our edit-distance analysis.

Finally, w/o label smoothing and para ft models demonstrate strong potential in reducing model errors. Since these two methods both improve the model confidence, we guess that confidence is highly related to model errors, and leave it as a future work.

4.3 Understanding Search Regularization via ME

Recent research has reported that regularization terms are essential in the success of beam search algorithms. Regularization terms, like length penalty [2, 27], UID penalties [13], typically modify the log-probability produced by model. In this section, we study how these regularization terms (or called penalties) affect model errors. These regularizations are commonly considered as inductive biases to help beam search avoid errors. As a result, these regularization terms are commonly regarded as fixes for the beam search algorithm. Nonetheless, we argue that these regularization terms substantially improve the model’s ranking capability and can be evaluated using the proposed CR-based model error metrics. Recall that given a candidate-level distribution \( \log P(y|x) \), the model’s regularized ranked list is defined by:

\[
I_M = \text{argsort}([\log P(y_1|x), \cdots, \log P(y_n|x)]),
\]

\[
Y_M = [y_I^{I_M}, y_I^{I_M}, \cdots, y_I^{I_M}],
\]

(19)

Then, a certain regularization term \( \mathcal{R}(y) \) changes model rankings to:

\[
I_{MR} = \text{argsort}([\log P(y_1|x) + \mathcal{R}(y_1), \cdots, \log P(y_n|x) + \mathcal{R}(y_n)]),
\]

\[
Y_{MR} = [y_{I_{MR}}^{I_{MR}}, y_{I_{MR}}^{I_{MR}}, \cdots, y_{I_{MR}}^{I_{MR}}],
\]

(21)

(22)
 Accordingly, search penalties is closely related with ranking capability of NMT model. We conduct experiments using search penalties to rerank the exact search outputs for Transformer(base) model, to see how search penalties changes the ranking and over all model errors. For search penalties, we choose length normalization \cite{27} and UID regularizations \cite{15}. Results are shown in Table 2.

As we can see, all regularization terms substantially improve the model errors by a strong margin, from 50.33 to 62+ in Rank-nDCG and from 10.50 to 11.79+ in Norm-DCG. It proves our point that search penalties indeed influence model errors. We find that length normalization performs the best among all terms among all penalties, which proves length bias is an important issue in model errors. The UID terms have lower performance in the ranking ability (Rank-nDCG) but get similar results in Norm-DCG, compared with length normalization, demonstrating that UID terms improve in a partially orthogonal direction with length norm term.

## 5 Approximate Exact Decoding

The ranking-based ME enables us to evaluate the quality of NMT models and find new problems from a different perspective. A fact is that the algorithm of an evaluation protocol should be consistent with the algorithm used in production. For instance, the beam search with BLEU evaluation protocol is widely used because beam search is commonly adopted in production. Otherwise, the evaluation is hard to provide informative clues for improving the quality of production models. Nevertheless, our proposed ME relies on the proposed exact top-k decoding, and the exact decoding methods are still far from the beam search decoding with regard to the computational cost. We argue that the future of sequence decoding should be either a super-fast exact decoding approach or an approximate algorithm that decodes as close as exact algorithms. In this section, we propose a solution based on beam search to approximate exact algorithms while not sacrificing computational time.

Beam search is an improved version of greedy algorithm, it uses a limited breadth \( b \in \mathbb{Z}_+ \) to prune breadth-first search (BFS) algorithm. Specifically, at each step of expansion, only \( b \) best candidates are stored and others are pruned. We follow the notations defined in Section 4 here. The target of beam search decoding is to find a target sentence \( y^* = \arg \max \log P(y \mid x) \) overall all candidate sets. Let \( Y_t \) be the prioritized hypotheses at step \( t \), then it can be expressed as:

\[
Y_0 = \{ \text{BOS} \} \\
Y_t = \text{arg top}_b \{ \log P(y^t_i \mid x) \mid y^t_i \in B_t \} 
\]

where \( B_t \) denotes all candidates from which beam search can select, and it can be defined as:

\[
B_t = \{ y^{t-1}_i \circ v \mid y^{t-1}_i \in Y_{t-1}, v \in V \} 
\]

Beam search terminates after a predefined number of iterations, or if all candidates end with EOS, or satisfying a specific early-stopping criterion. The output of beam search is \( Y_T \) where \( T \) is the end time step. The design philosophy of beam search algorithm discards candidate \( y_i \) with the following form on purpose:

\[
y_i^t = \{ y_i^{t-1} \circ \text{EOS} \} \quad \text{and} \quad y_i^t \not\in Y_t, 
\]

where \( \circ \) denotes string concatenation. The above case often happens at the beginning of decoding; that is, an empty sentence \( y_{\text{emp}} \)’s score is overall the highest, but it is pruned because it is worse than
Table 3: Search error statistics for beam search, min-heap beam search, and exact search in WMT’14 En-De task. All numbers range in [0, 100%.

| Method                      | Beam Search (↓) | Min-heap Beam Search (↓) | Exact Search |
|-----------------------------|-----------------|--------------------------|-------------|
| Transformer(base)           | 67.53%          | 2.20%                    | 0%          |
| - label smoothing           | 48.01%          | 12.49%                   | 0%          |
| + para ft                   | 4.10%           | 3.03%                    | 0%          |
| Transformer(Dim 768)        | 57.61%          | 6.13%                    | 0%          |

Table 4: BLEU scores of beam search and our min-heap beam search using different regularization terms in WMT’14 En-De task. All numbers range in [0, 100].

| Method                      | Beam Search | Min-heap Beam Search |
|-----------------------------|-------------|----------------------|
| Transformer(base)           | 27.22       | 0.40                 |
| + length normalization      | 26.72       | 26.73                |
| + greedy regularization     | 27.38       | 27.36                |
| + max regularization        | 27.44       | 26.18                |
| + square regularization     | 27.43       | 27.21                |
| + variance regularization   | 27.35       | 26.37                |

The chosen $k$ candidates. This explains why many empty sentences are not captured by beam search algorithm but count for the most percentage by [22].

We make a simple yet effective modification to the original beam search algorithm by adding a minimum heap $H$. The capacity of $H$ is identical to the beam size. Unlike the original beam search, we propose to push all candidates in $B_t$ with EOS to $H$. When beam search terminates, we replace the output $Y_T$ of beam search with $H$ as the final output.

**Theorem:** The target sentences in $H$ are not worse than the target sentences in $Y_T$.

**Proof:** If there exists a sentence $\bar{y} \in Y_T$ which has a better score than any sentence in $H$, its score must be lower than the minimum score of $H$. However, the minimum score of $H$ is monotonically increased. □

We conduct an experiment to compare the search errors using the definition proposed in [22]. Table 3 shows the results that the percentage of exact matched sentences is significantly increased compared to the ones of original beam search. The results empirically demonstrate that our proposed min-heap beam search approximates exact search decoding well.

We conduct an additional experiment on comparing search regularization terms (see Table 4). Exact decoding is impossible to achieve since the regularization usually makes the scoring function non-monotonic. Thus we use the proposed min-heap beam search to investigate this problem. The experimental results show that length normalization and greedy regularization might be more suitable for NMT compared to other regularization techniques.

Min-heap beam search is an efficient approximation to the exact decoding, and it is effortlessly to replace beam search with min-heap beam search. There are many unknown areas to explore by revisiting previously proposed techniques using the min-heap beam search as an approximation, such as schedule sampling [29], reinforcement-learning-based training [26], and so on.

6 Conclusion and Future Directions

This paper proposes a new evaluation protocol to avoid search errors and analyze model errors from the perspective of candidate space. We argue that ranking capability is key to model errors, and prove the state-of-the-art Transformer models are facing serious ranking problems. With the help of our proposed exact top-$k$ decoding and ranking-based model error metrics, we evaluate various techniques and different model architectures in the WMT’14 English-German task. In addition, we show that commonly adopted search regularization terms in beam search are also connected with
ranking-based model errors. Finally, to effectively approximate the exact top-\( k \) search, we propose a minimum heap augmented beam search algorithm that reduces search errors.

From our point of view, evaluating NMT models without search errors is the future direction. It might save researchers a large amount of time for tuning their models where the beam search blessing is not necessarily existing. The corresponding decoding algorithms for NMT systems should either be a super-fast exact decoding approach or an approximate algorithm that decodes as close as exact algorithms. We hope our evaluation metrics and experimental results can shed light on future directions for model design and make researchers rethink the ranking problem of NMT model specification.

### A Experimental Details

#### A.1 Datasets

For our WMT’14 En-De task, we use 4.5M preprocessed data, which is tokenized and split using byte pair encoded (BPE) [20] with 32K merge operations and a shared vocabulary for English and German. We use newstest2013 as the validation set and newstest2014 as the test set, which contain 3,000 and 3,003 sentences respectively.

#### A.2 Training and Evaluation

Our models are trained using the fairseq toolkit [4]. We train each of our Transformer models for 300k steps, and evaluate each model for 5000 steps. The default label smoothing hyperparameter is set to 0.1. The dropout rates for different Transformer models are ranging from 0.1 to 0.3. We train each model with 8 NVIDIA V100 GPUs and a batch size of 4096 tokens on each GPU. All our Transformer models are pre-norm models. Other hyperparameter settings are the same as in [25]. For evaluation, we report tokenized BLEU scores using multi-bleu.perl [5]. We select the checkpoint performed the best on the valid set and report its performance on the test set.

### B Implementation Details of Exact Top-\( k \)

Here we explain the implementation details of our exact top-\( k \) algorithm. The detailed algorithm is shown in Algorithm [1]. Our implementation is based on uid-decoding [6] and sgnmt [7] projects, and compatible with the models trained with fairseq. The original implementation of exact top-1 decoding heavily relies on CPU operations, and our top-\( k \) version significantly improves the speed. Specifically, we use the following implementation tricks.

- **Optimizing the iterating process.** As defined the 13-th line of our Algorithm [1], we need to iterate through all words in the vocabulary. However, the order of iterations strongly influences the speed, because of the existence of lower bounds. Empirically, we find that iterating the vocabulary greedily substantially reduces the run-time.

- **Batching the candidates for each time step.** As stated at the 14-th line of Algorithm [1], we iterate one word and perform one model forward pass at a time. However, we observe that the GPU utilization of this scheme is extremely low. Thus, we use batch technique and batch \( b \) different words for one model forward pass, which significantly increases the GPU utilization.

- **Good lower bounds facilitate the search process.** Empirically, we find better lower bounds vastly reduce the search time. In our implementation, we use the \( n \)-best list output by Min-heap Augmented Beam Search (ref. Section 5 of the paper) as our lower bounds.

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[1] https://github.com/pytorch/fairseq
[2] https://github.com/moses-smt/mosesdecoder/blob/master/scripts/generic/multi-bleu.perl
[3] https://github.com/rycolab/uid-decoding
[4] https://github.com/ucam-smt/sgnmt
Algorithm 1: DFS-based Top-k Exact Search.

Input: x: Source sentence, y: Translation prefix (default: []), p: log \( P(y|x) \) (default 0.0), k: Top-k candidates to output

Output: List \( l \) contains top-k candidates with log-probabilities.

1. \( \text{global heap } \gamma \leftarrow \text{inf} \)
2. \( \text{Function DFS_Top_k}(x, y, p): \)
3. \( \text{if } |y| - 1 < k \text{ then} \)
4. \( \text{Push } (p, y) \text{ to heap} \)
5. \( \text{if } \text{len}(\text{heap}) > k \text{ then} \)
6. \( \text{pop(heap)} \)
7. \( \text{end} \)
8. \( \text{end} \)
9. \( \text{if } \text{len}(\text{heap}) = k \text{ then} \)
10. \( \gamma \leftarrow \text{heap}[0][0] \)
11. \( \text{end} \)
12. \( \text{end} \)
13. \( \text{for } v \in V \text{ do} \)
14. \( p' \leftarrow p + \log P(v|x, y) \)
15. \( \text{if } p' \geq \gamma \text{ then} \)
16. \( \text{DFS_Top_k}(x, [y; v], p') \)
17. \( \text{end} \)
18. \( \text{end} \)
19. \( \text{return heap; } \)
20. \( l \leftarrow \text{DFS_Top_k}(x, [], 0.0) \text{ return } l \)

B.1 Worst-Case Analysis for Exact Search algorithms

In this section, we analyze the worst-case behaviors of exact search algorithms. First, let us discuss a simple case when exact searches do not use lower bounds. Given a target sentence set \( Y_l = \{y|\text{len}(y) = l\} \) where all candidates in that set have a length \( l \), it is evident that the search operations needed for exact top-1 and exact top-k algorithms are the same, i.e., \( N_l = |Y_l| = |V|^l \). Then, the total search operations for all lengths \( l \in [1, l_{\text{max}}] \) can be computed by \( N = \sum_{l \in [1, l_{\text{max}}]} N_l \).

Next, we consider the case with lower bounds. Since lower bounds help trim the search space, the worst case with lower bounds happens when the search algorithm finds the candidates in a reversed order. In that case, lower bounds could not trim any search space and have to iterate through all candidates. Hence, the numbers of search operations needed for both top-1 and top-k algorithms are identical, i.e., \( N = \sum_{l \in [1, l_{\text{max}}]} N_l \) operations. Besides, both the top-1 and our top-k algorithms are similar to Branch&Bound algorithm [9], which cannot lower the time complexity in the worst case, and its time complexity is the same with the one of depth-first-search (DFS) algorithm [14]. However, it is very useful in real-life cases because it is proved to be able to significantly improve the search speed.

C Empirical Computational Cost

C.1 Compared with Different Decoding Algorithms

This section provides some empirical results to show how different decoding methods perform in terms of computational time. We randomly sample 100 sentences in newstest2014 and report the corresponding run time as well as the number of expansion operations. The expansion operation, i.e., model’s forward pass, is the most time-consuming operation in the exact search algorithm. We report the computational costs for four different algorithms, including Beam Search, Exact Top-1, Exact Top-10 and Exact Top-10 with min-heap lower bounds. Each reported number is the average over four runs with different samples as inputs.

The results are shown in Table [5]. First, we can see that Beam Search is about ten to twenty times faster than exact search algorithms. Second, compared with previous Exact Search implementation,
Table 5: Time cost and number of expansions for exact search algorithms with 4 sampled runs on 100 test sentences.

| Method                                      | Time Cost (seconds) | Num Expansions |
|---------------------------------------------|---------------------|----------------|
| Beam Search                                 | 453.0               | -              |
| Stahlberg and Byrne [22]                    | 8,064.0             | 2,769.6        |
| Exact Top-10 w/ BS lower bounds             | 19,312.8            | 13,344.9       |
| Exact Top-10 w/ Minheap BS lower bounds     | 18,908.4            | 12,918.9       |

Table 6: Computational time and expansions for exact search algorithms when \( k \) increases.

| Method                                      | Time Cost (seconds) | Num Expansions |
|---------------------------------------------|---------------------|----------------|
| Stahlberg and Byrne [22]                    | 8,064.0             | 2,769.6        |
| Exact Top-5 w/ Minheap BS lower bounds      | 8,914.4             | 6,029.4        |
| Exact Top-10 w/ Minheap BS lower bounds     | 15,916.2            | 10,865.9       |
| Exact Top-20 w/ Minheap BS lower bounds     | 28,313.9            | 19,155.8       |

our implementation of top-10 search is only two times slower, which is a reasonable extra cost for our newly proposed decoding methods. Third, we find that using min heap beam search generated lower bounds can accelerate our decoding algorithm, from 19,312.8 seconds to 18,908.4 seconds.

By taking the number of expansions into account, we notice another two interesting facts – On the one hand, the number of expansions is not linear to \( k \). Our top-\( k \) algorithm explores only about five times the search space compared with top-1 algorithm. On the other hand, our algorithms are significantly more efficient than the original implementation, with four times in terms of the number of expansions and only about two times in terms of the computational cost.

C.2 Compared with Different \( k \)

We also report results with different \( k \), shown in Table 6. The computational time and the number of expansions grow as \( k \) increases. When we enlarge the number of \( k \) from 5 to 10, the time costs grow by about 1.9 times \((15,916.2/8,914.4)\), which denotes an almost linear time cost with regard to \( k \). Compared with [22], our algorithms are more efficient – Our top-5 algorithm operates two times of expansions and performs comparably with their algorithm in terms of computational time.

In the main content of our paper, we mainly use top-10 results for our evaluation method for the trade-off between efficiency and effectiveness.

D Case Study

This section provides a case study for English-German translation outputs for our Exact Top-\( k \) decoding algorithm. The generated candidates, their corresponding log probabilities, and BLEU scores are shown in Table 7.

We conclude several problems of models’ generated outputs based on the example: First, the ranking problem we argue in the main content apparently exists, which is demonstrated in our provided example. For instance, the model gives the highest score to an empty candidate (only <EOS>), which ranks the model’s mode candidate the worst in the whole candidate space. Second, the model ranks some suitable candidates in the top-10 rankings, like 2-nd, 4-th, 7-th, 10-th. However, the best candidate among them is ranked only at the 10-th position. It can also prove the existing of the ranking problem. Third, the model favors shorter candidates. The candidates at rank positions 1-st, 6-th, and 9-th are much shorter than the others. The short candidates have roughly the similar scores as the longer ones. Furthermore, most of the candidates have a similar prefix, which is similar to the reference, demonstrating that the model can find proper translations with incorrect log probabilities. It might indicate an under-confidence problem exists, which beyond this paper’s scope but needs more attention in the future.
### Table 7: The generated translations with top-10 decoding. The source sentence is "Two sets of lights so close to one another: intentional or just a silly error?"

| Rank | LogProb | BLEU | Candidate |
|------|---------|------|-----------|
| Ref  | -       | 100.00 | Zwei Anlagen so nah beieinander: Absicht oder Schildbürgerstreich? <EOS> |
| 1    | -9.04  | 00.00 | <EOS> |
| 2    | -10.13 | 20.45 | Zwei Leuchten so nah beieinander: absichtlich oder einfach nur ein dummer Fehler? <EOS> |
| 3    | -10.40 | 07.47 | Zwei Leuchten so nahe beieinander: absichtlich oder einfach nur ein dummer Fehler? <EOS> |
| 4    | -10.56 | 22.24 | Zwei Leuchten so nah beieinander: absichtlich oder nur ein dummer Fehler? <EOS> |
| 5    | -10.92 | 08.13 | Zwei Leuchten so nahe beieinander: absichtlich oder nur ein dummer Fehler? <EOS> |
| 6    | -10.94 | 05.89 | Zwei Leuchten so nahe beieinander? <EOS> |
| 7    | -11.10 | 22.24 | Zwei Leuchten so nah beieinander: absichtlich oder einfach nur ein dummer Fehler? <EOS> |
| 8    | -11.15 | 37.60 | Zwei Leuchten so nah beieinander: Absicht oder einfach nur ein dummer Fehler? <EOS> |
| 9    | -11.21 | 17.63 | Zwei Leuchten so nah beieinander? <EOS> |
| 10   | -11.39 | 40.90 | Zwei Leuchten so nah beieinander: Absicht oder nur ein dummer Fehler? <EOS> |

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