

BPE Gets Picky: Efficient Vocabulary Refinement During Tokenizer Training

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Abstract

Language models can largely benefit from efficient tokenization. However, they still mostly utilize the classical BPE algorithm, a simple and reliable method. This has been shown to cause such issues as under-trained tokens and sub-optimal compression that may affect the downstream performance. We introduce Picky BPE, a modified BPE algorithm that carries out vocabulary refinement during tokenizer training. Our method improves vocabulary efficiency, eliminates under-trained tokens, and does not compromise text compression. Our experiments show that our method does not reduce the downstream performance, and in several cases improves it.

1 Introduction

Tokenization is a relatively understudied area, but it can greatly impact model performance and efficiency (Rust et al., 2021; Hofmann et al., 2022; Ali et al., 2023; Toraman et al., 2023; Petrov et al., 2023; Singh and Strouse, 2024; Rajaraman et al., 2024; Shao et al., 2024; Wang et al., 2024). Vocabularies should be efficient, as every additional token in the vocabulary increases embedding parameters, and thus model size. Each vocabulary item should contribute enough to model performance to justify the use of parameters.

In this paper, we focus on Byte-Pair Encoding (BPE; Gage (1994); Sennrich et al. (2016)) tokenizers. BPE tokenization works by breaking down a text into each of its characters or bytes and then building tokens in the vocabulary through a series of merges. The result of each merge must be stored as a token in the vocabulary. Tokens which are used only to execute merges are sometimes referred to as intermediate “junk” tokens (Bostrom and Durrott, 2020). An example is illustrated in Figure 1. Intermediate tokens clutter the vocabulary and are hardly ever used during tokenization.

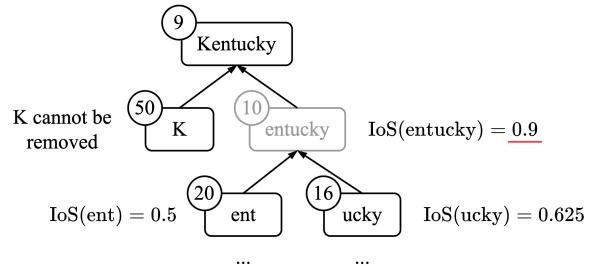


Figure 1: An example of a series of merges to produce a token Kentucky. The pre-merge token frequencies are demonstrated in corresponding circles. In the vanilla BPE algorithm, entucky should also be stored in the vocabulary, whereas it is redundant after the merge. In this example, the IoS metric effectively captures the intermediate token, as $\text{IoS}(\text{entucky}) \geq \mathcal{T} = 0.9$.

In addition to efficiency, we consider other model behaviors that may be driven by tokenization. Land and Bartolo (2024) recently showed that very low-frequency tokens in the vocabulary may be under-trained by a model. This leads to worse downstream performance and unwanted outputs, such as hallucinations. Under-trained tokens can also potentially be exploited to avoid safety measures through the use of these out-of-distribution items. These tokens are also called “glitch tokens” (Rumbelow and Watkins, 2023; Geiping et al., 2024; Li et al., 2024).

Vocabulary trimming, which entails removing items from a tokenizer’s vocabulary, has been proposed as a method to remove unnecessary tokens, e.g., language- or domain-specific tokens. Trimming has been shown to reduce embedding parameters without degrading downstream performance (Ushio et al., 2023; Pang and Vulić, 2024). Under-trained token indicators were shown to be correlated with token frequency in the training corpus, where less frequent tokens are more likely to be under-trained (Land and Bartolo, 2024). Vocabulary trimming, thus, is well suited to address the issue of under-trained tokens.

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Vocabulary trimming has mostly been implemented after tokenizer training (Yang et al., 2022; Cognetta et al., 2024). This means that it is difficult to determine the vocabulary size in advance because it is not known in advance how many tokens will be removed by the trimming procedure. Setting a fixed vocabulary size might be important, for example, in increasing training throughput (Groeneveld et al., 2024).

In this paper, we introduce **Picky BPE**¹ — a modified BPE tokenizer that implements vocabulary refinement during tokenizer training. Unlike other trimming procedures, Picky BPE effectively removes intermediate tokens once they become useless and seamlessly collects the vocabulary of the desired size without data-specific heuristics. Our method leads to more efficient usage of the limited vocabulary, and thus the embedding parameters. We show that our method leads to equal or better performance on a downstream translation task (§4). Furthermore, we reduce the number of tokens that are likely to be under-trained (§5) and free space for higher-quality word-initial tokens. Due to the improved quality of the desired-size vocabulary, Picky BPE does not compromise text compression (§6) unlike other trimming methods, which makes it suitable for practical use.

2 Related Work

Several common alternatives to BPE tokenization implicitly address the issue of intermediate low-frequency tokens. For instance, WordPiece tokenization (Wu et al., 2016) is based on a series of merges akin to BPE, but along with the pair frequency, it also takes individual token frequencies into account. Thus, the tokenizer is less likely to add merges that would leave redundant tokens. However, this does not guarantee that the tokenizer adds merges in an optimal order, nor does it facilitate the retrospective removal of intermediate tokens that might eventually appear.

Another popular algorithm is Unigram tokenization (Kudo, 2018) used in SentencePiece (Kudo and Richardson, 2018). The core of this algorithm is different from BPE-like solutions. Unigram works by creating a large vocabulary and iteratively pruning it until it reaches the desired size. The pruning is performed according to how much the token removal affects the likelihood of the subword sequence, and takes into account individual token fre-

quencies. Intermediate tokens are also less likely to appear in such a scenario, which might suggest that Unigram tokenization implicitly performs a form of vocabulary trimming. We compare our method with Unigram tokenization in §6.

There are also several proposed modifications to BPE, which address the issues raised in §1. BPE-Dropout was proposed to mitigate the issue of rare subwords by dropping merges randomly during tokenizer training (Prosvilov et al., 2020). This method regularizes the BPE training to expose a model to alternate tokenizations of the same strings, making it more robust to noisy input, such as misspellings. BPE-dropout also helps in reducing the under-training of low-frequency tokens. However, this method does not change the tokenizer vocabulary that is used during inference, and ultimately does not bear on the issue of vocabulary efficiency.

Sennrich et al. (2017) use an absolute frequency cut-off to prevent very low-frequency tokens from being added to the vocabulary. Similarly, Vilar and Federico (2021) propose a stopping criterion in order to select the optimal vocabulary for BPE. The authors propose a maximum likelihood constraint, where BPE stops adding merges during training if a merge decreases the overall likelihood of the token sequence.

Cognetta et al. (2024) implemented a vocabulary trimming method for BPE. They found that they were able to reduce the vocabulary size without significantly reducing downstream translation performance. Their method, however, did worsen compression. In some cases, when they showed the greatest task improvement, they found an increase of over 13% in sequence length, *i.e.*, text length in number of tokens. Better compression has been shown to correlate with better model performance (Gallé, 2019; Liang et al., 2023; Goldman et al., 2024) and lead to faster inference time (Song et al., 2021; Petrov et al., 2023; Yamaguchi et al., 2024).

Our Picky BPE differs from this method as we do not reduce the final vocabulary size. In addition, our trimming is performed during training, which preserves the overall distribution of token frequencies and does not require heuristic data-related post-processing, *i.e.*, choosing an absolute frequency threshold that is different for every dataset (Cognetta et al., 2024).

In a concurrent work, Lian et al. (2024) also identify the issue of intermediate (“scaffold”) tokens and introduce Scaffold-BPE. The authors propose to identify intermediate tokens when they are be-

¹https://github.com/pchizhov/picky_bpe

Algorithm 1 Picky BPE Training Step

```
1: Input: Vocabulary  $\mathcal{V}$ ; Tokenized corpus  $\mathcal{C}$ ;  
   Events order  $\mathcal{E}$ ; IoS threshold  $\mathcal{T}$   
2: Output: Updated  $\mathcal{V}, \mathcal{C}, \mathcal{E}$   
3:  $x_1, x_2 \leftarrow$  the most frequent pair in  $\mathcal{C}$   
4:  $x_3 = x_1 + x_2$   
5:  $\mathcal{V} \leftarrow \mathcal{V} + \{x_3\}$   
6:  $\mathcal{E} \leftarrow \mathcal{E} + \{\text{Merge, } (x_1, x_2)\}$   $\triangleright$  new event  
7: if  $\text{IoS}(x_1 | x_1, x_2) \geq \mathcal{T}$  then  
8:    $\mathcal{V} \leftarrow \mathcal{V} \setminus \{x_1\}$   $\triangleright$  remove  $x_1$   
9:    $\mathcal{E} \leftarrow \mathcal{E} + \{\text{Remove, } x_1\}$   $\triangleright$  new event  
10: end if  
11: if  $x_2 \neq x_1$  and  $\text{IoS}(x_2 | x_1, x_2) \geq \mathcal{T}$  then  
12:    $\mathcal{V} \leftarrow \mathcal{V} \setminus \{x_2\}$   $\triangleright$  remove  $x_2$   
13:    $\mathcal{E} \leftarrow \mathcal{E} + \{\text{Remove, } x_2\}$   $\triangleright$  new event  
14: end if  
15: Update  $\mathcal{C}$  based on events from this iteration  
16: return  $\mathcal{V}, \mathcal{C}, \mathcal{E}$ 
```

low the current range of frequencies during the tokenizer training. Compared to our method that uses a thresholding hyperparameter (see §3), there is no way to regulate the strength of Scaffold-BPE. In addition, the authors propose to run inference by first tokenizing the input text using both vocabulary and scaffold tokens and then splitting the scaffold tokens into the shortest valid token sequences. This approach does not strictly adhere to the training process and leads to inaccuracies in tokenization and worse compression (see the example and the comparison in Appendix A).

Another contemporaneous work by Bauwens and Delobelle (2024) also proposes a method of pruning merges that lead to undesired segmentation and bloated vocabularies. This approach differs in at least two key ways from Picky BPE: 1) it allows merges of more than two tokens and 2) it uses a semi-supervised method to determine which merges to remove, based on manually annotated language-specific morphological segmentations.

3 Picky BPE

Our method is a modification of the original BPE algorithm (Gage, 1994; Sennrich et al., 2016). The intuition behind our modification is that we can identify intermediate tokens based on their individual frequency and frequency within a larger token. Intermediate tokens should have low frequency outside of the context of the token that contains them. For example, in Figure 1, an intermediate token entucky is almost always a part of Kentucky,

Algorithm 2 Picky BPE Tokenization

```
1: Input: Word  $w$ ; Vocabulary  $\mathcal{V}$ ; Events order  $\mathcal{E}$   
2: Output: Tokenized word  $\mathcal{W}$   
3:  $\mathcal{W} \leftarrow$  split  $w$  into symbols  $\in \mathcal{V}$   
4:  $\mathcal{M} \leftarrow$  possible merges in  $\mathcal{W}$   
5:  $\mathcal{R} \leftarrow$  possible removals in  $\mathcal{W}$   
6: while  $\mathcal{M} \neq \emptyset$  or  $\mathcal{R} \neq \emptyset$  do  
7:    $\varepsilon \leftarrow$  earliest event in  $\mathcal{E}$ ,  $\varepsilon \in \mathcal{M} \cup \mathcal{R}$   
8:   perform  $\varepsilon$   
9:   update  $\mathcal{M}, \mathcal{R}$   
10:  exclude events from  $\mathcal{E}$  earlier than  $\varepsilon$   
11: end while  
12: return  $\mathcal{W}$ 
```

which is easy to capture by comparing the frequencies of Kentucky and entucky. To formalize this approach, we introduce a measure called *Intersection over Self (IoS)*, which is computed as follows:

$$\text{IoS}(x_1 | x_1, x_2) = \frac{f_p(x_1, x_2)}{f_t(x_1)}; \quad (1)$$

$$\text{IoS}(x_2 | x_1, x_2) = \frac{f_p(x_1, x_2)}{f_t(x_2)}. \quad (2)$$

Here x_1 and x_2 are the tokens being merged, f_t is token frequency, and f_p is pair frequency. $\text{IoS}(x_1 | x_1, x_2)$ shows how often token x_1 occurs as part of a pair $\{x_1, x_2\}$ compared to all occurrences of x_1 . If this value is too high, *i. e.*, close to 1, x_1 is highly likely an intermediate token, an integral part of a longer, more meaningful token $x_1 + x_2$. Adding $x_1 + x_2$ to the vocabulary makes x_1 redundant and we can consider removing it.

3.1 Algorithm description

The training of Picky BPE follows the main steps of the vanilla BPE training. The text is first split into a sequence of characters/bytes, initializing the vocabulary with unique symbols. Optionally, the coverage parameter (we use 0.9999 in our experiments) is used to replace the rarest symbols with <unk>. After that, the algorithm iteratively chooses the most frequent pair of tokens to merge and adds it to the vocabulary. The difference comes after each merge when we check whether we can remove any of the merged tokens judging by the IoS value. The pseudocode for a training step is demonstrated in Algorithm 1. We integrate the IoS metric into the merging stage. When a pair of tokens is merged, we check whether we can safely remove either of the two tokens from the vocabulary. For

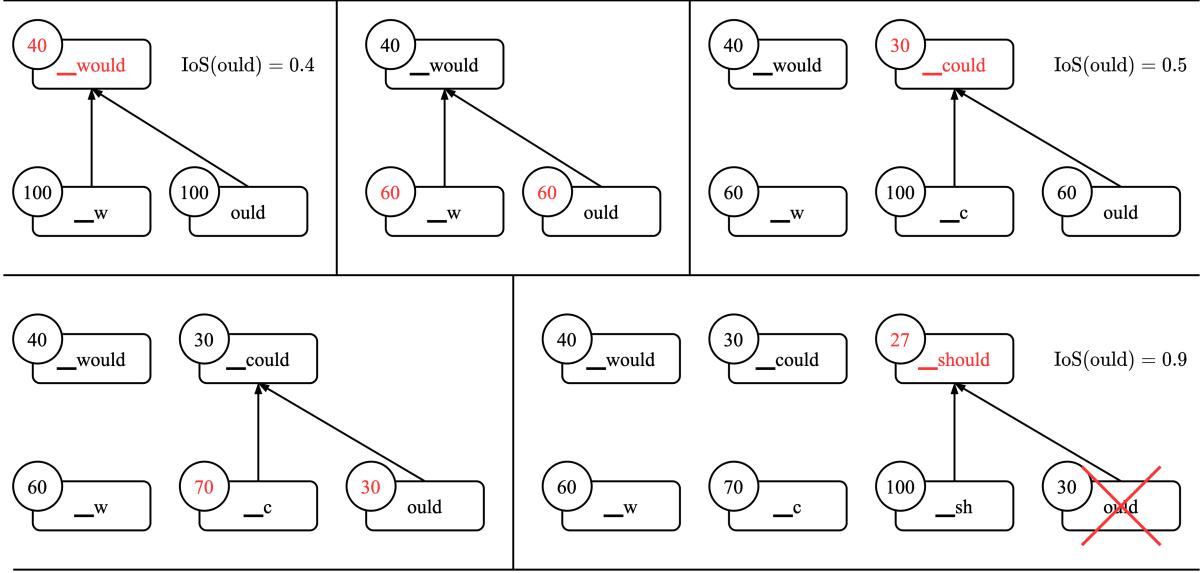


Figure 2: Picky BPE tokenization example. Token frequencies are demonstrated in the corresponding circles and are updated on merges. Token “ould” is removed only after merging into three common tokens containing it. The corresponding IoS values are visualized on every merge. Once IoS becomes greater or equal to the threshold \mathcal{T} , 0.9 in this example, the token “ould” is removed.

this, we introduce a hyperparameter \mathcal{T} , the IoS threshold. If $\text{IoS}(x_1 | x_1, x_2) \geq \mathcal{T}$, we remove x_1 . Thus, \mathcal{T} leverages the strength of the removal policy: \mathcal{T} is a positive value ≤ 1 , and the closer it is to 1, the less strict becomes the removing criterion. For instance, $\mathcal{T} = 0.9$ means that only the tokens present not more than 10% of the time outside of the current merge will be removed. In an extreme case, $\mathcal{T} = 1$ means that no removals are possible, thus the algorithm becomes the vanilla BPE. Another unique feature of our algorithm is that the merges and removals are stored in the events order array \mathcal{E} in the order of happening. The events order is crucial for the tokenization step.

The tokenization (inference) step is described in Algorithm 2. We first split the input word into a series of in-vocabulary symbols. Then we collect the sets of possible merges and removals in the current tokenization and iteratively greedily choose the earliest possible event using event order \mathcal{E} . The action associated with the chosen event is performed and the sets of possible merges and removal are updated. This process strictly follows the tokenizer training and avoids compression issues happening in the approximation methods (see Appendix A).

3.2 Algorithm analysis and justification

The training of Picky BPE is longer than that of the original vanilla BPE. However, the difference is not drastic. When a token is removed, recalcula-

lating the distances requires a constant number of operations, which makes the training time depend linearly on the number of events (merges and removals). With threshold \mathcal{T} values of 0.6 and higher, the proportion of removed tokens generally does not surpass 10% (for details refer to Appendix D), which makes the number of removals inferior to the number of merges. On the tokenization stage, the time depends on the number of events, just as the tokenization time of the vanilla BPE depends on the number of merges. As we show in Appendix D, merges comprise the largest partition of overall events, therefore removal events do not significantly slow down the inference. Depending on the programming language and the implementation, the astronomical time of both stages of the algorithm can differ significantly.

Here we also enumerate several algorithmic advantages of the proposed method.

Universal threshold. The threshold \mathcal{T} is relative and does not depend on the size of the training corpus or the desired vocabulary. This is one of the advantages of our method compared to the main counterparts, such as Cognetta et al. (2024). Furthermore, the removals happen during training resulting in the desired vocabulary size that does not require any post-processing.

Variety of intermediate tokens. An intermediate token may be part of more than one token, as

shown in Figure 2. Our algorithm handles these cases, removing the token only after there are few to no words it can be merged into.

Second chances. Any removed token may be merged again if its frequency is higher at a later point in the order of merges. This is usually the case for tokens removed in the very beginning when the frequencies of new tokens are very high. For example, (“t”, “he”) is likely to be merged early in tokenizer training because “the” is a frequent word. Because the relative frequency of “he” is lower, “he” may be split into (“h”, “e”). But because “he” is still a high-frequency word, it is likely to be merged again. If a previously removed token is restored, it is re-activated to keep its original place in the list of merges. This is essential to the merge order during tokenization.

4 Machine Translation Experiments

To evaluate the downstream performance of our algorithm, we conduct several machine translation (MT) experiments. We experiment with three translation directions: English–German (EN–DE), German–Estonian (DE–ET), and Ukrainian–Estonian (UK–ET). With this choice of language pairs, we aim to cover diverse MT tasks of varying difficulty. German and English are related languages and share the same script. This language pair represents an easier translation task. German and Estonian use the same script, but are much less closely related, belonging to different language families. Translation for this pair should be more difficult. Finally, Ukrainian and Estonian represent the most difficult translation pair in our experiments. These languages are not only distant but also use different scripts.

To train the EN–DE models, we use the training corpus from the WMT16 news translation task (Bojar et al., 2016), with newstest2016 corpus for evaluation. For DE–ET and UK–ET, we use the mixtures of parallel corpora assembled by Korotkova and Fishel (2024). For the evaluations of outputs in Estonian, we use the development set of the FLORES benchmark (Goyal et al., 2022).

We test our method with several thresholds: 0.6, 0.7, 0.8, 0.9. We did not consider lower thresholds as they would remove too many useful tokens. For the baseline, we chose vanilla BPE, which we obtained by training our Picky BPE with $\mathcal{T} = 1$ to ensure effects are not driven by implementation differences. We use the transformer-iwslt model

Experiment	\mathcal{T}	BLEU (\uparrow)	COMET (\uparrow)
EN–DE	1.0*	30.1 ± 0.7	0.431
	0.9	30.3 ± 0.7	0.431
	0.8	30.0 ± 0.7	0.431
	0.7	30.6 ± 0.7	0.434
	0.6	30.3 ± 0.7	0.431
DE–ET	1.0*	19.4 ± 1.0	0.516
	0.9	19.9 ± 1.0	0.520
	0.8	19.8 ± 1.0	0.520
	0.7	19.9 ± 1.0	0.520
	0.6	19.9 ± 1.1	0.520
UK–ET	1.0*	16.9 ± 1.0	0.506
	0.9	15.8 ± 1.5	0.508
	0.8	16.7 ± 1.3	0.511
	0.7	17.2 ± 1.0	0.509
	0.6	16.9 ± 0.9	0.511

Table 1: Machine translation results with vocabulary size 8192 on newstest2016 set (Bojar et al., 2016) for EN–DE, and on FLORES-dev (Goyal et al., 2022) for DE–ET and UK–ET. For every threshold \mathcal{T} , we report BLEU (Papineni et al., 2002) and COMET (Rei et al., 2020) scores on the translation task. The best scores are highlighted in **bold**. Other scores that are not statistically significantly different from the best are also highlighted in **bold**. If neither of the scores is significantly better, nothing is highlighted. * $\mathcal{T} = 1.0$ represents the baseline vanilla BPE without intermediate token removal.

from fairseq (Ott et al., 2019) for all translation tasks. The architecture and training details can be found in Appendix B.

For generation, we use beam search with beam size 5 in all our experiments. We use BLEU (Papineni et al., 2002) from sacreBLEU (Post, 2018) and COMET (Rei et al., 2020) scores for automatic evaluation. We compute paired t-Test with bootstrapping² to compare the obtained translation systems with statistical significance (Koehn, 2004).

Smaller vocabularies. First, we conduct experiments on all three language pairs with a small vocabulary size of 8192. We chose such a restrictive setting to make sure all the tokens are sufficiently trained, as the relatively small training datasets we used ($\sim 1\text{--}4\text{M}$ sentence pairs) do not necessitate large vocabularies (Sennrich and Zhang, 2019)

²We evaluate 1000 bootstrap resamples and use t-Test with confidence level 0.95.

and the effect of using our method might be less pronounced. The results are presented in Table 1. Overall, the models trained with Picky BPE vocabulary performed comparably to the vanilla BPE, with at least one Picky BPE threshold significantly outperforming it for all three translation directions according to the COMET metric. COMET scores for the DE–ET experiment show that all Picky BPE models were better than the vanilla baseline.

Larger vocabularies. We also tested Picky BPE with larger vocabularies for the EN–DE task. We used two settings: separate vocabularies for input and output, and joint vocabularies. In both cases, we used total vocabulary sizes 16384, 32768, and 65536. The results for all these experiments are presented in Table 2. As with the smaller vocabulary setting, we see models based on Picky BPE tokenization performing on par with the ones based on the vanilla BPE. In most experiments, our method brings downstream improvements judging by the values of the COMET metric. We also observe by the BLEU scores that for the largest vocabularies of sizes 32768 + 32768 and 65536 the performance is generally worse than with the smaller vocabularies, regardless of the tokenization method. This is likely due to the volume of training data being insufficient for such a large vocabulary. However, in this setting Picky BPE still outperforms vanilla BPE by COMET.

5 Under-Trained Tokens

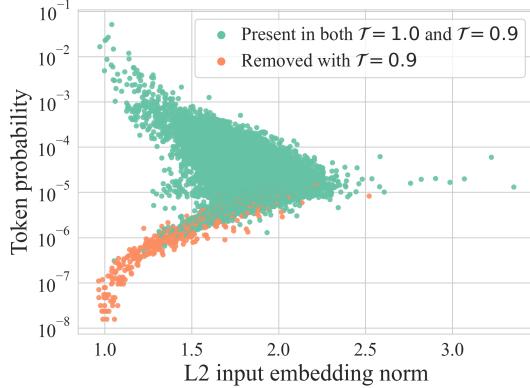
We also test whether Picky BPE decreases the number tokens likely to be under-trained. These tokens can be identified by looking for very low L2 norm of the token embeddings (Land and Bartolo, 2024). We plot L2 norms for $\mathcal{T} = 0.9$ in Figure 3 and those for the remaining thresholds in Appendix C. There are two groups of low-L2 norm tokens: the first is the low-frequency tokens, which can be seen in the lower left of Figure 3a. According to Land and Bartolo (2024), these are the candidates for under-training. There is also a group of the highest-frequency tokens with low L2 norms (top left, Figure 3a). We posit that these are general-purpose tokens that occur in a wide variety of contexts, and thus their representations are less specific. It has long been observed that high-frequency words are more likely to have more senses, *i.e.*, meanings (Zipf, 1945), and thus be more general-purpose.

A large portion of the tokens removed by Picky BPE (Figure 3a) are likely to become under-trained.

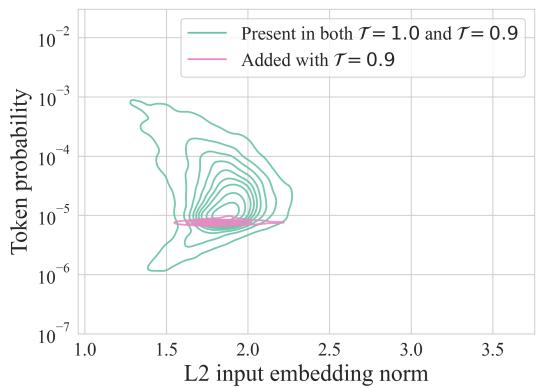
Vocabulary	\mathcal{T}	BLEU (\uparrow)	COMET (\uparrow)
	1.0*	30.7 ± 0.7	0.431
8192	0.9	30.4 ± 0.7	0.431
	0.8	30.3 ± 0.7	0.430
	0.7	30.3 ± 0.7	0.430
	0.6	30.8 ± 0.7	0.432
	1.0*	31.1 ± 0.7	0.433
16384	0.9	31.1 ± 0.7	0.433
	0.8	31.0 ± 0.7	0.435
	0.7	31.4 ± 0.7	0.435
	0.6	31.1 ± 0.7	0.435
	1.0*	29.8 ± 0.7	0.418
32768	0.9	29.6 ± 0.8	0.428
	0.8	30.5 ± 0.7	0.430
	0.7	30.4 ± 0.7	0.430
	0.6	28.3 ± 0.8	0.416
	1.0*	31.1 ± 0.7	0.436
16384	0.9	31.2 ± 0.7	0.436
	0.8	30.9 ± 0.6	0.434
	0.7	31.1 ± 0.7	0.436
	0.6	31.3 ± 0.7	0.438
	1.0*	30.9 ± 0.7	0.435
32768	0.9	31.1 ± 0.7	0.434
	0.8	31.1 ± 0.7	0.437
	0.7	30.9 ± 0.7	0.436
	0.6	30.9 ± 0.7	0.431
	1.0*	28.5 ± 0.7	0.421
65536	0.9	28.4 ± 0.7	0.427
	0.8	28.6 ± 0.7	0.425
	0.7	28.0 ± 0.7	0.416
	0.6	28.8 ± 0.7	0.420

Table 2: Machine translation results on EN–DE newstest2016 set (Bojar et al., 2016) with larger vocabularies: 8192 for each language separately, and joint vocabularies of sizes 16384, 32768, and 65536 for both languages. For every threshold \mathcal{T} , we report BLEU (Papineni et al., 2002) and COMET (Rei et al., 2020) scores on the translation task. The best scores are highlighted in **bold**. Other scores that are not statistically significantly different from the best are also highlighted in **bold**. If neither of the scores is significantly better, nothing is highlighted. * $\mathcal{T} = 1.0$ represents the baseline vanilla BPE without intermediate token removal.

By contrast, the added tokens (Figure 3b) have higher L2 norms and higher probability. The high-



(a) Picky BPE tokens when $\mathcal{T} = 1.0$. The tokens that are present when $\mathcal{T} = 1.0$ but removed when $\mathcal{T} = 0.9$ (orange) are generally infrequent and have low L2 embedding norms, thus the majority of them are likely to be under-trained ([Land and Bartolo, 2024](#)).



(b) Picky BPE tokens when $\mathcal{T} = 0.9$. The tokens that are present when $\mathcal{T} = 0.9$ but not when $\mathcal{T} = 1.0$ (pink) have frequencies and L2-norms of the embeddings close to the blob center and thus are less likely to be under-trained ([Land and Bartolo, 2024](#)).

Figure 3: Input embedding vectors for Picky BPE tokens with (a) $\mathcal{T} = 1$ and (b) $\mathcal{T} = 0.9$ for English vocabularies of size 16384 in EN–DE experiments with separate vocabularies. For each token we compute its probability in the training corpus (y-axis), and the L2 norm of its embedding vector in the trained model (x-axis).

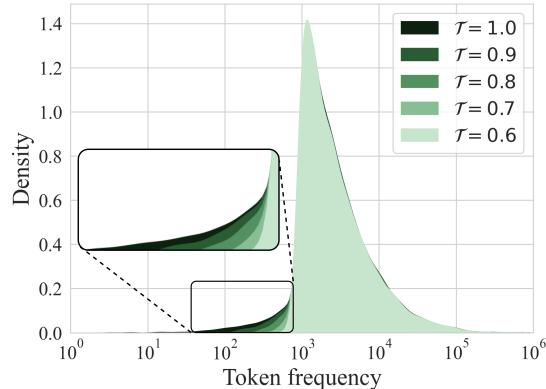


Figure 4: Token frequency distributions for English vocabularies of size 16384 in EN–DE experiments with separate vocabularies for input and output. The left tail becomes less heavy as we decrease the threshold.

frequency general tokens are not removed by Picky BPE. We argue that Picky BPE reduces the likelihood of under-trained tokens and the risks that come with them, such as increased hallucinations.

We also find that as we lower the threshold for Picky BPE, there is a decrease in the left tail of the token frequency distribution, which represents the low-frequency tokens (Figure 4). Trimming methods that involve an absolute frequency cut-off, such as the one used by [Cognetta et al. \(2024\)](#) and originally proposed in [Sennrich et al. \(2017\)](#), would completely eliminate the left tail and leave an abrupt fall-off on the distribution. We observe that Picky BPE preserves the overall distribution and does not eliminate the left tail. This shows that

\mathcal{T}	# unique tokens vs vanilla BPE	# unique tokens vs vanilla BPE + post-trimming
0.9	168 (2.1%)	115 (1.4%)
0.8	391 (4.8%)	248 (3.0%)
0.7	625 (7.6%)	393 (4.8%)
0.6	869 (10.6%)	588 (7.2%)

Table 3: Comparison of tokens from picky BPE and vanilla BPE for joint EN–DE vocabularies of size 8192. For each threshold \mathcal{T} , we report the number of unique tokens in the Picky BPE vocabulary compared to the vanilla BPE ($\mathcal{T} = 1$) with and without low-frequency token trimming on post-processing.

Picky BPE is not another implementation of the post-training trimming of low-frequency tokens.

Table 3 shows the difference between Picky BPE and vanilla BPE with and without post-processing trimming. By post-trimming we mean training the vanilla BPE to have a larger vocabulary with further trimming low-frequency tokens to achieve the desired vocabulary size. We train the initial tokenizer so the number of additional tokens is the number of replaced tokens from the corresponding Picky BPE tokenizer. Through both differences in the number of replaced tokens in the two different strategies, we show that Picky BPE is not simply a different implementation of the post-trimming akin to [Cognetta et al. \(2024\)](#), but it leads to a fundamentally different resulting vocabulary.

Threshold	# removed	Compression (↓)		% Word-Initial Tokens			Mean Token Length (↑)
		German	English	Dropped (↓)	Added (↑)	Overall (↑)	
1.0*	0	1.000	1.000	—	—	61.5	5.38
0.9	160	0.997	0.996	43.8	65.5	61.9	5.40
0.8	358	0.995	0.993	41.1	67.5	62.7	5.44
0.7	588	0.994	0.991	42.0	66.9	63.3	5.47
0.6	805	0.992	0.989	42.1	64.2	63.6	5.50

Table 4: Token quality evaluation on EN–DE tokenizers with joint vocabularies of size 8192. Compression scores are reported as corpus token counts of the newstest2016 set relative to the vanilla BPE, such that 1 indicates the same compression rate. We report the proportion of word-initial tokens out of dropped tokens, added tokens, and out of the whole vocabulary along with the mean token length in characters. * $\mathcal{T} = 1.0$ represents the baseline vanilla BPE without intermediate token removal.

6 Features of Picky BPE

Text Compression. Text compression is generally considered to be an important aspect of tokenizer evaluation (Gallé, 2019; Goldman et al., 2024), and language models that compress more have been shown to have better performance (Liang et al., 2023; Goldman et al., 2024). We use *corpus token count* (CTC; Schmidt et al. (2024)) to measure compression. CTC, also called sequence length, is the number of tokens needed to represent a given text. The fewer tokens are needed, the better the compression.

Table 4 shows the changes in compression as a percentage relative to the tokenizer of the same vocabulary size with a threshold of 1, all for EN–DE vocabularies of size 8192. We report additional compression rates in Appendix E. We find that Picky BPE shows no loss in compression. This is an improvement over the method in Cognetta et al. (2024), which shows worse compression after vocabulary trimming.

Token Qualities. In addition to the above metrics, we compare the tokens themselves. One quality of interest is the proportion of word-initial tokens, which are stored in the tokenizer with an underscore at the beginning to represent a space character. Yehezkel and Pinter (2023) also notice that their trimming procedure leads to an increased number of word-initial tokens.

In Table 4, we also report the percentage of word-initial tokens from the added and removed tokens as well as overall proportions for the EN–DE vocabulary of size 8192. We report results for the other experiments in Appendix F. We find that dropped tokens are far less likely to be word-initial

than added tokens. Therefore, Picky BPE is adding more word-initial tokens than it is removing. As the threshold is lowered, we see slightly fewer word-initial tokens added to the vocabulary. This might be due to the intensive removals happening with lower thresholds. In the overall rates of word-initial tokens, we see a slight increase as \mathcal{T} goes down.

Upon inspection of the added tokens, we see that many of the word-initial tokens are also complete, meaningful words, for example `_renovated`, `_overcoat`, `_cognition`, and `_unconventional`. Increased rates of word-initial tokens may be indicative of improved token quality.

We also found that many of the tokens removed by Picky BPE were intermediate, much like entucky (Figure 1). These tokens are relatively long and only occur in the context of a longer token that is also present in the vocabulary. Often, these tokens are missing only one or two characters relative to the full word. We find word-initial and word-medial intermediate tokens, e.g., `_Chicag`, `_algorith`, `roprietary`, `omenclature` (cf. ‘Chicago’, ‘algorithm’, ‘proprietary’, ‘nomenclature’).

Following Bostrom and Durrett (2020), we also measure mean token length. They argue that longer mean token length is associated with gold-standard morphologically-aligned tokenization, and thus with better token quality. Additionally, longer tokens on average will lead to increased compression, as a text of a fixed length can be represented with fewer, longer tokens. We find that the mean token length slightly but consistently increases as we lower the threshold (see Table 4). We report additional mean token length results in Appendix G.

We additionally compare Picky BPE with Uni-

Method	CTC (\downarrow)		% Word-initial (\uparrow)	Mean len (\uparrow)
	EN	DE		
Unigram	1.143	1.124	75.6	7.73
$\mathcal{T} = 1.0$	1.000	1.000	72.2	6.85
$\mathcal{T} = 0.9$	0.997	0.998	72.8	6.88
$\mathcal{T} = 0.8$	0.996	0.998	73.2	6.91
$\mathcal{T} = 0.7$	0.994	0.997	73.6	6.94
$\mathcal{T} = 0.6$	0.992	0.996	73.9	6.95

Table 5: Comparing Picky BPE and Unigram (Kudo, 2018) on joint EN–DE vocabularies of size 32768. We report corpus token counts (CTC) on the newstest2016 set relative to the vanilla BPE ($\mathcal{T} = 1.0$), percentage of word-initial tokens, and mean token length (“Mean len” in the Table).

gram tokenization in Table 5. Unigram tokenization seems to have longer tokens with a higher proportion of word-initial tokens. However, it drastically worsens the compression. We hypothesize that Unigram adds many meaningful full-word tokens which are not optimal for the text compression under the restriction of the vocabulary size.

7 Discussion

We believe Picky BPE would be beneficial for Large Language Models (LLMs), however, the lack of computational resources does not allow us to carry out a side-by-side comparison. Instead, we provide a series of experiments that we believe illustrate key properties of the proposed method. To put these results into perspective, we want to reiterate two core aspects of the provided experiments: first, there is no universal methodology that could assess tokenizer quality; second, the inefficiencies associated with undertrained tokens discussed by Land and Bartolo (2024) depend on the size of vocabulary relative to the size of training data.

Evaluating tokenizers. It is not always clear how to best compare different tokenizers (Zouhar et al., 2023). One approach is training models for each tokenizer and evaluating downstream performance, *e.g.*, Goldman et al. (2024). However, these results may be driven by confounding factors, such as differences in compression leading to the model effectively being trained on less text (Petrov et al., 2023), and downstream task results may also be task-specific. The second general approach to evaluating tokenizers is to evaluate some quality of the

tokenizer’s output such as fertility (average number of tokens per word; Rust et al. (2021)), similarity of tokenizer boundaries to morphological boundaries (Hofmann et al., 2021), and cognitive plausibility of tokens (Beinborn and Pinter, 2023). There is no consensus about which metric(s) provide the best overall estimation of tokenizer quality.

Role of undertrained tokens. We achieved better or equal performance on machine translation with small vocabularies compared to the vanilla BPE. However, we did not improve the performance with a large vocabulary. The restriction on vocabulary size was set intentionally to reduce redundancy and ensure all tokens receive enough training. We expect to see the same effect with LLMs as their large vocabulary size corresponds to the massive scale of training data and model size. This is well-justified by our analysis of under-trained tokens in response to the exploration of LLMs by Land and Bartolo (2024). We also witness improved token quality that comes with our method, which does not affect text compression, see comparison to the Unigram tokenization in §6.

8 Conclusion

In this paper, we propose a novel tokenization algorithm, Picky BPE, which refines vocabulary during tokenizer training targeting intermediate tokens. Our results show that our algorithm may improve downstream performance in a setting of limited vocabulary, which we can extrapolate on larger vocabularies given enough training. Our method also mitigates the issue of under-trained tokens, efficiently removing them during training, and improves token quality and text compression, filling the freed vocabulary space with meaningful tokens with higher frequency. These factors suggest that Picky BPE can be considered for larger models to improve downstream performance and safety and avoid undesired behavior, *e.g.*, hallucinations.

9 Limitations

Picky BPE behavior depends on the choice of threshold \mathcal{T} . Even though the threshold is relative and mostly intuitive in use, one must consider that with lower thresholds the probability of eliminating useful tokens grows and the behavior becomes less stable. Therefore, it is important to start with safer larger thresholds, analyzing the tokenization using vocabulary-related measures.

In this paper, the only downstream task we evaluate our models on is translation. Training a larger language model and evaluating it on other downstream tasks may show different patterns. This may allow us to better understand the contribution of Picky BPE as well as its potential drawbacks.

Rust et al. (2021) show that different tasks have variable correlation with tokenizer evaluations like fertility. To the best of our knowledge, there is not enough empirical work to determine which tasks would be most informative for evaluating tokenizer quality. This is an important area for future work.

Our experiments are also limited to a relatively small set of languages. We selected pairs of languages that were typologically varied and used different writing systems, however, all the languages are spoken in Europe. Future work should evaluate whether a larger and more diverse sample of languages exhibit the same trends as in this paper.

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A Inference options

Picky BPE inference strictly follows the training order of events and executes merges and removals in the same chronological order (Algorithm 2). Concurrent works use a different approach to inference: the input text is first tokenized with a vanilla BPE tokenizer using both active and removed tokens and then the low-frequency (Cognetta et al., 2024) or scaffold (Lian et al., 2024) tokens are split into the shortest available sequences of valid tokens. The

τ	BPE inference with post-removal	Picky BPE inference
1.0	1.000	1.000
0.9	0.998	0.997
0.8	0.998	0.996
0.7	1.000	0.994
0.6	1.005	0.992

Table 6: Comparison of compression rates (\downarrow) for the vanilla BPE inference followed by splitting undesired tokens and Picky BPE inference by events order for EN-DE vocabularies of size 32768. The compression rates are shown for English.

latter approach is suboptimal, as the training events order is likely to be broken.

For example, imagine the token sequence [t, h, e, r, e] on a certain training step. Tokens (h, e) are merged into he (event e_{i_1}). The sequence becomes [t, he, r, e]. Later, token he becomes useless and is removed (event $e_{i_2}, i_2 > i_1$). Thus, the sequence returns to [t, h, e, r, e]. It can happen now that tokens (e, r) are merged into a new token er (event $e_{i_3}, i_3 > i_2$). The resulting tokenization is [t, h, er, e]. Picky BPE tokenization will follow event order $e_{i_1}, \dots, e_{i_2}, \dots, e_{i_3}$ and result in [t, h, er, e]. The tokenization when the tokens are removed after the vanilla BPE process will first achieve [t, he, r, e], as it will execute all the available merges. In a simplified example, there are no merges to perform after this step, and the algorithm will move to the removals phase: he will be split, and the resulting tokenization will become [t, h, e, r, e]. Therefore, er will not be merged, as it happened after the removal and contains a part of the removed token.

When repeated several times, the described issue may lead to undesired tokenization results and compromise compression. In Table 6, we compare the compression rates of the two methods. The compression issues become more pronounced with lower thresholds as more tokens are removed.

Apart from the described inference methods, Picky BPE can use any inference method requiring a fixed vocabulary: for example, greedy left-to-right decoding (Wu et al., 2016) or recently introduced PathPiece (Schmidt et al., 2024).

Parameter	Value
Encoder layers	6
Decoder layers	6
Embedding dim	512
Hidden dim	1024
Attention heads	4
Max tokens in a batch	4096
Optimizer	Adam
Weight decay	1e-4
Learning rate (LR)	5e-4
LR Scheduler	inverse sqrt
Warmup steps	4000
Precision	fp16

Table 7: transformer-iwslt architecture and training details configuration from fairseq (Ott et al., 2019).

B Training details

Table 7 shows the main model and training hyperparameters we used in every machine translation experiment. We trained every model for 20 epochs, except for a larger vocabulary of 32768 tokens where we trained for 25 epochs, on a single NVIDIA A40 GPU (driver version 555.42.02, CUDA version 12.5).

C Under-trained tokens inspection

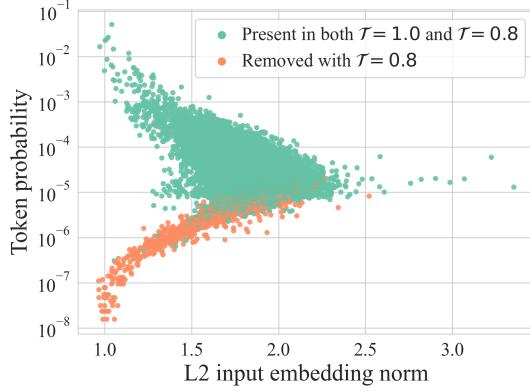
Figure 5 shows examples of token embedding norm distributions for thresholds 0.6, 0.7, and 0.8. As we lower the threshold, the proportion of unique tokens gets larger. However, there is no change in their nature: we remove mostly infrequent tokens and add more frequent tokens with higher norms that are close to the overall distribution.

D Number of Added/Removed Tokens

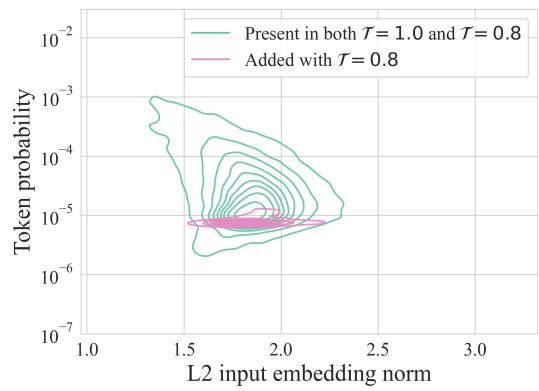
Tables 8, 9, and 10, report the number of added/removed tokens for each tokenizer. This is equivalent to the size of V_i , discussed in §3.1.

E Compression

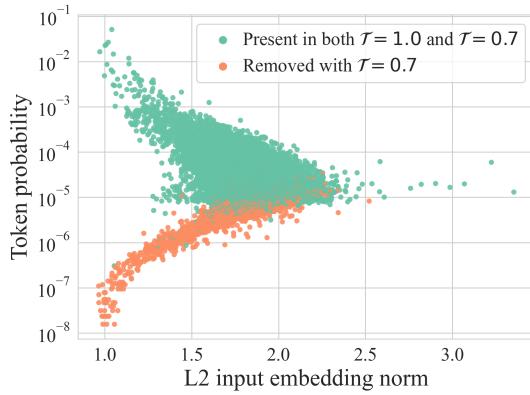
In Tables 11, 12, and 13, we show compression metrics for Picky BPE tokenizers relative to the vanilla BPE. We notice that compression is most pronounced in smaller vocabularies, as for the sizes of the datasets that we used larger vocabularies have large redundancy and a larger partition of tokens is allowed to be unused.



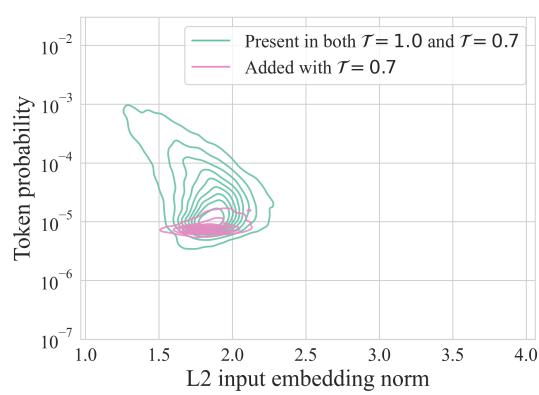
(a) Picky BPE tokens when $\mathcal{T} = 1.0$. The tokens that are present when $\mathcal{T} = 1.0$ but are removed when $\mathcal{T} = 0.8$ (orange) are generally infrequent and have low L2 embedding norms, thus the majority of them are likely to be under-trained ([Land and Bartolo, 2024](#)).



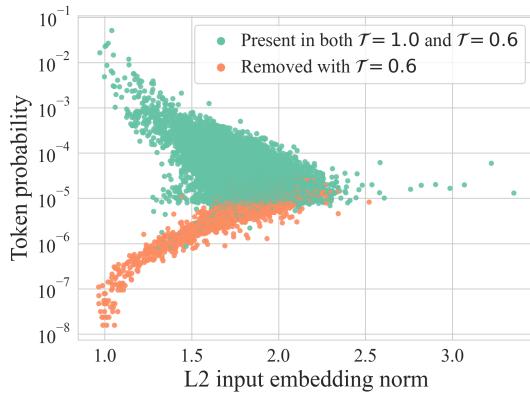
(b) Picky BPE tokens when $\mathcal{T} = 0.8$. The tokens that are present when $\mathcal{T} = 0.8$ but not when $\mathcal{T} = 1.0$ (pink) have frequencies and L2-norms of the embeddings close to the blob center and thus are less likely to be under-trained ([Land and Bartolo, 2024](#)).



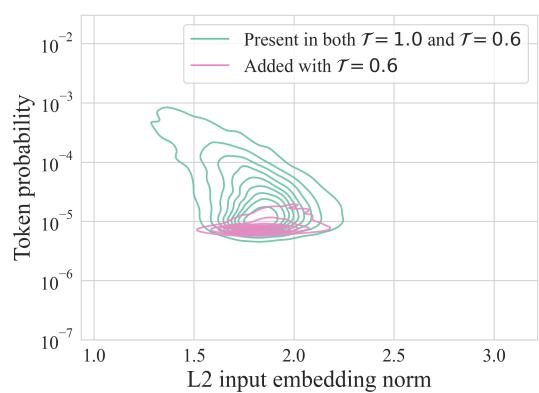
(c) Picky BPE tokens when $\mathcal{T} = 1.0$. The tokens that are present when $\mathcal{T} = 1.0$ but are removed when $\mathcal{T} = 0.7$ (orange) are generally infrequent and have low L2 embedding norms, thus the majority of them are likely to be under-trained ([Land and Bartolo, 2024](#)).



(d) Picky BPE tokens when $\mathcal{T} = 0.7$. The tokens that are present when $\mathcal{T} = 0.7$ but not when $\mathcal{T} = 1.0$ (pink) have frequencies and L2-norms of the embeddings close to the blob center and thus are less likely to be under-trained ([Land and Bartolo, 2024](#)).



(e) Picky BPE tokens when $\mathcal{T} = 1.0$. The tokens that are present when $\mathcal{T} = 1.0$ but are removed when $\mathcal{T} = 0.6$ (orange) are generally infrequent and have low L2 embedding norms, thus the majority of them are likely to be under-trained ([Land and Bartolo, 2024](#)).



(f) Picky BPE tokens when $\mathcal{T} = 0.6$. The tokens that are present when $\mathcal{T} = 0.6$ but not when $\mathcal{T} = 1.0$ (pink) have frequencies and L2-norms of the embeddings close to the blob center and thus are less likely to be under-trained ([Land and Bartolo, 2024](#)).

Figure 5: Input embedding vectors for Picky BPE tokens with (a, c, e) $\mathcal{T} = 1.0$, (b) $\mathcal{T} = 0.8$, (d) $\mathcal{T} = 0.7$, and (f) $\mathcal{T} = 0.6$ for English vocabularies of size 16384 in EN-DE experiments with separate vocabularies. For each token we compute its probability in the training corpus (y-axis), and the L2 norm of its embedding vector in the trained model (x-axis).

Vocabulary Size	Threshold	Added / Removed Tokens
8192	0.9	160
	0.8	358
	0.7	588
	0.6	805
16384	0.9	342
	0.8	707
	0.7	1092
	0.6	1468
32768	0.9	677
	0.8	1280
	0.7	1970
	0.6	2563
65536	0.9	1149
	0.8	2165
	0.7	3312
	0.6	4431

Table 8: Numbers of added (removed) tokens at different thresholds for the EN–DE tokenizers used for the translation experiments.

Vocabulary Size	Threshold	Added / Removed Tokens
8192	0.9	133
	0.8	313
	0.7	506
	0.6	718

Table 9: Numbers of added (removed) tokens at different thresholds for the DE–ET tokenizers used for the translation experiments.

Vocabulary Size	Threshold	Added / Removed Tokens
8192	0.9	107
	0.8	255
	0.7	446
	0.6	605

Table 10: Numbers of added (removed) tokens at different thresholds for the UK–ET tokenizers used for the translation experiments.

F Word-Initial Tokens

In Tables 14, 15, and 16, we show the proportions of added and removed word-initial tokens for different vocabulary sizes and language pairs. In Ta-

Vocabulary size	T	Compression (\downarrow)	
		English	German
8192	1.0	1.000	1.000
	0.9	0.997	0.996
	0.8	0.995	0.993
	0.7	0.994	0.991
16384	0.6	0.992	0.989
	1.0	1.000	1.000
	0.9	0.996	0.998
	0.8	0.994	0.996
32768	0.7	0.993	0.995
	0.6	0.991	0.993
	1.0	1.000	1.000
	0.9	0.997	0.998
65536	0.8	0.996	0.998
	0.7	0.994	0.997
	0.6	0.992	0.996
	1.0	1.000	1.000
	0.9	0.998	0.998
	0.8	0.997	0.998
	0.7	0.997	0.998
	0.6	0.996	0.997

Table 11: Compression for EN–DE tokenizers with different vocabulary sizes. The score is computed as corpus token count relative to the vanilla BPE (T = 1)

Vocabulary size	T	Compression (\downarrow)	
		German	Estonian
8192	1.0	1.000	1.000
	0.9	0.998	0.998
	0.8	0.994	0.996
	0.7	0.991	0.993
	0.6	0.989	0.991

Table 12: Compression for DE–ET tokenizers with a vocabulary size of 8192. The score is computed as corpus token count relative to the vanilla BPE (T = 1)

bles 17, 18, and 19, we show overall proportions of word-initial tokens.

G Token Length

In Tables 20, 21, and 22, we show mean token lengths over different vocabulary sizes that we used in the translation experiments.

Vocabulary size	T	Compression (\downarrow)	
		Ukrainian	Estonian
8192	1.0	1.000	1.000
	0.9	0.998	0.998
	0.8	0.996	0.996
	0.7	0.993	0.994
	0.6	0.992	0.993

Table 13: Compression for UK–ET tokenizers with a vocabulary size of 8192. The score is computed as corpus token count relative to the vanilla BPE (T = 1)

Vocabulary size	T	% Word-Initial Tokens	
		Dropped	Added
8192	0.9	43.8	65.5
	0.8	41.1	67.5
	0.7	42.0	66.9
	0.6	42.1	64.2
16384	0.9	43.9	69.6
	0.8	43.7	67.1
	0.7	45.3	68.1
	0.6	45.3	65.8
32768	0.9	46.7	73.3
	0.8	44.8	68.3
	0.7	47.5	68.5
	0.6	48.7	67.9
65536	0.9	50.6	74.6
	0.8	49.2	71.0
	0.7	51.5	69.9
	0.6	52.0	69.0

Table 14: Percent of word-initial tokens out of added and removed tokens for the EN–DE tokenizers. Added tokens are relative to the vanilla (T = 1) tokenizer of the same vocabulary size and language pair.

Vocabulary size	T	% Word-Initial Tokens	
		Dropped	Added
8192	0.9	33.1	60.9
	0.8	32.3	63.3
	0.7	37.0	60.3
	0.6	40.4	58.4

Table 15: Percent of word-initial tokens out of added and removed tokens for the DE–ET tokenizers. Added tokens are relative to the vanilla (T = 1) tokenizer of the same vocabulary size and language pair.

Vocabulary size	T	% Word-Initial Tokens	
		Dropped	Added
8192	0.9	31.8	73.6
	0.8	33.3	66.3
	0.7	37.4	61.8
	0.6	39.0	61.3

Table 16: Percent of word-initial tokens out of added and removed tokens for the UK–ET tokenizers. Added tokens are relative to the vanilla BPE (T = 1) of the same vocabulary size and language pair.

Vocabulary Size	Threshold	% Word-Initial Tokens	
		Dropped	Added
8192	1.0	61.5	
	0.9	61.9	
	0.8	62.7	
	0.7	63.3	
16384	0.6	63.6	
	1.0	68.0	
	0.9	68.6	
	0.8	69.2	
32768	0.7	69.7	
	0.6	70.0	
	1.0	72.2	
	0.9	72.8	
32768	0.8	73.2	
	0.7	73.6	
	0.6	73.9	
	1.0	75.2	
65536	0.9	75.7	
	0.8	76.1	
	0.7	76.3	
	0.6	76.6	

Table 17: Overall proportion of word-initial tokens at different thresholds for the EN–DE tokenizers used for the translation experiments.

Vocabulary Size	Threshold	% Word-Initial Tokens	
		Dropped	Added
8192	1.0	58.1	
	0.9	58.6	
	0.8	59.4	
	0.7	59.8	
8192	0.6	60.0	

Table 18: Proportion of word-initial tokens at different thresholds for the DE–ET tokenizers used for the translation experiments.

Vocabulary Size	Threshold	% Word-Initial Tokens
8192	1.0	59.8
	0.9	60.4
	0.8	60.9
	0.7	61.1
	0.6	61.5

Table 19: Proportion of word-initial tokens at different thresholds for the UK–ET tokenizers used for the translation experiments.

Vocabulary Size	Threshold	Mean Token Length (Chars) (\uparrow)
8192	1.0	5.38
	0.9	5.40
	0.8	5.44
	0.7	5.47
	0.6	5.50
16384	1.0	6.19
	0.9	6.21
	0.8	6.24
	0.7	6.26
	0.6	6.28
32768	1.0	6.85
	0.9	6.88
	0.8	6.91
	0.7	6.94
	0.6	6.95
65536	1.0	7.44
	0.9	7.46
	0.8	7.49
	0.7	7.51
	0.6	7.53

Table 20: Mean token length at different thresholds for the EN–DE tokenizers used for the translation experiments.

Vocabulary Size	Threshold	Mean Token Length (Chars) (\uparrow)
8192	1.0	4.84
	0.9	4.85
	0.8	4.86
	0.7	4.88
	0.6	4.90

Table 22: Mean token length at different thresholds for the UK–ET tokenizers used for the translation experiments.

Vocabulary Size	Threshold	Mean Token Length (Chars) (\uparrow)
8192	1.0	5.35
	0.9	5.38
	0.8	5.40
	0.7	5.41
	0.6	5.42

Table 21: Mean token length at different thresholds for the DE–ET tokenizers used for the translation experiments.