Data Mixture Inference: What do BPE Tokenizers Reveal about their Training Data?

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Abstract

The pretraining data of today's strongest language models remains opaque, even when their parameters are open-sourced. In particular, little is known about the proportions of different domains, languages, or code represented in the data. While a long line of membership inference attacks aim to identify training examples on an instance level, they do not extend easily to *global* statistics about the corpus. In this work, we tackle a task which we call *data mixture inference*, which aims to uncover the distributional make-up of training data. We introduce a novel attack based on a previously overlooked source of information — byte-pair encoding (BPE) tokenizers, used by the vast majority of modern language models. Our key insight is that the ordered list of merge rules learned by a BPE tokenizer naturally reveals information about the token frequencies in its training data: the first merge is the most common byte pair, the second is the most common pair after merging the first token, and so on. Given a tokenizer's merge list along with data samples for each category of interest (e.g., different natural languages), we formulate a linear program that solves for the relative proportion of each category in the tokenizer's training set. Importantly, to the extent to which tokenizer training data is representative of the pretraining data, we indirectly learn about the pretraining data. In controlled experiments, we show that our attack recovers mixture ratios with high precision for tokenizers trained on known mixtures of natural languages, programming languages, and data sources. We then apply our approach to off-the-shelf tokenizers released with recent LMs. We confirm much publicly disclosed information about these models, and also make several new inferences: GPT-4O is much more multilingual than its predecessors, training on 10× more non-English data than GPT-3.5; GPT-3.5 and CLAUDE are trained on predominantly code; many recent models (or at least their tokenizers) are trained on 7-23% English books. We hope our work sheds light on current design practices for pretraining data, and inspires continued research into data mixture inference for LMs.

1. Introduction

Pretraining data is at the heart of language model development, yet it remains a trade secret for today's strongest models. While it has become more common for model-producing organizations to open-source model parameters, they rarely share the pretraining data or many details about its collection. In particular, little is known about the proportion of different languages, code, or data sources present in the data; these design decisions require extensive experimentation that few organizations have the resources to perform, and have a significant impact on the resulting LM (Albalak et al., 2024; MA et al., 2024; Li et al., 2022; Longpre et al., 2023; Schäfer et al., 2024; Xie et al., 2023).

While a long line of membership inference attacks (Carlini et al., 2021; Shi et al., 2024; Mireshghallah et al., 2023; Shokri et al., 2017; Carlini et al., 2022; Choquette-Choo et al., 2021) aim to reveal information about the model's pretraining data, they typically focus on testing whether particular instances, authors, or websites contributed to the data. In this work, we tackle a different task we call *data mixture inference*, which, given a set of disjoint categories that cover the pretraining data (e.g., the set of natural and programming languages), aims to uncover the proportion of each one.

To this end, we identify a previously overlooked source of information — trained byte-pair encoding tokenizers (BPE; (Sennrich et al., 2016)), which are the near-universal choice for modern language models. Our key insight is that the *ordered merge rules* learned by a BPE tokenizer *naturally reveal information about the frequency of tokens* in the

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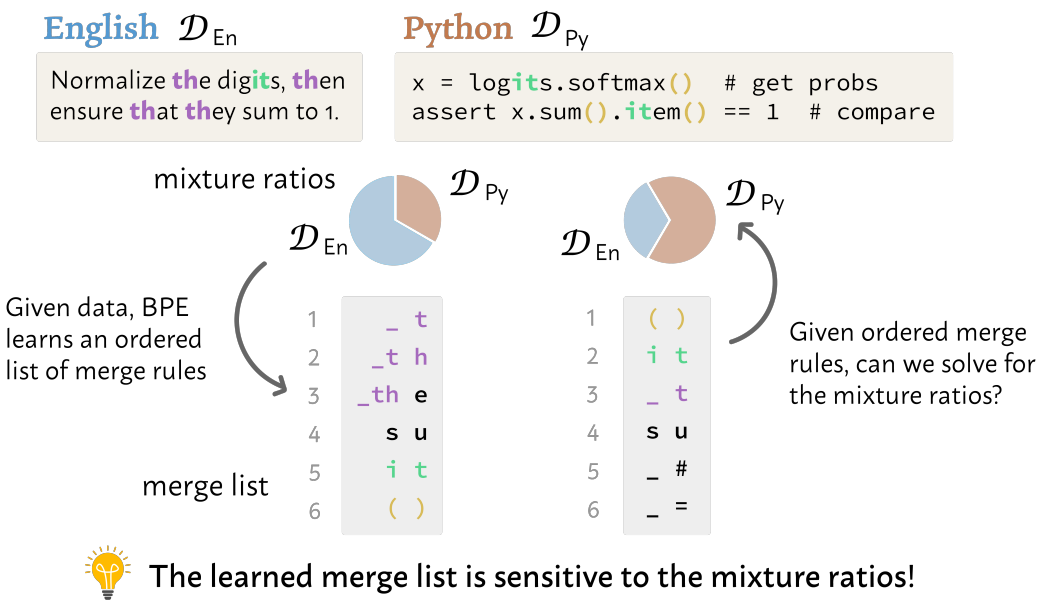

Figure 1. **Illustration of our problem statement** on a simple example where two tokenizers are trained on different mixtures of English and Python data. During training, the BPE algorithm iteratively finds the pair of tokens with the highest frequency in the training data, adds it to the merge list, then applies it to the dataset before finding the next highest-frequency pair. To encode text at inference time, the learned merge rules are applied in order. The resulting order of merge rules is extremely sensitive to the proportion of different data categories present. Our goal is to solve for these proportions, a task which we call *data mixture inference*.

tokenizer's training data. During training, BPE tokenizers iteratively find the ordered pair of tokens with the highest frequency, add it to the merge list, and apply this merge to the dataset before finding the next highest-frequency pair. Therefore, if the pair `(;, \n)` was merged in the 51st step (as in the case of GPT-4O), then it must be the most frequent pair in the data after applying the 50 preceding merges; in this case, it is a signature of substantial code data. Our method builds a linear program where the constraints are derived from the true most-frequent merge at every step in the merge list, and solves for the proportions of each category.

Importantly, the tokenizer training data is ideally representative of the LM's pretraining data (Workshop, 2023); disconnects lead to poor encoding of the pretraining text (Ahia et al., 2023) and potential for "glitch tokens" that trigger degenerate model behavior (Rumbelow & Watkins, 2023; Geiping et al., 2024; Land & Bartolo, 2024). Note that at inference-time, new text is tokenized by applying the learned merge rules in-order. Open-source models require open tokenizers; even for closed models, tokenizers are often open for the purpose of estimating query cost ahead of time.

We first demonstrate the effectiveness of our method in controlled experiments where we train tokenizers on known mixtures of data. We consider three kinds of data mixtures: natural languages, programming languages, and data sources. Our method is highly effective, achieving between three and six orders of magnitude better accuracy than random guessing.

Then, we apply our method to infer previously unknown distributional information about off-the-shelf, commercial tokenizers (the top of these merge lists are shown in §F.1 for qualitative inspection). We consider the tokenizers released with GPT-2, GPT-3.5, GPT-4O, LLAMA 3, and CLAUDE. We corroborate reported information and public intuition about these tokenizers with exact numbers – GPT-2 is trained on predominantly English (98.2%), and GPT-3.5 is the first in the GPT family to be trained extensively on code (62.1%). We also make several new inferences: GPT-4O is trained on 10× more non-English data than GPT-3.5 (39.0% compared to 4.4%), LLAMA 3 and CLAUDE are both trained on ∼60% code, and all the models we study are trained on at least 7% book data.

Inferring pretraining data mixtures of LMs has several important implications. It leaks technical information about the model construction, which model producers may intend to keep proprietary. Identifying the exact data sources can potentially enable targeted data poisoning attempts if the LM is further trained on the same sources (Carlini et al., 2024). Finally, data mixture inference can enable external auditing of the pretraining data for biases, such as identifying under-represented languages or data sources.

2. Background: BPE tokenizers

Byte-pair encoding (BPE), introduced by Sennrich et al. (2016) for NLP,[1] is a tokenization algorithm that learns subword-based encodings from training data. Broadly, the algorithm first separates the training corpus into individual bytes (which are used to initialize the vocabulary), and then iteratively merges frequently co-occurring pairs of tokens until the desired vocabulary size is reached.

More precisely, the training text is first *pretokenized*, that is, split into "word" units that give an upper bound on what tokens can look like. Merges cannot bridge these words, and the final learned tokens will be *parts* of these words. Pretokenization can be simple as splitting on whitespace, so that common sequences of words (e.g., "*it is*") do not become a single token.

After pretokenization, all of the words are split into bytes, which form the starting vocabulary. Then, the BPE algorithm iteratively counts the frequency of each neighboring pair of tokens and picks the most frequent to be the next merge. This merge is added to the merge list and applied to the entire text, and the merged token is added to the vocabulary. For instance, if the merge is (`th`, `e`), then all instances of "`th e`" will be replaced with `the`, which is added to the vocabulary. BPE then updates the frequencies of all pairs, and identifies the next most frequent. This continues until the desired vocabulary size is reached. At the end of training, the algorithm has learned an ordered list of merge rules $m^{(1)}, ..., m^{(M)}$.

To tokenize new text, the tokenizer splits the text into bytes and applies the learned merge rules, in order. As we will see, the merge list reflects rich distributional information about the training data.

3. Data mixture inference attack

Suppose we have a set of n data categories of interest, and data distributions $\{\mathcal{D}_i\}_{i=1}^n$ for each one. Then suppose we receive a BPE tokenizer, which was obtained by training on a large sample of text from the mixture $\sum_{i=1}^n \alpha_i^* \mathcal{D}_i$ where the nonnegative weights $\alpha^* \in \mathbb{R}^n$ satisfy $\sum_{i=1}^n \alpha_i^* = 1$. Given corpora $\{D_i\}_{i=1}^n$ sampled from each of the $\mathcal{D}_i$ respectively, the goal of *data mixture inference* is to produce a good estimate $\hat{\alpha}$ of α^*.

Now we describe how to set up the set of constraints that make up a linear program whose solution is this estimate (§A.1), reduce the storage requirement (§A.2), and improve efficiency (§A.3, §A.4).

[1] Though, it originated in 1994 in the field of data compression (Gage, 1994).

4. Experiments

In our initial experiments, we train tokenizers on known data mixtures and measure the accuracy of our attack's prediction. We consider mixtures of natural languages, programming languages, and data sources (which we also refer to as domains). For more detail about each of these datasets, see Appendix E.

4.1. Setup

Because BPE tokenizers operate on bytes, we measure the proportion of each language in terms of bytes. Each tokenizer is trained on a mixture of n categories, where n varies from 5 and 112. We randomly sample the n categories and their weights (using an algorithm from (Smith & Tromble, 2004)) to train 100 tokenizers on 10 GB of data. The data for each category is sampled from the corresponding corpus; if there is not enough data for any category (e.g., we have many low-resource languages), we duplicate the data until the necessary amount is achieved, to preserve the desired mixture ratio. We train tokenizers using the HuggingFace `tokenizers` library with a maximum vocabulary size of 30,000, and apply a minimal set of common pretokenization operations: we encode strings into bytes using UTF-8, split on whitespace, and only allow digits to be merged with other contiguous digits.

After training the tokenizers, we apply our attack. We estimate merge frequencies for each category by sampling 1 GB of data per category, or less if there is not that much data. Note that the data used for training the tokenizer and estimating pair frequencies are sampled from the same distribution, but are not necessarily the same data. We use **mean squared error** to evaluate the estimated proportions, $\text{MSE} := \frac{1}{n}\sum_{i=1}^n (\hat{\alpha}_i - \alpha_i^*)^2$. In practice, we report $\log_{10}(\text{MSE})$. We empirically calculate the accuracy of random guessing as a baseline.

We use the Oscar v23.01 corpus (Abadji et al., 2022), which is based on the Nov/Dec 2022 dump from Common Crawl. We consider the 112 languages with at least 1 MB of data.

Programming Language Mixtures We use the GitHub split of RedPajama (Computer, 2023). To determine the programming language for each record, we map the file extension to its associated language (e.g., `.py` → `Python`). This leads to a total of 37 programming languages.

Domain Mixtures We consider the following five English domains (adapted from (Longpre et al., 2023)), instantiated by data from the RedPajama dataset: **Wikipedia**, containing English Wikipedia dumps from Jun-Aug 2022, **Web**, Common Crawl data that was de-duplicated and filtered for English, **Books** from the Gutenberg Project and Books3 of The Pile, **Code** from GitHub, and **Academic**, which

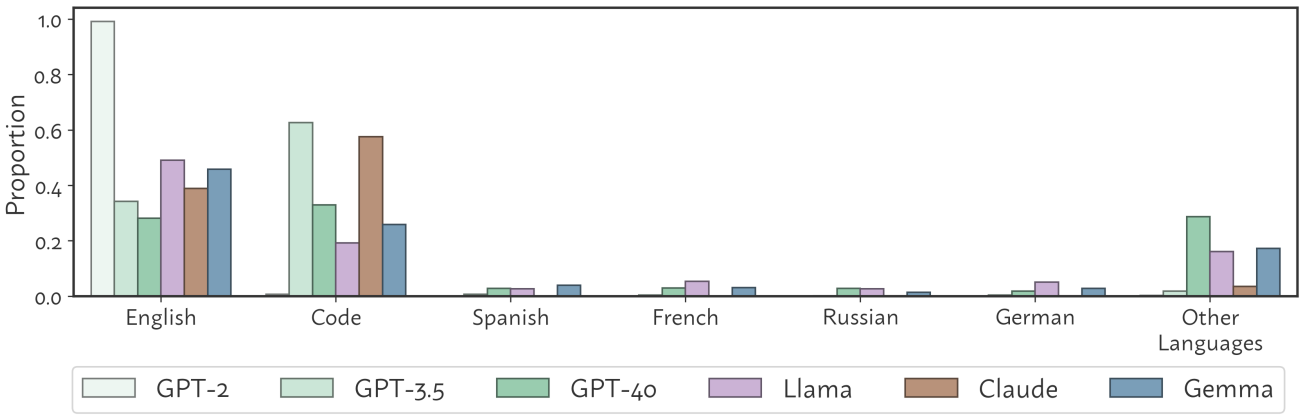

Figure 2. **Our inference for the data mixtures of several commercial tokenizers.**

Table 1. **Experimental results for controlled experiments.** The settings we consider are mixtures of natural languages, mixtures of programming languages, and mixtures of data sources. In each cell, we report the mean and standard deviation of $\log_{10}(\text{MSE})$ over 100 trials. Note that a decrease by 1 corresponds to a $10\times$ improvement in the MSE. **Random** shows the random-guessing baseline. In total, we have 112 natural languages, 37 programming languages, and 5 data sources.

n	Random	**Languages**	**Code**	**Data Sources**
5	-1.39	$-7.30_{\pm 1.31}$	$-6.46_{\pm 0.79}$	$-3.74_{\pm 0.94}$
10	-1.84	$-7.66_{\pm 1.04}$	$-6.30_{\pm 0.64}$	–
30	-2.70	$-7.73_{\pm 1.12}$	$-5.98_{\pm 1.11}$	–
112	-3.82	$-7.69_{\pm 1.28}$	–	–

contains LateX files of scientific papers on ArXiv.

For dataset details, such as the full list of categories and the corresponding amount of data, please see Appendix E.

4.2. Results

Shown in Table 1, our attack is highly effective. Across all mixture types and values of n, we achieve mean MSE 3 to 5 orders of magnitude better than random guessing. We observe that the easiest setting (with the highest attack success) is mixed languages, whereas the most challenging is mixed (English) domains. This is perhaps unsurprising when considering the source of signal for our attack, which is the different token pair frequencies in different categories of data. Intuitively, we would expect these to be very different for different natural languages, which have distinct vocabularies. In contrast, programming languages can share many syntactic features, such as using indents, semicolons, curly brackets `{}`, and control structures like `if`, `for`, and `while`. More so, different English domains should largely share the same vocabulary, but have more subtle differences in token frequencies. Nonetheless, even in this most challenging setting, we achieve accuracy $1000\times$ better than random.

5. Attacking commercial tokenizers

After validating our attack in synthetic experiments (§4), we apply it to infer training data mixtures of off-the-shelf commercial tokenizers. We refer to tokenizers by the name of the model they were first released with, whose pretraining data they most likely reflect. We consider GPT-2 (Radford et al., 2019), GPT-3.5 (OpenAI, 2022), GPT-4o (OpenAI, 2024), LLAMA (Touvron et al., 2023), LLAMA 3 (Meta, 2024), CLAUDE (Anthropic, 2023a), and GEMMA (Team, 2024). While some of these are closed models, all tokenizers are publicly shared so that customers can estimate the cost of queries ahead of time. We note that the LLAMA and GEMMA tokenizers use *characters* rather than bytes as the base vocabulary for the BPE algorithm; we apply our attack in the same way, and discuss this distinction further in Appendix G.

For these experiments, we aim to infer the proportion of natural languages and code (where code is a single category, not split into separate programming languages), as well as the proportion of English domains that make up the English data. We merge code into one category because some programming languages, like `Markdown` and `Pod6`, are almost entirely English, and we do not expect the distribution of programming languages in pretraining data to differ substantially from that of GitHub, which is the largest

public code hosting platform. To infer the distribution of English domains, we replace the English category with the four English domains from §4 (web, books, Wikipedia, and academic). We expect these to approximately cover the English data.

Our predictions are shown in Figure 2, with specific numbers in §E.3. Below, we discuss our findings in comparison with publicly disclosed information about these models.

5.1. GPT models

The GPT tokenizers are open-source on `tiktoken`. There are three such tokenizers, released with GPT-2, GPT-3.5, and the very recent GPT-4O.

GPT-2 GPT-2 (Radford et al., 2019) was trained on WebText, consisting of text scraped from outbound links from Reddit, and filtered to be English-only. Indeed, we confirm the training data consists of 98.2% English. However, we surprisingly estimate that only 57.5% of the data was web, with another 39.4% being books — even though books were not explicitly included in WebText. In a data contamination analysis, the authors indeed report that they find books in WebText, but our estimate suggests the contamination is much deeper. We note that books were a popular source of pretraining data for early Transformer language models, with GPT-1 being trained entirely on BooksCorpus (Zhu et al., 2015). The GPT-2 tokenizer was reused for GPT-3.

GPT-3.5 The GPT-3.5 family of models is known to depart from its predecessors by training on large amounts of code: the first two models in this family were `code-davinci-002` (trained on text and code) and `text-davinci-002`, with the latter being instruction-tuned from the former. In fact, some evidence suggests that GPT-3.5's large leap in reasoning abilities comes from this code data, which intuitively requires similar procedural skills (Fu & Khot, 2022).

Indeed, we estimate that GPT-3.5 is trained on 62.1% code, compared to $< 1\%$ for GPT-2. In the domain breakdown, we see that 25.2% is of the data is web, 7.7% books, and 0.6% academic articles. The substantial representation of books (though much lower than GPT-2) is consistent with findings that this model has memorized a wide collection of copyrighted books (Chang et al., 2023).

GPT-4O Released on May 13, 2024, GPT-4O (OpenAI, 2024) is a multimodal model announced as more multilingual than its predecessors; its tokenizer achieves a better compression rate on non-English languages, and the model has notably better non-English performance.

Our findings support this. We estimate that GPT-4O was trained on 39.0% non-English data, compared to only 4.3% for GPT-3.5, making it the most multilingual model we study. The language distribution has a thick non-English tail, with 58 languages that make up at least 0.1% of the data: the most common are French (3.2%), Spanish (2.5%), Russian (2.4%), Portuguese (2.4%), and German (1.8%). Additionally, GPT-4O was trained on 9.4% books.

5.2. CLAUDE

Finally, we consider the CLAUDE tokenizer. Very little is known about tokenizers from the CLAUDE family, but a remark in the Anthropic SDK suggests that Claude 1 (Anthropic, 2023a) and 2 (Anthropic, 2023b) share the same tokenizer, which is open-source, while Claude 3 (**?**) uses a different (closed) tokenizer. Nothing is shared about the pretraining data of these models. We estimate that CLAUDE was trained on 57.0% code, 36.1% English, and 6.9% other languages. Moreover, more than half of its English data comes from books.

6. Conclusion

In this work, we present a data mixture inference attack that solves for the distributional make-up of a tokenizer's training data, which is commonly representative of the language model's pretraining data. Although we are able to infer some basic properties of commercial LLM tokenizers, we believe there is still a wealth of information hidden in their merge lists. This can shed light on the secretive and often contentious design decisions surrounding pretraining data today, potentially enabling external auditing for safety, copyright issues, and distributional biases. We hope our work will inspire continued research into various forms of distribution inference for tokenizers, as well as data mixture inference for language models more generally.

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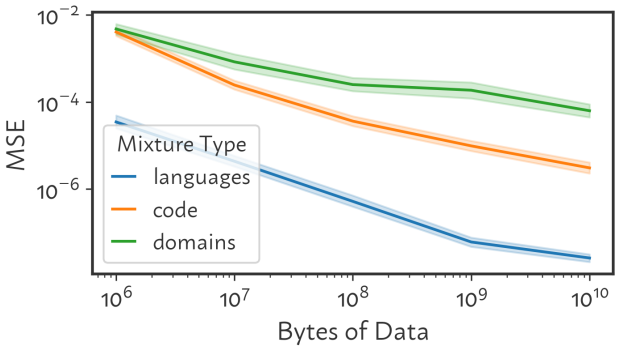

Figure 3. **Analysis of scaling with the amount of data used for estimating pair frequencies** (§B.1). Sampling more data per category consistently produces more precise inferences.

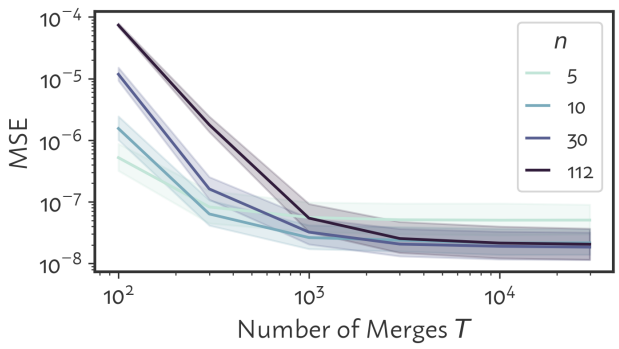

Figure 4. **Analysis of scaling with the number of merges** T used in the merge list (§B.2). Attack performance saturates at around 1000 merges.

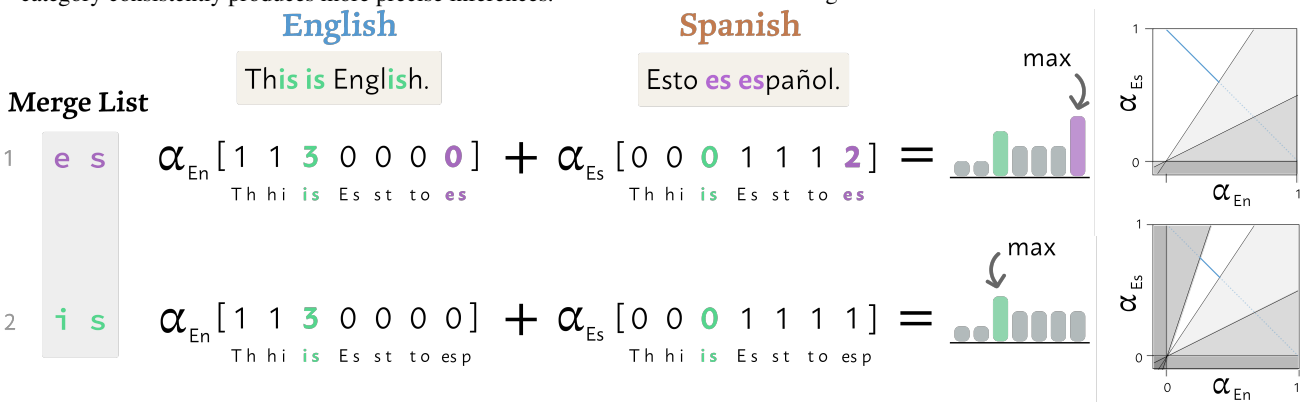

Figure 5. **Illustration of our method** on a simple example. We know that after applying in the first $t-1$ merges to the training data, the t^{th} merge be the most common pair. More explicitly, this means that α_i should give a vector in which the value corresponding to the true next merge is the maximum. Our attack collects these inequalities at every time step to construct the linear program.[3]

A. Implementation

In this section, we describe the implementation of our algorithm, introduced in §3.

A.1. Data mixture inference via linear programming

We build a linear program (LP) with variables α and constraints derived using information from the tokenizer and our sample corpora. The given tokenizer can be represented by an ordered list of merge rules $m^{(1)}, \ldots, m^{(M)}$. For each time step $t \in [M]$, we apply all preceding merge rules $m^{(1)}, \ldots, m^{(t-1)}$ to our corpora D_i and use $c_{i,p}^{(t)}$ to denote how many times the token pair p occurred in the partially merged text. We know that when the tokenizer was trained, the pair $m^{(t)}$ was more frequent at time t than any other pair. In other words,

$$\sum_{i=1}^{n} \alpha_i c_{i,m^{(t)}}^{(t)} \geq \sum_{i=1}^{n} \alpha_i c_{i,p}^{(t)} \qquad \text{for all } p \neq m^{(t)}.$$

Collecting these constraints for all t and p defines a set of possible α's.

Of course, because we only have samples from the the category distributions and not the exact data the tokenizer was trained on, the linear program we described above may not be feasible, as the counts will be noisy due to sampling. To address this, we relax the constraints by introducing new non-negative variables $v^{(t)}$ for all $t \in [M]$, and v_p for all pairs p, which

[5]Technically, the elements of the vectors should be normalized by size of the language data, but in this case they are the same for the two languages so we show the unnormalized counts for readability.

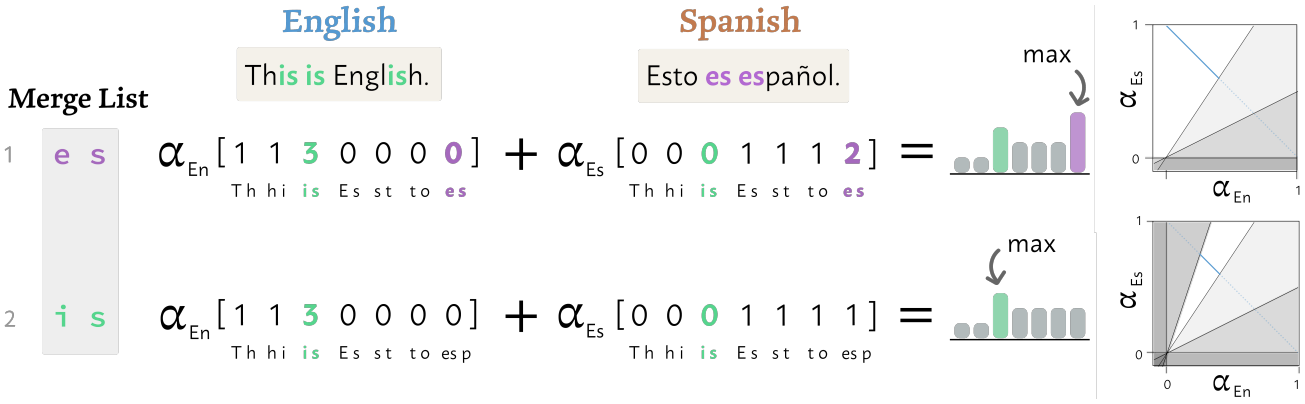

Figure 6. **Illustration of our method** on a simple example. We know that after applying in the first $t-1$ merges to the training data, the t^{th} merge be the most common pair. More explicitly, this means that α_i should give a vector in which the value corresponding to the true next merge is the maximum. Our attack collects these inequalities at every time step to construct the linear program.[5]

represent the degree of constraint violation for each merge and pair, respectively. We replace our constraints with new ones of the form

$$v^{(t)} + v_p + \sum_{i=1}^{n} \alpha_i c_{i,m^{(t)}}^{(t)} \geq \sum_{i=1}^{n} \alpha_i c_{i,p}^{(t)} \qquad \text{for all } p \neq m^{(t)}.$$

In general, we expect $v^{(t)}$ to be large when $m^{(t)}$ is over-represented in the tokenizer training data and v_p to be large when p is over-represented in the mixture defined by α. This new system of constraints is guaranteed to be feasible as the v's can be made arbitrarily large. To produce the best possible estimate, our objective is to minimize the total constraint violation $\sum_{t=1}^{M} v^{(t)} + \sum_p v_p$. We call the resulting linear program `LP1`. To estimate α, we solve `LP1` and report the optimal value of α as our $\hat{\alpha}$.

As written, `LP1` can be prohibitively large. If our vocabulary has size V, the total number of constraints scales like $O(V^3)$ since there are $O(V)$ time steps t to consider and $O(V^2)$ competing byte pairs $p \neq m^{(t)}$. Additionally, there are $O(V^2)$ variables v_p. The first step to reduce the size is to limit t to the first T merges. We will call this truncated program $\texttt{LP1}_T$. However, even for modest choices of T, $\texttt{LP1}_T$ can still have millions of variables and tens of billions of constraints. In the following sections, we will describe how to efficiently solve $\texttt{LP1}_T$ using simultaneous delayed row (constraint) and column (variable) generation (Benders, 1962; Dantzig & Wolfe, 1960).

A.2. Efficient storage of pair counts

First, as a preprocessing step, we apply the target tokenizer to each language corpus D_i, recording the pair counts $c_{i,p}^{(t)}$ after each merge is applied for later use. Naively, this would require a large amount of space, since the number of possible pairs p scales like $O(V^2)$. However, note that $c_{i,p}^{(t)} \neq c_{i,p}^{(t+1)}$ only when p overlaps with $m^{(t)}$. In other words, bigrams with no overlap with the most recent merge will have their counts unaffected. Thus, there are only $O(V)$ differences between $c_{i,\cdot}^{(t)}$ and $c_{i,\cdot}^{(t+1)}$. In practice, the number of changes caused by a single merge is usually a few hundred at most. By saving only the incremental changes from each set of pair counts to the next, we can efficiently record the pair counts at every iteration of the tokenization process.

A.3. Efficient constraint violation detection

Our plan is to solve $\texttt{LP1}_T$ using only a subset of its constraints, giving a potential solution (α, v). We can check whether (α, v) violates any of the constraints of $\texttt{LP1}_T$ and if it does, we can add them to the subset. This requires an efficient method to detect violated constraints, which we describe below.

For convenience, let $s_p^{(t)} := \sum_{i=1}^{n} \alpha_i c_{i,p}^{(t)}$ and recall that, for a given time step t, we want to check whether $v^{(t)} + s_{m^{(t)}}^{(t)} \geq \max_p(s_p^{(t)} - v_p)$. Naively, we would do so by iterating over all possible $p \neq m^{(t)}$ to see if the constraint is violated, which can be quite costly. Moreover, we must do this for all $t \leq T$. However, by taking advantage of the structure of the $s_p^{(t)}$ as t

varies, we can reduce our work substantially.

The first step is to take each initial pair p and add it to a priority queue with priority $s_p^{(0)}$. This can be done in aggregate in $O(V^2)$ time using a fast heap building algorithm. Now, we can scan through the pairs in order of descending $s_p^{(0)}$ using the queue's `delete-min` operation. For each pair p, we can check whether $v^{(t)} + s_{m^{(t)}}^{(t)} > s_{p^*}^{(t)} - v_{p^*}$ and if not, we mark the corresponding constraint as violated. Once we find $p = m^{(t)}$, we stop, since the remaining constraints must be satisfied. If there were k pairs before $m^{(t)}$ in the queue, then the total time taken is $O(k \log V)$.

Crucially, we can quickly update the priority queue to reflect the state at $t = 1$. Since we precomputed all count changes from $c_{i,p}^{(0)}$ to $c_{i,p}^{(1)}$, we know what queue entries need to be updated or inserted. If k_{new} new pairs were created and k_{old} pairs had their counts changed when pair $m^{(0)}$ was merged, then we can update the priority queue using k_{new} `insert` operations and k_{old} `decrease-priority` operations, which can be done in $O((k_{\text{new}} + k_{\text{old}}) \log V)$ time. Now that we have updated the priority queue, it is easy to check for any constraint violations for $t = 1$. By iterating this process, we can quickly check for violated constraints for all $t \leq T$.

A.4. Lazy constraint generation

Now we are ready to solve $\texttt{LP1}_T$ in an efficient way. We begin by guessing uniform proportions for α, and $v^{(t)} = v_p = 0$ for all t, p. Then we use our constraint checker to identify violated constraints of $\texttt{LP1}_T$ and construct a lazy version of $\texttt{LP1}_T$, denoted $\texttt{LP2}_T$, using only those constraints and the variables they contain. We then solve $\texttt{LP2}_T$, which gives us a new guess for α. We iterate the above process, adding progressively more constraints to $\texttt{LP2}_T$ until we find a solution that is also feasible for $\texttt{LP1}_T$. It follows that this solution is optimal for $\texttt{LP1}_T$ since the two programs share the same objective. This is guaranteed to happen eventually because there are a finite number of constraints to add.

In practice, the constraint violation detection can typically check $T = 30000$ merges in less than 10 seconds. On difficult instances, such as those for commercial tokenizers in §5, the full solve can take up to a day to complete. Easier instances like those in Table 1 can be solved in a few minutes.

B. Scaling analysis

Using the natural language mixture setup from §4 with $n = 10$ languages, we analyze how our attack's performance varies with the amount of data used (§B.1) and the number of merges we apply from the merge list (§B.2).

B.1. How many data samples should we use from each category?

We explore how the attack's performance scales with the amount of data sampled from each distribution $\mathcal{D}_i$ for calculating pair counts. For each type of mixture considered in §4, we train 100 new tokenizers considering only categories with at least 10 GB of data available. For our attack, we compare sampling 1 MB, 10 MB, 100 MB, 1 GB, and 10 GB of data for each language, and use $T = 3000$ merges. Shown in Figure 3, more data consistently improves the accuracy of predictions.

B.2. How many merges should we consider?

Next, we investigate how performance scales with the number of merges T that we apply from the merge list. Using the same 100 tokenizers from §4, we solve for the data mixture using various choices of $T \in [30, 30000]$. Shown in Figure 4, we find that when there are more categories, it is useful to consider more merges. This makes sense because more constraints may be needed to bound the solutions in higher dimensions.

C. Discussion of possible defenses

We discuss some possible approaches for defenses to our attack, which we believe would all have limited effectiveness.

Post-hoc changing the order of merge rules Model producers may consider changing the order of merge rules, which is the source of signal for our attack, after the tokenizer is trained. However, naively re-ordering merge rules for a tokenizer would be damaging, as it can lead to unfamiliar encodings of words as well as entirely unreachable tokens. The only functionally-equivalent re-ordering would be *within contiguous sections* of merge rules where each token appears exclusively

on the left or right side of all merges it appears in. In this case, we can easily adapt our method by working at the level of contiguous non-conflicting sections instead of individual merge rules, as we know that each section has higher frequencies than the next.

Hiding pretokenization rules Our method relies on a reasonable reconstruction of the pretokenization rules, which control what kinds of merge rules are considered. It is not necessary to share pretokenization rules as they are not strictly necessary for inference. However, we find that important pretokenization rules (like whether to pre-tokenize on spaces, digits, and punctuation) are easy to infer from manual inspection. Moreover, organizations are incentivized to release pretokenization rules as it greatly enhances the speed of encoding by enabling parallelism.

Not using BPE tokenizers Model producers may choose to forgo BPE tokenizers entirely in future models. Despite the current popularity of BPE, there is a lively area of research into alternative methods of tokenization or doing without tokenization entirely (Wang et al., 2024; Yang, 2024; Limisiewicz et al., 2024). While we only explore BPE tokenizers in this paper, it is plausible that any tokenizer learning algorithm will leak information about its training data, as they are specifically developed to best encode the given data.

D. Experiment details

E. Experiment details & additional results

E.1. Data details

The full set of categories that we use in §4 and the amount of data available for each category are shown in Table 4, Table 5, and Table 6.

Language mixtures We use OSCAR-23.01, which is the January 2023 version of the OSCAR Corpus based on the November/December 2022 dump of Common Crawl. We only keep languages with at least 1 MB of data.

Code mixtures We use the GitHub split of RedPajama-Data-1T, which is an open reproduction of LLAMA's training data.

Domain mixtures We use five splits of RedPajama, namely Wikipedia, Common Crawl, Books, Github, and ArXiv. To reduce disk usage, we download only 8% of the CC URLs.

Below, we enumerate the licenses for these datasets.

- Oscar: CC0 1.0 Universal
- RedPajama has different licenses for each subset
  - C4: ODC-BY
  - GitHub: MIT, BSD, or Apache
  - Books3: MIT
  - Project Gutenberg: Apache 2.0
  - ArXiv: CCo 1.0
  - Wikipedia: CC-BY-SA-3.0

E.2. Compute details

We run all of our experiments on CPUs. For training tokenizers and calculating pair frequencies, we use 16-32 CPUs and a variable amount of memory (ranging from 4 GB to 64 GB) depending on the data. Training a tokenizer on 10 GB of data (as in our experiments) usually takes around 10 minutes, while calculating pair counts takes between 1 minute and 2 hours, again depending on the data. To solve our linear programs, we use Gurobi (Gurobi Optimization, LLC, 2023).

E.3. Full results for commercial tokenizers

We report the full inferences from §5 in Table 3.

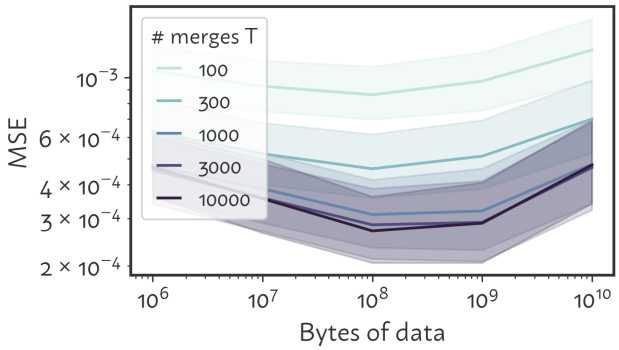

Figure 7. **Scaling the amount of data used for estimating pair frequencies** for distribution shift experiments from **??**.

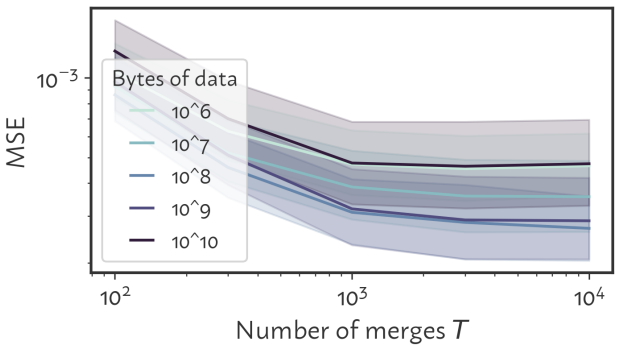

Figure 8. **Scaling the top T merges used in the merge list** for distribution shift experiments from **??**.

E.4. Scaling analysis under distribution shift

We show additional scaling analysis for experiments in **??** in Figure 7 and Figure 8. Surprisingly, we find a U-shaped curve for how performance scales with the amount of data used for calculating pair frequencies, unlike our main experiments in §4.

F. Commercial tokenizers

F.1. Snapshot of commercial tokenizer merge lists

We show the first 50 merges of the commercial tokenizers we study in Table 2

F.2. Handling redundant merges

We observe that the merge list of LLAMA, LLAMA 3, and GEMMA contain clusters of redundant merge rules. For instance, in the LLAMA 3 merge list, we see the sequence of merges `_ the`, `_t he`, and `_th e`, as well as `_ and`, `_a nd`, and `_an d`. Because the merge path for every token is unique, it is impossible for more than one of these merges to ever be used, and we empirically verify this by applying the tokenizer to a large amount of text.

We find that this is an artifact of the conversion from `sentencepiece` to Huggingface `tokenizers` format. To construct the merge list, the conversion algorithm naively combines every pair of tokens in the vocabulary, and then sorts them by token ID, which represents order of creation. While this is functionally correct, because the redundant merges are not products of the BPE algorithm (i.e., they do not actually represent the most-likely next-merge), we need to remove them for our algorithm. To do this, we do some simple pre-processing: for every cluster of redundant merges, we record the path of merges that achieves each merge; the earliest path is the one that would be taken, so we keep that merge and remove the rest.

As an aside, note that this means the merge list can be completely reconstructed from the vocabulary list, if the order of token creation is provided. Namely, given only the resulting token at each time step, we can derive the merge that would have produced it.

F.3. Manual merges in GEMMA

For GEMMA, we notice large contiguous blocks of merges consisting entirely of `\n`, `\t`, and the whitespace character `_`. They appear to be manually inserted and not organically learned by the BPE algorithm, as they do not correspond to increasing vocabulary IDs. Therefore, we remove these merges so that the remaining ordered merge rules align with monotonically increasing vocabulary ID.

F.4. GPT tokenizers

While GPT tokenizers are open source on `tiktoken`, they are not released in a format compatible with HuggingFace tokenizers. We used the `tokenizers`-compatible files uploaded by a HuggingFace user named `Xenova`. For instance,

the GPT-4O tokenizer can be found at https://huggingface.co/Xenova/gpt-4o.

G. `sentencepiece` tokenizers

The LLAMA and GEMMA tokenizers are trained with the `sentencepiece` library, which uses the same BPE algorithm, except the units of the base vocabulary are characters rather than bytes. In other words, the merge rules learned will apply to pairs of character sequences instead of byte sequences. While byte-level tokenizers always start with the same base vocabulary of 256 bytes, character-level tokenizers determine the base vocabulary using a *character coverage* hyperparameter (usually set to $\sim$0.9995), which determines what proportion of characters that appear in the training text will be in the base vocabulary. Byte fallback is used to represent the out-of-vocabulary characters using bytes.

To empirically test our attack on character-level BPE tokenizers, we train 100 `sentencepiece` tokenizers on mixtures of $n = 10$ natural languages. We apply our attack using the top $T = 3000$ merges, but otherwise use the same settings as §4.

With character-level tokenizers, we achieve log MSE of -4.09 compared to -1.39 for random guessing and -7.65 for byte-level tokenizers. That is, character-level tokenizers are harder for our algorithm to reverse than byte-level tokenizers! We believe this is because different languages have widely varying numbers of characters in their writing systems. For languages with many characters, their merges will appear lower in the merge list due to their lower average frequency compared to languages with fewer characters. This leads to a bias in representation among the first T merges considered by our approach.

G.1. Miscellaneous observation: how ties in pair count frequencies are broken

We observe that in `sentencepiece` tokenizers, after going deep in the merge list (about halfway), the merges begin forming groups, in which the length of the merge is ordered from shortest to longest. We trace this to how ties in pair counts are broken in `sentencepiece`, which is by length of the merge. In terms of reverse engineering, this points to a way to infer the size of the tokenizer training data, since exact ties in frequency become less likely as more training data is considered. We leave this direction to future work.

Table 2. **The first 50 merges of the commercial tokenizers we study.** For readability, we replace the space token Ġ with _ and the newline Ċ with \n. To a careful observer, there are many interpretable signatures of training sources. For instance, consecutive whitespace is common in code, as indents are equivalent to four spaces by most coding standards. Indeed, _ _ is the first merge of all tokenizers except GPT-2, which is likely the only tokenizer not trained on code. The merges ; \n, _ =, and sel f are also common token pairs in code. The odd-looking symbols are encodings of bytes that make up *parts* of single characters in many languages. For instance, à ¤ encodes the prefix for the first half of the Devanagari Unicode block (used for writing Hindi, Nepali, Sanskrit, among others), Ð ° encodes the Cyrillic "a", and á ĥ encodes the prefix for the second half of the Georgian Unicode block. The early presence of these in GPT-4O is a sign of its multilingual training data.

GPT-2	GPT-3.5	GPT-4O	LLAMA	GEMMA	CLAUDE
_ t	_ _	_ _	_ t	i n	_ _
_ a	__ __	__ __	e r	_ t	__ __
h e	i n	i n	i n	e r	i n
i n	_ t	e r	_ a	_ a	__ _
r e	____ ____	_ t	e n	o n	_ t
o n	e r	_ a	o n	r e	e r
_t he	__ _	e n	_t h	e n	____ ____
e r	o n	o n	e s	h e	o n
_ s	_ a	r e	_ s	a n	_ a
a t	r e	_ s	_ d	a t	r e
_ w	a t	a t	a t	o r	a t
_ o	s t	o r	o r	e s	s e
e n	e n	e s	a n	_ s	h e
_ c	o r	____ ____	_ c	a r	o r
i t	_t h	a n	i s	t i	s t
i s	\n \n	__ _	r e	t e	e n
a n	_ c	_ d	i t	t h	____ ___
o r	l e	h e	_th e	s t	a l
e s	_ s	_ c	a r	n d	_t he
_ b	i t	_ p	l e	a l	i t
e d	a n	i s	_ w	_ o	_ c
_ f	a r	a r	_ p	l e	a n
in g	a l	i t	o u	d e	l e
_ p	_th e	\n \n	a l	_ i	_ =
o u	; \n	a l	_ f	s e	d e
_a n	_ p	à ¤	_ m	_ c	a r
a l	_ f	l e	e d	_ d	\n _____
a r	o u	o u	_ o	i t	_ f
_t o	_ =	_ m	_ b	n t	_ p
_ m	i s	_ f	o m	i s	\n _____
_o f	____ ___	_ w	i on	_ p	_ o
_ in	in g	_ b	in g	m e	_ s
_ d	e s	a s	i c	r i	_ w
_ h	_ w	in g	a s	r a	m e
_an d	i on	_t he	e l	o u	\n ___
i c	e d	i c	en t	a s	r o
a s	i c	e t	_ in	e d	i on
l e	_ b	_ o	_ h	n e	in g
_t h	_ d	i on	n d	t o	i s
i on	e t	e d	e t	n g	_ in
o m	_ m	e l	_ l	_ w	_ b
l l	_ o	_ n	_ n	r o	i c
en t	ĉ ĉ	r o	s t	l i	se l
_ n	r o	en t	_t o	t a	o u
_ l	a s	_ Ð	c h	_ f	sel f
s t	e l	n d	_ I	_ b	e d
_ re	c t	s t	r o	_ m	- -
v e	n d	á ĥ	i l	i c	n d
_ e	_ in	Ð °	_o f	e l	e s
r o	_ h	_ l	d e	l a	_ m

Table 3. **The full set of inferences** we make for commercial tokenizers. Note that instead of one English category, we split it into four English domains: web, books, academic, and Wikipedia. For the sake of space, only categories with at least cumulative 0.2% representation across the models are shown.

Category	GPT-2	GPT-3.5	GPT-4O	LLAMA	CLAUDE	GEMMA
Web	83.6	27.3	20.7	11.3	12.7	25.7
Code	0.7	62.6	32.8	19.2	57.5	25.9
Books	15.4	6.8	7.4	23.1	17.4	12.8
Academic	0.1	0.2	0.0	8.0	5.1	4.3
Wiki	0.0	0.0	0.0	6.7	3.7	3.0
French	0.0	0.3	2.9	5.3	0.0	3.0
German	0.0	0.4	1.8	5.1	0.1	2.8
Spanish	0.0	0.6	2.8	2.7	0.0	3.9
Russian	0.0	0.1	2.8	2.6	0.1	1.4
Italian	0.0	0.3	0.5	2.6	0.3	1.6
Portuguese	0.0	0.3	2.3	1.1	0.5	1.5
Dutch	0.0	0.1	2.0	1.2	0.1	0.6
Japanese	0.1	0.0	0.4	0.3	0.0	1.6
Arabic	0.0	0.0	1.6	0.0	0.0	0.3
Polish	0.0	0.1	0.5	1.4	0.0	0.7
Hindi	0.0	0.0	1.4	0.0	0.0	0.1
Ukrainian	0.0	0.0	0.3	1.3	0.0	0.2
Catalan	0.0	0.0	0.3	1.1	0.3	0.4
Georgian	0.0	0.0	0.8	0.0	0.0	0.0
Indonesian	0.0	0.1	0.4	0.1	0.0	0.8
Chinese	0.0	0.0	0.8	0.0	0.1	0.1
Swedish	0.0	0.0	0.3	0.7	0.0	0.1
Korean	0.0	0.0	0.7	0.1	0.1	0.2
Estonian	0.0	0.1	0.5	0.1	0.2	0.6
Czech	0.0	0.0	0.3	0.6	0.0	0.3
Low German	0.0	0.0	0.0	0.6	0.0	0.0
Turkish	0.0	0.0	0.6	0.0	0.0	0.6
Gujarati	0.0	0.0	0.6	0.0	0.0	0.0
Greek	0.0	0.0	0.6	0.0	0.0	0.1
Finnish	0.0	0.0	0.5	0.2	0.0	0.6
Malayalam	0.0	0.0	0.6	0.0	0.0	0.0
Bangla	0.0	0.0	0.5	0.0	0.0	0.0
Vietnamese	0.0	0.0	0.5	0.1	0.0	0.4
Hebrew	0.0	0.0	0.5	0.0	0.0	0.1
Basque	0.0	0.0	0.1	0.0	0.1	0.5
Serbian	0.0	0.0	0.1	0.5	0.0	0.0
Armenian	0.0	0.0	0.5	0.0	0.0	0.0
Filipino	0.0	0.0	0.3	0.1	0.1	0.5
Lithuanian	0.0	0.0	0.1	0.0	0.0	0.5
Persian	0.0	0.0	0.4	0.0	0.0	0.3
Thai	0.0	0.0	0.4	0.0	0.0	0.1
Kannada	0.0	0.0	0.4	0.0	0.0	0.0
Romanian	0.0	0.0	0.3	0.4	0.1	0.3
Telugu	0.0	0.0	0.4	0.0	0.0	0.0
Danish	0.0	0.0	0.4	0.3	0.3	0.2
Welsh	0.0	0.0	0.1	0.1	0.0	0.4
Slovenian	0.0	0.1	0.3	0.2	0.2	0.1
Urdu	0.0	0.0	0.3	0.0	0.0	0.0
Malagasy	0.0	0.0	0.1	0.1	0.1	0.3
Tamil	0.0	0.0	0.3	0.0	0.0	0.0
Irish	0.0	0.0	0.3	0.1	0.0	0.2
Tajik	0.0	0.0	0.3	0.0	0.0	0.0
Nepali	0.0	0.0	0.3	0.0	0.0	0.0
Kazakh	0.0	0.0	0.3	0.0	0.0	0.0
Belarusian	0.0	0.0	0.3	0.1	0.0	0.0
Afrikaans	0.0	0.0	0.3	0.2	0.1	0.2
Tatar	0.0	0.0	0.3	0.0	0.0	0.0
Galician	0.0	0.0	0.2	0.3	0.2	0.0
Uzbek	0.0	0.0	0.1	0.1	0.1	0.2
Bulgarian	0.0	0.0	0.2	0.2	0.0	0.1
Norwegian Nynorsk	0.0	0.1	0.1	0.2	0.0	0.1
Slovak	0.0	0.0	0.2	0.0	0.0	0.2
Lojban	0.1	0.0	0.2	0.0	0.0	0.0
Icelandic	0.0	0.0	0.2	0.1	0.0	0.1
Esperanto	0.0	0.0	0.0	0.2	0.0	0.1
Kyrgyz	0.0	0.0	0.2	0.0	0.0	0.0
Pashto	0.0	0.0	0.2	0.0	0.0	0.0
Breton	0.0	0.0	0.1	0.1	0.0	0.2
Yiddish	0.0	0.0	0.2	0.0	0.0	0.0
Bashkir	0.0	0.0	0.2	0.0	0.0	0.0
Norwegian	0.0	0.0	0.2	0.0	0.0	0.1
Hungarian	0.0	0.0	0.0	0.1	0.0	0.0
Latvian	0.0	0.0	0.1	0.0	0.0	0.2

Table 4. The 112 natural languages considered in §4. The data is from Oscar v23.01, which performs language identification at the document level.

Language	Size (MB)	Language	Size (MB)	Language	Size (MB)	Language	Size (MB)
Chinese	776494.9	Bangla	19055.4	Icelandic	2194.7	Sanskrit	56.3
English	666955.4	Hebrew	17970.6	Slovenian	1398.1	Ossetic	50.7
Russian	531902.4	Tamil	15776.8	Punjabi	1377.2	Chuvash	42.3
Spanish	424143.2	Catalan	15346.5	Basque	1195.9	Cebuano	41.1
French	371967.1	Danish	14843.6	Tajik	1028.4	Afrikaans	37.2
German	356683.7	Lithuanian	14518.6	Tatar	834.1	Breton	31.4
Italian	214768.2	Georgian	8388.2	Central Kurdish	773.1	South Azerbaijani	28.4
Japanese	181299.8	Estonian	8026.9	Filipino	719.4	Croatian	26.5
Hungarian	150134.4	Serbian	7666.2	Odia	543.2	Eastern Mari	22.9
Polish	146001.9	Latvian	7411.5	Tibetan	531.6	Luxembourgish	18.4
Vietnamese	139298.4	Malayalam	5815.1	Amharic	513.0	Uzbek	15.3
Dutch	135078.1	Mongolian	5777.3	Kyrgyz	489.5	Chechen	13.9
Arabic	110728.5	Gujarati	5593.9	Esperanto	475.1	Malagasy	11.2
Portuguese	105065.0	Nepali	4950.5	Lao	472.3	Low German	10.7
Greek	95750.9	Armenian	4884.7	Assamese	412.2	Mingrelian	6.1
Persian	93225.0	Macedonian	4745.4	Bashkir	363.9	Bishnupriya	5.4
Thai	91968.7	Marathi	4478.3	Welsh	333.1	Newari	4.0
Czech	76987.1	Telugu	3873.8	Pashto	261.7	Minangkabau	3.8
Turkish	72207.2	Urdu	3761.3	Galician	255.9	Egyptian Arabic	3.7
Swedish	50001.1	Kazakh	3325.4	Uyghur	219.8	Norwegian Nynorsk	3.7
Romanian	45590.6	Albanian	3224.9	Divehi	200.2	Turkmen	3.3
Ukrainian	44746.7	Khmer	3155.2	Kurdish	174.2	Piedmontese	3.1
Bulgarian	44118.5	Azerbaijani	3038.3	Yiddish	171.8	Malay	2.6
Finnish	41143.7	Burmese	3035.4	Sindhi	131.7	Goan Konkani	2.3
Korean	38158.4	Sinhala	2599.3	Western Panjabi	105.8	Latin	2.0
Hindi	32615.5	Norwegian	2583.2	Western Frisian	70.5	Lojban	1.5
Indonesian	23416.0	Kannada	2574.4	Sakha	68.8	Maltese	1.3
Slovak	21460.7	Belarusian	2339.5	Irish	63.2	Swahili	1.0

Table 5. The 37 programming languages considered in §4. Data is sourced from the Github split of RedPajama, and classified into a language based on the file extension.

Language	Size (in MB)	Language	Size (in MB)
Java	29493.0	Haskell	547.6
JavaScript	27910.4	TSQL	489.5
HTML	25864.1	Lua	393.4
XML	18804.0	Dockerfile	272.7
C++	15543.1	Makefile	265.7
Python	12970.1	TeX	256.9
Smalltalk	11580.5	XPixMap	248.7
Objective-C	10909.5	PowerShell	240.7
PHP	9837.4	CMake	118.5
Go	6287.2	Raku	106.9
Markdown	6137.3	Hack	79.1
C	6045.0	Julia	72.3
CSS	4084.9	Batchfile	60.9
Ruby	3381.4	Pod6	46.6
Scala	1376.8	FortranFreeForm	40.8
Smali	978.3	Fortran	31.2
reStructuredText	891.4	Motorola68KAssembly	22.7
VisualBasic.NET	563.0	Perl	2.0
Shell	551.6		

Table 6. The 5 domains considered in §4. Data is sourced from RedPajama.

Domain	Size (in MB)
Web	305139.9
Code	196506.0
Books	104975.0
Academic	89044.9
Wikipedia	20505.8