FROM LANGUAGE MODELS OVER TOKENS TO LANGUAGE MODELS OVER CHARACTERS

Tim Vieira*,1Ben LeBrun2Mario Giulianelli1Juan Luis Gastaldi1Brian DuSell1John Terilla4Timothy J. O'Donnell3,2,5Ryan Cotterell11ETH Zürich2Mila – Quebec Artificial Intelligence Institute3McGill University4City University of New York5Canada CIFAR AI Chair, Mila

ABSTRACT

Modern language models are internally—and mathematically—distributions over *token* strings rather than *character* strings, posing numerous challenges for programmers building user applications on top of them. For example, if a prompt is specified as a character string, it must be tokenized before passing it to the token-level language model. Thus, the tokenizer and consequent analyses are very sensitive to the specification of the prompt (e.g., if the prompt ends with a space or not). This paper presents algorithms for converting token-level language models to character-level ones. We present both exact and approximate algorithms. In the empirical portion of the paper, we benchmark the practical runtime and approximation quality. We find that—even with a small computation budget—our method is able to accurately approximate the character-level distribution (less than 0.00021 excess bits / character) at reasonably fast speeds (46.3 characters / second) on the Llama 3.1 8B language model.

https://github.com/rycolab/token-to-char-lm

1 INTRODUCTION

For various technical reasons, modern language models are engineered as probability distributions over strings of *tokens* rather than strings of *characters*. However, this leads to a fundamental tension between the users of large language models and the engineers who build them. Specifically, token-level models are rife with unintuitive behaviors that—without a technical fix—baffle users. As an illustrative example of a common user complaint, we exhibit the prompt boundary problem (see below). This paper provides a principled solution to the prompt boundary problem as well as other oddities that make interfacing with token-level language models with character-level prompts hard for users.

Tokenized language models: A brief overview. Let Σ be an alphabet of characters, and let Σ^* denote the set of all strings that can be built from it. Suppose there is a true distribution p_{Σ}^* over Σ^* that we seek to model. We observe a training corpus of character strings: $\sigma^{(1)}, \ldots, \sigma^{(M)} \stackrel{\text{i.i.d.}}{\sim} p_{\Sigma}^*$. However, rather than estimating a language model that approximates p_{Σ}^* directly, we employ a (possibly stochastic)¹ tokenizer τ that transforms the training corpus into a corpus of *token* strings. $\delta^{(1)} \sim \tau(\cdot | \sigma^{(1)}), \ldots, \delta^{(M)} \sim \tau(\cdot | \sigma^{(M)})$. Next, we estimate a token-level language model to fit the strings $\delta^{(1)}, \ldots, \delta^{(M)}$. Lastly, we use p_{Δ} to generate character strings by means of the following generative process: (i) sample $\delta \sim p_{\Delta}$ and (ii) return $\sigma = \kappa(\delta)$ where κ is a decoding function. Let p_{Σ} denote the resulting distribution of this process. Practically, we hope that the choice of τ and κ should aid in our ability to estimate p_{Σ}^* in the sense that $p_{\Sigma}^* \approx p_{\Sigma}$.² Commonly used tokenizers in the realm of LLMs use tokenizers τ that break long strings into chunks. Intuitively, generating chunks

^{*}Please direct correspondence to tim.f.vieira@gmail.com and ryan.cotterell@inf.ethz.ch.

¹The tokenizer τ is often deterministic (e.g., byte-pair encoding (Sennrich et al., 2016)), but stochastic tokenizers (e.g., UnigramLM (Kudo, 2018)) are also of interest to the community.

²Gastaldi et al. (2024) give a general characterization of which tokenizers allow consistent statistical estimation.

instead of individual characters helps because it effectively shortens strings without obfuscating them using a complicated encoding.

The prompt boundary problem. Consider the case of GPT2 (Radford et al., 2019), which was trained over token strings created from byte-pair encoding (BPE; Sennrich et al. (2016); Gage (1994)). Suppose we wish to generate continuations of the prompt:

"In_the_kingdom_of_the_blind,_the

Unfortunately, the language model p_{Δ} does not accept a *character* string; thus, it is common to encode it as a *token* string with an encoding function τ_{BPE} :^{3,4}

 $\tau_{\rm BPE}("{\tt In_the_kingdom_of_the_blind,_the}) = [\stackrel{"}{_1}, \stackrel{{\tt In_the_kingdom_of_the_blind}}_{13239}, \stackrel{{\tt of_the_blind}}_{262}, \stackrel{{\tt of_the_blind}}_{7770}, \stackrel{{\tt the}}_{11, 262}]$

If we complete the prompt by taking the most likely next token (also known as *greedy completion*), we generate the following continuation:

Now that we have our generated output, we can apply the decoding function κ that maps token strings to character strings as part of the tokenization protocol:

```
\kappa_{\rm BPE}(["In _the _kingdom _of _the _blind , _the _one - eyed _man _is _king ."])
```

= "In_the_kingdom_of_the_blind,_the_one-eyed_man_is_king."

This is a good completion, as the string is a well-known proverb. However, if we tweak the prompt *ever so slightly* by inserting a trailing whitespace:

 $\tau_{\rm BPE}("{\tt In_the_kingdom_of_the_blind,_the_}) = [\stackrel{"}{\underset{1,818}{,}_{262}}, \stackrel{{\tt Lhe_kingdom_of_the_blind}{,}_{286}, \stackrel{{\tt Che_blind}{,}_{262}}, \stackrel{{\tt Lhe_blind}{,}_{286}, \stackrel{{\tt Che_blind}{,}_{262}}, \stackrel{{\tt Lhe_blind}{,}_{262}, \stackrel{{\tt Lhe_blind}{,}_{262}, \stackrel{{\tt Lhe_blind}{,}_{262}}, \stackrel{{\tt Lhe_blind}{,}_{262}, \stackrel{{\tt Lhe_blind}{,}_{266}, \stackrel{{\tt Lhe_blind}{,}_{262}, \stackrel{{\tt Lhe_blind}{,}_{262}$

greedy completion returns

[ills _of _the _world _are _seen ____] [2171, 286, 262, 995, 389, 1775, ...]

This happens because the conditional probability $(\overrightarrow{p_{\Delta}})$ of generating the characters we want becomes extremely unlikely:

Hence, the trailing white space undesirably impacts the output, which no longer corresponds to the proverb. This behavior is odd, as we would expect the most likely continuation (shown above) to be invariant to whether or not the whitespace character ($_{\sim}$) is in the prompt or the continuation. More broadly, the *prompt boundary problem* may be generally characterized as an unwanted sensitivity to the characters at the boundary and the continuation. Our perspective is that the prompt boundary problem arises from incorrectly conditioning the *token-level* language model on a string of *characters* by using $\tau(\sigma)$ rather than finding token strings that best match the prompt σ .

 \hookrightarrow The token healing heuristic: Lundberg & Ribeiro (2023) present token healing as a heuristic that mitigates the prompt boundary problem. Token healing works as follows: (1) Tokenize (i.e., encode) the prompt. (2) Backup the tokenized prompt to the penultimate token. (3) Generate the next token subject to the constraint that it starts with the unmatched substring at the end of the prompt. (4) Continue generating as usual. Now, we can see how token healing patches the running example:

 $\tau_{\rm BPE}("{\tt In_the_kingdom_of_the_blind_}) = [" {\tt In_the_kingdom_of_the_blind_}, {\tt the_kingdom_of_the_blind_}) = [" {\tt In_the_kingdom_of_the_blind_}, {\tt the_kingdom_of_the_blind_}]$

The most probable next token starting with $_$ is $\frac{_one}{_{530}}$. From here, generating the remaining tokens recovers the desired output because it matches the prompt before we added the whitespace.

³In practice, τ_{BPE} outputs an integer sequence; however, we provide the substring gloss for readability. ⁴Here we write $\delta = \tau(\sigma)$ instead of $\delta \sim \tau(\cdot | \sigma)$ since τ is deterministic (i.e., a function).

Unfortunately, backing up one token is insufficient for the general case, as the following example will illustrate. Consider generating from GPT2 using the prompt Hello,_worl:

 $au_{\mathrm{BPE}}(\mathrm{Hello}, \mathrm{worl}) = [^{\mathrm{Hello}}_{15496}, \mathrm{Hello}, \mathrm{Hello}$

The most likely next *character* ought to be d as Hello, _world is a common expression (popularized in educational material). However, the most likely token is Hello, _worlwide, an apparent misspelling of worldwide.⁵ Unfortunately, token healing's strategy of backing up by a single token cannot salvage

the poor tokenization as $\frac{1}{75}$ is still the most common next token that is consistent with the string 1.

Thus, after generating $\frac{1}{75}$, we are back where we started, generating $\begin{bmatrix} Hello \\ 15496 \\ 11 \end{bmatrix}$, wor $\frac{1}{476}$, $\frac{1}{75}$, $\frac{wide}{422}$].

 \hookrightarrow Getting it right: A simple "probability 101" expression tells us the correct solution to the prompt boundary problem. Consider a Δ^* -valued random variable Y, distributed according to p_{Δ} . Then, the correct way to sample from p_{Δ} conditioned on a character string σ is according to

$$p_{\Delta\mid\Sigma}(\boldsymbol{\delta}\mid\boldsymbol{\sigma}) \stackrel{\text{def}}{=} \mathop{\mathbb{P}}_{Y \sim p_{\Delta}}[Y = \boldsymbol{\delta} \mid \kappa(Y) \succeq \boldsymbol{\sigma}]$$
(1)

where we have conditioned on the event that the decoded string $\kappa(Y)$ has σ as a prefix (i.e., $\kappa(Y) \succeq \sigma$). While innovative with respect to the literature, the expression $\mathbb{P}_{Y \sim p_{\Delta}}[Y = \delta | \kappa(Y) \succeq \sigma]$ conveys the probability we are interested in precisely and concisely. For the more procedurally minded, this corresponds to the following generation process:⁶

```
1 def conditional_token_generation(\sigma):

2 while True:

3 sample \delta \sim p_{\Delta}

4 if \kappa(\delta) \succeq \sigma: # accept

5 return \delta

6 else:

7 pass # try again...
```

This is, of course, very inefficient, but fear not-we will provide an equivalent, efficient algorithm.

Our method finds a set of token strings that form a *covering*, a key technical concept we introduce in this paper. Once we have the covering, we can pick a member of the covering in proportion to its (normalized) prefix probability⁷ and then repeatedly sample subsequent tokens until the end-of-string event EOS is generated. We give a complete algorithm with correctness guarantees in §3.4. Notice that each token string in the covering (shown on the right) includes the character string Hello, worl as a prefix, but it may have some extra characters (marked by underlining) in the partially matched last token—just like token healing. The size of the complete covering may, in general, be exponential in the length of the character string. However, we can enumerate its high-probability members very quickly in practice. Since the worst-case time to find the top-*K* elements of the covering

(0.9820714) : [15496, 11, 995]
Hello , _worl <u>ds</u> (0.0106702) :[15496,11, 11621]
Hello , _worl <u>dwide</u> 1(0.0070749) :[15496,11, 8688]
Hello , _worl <u>dly</u> I(0.0000830) : [₁₅₄₉₆ , ₁₁ , ₄₃₂₄₉]
Hello , _worl <u>dview</u> 1(0.0000369) :[15496,11, 29081]
Hell o , _world [28254,78,11, 995]
Hello , _wor 1 (0.0000179) : [15496, 11, 476, 75]
Hello , _wor ls (0.0000036) : [15496, 11, 476, 7278]

might be exponential, we provide a more aggressive approximation based on beam search that gives a good approximation even with small beam sizes. Unlike token healing, the sequence $\begin{bmatrix} Hello \\ 15496 \\ 11, 11 \end{bmatrix}$ is the highest probability member of the covering; thus, it is not pruned away by the aggressive heuristics based on τ , as in token healing. The covering is defined only in terms of κ , and the pruning is based on the language model probability, which typically prioritizes the kinds of token strings that τ generates, as they are the most reflective of the language model's training data. We provide an algorithm for correctly conditioning a token-level model on a character string in §3.4.

⁵The misspelling is a testament to the extent to which the tokenized prompt is out-of-distribution.

⁶We adopt the common notational convention of probability theory where random variables are denoted by upper-case symbols (e.g., Y), and values by lower-case symbols (e.g., δ).

⁷In the diagram, we have normalized the prefix probability to make it a distribution over the covering.

Character-level model. Reasoning at the character level is intuitive. Consider again our example illustrating the prompt boundary problem. Appending whitespace behaves intuitively at the character level, as it satisfies the *probabilistic chain rule*:

 $\overrightarrow{p_{\Sigma}}(_one \mid "In_the_kingdom_of_the_blind,_the)$ $= \overrightarrow{p_{\Sigma}}(_ \mid "In_the_kingdom_of_the_blind,_the) \cdot \overrightarrow{p_{\Sigma}}(one \mid "In_the_kingdom_of_the_blind,_the_)$

Here $\overrightarrow{p_{\Sigma}}$ denotes the character-level model's conditional distribution. Similarly, recall the Hello,_world example above. The character-level model correctly infers that d is the most likely next character given Hello,_worl. The computation of this conditional probability is simply the total probability of the covering of Hello,_world divided by the total probability of the covering of Hello,_world divided by the total probability of the covering of Hello,_world in algorithm for determining the distribution over possible next characters. Beyond the prompt boundary problem, computing the conditional probability of a character string given a token-level language model has many applications.

Applications. Aside from making character-level conditioning well-behaved, we highlight a few applications of language models requiring careful reasoning about character strings.

 \hookrightarrow *Character-level constraints:* Enforcing character-level constraints on allowed strings is a promising area that has received much recent attention (e.g., Scholak et al., 2021; Poesia et al., 2022; Geng et al., 2023; Microsoft, 2023; Willard & Louf, 2023; Koo et al., 2024).

 \hookrightarrow Computational psycholinguistics: Computing the contextual surprisal (negative log probability) of a character substring to predict human reading times (Hale, 2001; Levy, 2008). Two recent papers (Oh & Schuler, 2024; Pimentel & Meister, 2024) have given algorithms for computing the surprisal of whitespace-separated *words* under a number of strong assumptions. Our algorithms can compute the contextual surprisal of arbitrary character strings. Giulianelli et al. (2024) show experimentally that having the flexibility to compute character substring surprisals leads to a more predictive model of reading behavior than a fixed notion of a word.

Does it work? In the experimental portion of our paper (§4), we report the empirical runtime of our algorithm for converting token-level language models to character-level ones and quantify its accuracy in estimating the conditional distribution over characters. We find that even with a limited computational budget, our method is able to provide an accurate estimate of the conditional distribution over the next character under two publicly available language models (GPT2-large and Llama 3.1 8B). We defer further discussion to §4. s

2 BACKGROUND

2.1 ALPHABETS AND STRINGS

An **alphabet** Γ is a non-empty, finite set of elements called **symbols**. A **string** γ over alphabet Γ is a finite sequence $\gamma = \gamma_1 \cdots \gamma_N$ for some $0 \leq N < \infty$ of symbols where $\gamma_1, \ldots, \gamma_N \in \Gamma$. Let $|\gamma|$ denote the string's length N. We denote the empty string as ε . For any alphabet Γ , let Γ^* denote the set of all strings over Γ , and let Γ^+ denote the set of all non-empty strings over Γ . For any two strings $\gamma', \gamma'' \in \Gamma^*$, we denote their concatenation as $\gamma' \cdot \gamma''$. Additionally, we define $S \cdot S' \stackrel{\text{def}}{=} \{\gamma \cdot \gamma' \mid \gamma \in S, \gamma' \in S'\}$ for any $S, S' \subseteq \Gamma^*$. Given a string γ such that $|\gamma| \geq t$, let $\gamma_{<t}$ denote the string of the first t-1 characters of γ . We write $\gamma \preceq \gamma'$ if γ is a prefix⁸ of γ' and $\gamma \prec \gamma'$ if γ is a proper prefix of γ' . The relation \preceq defines a partial order on Γ^* . We write \succeq and \succ to refer to the relations \preceq and \prec with their respective arguments transposed.

2.2 LANGUAGE MODELS AND PREFIX PROBABILITY

A language model p_{Γ} is a probability distribution over Γ^* where Γ is an alphabet. Let Y be a Γ^* -valued random variable distributed according to p_{Γ} and $\gamma \in \Gamma^*$. We define the **prefix probability**

⁸Formally,
$$(\gamma \preceq \gamma') \stackrel{\text{def}}{=} (\exists \gamma'' \in \Gamma^* : \gamma' = \gamma \cdot \gamma'') \text{ and } (\gamma \prec \gamma') \stackrel{\text{def}}{=} (\exists \gamma'' \in \Gamma^+ : \gamma' = \gamma \cdot \gamma'').$$

 $\overrightarrow{p_{\Gamma}}(\gamma)$ as the probability that Y has γ as a prefix:

$$\overrightarrow{p_{\Gamma}}(\boldsymbol{\gamma}) \stackrel{\text{def}}{=} \mathop{\mathbb{P}}_{Y \sim p_{\Gamma}}[Y \succeq \boldsymbol{\gamma}] = \sum_{\boldsymbol{\gamma}' \in \Gamma^*} \mathbb{1}\{\boldsymbol{\gamma}' \succeq \boldsymbol{\gamma}\} p_{\Gamma}(\boldsymbol{\gamma}')$$
(2)

We also define the following shorthand for the **conditional prefix probability** $\overrightarrow{p_{\Gamma}}(\gamma' \mid \gamma)$ as the probability of the event $Y \succeq \gamma \cdot \gamma'$ provided that $Y \succeq \gamma$:

$$\overrightarrow{p_{\Gamma}}(\gamma' \mid \gamma) \stackrel{\text{def}}{=} \mathbb{P}_{Y \sim p_{\Gamma}}[Y \succeq \gamma \cdot \gamma' \mid Y \succeq \gamma] = \frac{\overrightarrow{p_{\Gamma}}(\gamma \cdot \gamma')}{\overrightarrow{p_{\Gamma}}(\gamma)} = \frac{\sum_{\gamma'' \in \Gamma^*} \mathbb{1}\{\gamma'' \succeq \gamma \cdot \gamma'\} p_{\Gamma}(\gamma'')}{\sum_{\gamma'' \in \Gamma^*} \mathbb{1}\{\gamma'' \succeq \gamma\} p_{\Gamma}(\gamma'')} \quad (3)$$

Note that the conditional prefix probability above is only well-defined when $\overrightarrow{p_{\Gamma}}(\gamma) > 0.^9$ Usefully, we may express the probability of γ as a product of conditional prefix probabilities:¹⁰

$$p_{\Gamma}(\boldsymbol{\gamma}) = \overrightarrow{p_{\Gamma}}(\text{EOS} \mid \boldsymbol{\gamma}) \prod_{t=1}^{|\boldsymbol{\gamma}|} \overrightarrow{p_{\Gamma}}(\gamma_t \mid \boldsymbol{\gamma}_{< t})$$
(4)

where each $\overrightarrow{p_{\Gamma}}(\gamma_t \mid \boldsymbol{\gamma}_{< t})$ is an instance of Eq. (3), and

$$\overrightarrow{p_{\Gamma}}(\text{EOS} \mid \gamma) \stackrel{\text{def}}{=} \frac{p_{\Gamma}(\gamma)}{\overrightarrow{p_{\Gamma}}(\gamma)}$$
(5)

Here, EOS is a distinguished **end-of-string symbol** that cannot appear in any alphabet. Of particular interest are the single-symbol conditional prefix distributions $\overrightarrow{p_{\Gamma}}(\cdot | \boldsymbol{\gamma}_{< t})$, as they may each be interpreted as a probability distribution over the set $\Gamma \cup \{\text{EOS}\}$ —in fact, modern language models¹¹ are *defined* via the product in Eq. (4) where each single-symbol conditional prefix probability comes from the learned parametric model.¹²

An apparent chicken and egg problem. The reader may notice that the equations for $p_{\Gamma}(\gamma)$, $\overrightarrow{p_{\Gamma}}(\gamma' | \gamma)$, and $\overrightarrow{p_{\Gamma}}(EOS | \gamma)$ may appear cyclical. The key to resolving the concern is to recognize that the apparent cycle just needs a base case. In our presentation, we assumed that p_{Γ} is the base case. Some readers may view Eq. (4) as the *definition* of the language model p_{Γ} , i.e., they take the components on the right-hand side of Eq. (4) as the base case.

2.3 TOKENIZATION

We now discuss our basic formalization for tokenization.

Definition 1. An (exact) tokenization model is a tuple $(\Sigma, \Delta, \tau, \kappa)$ where

- Σ is an alphabet of **character** symbols
- Δ is an alphabet of **token** symbols
- τ is a (possibly) stochastic **encoder**: $\tau(\cdot | \sigma)$ is a probability distribution over Δ^* for each $\sigma \in \Sigma^*$
- $\kappa: \Delta^* \to \Sigma^*$ is a **decoder** function mapping token strings to character strings satisfying

$$\sum_{\boldsymbol{\delta}\in\Delta^*} \mathbb{1}\{\kappa(\boldsymbol{\delta}) = \boldsymbol{\sigma}\}\tau(\boldsymbol{\delta} \mid \boldsymbol{\sigma}) = 1, \quad \text{for all } \boldsymbol{\sigma}\in\Sigma^*$$
(6)

The condition between τ and κ expressed in Eq. (6) is called **exactness**. One may consider more general tokenization models in which κ is possibly stochastic and for which Eq. (6) may not hold. All tokenization models considered in this paper will be exact and will be called simply *tokenization*

⁹Such a caveat is common of conditional probabilities. We note that the condition is always satisfied in practice for softmax-normalized language models, as they place nonzero probability on all elements of Γ^* ; hence, every string in Γ^* has a nonzero prefix probability.

¹⁰Note that conditional prefix probabilities satisfy the following chain rules: $\overrightarrow{p_{\Gamma}}(\gamma \cdot \gamma') = \overrightarrow{p_{\Gamma}}(\gamma) \overrightarrow{p_{\Gamma}}(\gamma' \mid \gamma)$ for all $\gamma, \gamma' \in \Gamma^*$, and $\overrightarrow{p_{\Gamma}}(\gamma' \cdot \gamma'' \mid \gamma) = \overrightarrow{p_{\Gamma}}(\gamma' \mid \gamma) \overrightarrow{p_{\Gamma}}(\gamma'' \mid \gamma \cdot \gamma'')$ for all $\gamma, \gamma', \gamma'' \in \Gamma^*$. ¹¹E.g., transformers (Vaswani et al., 2017), RNNs (e.g., Mikolov et al., 2010; Sundermeyer et al., 2015), and

¹¹E.g., transformers (Vaswani et al., 2017), RNNs (e.g., Mikolov et al., 2010; Sundermeyer et al., 2015), and *n*-gram models (e.g., Shannon, 1948). These models are often called *autoregressive*, as they directly predict the probability of the next symbol in the string based on its previous symbols using a parametric model.

¹²Note that this can lead to the issue of *tightness* (see, for example, Cotterell et al. (2024)) where probability is lost to infinite sequences—leading to a probability model summing to less than one over Γ^* .

models rather than *exact tokenization models*. Exactness is satisfied by lossless tokenizers, including BPE (Sennrich et al., 2016), UnigramLM (Kudo, 2018)), and SentencePiece (Kudo & Richardson, 2018). Lossy tokenizers, such as those leveraging out-of-vocabulary (OOV) tokens, are not exact. See Gastaldi et al. (2024) for the general case; in particular, for a proof that Eq. (6) implies that an *a priori* stochastic κ must, in fact, be deterministic.

Definition 2. A tokenized language model p_{Σ} is a language model over Σ^* that is parameterized by a language model p_{Δ} over Δ^* and a decoding function $\kappa \colon \Delta^* \to \Sigma^*$. This tokenized language model generates character strings via the following process: (i) $\delta \sim p_{\Delta}$, (ii) $\sigma \leftarrow \kappa(\delta)$. Thus, the character strings σ generated have the following distribution:

$$p_{\Sigma}(\boldsymbol{\sigma}) \stackrel{\text{def}}{=} \mathbb{P}_{Y \sim p_{\Delta}}[\kappa(Y) = \boldsymbol{\sigma}], \quad \forall \boldsymbol{\sigma} \in \Sigma^{*}$$
(7)

Note that $p_{\Sigma}(\sigma)$ accounts for the fact that many token strings may be associated with a given character string through κ .¹³ To describe that association, we define $\mathcal{E}(\sigma) \stackrel{\text{def}}{=} \{\delta \in \Delta^* : \sigma = \kappa(\delta)\}$ denote the set of **encodings** for any character string $\sigma \in \Sigma^*$.¹⁴

What about τ ? The reader may notice that τ does not appear in Eq. (7). Although τ is essential for generating training data, once the model p_{Δ} has been trained, the information in τ is not of immediate practical use. Moreover, attempts to leverage τ seem to lead to faulty heuristics, as we discussed in the introduction. We note that under exactness (Eq. (6)), $\tau(\sigma)$ must be present in $\mathcal{E}(\sigma)$. This is because exactness *indirectly* implies that $\mathcal{E}(\sigma) \supseteq \{\delta \in \Delta^* : \tau(\delta \mid \sigma) > 0\}$ for all $\sigma \in \Sigma^*$. In the common case where τ is **deterministic** (i.e., $\tau(\delta \mid \sigma) \in \{0, 1\}$ for all $\delta \in \Delta^*, \sigma \in \Sigma^*$), we emphasize that $\mathcal{E}(\sigma)$ is only *lower bounded* by $\{\tau(\sigma)\}$. The tokenization model would need to be bijective for $\mathcal{E}(\sigma) = \{\tau(\sigma)\}$. Unfortunately, common tokenizers (e.g., BPE) are *not* bijective because they do *not* satisfy $\tau(\kappa(\delta)) = \delta$ for all $\delta \in \Delta^*$. We illustrate this in Example 1 below.

The mirage of the canonical tokenization. Consider the case when the encoder τ is deterministic. In that case, we write $\delta = \tau(\sigma)$, and we call this δ the **canonical** tokenization of σ . Note that even if τ is deterministic, there may exist many **noncanonical** tokenizations $\delta' \in \mathcal{E}(\sigma)$ such that $\delta' \neq \tau(\sigma)$ with nonzero probability $p_{\Delta}(\delta') > 0$. Thus, the character string generation process includes a mix of canonical and noncanonical token strings—making it incorrect to only consider a character string's canonical tokenization when assessing its probability. In practice, the conditional probability $\mathbb{P}_{Y \sim p_{\Delta}}[Y = \delta | \kappa(Y) = \sigma]$ over the encodings δ of a character string σ tends to be highly concentrated around the canonical tokenizations, as illustrated in Example 1 below.

Example 1.

On the right, we show the top-8 encodings $\mathcal{E}(\text{Hello}, world)$ under GPT2 ranked by their conditional probability. This short string has 78 tokenizations, which arise because there are many ways to break up Hello, world into substrings from the tokenization alphabet Δ :

$$\Delta \supseteq \{ \begin{array}{c} , \text{ H o } , \text{ W ld wor ell world} \\ 11, 39, 78, 220, 266, 335, 476, 695, 995 \end{array} , \\ \text{He orld world ello Hell Hello llo} \\ 1544, 1764, 6894, 11109, 28254, 15496, 18798 \end{array}$$

On the right, we see that the probability assigned to these tokenizations is heavily concentrated on the canonical tokenization: $\tau_{BPE}(Hello, world) = \begin{bmatrix} Hello, , , world \\ 15496, 11, 995 \end{bmatrix}$.

¹⁴Note that $|\mathcal{E}(\sigma)|$ can be very large, e.g., infinite in the worst case. In the case of BPE, it is exponential in $|\sigma|$.

^{(0.9999719): [}Hello , _world [15496.11, 995] Hell o , _world [28254.78.11, 995] (0.0000229): [28254.78.11, 995] (0.0000024): [15496.11, 476, 335] (0.0000017): [15496.11, 476, 335] (0.00000017): [15496.11, 995] (0.0000004): [39, 695, 78.11, 995] (0.0000002): [15496.11, 266.1764] (0.0000002): [39, 11109.11, 995] (0.0000001): [15496.11, 220, 6894]

¹³Many authors (Cao & Rimell, 2021; Chirkova et al., 2023; Phan et al., 2024) have discussed the particular complications introduced by the fact that for a given character string of length N, there are many token strings that decode to it. Marginalizing over the token strings that generate a given character string improves perplexity, but sometimes the improvements are only modest (Chirkova et al., 2023). However, prior work has not given algorithms for inferring the distribution over the next character.

A character-level interface. A character-level interface to the token-level language model p_{Δ} is available in the following equations, which hold $\forall \sigma, \sigma' \in \Sigma^*$:

$$\overrightarrow{p_{\Sigma}}(\boldsymbol{\sigma}) = \Pr_{\boldsymbol{Y} \sim p_{\Delta}}[\kappa(\boldsymbol{Y}) \succeq \boldsymbol{\sigma}]$$
(8)

$$\overrightarrow{p_{\Sigma}}(\sigma' \mid \sigma) = \frac{\overrightarrow{p_{\Sigma}}(\sigma \cdot \sigma')}{\overrightarrow{p_{\Sigma}}(\sigma)}$$
(9)

$$\overrightarrow{p_{\Sigma}}(\text{EOS} \mid \boldsymbol{\sigma}) = \frac{p_{\Sigma}(\boldsymbol{\sigma})}{\overrightarrow{p_{\Sigma}}(\boldsymbol{\sigma})}$$
(10)

These equations show that we can have a complete character-level language model derived from the tokenized language model if we can compute—or approximate—the necessary summations implied by Eq. (7) and (8); specifically,

$$p_{\Sigma}(\boldsymbol{\sigma}) = \sum_{\boldsymbol{\delta} \in \Delta^*} \mathbb{1}\{\kappa(\boldsymbol{\delta}) = \boldsymbol{\sigma}\} p_{\Delta}(\boldsymbol{\delta})$$
(11)

$$\overrightarrow{p_{\Sigma}}(\boldsymbol{\sigma}) = \sum_{\boldsymbol{\delta} \in \Delta^{*}} \mathbb{1}\{\kappa(\boldsymbol{\delta}) \succeq \boldsymbol{\sigma}\} p_{\Delta}(\boldsymbol{\delta})$$
(12)

We will develop effective methods for these summations in the remainder of the paper. We will study a family of strict-prefix monotone decoders κ (described in §2.4) where Eq. (11) and Eq. (12) admit a finite summation. In §3.4, we give an algorithm for the prompt boundary problem using these concepts.

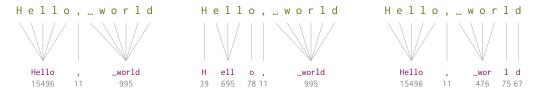
2.4 USEFUL PROPERTIES OF κ

This section provides a collection of definitions and basic results that are useful for characterizing tokenizers. We aim to capture only the essential properties of tokenizers, such as BPE, while committing to as few of its nuances as possible, as it will allow us to future-proof our methods.

Definition 3. We say that $\kappa: \Delta^* \to \Sigma^*$ is prefix monotone if $\delta \leq \delta' \implies \kappa(\delta) \leq \kappa(\delta')$ and strict-prefix monotone if $\delta \prec \delta' \implies \kappa(\delta) \prec \kappa(\delta')$.

In simpler terms, strict-prefix monotonicity says that concatenating a token to the encoding necessarily concatenates at least one character to the decoded character string.

Example 2. The diagrams below illustrate how GPT2's strict-prefix monotone κ gives rise to a certain alignment between three token strings and the character string Hello, _world:



More formally, every application $\sigma_1 \cdots \sigma_M = \kappa(\delta_1 \cdots \delta_M)$ of a strict-prefix monotone mapping has the following properties. Each token in $\delta_1 \cdots \delta_M$ maps to one or more contiguous characters in $\sigma_1 \cdots \sigma_M$. Moreover, the mappings do not exclude any characters, and no edges of the mapping cross one another. *Strict* prefix monotonicity, in contrast to prefix monotonicity, ensures that there are no deletions of tokens in the mapping, i.e., each token maps to *at least one* character.

Strict-prefix monotonicity is the key structural property that we require for the algorithms in §3, as it allows us to replace an infinite sum with a finite sum in Proposition 1. Before moving on to algorithms, we briefly mention multiplicative non-erasing decoders (defined below) as they are a common special case of strict-prefix monotone decoders, as they include BPE (Sennrich et al., 2016), WordPiece (Devlin et al., 2019), and SentencePiece (Kudo & Richardson, 2018). However, we will not leverage multiplicativity beyond the remainder of this subsection.

- We say that a decoder κ is multiplicative if κ(δ·δ') = κ(δ)·κ(δ') for all δ, δ' ∈ Δ*, and non-erasing if κ(δ) = ε ⇒ δ = ε.
- If κ is multiplicative, then κ is prefix monotone.
- If κ is multiplicative and non-erasing, then κ is strict-prefix monotone.
- If κ is multiplicative, then $\kappa(\delta_1 \cdots \delta_N) = \kappa(\delta_1) \cdots \kappa(\delta_N)$ for all $\delta_1 \cdots \delta_N \in \Delta^*$.

3 Algorithms

This section gives algorithms for $p_{\Sigma}(\sigma)$, $\overrightarrow{p_{\Sigma}}(\sigma)$, $\overrightarrow{p_{\Sigma}}(\sigma' | \sigma)$, $\overrightarrow{p_{\Sigma}}(EOS | \sigma)$, and conditional token generation (i.e., our solution to the prompt boundary problem). Unlike prior papers (Cao & Rimell, 2021; Chirkova et al., 2023; Phan et al., 2024) on the topic of marginalizing tokenization strings to compute, or estimate, the probability of character strings, i.e., compute $p_{\Sigma}(\sigma)$, we will provide algorithms for computing conditional probabilities $p_{\Sigma}(\sigma' | \sigma)$ for any strings $\sigma, \sigma' \in \Sigma^*$. Our approach is based on estimating the prefix probability $\overrightarrow{p_{\Sigma}}(\sigma)$, and it can be used in conjunction with Eq. (3) to compute $\overrightarrow{p_{\Sigma}}(\sigma' | \sigma)$. Throughout this section, we assume that κ is strict-prefix monotone.

3.1 COVERING

Our primary tool for the prefix probability $\overrightarrow{p_{\Sigma}}(\sigma)$ is the covering of σ . It is a subset of tokens associated with the given string σ that is sufficient to evaluate its prefix probability. As we will see experimentally (§4), this set's subset of high-probability token strings is often small enough to enumerate.

Eq. (12) shows that we can, in principle, compute the prefix probability $\overrightarrow{p_{\Sigma}}(\sigma)$ by summing over **prefix-encodings** of σ , $\mathcal{P}(\sigma) \stackrel{\text{def}}{=} \{\delta \in \Delta^* : \kappa(\delta) \succeq \sigma\}$. Unfortunately, $\mathcal{P}(\sigma)$ is infinitely large. Fortunately, we can exploit the prefix monotone structure of κ to find a different way to perform the summation by summing over a *finite* set.

Let $\delta \in \Delta^*$, and $\sigma \in \Sigma^*$. We say that δ covers σ if and only if $\kappa(\delta) \succeq \sigma$. Monotonicity ensures that for all $\delta \in \mathcal{P}(\sigma)$, we have that $\forall \delta' \in \Delta^* : \kappa(\delta \cdot \delta') \succeq \sigma$. In other words, any δ that decodes to an extension of σ (i.e., $\kappa(\delta) \succeq \sigma$) will continue to do so if we append tokens to it. Thus, we may additionally qualify the relationship as δ minimally covers σ if and only if $\kappa(\delta_1 \cdots \delta_{M-1}) \prec \sigma$. With that in mind, we define $\phi_{\sigma}(\delta)$ as the *shortest* prefix $\delta' \preceq \delta$ such that $\kappa(\delta') \succeq \sigma$, i.e., it maps any δ that covers σ to a (possibly equal) token string that minimally covers σ . Next, we define the set of *minimal* prefix encodings of $\mathcal{C}(\sigma)$, which we call the covering of σ , $\mathcal{C}(\sigma) \stackrel{\text{def}}{=} \{\phi_{\sigma}(\delta) \mid \delta \in \mathcal{P}(\sigma)\}$. A more convenient expression for the covering $\mathcal{C}(\sigma)$ of a string $\sigma \in \Sigma^*$ is equal to the following subset of Δ^* :

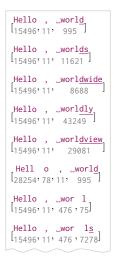
$$\mathcal{C}(\boldsymbol{\sigma}) = \begin{cases} \{\varepsilon\} & \text{if } \boldsymbol{\sigma} = \varepsilon \\ \{\delta_1 \cdots \delta_M \in \Delta^+ \colon \kappa(\delta_1 \cdots \delta_{M-1}) \prec \boldsymbol{\sigma} \preceq \kappa(\delta_1 \cdots \delta_M) \} & \text{otherwise} \end{cases}$$
(13)

Example 3.

Recall the example of a covering of $\sigma = \text{Hello}, worl from the introduction.$ We have repeated it on the right and couched it in our terminology. Note that the complete covering for this string contains 36,608 token strings; we only show the top-8 according to their respective $\overline{p_{\Delta}}$.

- The covering for any given string σ always has the property that each non-empty token string δ in the covering decodes to some string that is an extension of the character string $\sigma \leq \kappa(\delta)$. This is illustrated by the gloss string in the tokenization.
- However, it may include a partially matched token at its end (i.e., δ_M in Eq. (13)). We have marked the extra characters by underlining them. We note that the 7th member does not have a partially matched last token.
- Each token string in the covering has at most one partially matched token thanks to the condition $\kappa(\delta) \prec \sigma \preceq \kappa(\delta \cdot \delta)$. The 7th member of the cover has a completely matched last token; hence, there is no underlining.
- We see that if we were to extend any member $\delta \in C(\sigma)$ with an arbitrary string of additional tokens δ' , it would continue to decode to a string such that $\kappa(\delta \cdot \delta') \succeq \sigma$. Moreover, δ is minimal (i.e., $\phi_{\sigma}(\delta) = \delta$).

The notion of a covering is used to derive an algorithm for computing character-level probabilities given a token-level language model. We first show how it gives us the prefix probability and subsequently give equations for the remaining quantities of the character=level language model.



Proposition 1. Suppose $(\Sigma, \Delta, \tau, \kappa)$ is a tokenization model where κ is strict-prefix monotone and p_{Δ} is a token-level language model. Then, the prefix probability $\overrightarrow{p_{\Sigma}}(\sigma)$ for the character-level model Eq. (7) is given by the equation below.

$$\overrightarrow{p_{\Sigma}}(\sigma) = \sum_{\delta \in \mathcal{C}(\sigma)} \overrightarrow{p_{\Delta}}(\delta), \qquad \forall \sigma \in \Sigma^*$$
(14)

Proof. We prove the proposition directly through the following manipulations.

$$\overrightarrow{p_{\Sigma}}(\boldsymbol{\sigma}) = \sum_{\boldsymbol{\delta}' \in \Delta^*} \mathbb{1}\{\boldsymbol{\sigma} \preceq \kappa(\boldsymbol{\delta}')\} p_{\Delta}(\boldsymbol{\delta}')$$
(15)

$$= \mathbb{1}\{\boldsymbol{\sigma} = \varepsilon\} p_{\Delta}(\varepsilon) + \sum_{\boldsymbol{\delta}' \in \Delta^+} \mathbb{1}\{\boldsymbol{\sigma} \leq \kappa(\boldsymbol{\delta}')\} p_{\Delta}(\boldsymbol{\delta}')$$
(16)

$$= \mathbb{1}\{\boldsymbol{\sigma} = \boldsymbol{\varepsilon}\} p_{\Delta}(\boldsymbol{\varepsilon}) + \sum_{\boldsymbol{\delta} \cdot \boldsymbol{\delta}' \cdot \boldsymbol{\delta}'' \in \Delta^+} \mathbb{1}\{\kappa(\boldsymbol{\delta}) \prec \boldsymbol{\sigma} \preceq \kappa(\boldsymbol{\delta} \cdot \boldsymbol{\delta}' \cdot \boldsymbol{\delta}'')\} p_{\Delta}(\boldsymbol{\delta} \cdot \boldsymbol{\delta}' \cdot \boldsymbol{\delta}'')$$
(17)

$$= \mathbb{1}\{\boldsymbol{\sigma} = \varepsilon\} p_{\Delta}(\varepsilon) + \sum_{\boldsymbol{\delta} \cdot \boldsymbol{\delta}' \in \Delta^+} \mathbb{1}\{\kappa(\boldsymbol{\delta}) \prec \boldsymbol{\sigma} \preceq \kappa(\boldsymbol{\delta} \cdot \boldsymbol{\delta}')\} \sum_{\boldsymbol{\delta}'' \in \Delta^*} p_{\Delta}(\boldsymbol{\delta} \cdot \boldsymbol{\delta}' \cdot \boldsymbol{\delta}'')$$
(18)

$$= \mathbb{1}\{\boldsymbol{\sigma} = \boldsymbol{\varepsilon}\} p_{\Delta}(\boldsymbol{\varepsilon}) + \sum_{\boldsymbol{\delta} \cdot \boldsymbol{\delta}' \in \Delta^+} \mathbb{1}\{\kappa(\boldsymbol{\delta}) \prec \boldsymbol{\sigma} \preceq \kappa(\boldsymbol{\delta} \cdot \boldsymbol{\delta}')\} \overrightarrow{p_{\Delta}}(\boldsymbol{\delta} \cdot \boldsymbol{\delta}')$$
(19)

$$=\sum_{\boldsymbol{\delta}\in\mathcal{C}(\boldsymbol{\sigma})}\overrightarrow{p_{\Delta}}(\boldsymbol{\delta})\tag{20}$$

About the steps above: We start with the summation expression for the character-level prefix probability (i.e., Eq. (12)). We expand the summation into two cases (so that it will eventually match the two cases in the expression for the covering Eq. (13)). Next, for each summand, we consider its *unique* minimal prefix $\delta \cdot \delta'$ covering σ . We see why ε is handled separately, as it cannot be covered by a token sequence of that form. We exploit the key property of prefix monotone tokenizers (i.e., that once $\delta \cdot \delta'$ covers σ , each extension $\delta \cdot \delta' \delta''$ continues to cover it). This allows us to rearrange the summation to sum over the extension δ'' , which is conveniently equal to the prefix probability of $\delta \cdot \delta'$. The final step is to recognize that the summands can all be indexed by the covering $C(\sigma)$.

Eq. (14) is a substantial improvement over Eq. (8) for computing $\overrightarrow{p_{\Sigma}}(\sigma)$. Specifically, we now have a *finite* sum, as $|\mathcal{C}(\sigma)|$ is finite for all $\sigma \in \Sigma^*$. Bear in mind that the covering's size is likely too large to be practical, as there may still be a large number of summands; however, the set of high-prefix-probability elements of the covering tends to be reasonably small, an observation that we verify in §4, and leverage to develop practical algorithms in §3.

Given a covering, we filter it to the case of string equality, as

$$\mathcal{E}(\boldsymbol{\sigma}) = \left\{ \boldsymbol{\delta} \in \mathcal{C}(\boldsymbol{\sigma}) \colon \kappa(\boldsymbol{\delta}) = \boldsymbol{\sigma} \right\},\tag{21}$$

to give an expression of the string's probability

$$p_{\Sigma}(\boldsymbol{\sigma}) = \sum_{\boldsymbol{\delta} \in \mathcal{C}(\boldsymbol{\sigma})} \mathbb{1}\{\kappa(\boldsymbol{\delta}) = \boldsymbol{\sigma}\} p_{\Delta}(\boldsymbol{\delta}) = \sum_{\boldsymbol{\delta} \in \mathcal{E}(\boldsymbol{\sigma})} p_{\Delta}(\boldsymbol{\delta})$$
(22)

3.2 Algorithms for $\overrightarrow{p_{\Sigma}}(\sigma)$ and $p_{\Sigma}(\sigma)$

The enumeration algorithm will enumerate elements of the covering along with their prefix probability (for convenience). It filters prefixes of token strings that cannot eventually cover the target string σ . The strict-prefix monotonicity property is essential for this filtering.

Our algorithm enumerate_cover performs recursive enumeration of the members of the covering $\mathcal{C}(\boldsymbol{\sigma})$ along with some metadata. Specifically, the algorithm returns a collection of triples where each triple $(p', \boldsymbol{\sigma}', \boldsymbol{\delta}')$ satisfies $\boldsymbol{\delta}' \in \mathcal{C}(\boldsymbol{\sigma})$, $p' = \overrightarrow{p_{\Delta}}(\boldsymbol{\delta}')$, and $\boldsymbol{\sigma}' = \kappa(\boldsymbol{\delta}')$.

```
s def enumerate_cover(\sigma_1 \cdots \sigma_N):
            if N = 0: return [(1, \varepsilon, \varepsilon)]
 9
                                                                                                      # base case
10
            result = []
            for (p', \sigma', \delta') in enumerate_cover(\sigma_1 \cdots \sigma_{N-1}): # recurse
11
                                                                   # extend: \boldsymbol{\delta}' needs to be longer to cover \sigma_1 \cdots \sigma_N
                  if |\sigma'| < N:
12
                         for \delta'' \in \Delta:
13
                  \begin{array}{l} \mathbf{\sigma}'' \leftarrow \kappa(\mathbf{\delta}' \cdot \mathbf{\delta}'') \\ \mathbf{if} \ \mathbf{\sigma}''_N = \sigma_N : & \text{# filter: } N^{th} \text{ character matches} \\ \text{result.append}((p' \cdot \overrightarrow{p_{\Delta}}(\mathbf{\delta}'' \mid \mathbf{\delta}'), \mathbf{\sigma}'', \mathbf{\delta}' \cdot \mathbf{\delta}'')) \\ \mathbf{elif} \ \sigma'_N = \sigma_N : & \text{# filter: } N^{th} \text{ character matches} \\ \text{result.append}((p', \mathbf{\sigma}', \mathbf{\delta}')) \\ \end{array} 
14
15
16
17
18
            return prune(\sigma_1 \cdots \sigma_N, result)
19
```

Note that this method has an additional parameter, the function prune, which is used on the last line. This method, as the name suggests, is used to limit the size of the covering to prevent excessive growth. We will discuss this parameter shortly. For now, consider the following definition:

```
20 def prune_nothing(\sigma_1 \cdots \sigma_N, result):
21 return result
```

Below, we show how to use the output of the enumeration algorithm to compute several key quantities in the character-level interface.

```
22 def C(\sigma):

23 return {\delta' for (_,_,\delta') in enumerate_cover(\sigma)}

24 def \overrightarrow{p_{\Sigma}}(\sigma):

25 return sum(p' for (p',_,_) in enumerate_cover(\sigma))

26 def \mathcal{E}(\sigma):

27 return {\delta' for (_,\sigma', \delta') in enumerate_cover(\sigma) if \sigma' = \sigma}

28 def p_{\Sigma}(\sigma):

29 return sum(p' \cdot p_{\Delta}(\text{EOS} | \delta') for (p', \sigma', \delta') in enumerate_cover(\sigma) if \sigma' = \sigma)
```

This algorithm is specified at a fairly high level; thus, in order to meaningfully discuss its running time, we require some assumptions:

- κ : Our analysis assumes that $\kappa(\delta' \cdot \delta'')$ can be evaluated in constant time given $\kappa(\delta')$.
- $\overrightarrow{p_{\Delta}}$: Our analysis assumes that the cost of evaluating $\overrightarrow{p_{\Delta}}(\delta_t | \delta_{< t})$ is constant given that $\overrightarrow{p_{\Delta}}(\delta_s | \delta_{< s})$ has been computed for $0 \le s < t$.¹⁵

Under these assumptions, the running time of enumerate_cover($\sigma_1 \cdots \sigma_N$) can be exponential in N when no pruning is used. We provide detailed bounds on the covering's size in App. A. It is straightforward to verify that the space complexity is $\mathcal{O}(|\mathcal{C}(\sigma)|)$, and the running time is $\mathcal{O}(|\Delta| \cdot \sum_{t=1}^{|\sigma|} |\mathcal{C}(\sigma_{<t})|)$ which is dominated by the $|\Delta| \cdot |\mathcal{C}(\sigma)|$ term; thus, $\mathcal{O}(|\Delta| \cdot |\mathcal{C}(\sigma)|)$.

Pruning. We now consider some useful pruning heuristics for the algorithm, which make it an *approximation* but substantially improve its running time. We propose a heuristic based on beam search. This heuristic is very effective: it gives us a linear running time as a function of the character strings's length. It has a parameter K that controls the approximation quality. Larger K makes the approximation more accurate, and the approximation becomes exact as K approaches the size of the (largest intermediate) covering. For simplicity, we take K to be a global variable in the pseudocode.

 \hookrightarrow Our pruning heuristic: Our pruning heuristic enumerates $\leq K$ distinct token strings modulo their last token. This choice allows up to $|\Delta|$ versions of the last token to be enumerated. Thus, the work done at each step is $\mathcal{O}(K \cdot |\Delta|)$, and the size of the result list is at most that size. Therefore, the overall running time is $\mathcal{O}(N \cdot K \cdot |\Delta|)$ for a character string of length N.¹⁶

¹⁵In the case of the common transformer language model (Vaswani et al., 2017), this can be achieved with efficient caching and limiting context windows to a constant size.

¹⁶We note that finding the (unordered) collection of top-K elements from a set of size n is possible in O(n) time via the median-of-medians algorithm (Blum et al., 1973). This is faster asymptotically than the commonly used

30 **def** prune_top_K_buckets($\sigma_1 \cdots \sigma_N$, results): # Put items into buckets based on completely matched prefix 31 32 buckets = $\{\}$ 33 for item in results: $(p, \sigma', \delta_1 \cdots \delta_M) = \text{item}$ 34 # Exclude a partially matched last token from the key, if one exists 35 key = $\delta_1 \cdots \delta_{M-1}$ if $|\sigma'| > N$ else $\delta_1 \cdots \delta_M$ 36 buckets[key].append(item) # don't count last token 37 pruned = [] 38 for bucket in (top K buckets according to their total probability): 39 for item in bucket: 40 pruned.append(item) 41 return pruned 42

Bundled beam summing implementation. App. B describes an implementation strategy that improves the constant factors associated with the pseudocode above. The key idea is to group the token sequences that fall into the same bucket in prune_top_K_buckets into a *bundle* that represents them compactly. In particular, we can use a trie to efficiently filter out the next tokens that disagree with the next character. This improves the per-iteration cost of that filter as it can via the data structure, as it does the organizational work ahead of time in bulk. We can regard the trie as a local language model that generates the next token character-by-character according to the probability assigned by $\overrightarrow{p_{\Delta}}(\cdot | \delta)$. Each bundle can be unbundled (if necessary) into the respective tuples that the enumerate_cover algorithm maintains.

3.3 Algorithms for $\overrightarrow{p_{\Sigma}}(\sigma' \mid \sigma)$ and $\overrightarrow{p_{\Sigma}}(\text{eos} \mid \sigma)$

This section gives algorithms for computing the character-level conditional prefix probability. Recall the definition of the character-level conditional prefix probability, that is, Eq. (9) and (10), can be computed from a certain ratio of calls to $\overrightarrow{p_{\Sigma}}$ (and p_{Σ} in the case of EOS). Below is a direct translation of this into an algorithm that computes the distribution over $\Sigma \cup \{\text{EOS}\}$ given $\sigma \in \Sigma^*$:

```
43 def next_character_probability(\sigma): # slower version

44 Z = \overrightarrow{p_{\Sigma}}(\sigma); \ \overline{p} = \{\}

45 for \sigma' \in \Sigma:

46 \overline{p}(\sigma') = \overrightarrow{p_{\Sigma}}(\sigma \cdot \sigma')

47 \overline{p}(EOS) = p_{\Sigma}(\sigma)

48 return \overline{p}/Z
```

The algorithm below is semantically equivalent to the one above. However, it is more efficient because it reuses computations between iterations of the loop over $\sigma' \in \Sigma$. The duplicated work was caused by making separate calls to $\overrightarrow{p_{\Sigma}}$ and p_{Σ} for many related arguments; they are now fused in the method below.

```
49 def next_character_probability(σ):
                                                                                                                         # faster version
           N \leftarrow |\sigma|; Z = 0; \overline{p} = \{\sigma': 0 \text{ for } \sigma' \in \Sigma \cup \{\text{EOS}\}\}
50
            \begin{array}{l} \text{for } (p', \sigma', \delta') \in \texttt{enumerate\_cover}(\sigma) \colon \\ Z \ += \ p' \end{array} 
51
52
                 \tilde{\mathbf{if}} \ |\boldsymbol{\sigma}'| = N: # i.e., \boldsymbol{\sigma}' = \boldsymbol{\sigma}
53
                       \overline{p}(\text{EOS}) \stackrel{+=}{=} p' \cdot \overline{p_{\Delta}}(\text{EOS} \mid \boldsymbol{\delta})
for \delta'' \in \Delta: # extend
\sigma'' \leftarrow \kappa(\boldsymbol{\delta}' \cdot \boldsymbol{\delta}'')
54
55
56
                            \overline{p}(\sigma_{N+1}'') += p' \cdot \overrightarrow{p_{\Delta}}(\delta'' \mid \delta') # sum prefix prob. of (N+1)^{th} character
57
           else: # i.e., \sigma' \succeq \sigma

\overline{p}(\sigma'_{N+1}) \stackrel{\text{result}}{=} p' # sum prefix prob. of (N+1)^{th} character

return \overline{p}/Z # Z = \overrightarrow{p_{\Sigma}}(\sigma)
58
59
60
```

 $[\]mathcal{O}(n \log K)$ heap-based strategy. In practice, K is small enough that this is not an important detail. However, we sought to clarify why there is no log factor in our running time-bound. We also note that the cost of hashing a sequence of length N can be amortized to constant time in this pseudocode using the hashconsing pattern (see, Goubault, 1994, for an overview).

3.4 CONDITIONAL GENERATION $p_{\Delta|\Sigma}(\boldsymbol{\delta} \mid \boldsymbol{\sigma})$

This section gives a simple algorithm for correctly generating a token string Y that has a given character-level prompt σ as its prefix. This algorithm is equivalent to the algorithm in the introduction but significantly faster.

The algorithm works by enumerating the covering $C(\sigma)$, drawing a token string from it in proportion to its prefix probability, and finishing the token string by sampling a completion, which can be done from the token-level model.

```
61 def conditional_token_generation(σ):
       Z = \overrightarrow{p_{\Sigma}}(\boldsymbol{\sigma})
62
        # Sample from the covering
63
        \delta' \sim \text{Categorical}(\{\delta': p'/Z \text{ for } (p', \_, \delta') \text{ in enumerate_cover}(\sigma)\})
64
        return sample_completion(\delta')
65
66 def sample_completion(\delta'):
        \delta'' \leftarrow \varepsilon
67
        while True:
68
             \delta \sim \overrightarrow{p_{\Delta}}(\cdot \mid \boldsymbol{\delta}' \cdot \boldsymbol{\delta}'')
69
             if \delta = \text{EOS}: break
70
           \boldsymbol{\delta}'' \leftarrow \boldsymbol{\delta}'' \cdot \boldsymbol{\delta}
71
        return \delta' \cdot \delta''
72
```

The following proposition shows that the samples generated by the algorithm correctly condition on any character string prefix:

Proposition 2. The algorithm conditional_token_generation(σ) generates $Y \sim p_{\Delta|\Sigma}(\cdot | \sigma)$ for all $\sigma \in \Sigma^*$.

Proof (Sketch). Choose an arbitrary $\delta \in \Delta^*$.

$$p_{\Delta|\Sigma}(\boldsymbol{\delta} \mid \boldsymbol{\sigma}) = \Pr_{\boldsymbol{Y} \sim p_{\Delta}}[\boldsymbol{Y} = \boldsymbol{\delta} \mid \boldsymbol{\kappa}(\boldsymbol{Y}) \succeq \boldsymbol{\sigma}]$$
(23)

$$= p_{\Delta}(\delta) \frac{\mathbb{1}\{\kappa(\delta) \succeq \sigma\}}{\underset{Y \sim p_{\Delta}}{\mathbb{P}}[\kappa(Y) \succeq \sigma]}$$
(24)

$$= p_{\Delta}(\boldsymbol{\delta}) \frac{\mathbb{1}\{\kappa(\boldsymbol{\delta}) \succeq \boldsymbol{\sigma}\}}{\overrightarrow{p_{\Sigma}}(\boldsymbol{\sigma})}$$
(25)

Let $\delta' = \phi_{\sigma}(\delta)$ (i.e., the shortest prefix of δ such that $\kappa(\delta') \succeq \sigma$). Choose δ'' such that $\delta' \cdot \delta'' = \delta$.

$$= \underbrace{\overrightarrow{p_{\Delta}}(\text{EOS} \mid \delta' \cdot \delta'') \overrightarrow{p_{\Delta}}(\delta'' \mid \delta')}_{\text{sample completion}} \underbrace{\overrightarrow{p_{\Delta}}(\delta') \frac{\mathbb{1}\{\kappa(\delta') \succeq \sigma\}}{\overrightarrow{p_{\Sigma}}(\sigma)}}_{\text{sample from covering}}$$
(26)

We can see that the algorithm samples from this distribution because it samples a token string δ' from the covering in proportion to the right factor in Eq. (26) and then samples a completion δ'' of δ' in proportion to the left factor of the equation. Thus, the sample $\delta = \delta' \cdot \delta''$ has probability $p_{\Delta|\Sigma}(\delta \mid \sigma)$, and conditional_token_generation(σ) is a correct sampling procedure for it.

We also note the following corollary, as it gives an interpretation for the categorical distribution in the efficient conditional_token_generation algorithm.

Corollary 1. For all $\sigma \in \Sigma^*$, $\delta \in \Delta^*$,

$$\mathbb{P}_{Y \sim p_{\Delta}}[\phi_{\sigma}(Y) = \delta \,|\, \kappa(Y) \succeq \sigma] = \frac{\overline{p_{\Delta}}(\delta)}{\overline{p_{\Sigma}}(\sigma)} \mathbb{1}\{\delta \in \mathcal{C}(\sigma)\}$$
(27)

Thus, we have provided an efficient solution to the prompt boundary problem. We also note that generating from p_{Σ} a character at a time is also a correct solution to the prompt boundary problem; however, it is slower because it does not benefit from the fact that the generated string is shorter in token space. This is because once the minimally covering token string has been sampled, the method sample_completion will generate a complete sequence more efficiently than the character-at-a-time sample algorithm, as it does not have the overhead of marginalization that $\overrightarrow{p_{\Sigma}}(\cdot | \cdot)$ does.

4 **EXPERIMENTS**

In this section, we investigate our proposed algorithm's running time and accuracy.

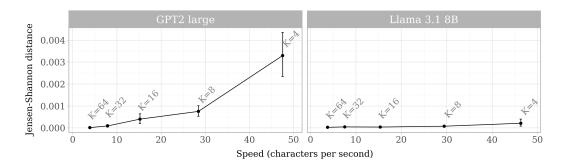
Setup.

- We use Llama 3.1 8B (Dubey et al., 2024) and GPT2 large (Radford et al., 2019) from the transformers library (Wolf et al., 2020). Both models were trained over token strings created from byte-pair encoding (BPE; Sennrich et al. (2016); Gage (1994)).
- We use the wikitext-103-v1 corpus as a source of character strings; we used the version in the ² datasets library. Specifically, we use the *test* portion.
- We use VLLM (Kwon et al., 2023) to perform the efficient, batched evaluation of transformer language models on GPUs. We batch the evaluation of all sequence extensions. All experiments were run an A100 GPU with 80GB of memory.
- Our implementation uses a trie to represent all items in each bucket efficiently (see App. B). We use the bucket-based pruning heuristic described in §3.

In the discussion below, let N denote $|\sigma|$ and let K denote the beam-size parameter.

Error vs. speed. To better understand the quality of the approximation that our method provides, we perform the following experiment. We use a large beam K = 128 as a reference model, and we measure the average per-character Jensen-Shannon distance (JSD) to the reference model's conditional distribution over the next character. The table below shows the average JSD between the character-level conditional distributions with beam sizes $K \in \{4, 8, 16, 32, 64\}$ and the reference model.¹⁷ The average is computed across the first 4000 characters of the wikitext-103-v1 test corpus. To quantify the speed of our method, we show the number of characters per second for each value of K, including the reference model.¹⁸ In parentheses, we provide a 95% confidence interval computed using bootstrapping. To aid in interpretation, we also show the same information graphically below.

	GPT2 large		Llama 3.1 8B	
K	average JSD / char	char / sec	average JSD / char	char / sec
4	0.00330 (0.00235, 0.00435)	47.51 (46.86, 48.17)	0.00021 (0.00008, 0.00041)	46.31 (45.82, 46.82)
8	0.00075 (0.00053, 0.00102)	28.45 (27.99, 28.94)	0.00008 (0.00006, 0.00010)	29.45 (29.03, 29.87)
16	0.00040 (0.00020, 0.00064)	15.23 (14.94, 15.54)	0.00004 (0.00003, 0.00005)	15.37 (15.13, 15.62)
32	0.00009 (0.00005, 0.00015)	7.90 (7.74, 8.06)	0.00005 (0.00004, 0.00006)	7.55 (7.42, 7.69)
64	0.00002 (0.00001, 0.00003)	3.88 (3.80, 3.96)	0.00003 (0.00003, 0.00003)	3.77 (3.70, 3.84)
128	(not applicable)	1.81 (1.77, 1.85)	(not applicable)	1.90 (1.87, 1.94)



Discussion. As expected, we observe that the character per second decreases with K. We observe an inverse relationship between error (JSD) and speed (chars/sec): as the processing speed (characters/sec) decreases, the JSD also decreases. Notably, this tradeoff is non-linear, with JSD increasing

¹⁷We note that if the beam size is too small, it is possible for the beam summing procedure to hit a *dead end* where no extension of the token sequences on the beam exist that match the next character of the input string. Indeed, for the very small beam size of K = 2, GPT2-large hits such a dead end after approximately 1700 characters; Llama 3.1 8B, on the other hand, manages to successfully complete the whole corpus with K = 2.

¹⁸Since the running time is linear, we can gain a good understanding of the total running time to process a string of any length N based on the measurement of the average characters per second.

more sharply at higher processing speeds compared to lower speeds. This trend is particularly evident for Llama 3.1 8B, where the JSD stabilizes around $K \ge 8$. This indicates diminishing returns in reducing error as K gets large. We hypothesize that this occurs because the language model's probability mass is concentrated around a limited set of tokenizations, which are adequately covered even with smaller beam sizes. A plausible explanation is that Llama 3.1 8B's larger model and training set size has made it better able to learn to assign much lower probabilities to non-canonical tokenizations; thus, mass tends to be concentrated around fewer tokenizations, making it possible to capture the distribution with a smaller value of K.

Comparing the two models, we observe that GPT2-large generally exhibits larger JSD from the reference distribution compared to Llama 3.1 8B across all K, with the exception of K = 64. This difference can be explained by GPT2-large spreading its probability mass across more tokenizations, requiring larger K to cover all probable tokenizations.

5 CONCLUSIONS, LIMITATIONS, AND FUTURE WORK

We have developed an effective method for ameliorating tensions between tokens and characters faced by engineers and users. We gave theory and algorithms that provide a character-level interface to tokenized language models. We characterized and resolved the prompt boundary problem. We investigated the empirical speed and error rates of our method on a modern language model.

The primary limitation of our beam summing method is that it will require a very large beam size K when the language model does not favor a small number of tokenizations. The models that we explored in our experiments concentrate mass on a few tokenizations; thus, we did not require large K to estimate their character-level prefix probabilities accurately. Future work may wish to investigate sampling-based estimation methods and possibly derive upper and lower bounds on the true values of the character-level prefix probability.

ACKNOWLEDGMENTS

The authors would like to thank Andreas Opedal, Alex Lew, Jacob Hoover Vigly, Luca Malagutti, Manuel de Prada Corral, and Vésteinn Snæbjarnarson for their helpful feedback and discussions. JT would like to thank Rycolab for its hospitality during a recent visit. The authors JLG and JT would like to thank Institut des Hautes Études Scientifiques (IHES) for their hospitality while revising this paper. MG was supported by an ETH Zürich Postdoctoral Fellowship. This research was enabled in part by compute resources provided by Mila (mila.quebec).

REFERENCES

- Manuel Blum, Robert W. Floyd, Vaughan R. Pratt, Ronald L. Rivest, and Robert Endre Tarjan. Time bounds for selection. *Journal of Computer and System Sciences*, 7(4), 1973. doi: 10.1016/ S0022-0000(73)80033-9. URL https://doi.org/10.1016/S0022-0000(73)80033-9.
- Kris Cao and Laura Rimell. You should evaluate your language model on marginal likelihood over tokenisations. In *Proceedings of the Conference on Empirical Methods in Natural Language Processing*, 2021. doi: 10.18653/v1/2021.emnlp-main.161. URL https://aclanthology.org/ 2021.emnlp-main.161.
- Nadezhda Chirkova, Germán Kruszewski, Jos Rozen, and Marc Dymetman. Should you marginalize over possible tokenizations? In *Proceedings of the Annual Meeting of the Association for Computational Linguistics*, 2023. doi: 10.18653/v1/2023.acl-short.1. URL https: //aclanthology.org/2023.acl-short.1.
- Ryan Cotterell, Anej Svete, Clara Meister, Tianyu Liu, and Li Du. Formal aspects of language modeling, 2024. URL https://arxiv.org/abs/2311.04329.
- Jacob Devlin, Ming-Wei Chang, Kenton Lee, and Kristina Toutanova. BERT: Pre-training of deep bidirectional transformers for language understanding. In *Proceedings of the Conference of the North American Chapter of the Association for Computational Linguistics: Human Language Technologies*, 2019. doi: 10.18653/v1/N19-1423. URL https://aclanthology.org/N19-1423.

- Abhimanyu Dubey, Abhinav Jauhri, Abhinav Pandey, Abhishek Kadian, Ahmad Al-Dahle, Aiesha Letman, Akhil Mathur, Alan Schelten, Amy Yang, Angela Fan, et al. The llama 3 herd of models. *arXiv preprint arXiv:2407.21783*, 2024.
- Philip Gage. A new algorithm for data compression. C Users Journal, 12(2), 1994. ISSN 0898-9788. URL https://web.archive.org/web/20230319172720/https://www.derczynski. com/papers/archive/BPE_Gage.pdf.
- Juan Luis Gastaldi, John Terilla, Luca Malagutti, Brian DuSell, Tim Vieira, and Ryan Cotterell. The foundations of tokenization: Statistical and computational concerns, 2024. URL https: //arxiv.org/abs/2407.11606.
- Saibo Geng, Martin Josifoski, Maxime Peyrard, and Robert West. Grammar-constrained decoding for structured NLP tasks without finetuning. In *Proceedings of the Conference on Empirical Methods in Natural Language Processing*, 2023. URL https://aclanthology.org/2023.emnlp-main. 674.pdf.
- Mario Giulianelli, Luca Malagutti, Juan Luis Gastaldi, Brian DuSell, Tim Vieira, and Ryan Cotterell. On the proper treatment of tokenization in psycholinguistics. In *Proceedings of the Conference on Empirical Methods in Natural Language Processing*, 2024. URL https://aclanthology.org/2024.emnlp-main.1032.
- Jean Goubault. Implementing functional languages with fast equality, sets and maps: An exercise in hash consing. *Journées Francophones des Langages Applicatifs*, 1994.
- John Hale. A probabilistic Earley parser as a psycholinguistic model. In *Meeting of the North American Chapter of the Association for Computational Linguistics*, 2001. URL https:// aclanthology.org/N01-1021.pdf.
- Terry Koo, Frederick Liu, and Luheng He. Automata-based constraints for language model decoding. In *Conference on Language Modeling*, 2024. URL https://openreview.net/forum?id= BDBdblmyzY.
- Taku Kudo. Subword regularization: Improving neural network translation models with multiple subword candidates. In *Proceedings of the Annual Meeting of the Association for Computational Linguistics*, 2018. doi: 10.18653/v1/P18-1007. URL https://aclanthology.org/P18-1007.
- Taku Kudo and John Richardson. SentencePiece: A simple and language independent subword tokenizer and detokenizer for neural text processing. In *Proceedings of the Conference on Empirical Methods in Natural Language Processing: System Demonstrations*, 2018. doi: 10.18653/v1/D18-2012. URL https://aclanthology.org/D18-2012.
- Woosuk Kwon, Zhuohan Li, Siyuan Zhuang, Ying Sheng, Lianmin Zheng, Cody Hao Yu, Joseph E. Gonzalez, Hao Zhang, and Ion Stoica. Efficient memory management for large language model serving with PagedAttention. In *Proceedings of the ACM SIGOPS Symposium on Operating Systems Principles*, 2023. URL https://arxiv.org/abs/2309.06180.
- Roger Levy. Expectation-based syntactic comprehension. Cognition, 106(3), 2008. ISSN 0010-0277. doi: https://doi.org/10.1016/j.cognition.2007.05.006. URL https://www.sciencedirect.com/ science/article/pii/S0010027707001436.
- Scott Lundberg and Marco Tulio Ribeiro. The art of prompt design: Prompt boundaries and token healing. *Medium*, 2023. URL https://towardsdatascience.com/ the-art-of-prompt-design-prompt-boundaries-and-token-healing-3b2448b0be38.

Microsoft. Guidance. https://github.com/microsoft/guidance, 2023.

Tomáš Mikolov, Martin Karafiát, Lukáš Burget, Jan Černocký, and Sanjeev Khudanpur. Recurrent neural network based language model. In *Proceedings of INTERSPEECH*, 2010. doi: 10.21437/Interspeech.2010-343. URL https://www.isca-archive.org/interspeech_2010/ mikolov10_interspeech.html.

- Byung-Doh Oh and William Schuler. Leading whitespaces of language models' subword vocabulary poses a confound for calculating word probabilities, 2024. URL https://arxiv.org/abs/2406. 10851.
- Buu Phan, Marton Havasi, Matthew J. Muckley, and Karen Ullrich. Understanding and mitigating tokenization bias in language models. In *ICML Workshop on Theoretical Foundations of Foundation Models*, 2024. URL https://openreview.net/forum?id=0qfdrBj1y1.
- Tiago Pimentel and Clara Meister. How to compute the probability of a word, 2024. URL https: //arxiv.org/abs/2406.14561.
- Gabriel Poesia, Alex Polozov, Vu Le, Ashish Tiwari, Gustavo Soares, Christopher Meek, and Sumit Gulwani. Synchromesh: Reliable code generation from pre-trained language models. In *The Tenth International Conference on Learning Representations, ICLR 2022, Virtual Event, April 25-29, 2022*. OpenReview.net, 2022. URL https://openreview.net/forum?id=KmtVD97J43e.
- Alec Radford, Jeffrey Wu, Rewon Child, David Luan, Dario Amodei, Ilya Sutskever, et al. Language models are unsupervised multitask learners. *OpenAI blog*, 1(8), 2019. URL https: //d4mucfpksywv.cloudfront.net/better-language-models/language-models.pdf.
- Torsten Scholak, Nathan Schucher, and Dzmitry Bahdanau. PICARD: parsing incrementally for constrained auto-regressive decoding from language models. In *Proceedings of the Conference on Empirical Methods in Natural*, 2021. doi: 10.18653/V1/2021.EMNLP-MAIN.779. URL https://doi.org/10.18653/v1/2021.emnlp-main.779.
- Rico Sennrich, Barry Haddow, and Alexandra Birch. Neural machine translation of rare words with subword units. In *Proceedings of the Annual Meeting of the Association for Computational Linguistics*, 2016. doi: 10.18653/v1/P16-1162. URL https://aclanthology.org/P16-1162.
- Claude E. Shannon. A mathematical theory of communication. *The Bell System Technical Journal*, 27(4), 1948. URL https://doi.org/10.1002/j.1538-7305.1948.tb00917.x.
- Martin Sundermeyer, Hermann Ney, and Ralf Schlüter. From feedforward to recurrent LSTM neural networks for language modeling. *IEEE/ACM Transactions on Audio, Speech, and Language Processing*, 23(3), 2015. URL https://ieeexplore.ieee.org/document/7050391.
- Ashish Vaswani, Noam Shazeer, Niki Parmar, Jakob Uszkoreit, Llion Jones, Aidan N Gomez, Łukasz Kaiser, and Illia Polosukhin. Attention is all you need. *Advances in Neural Information Processing Systems*, 30, 2017. URL https://arxiv.org/abs/1706.03762.
- Brandon T. Willard and Rémi Louf. Efficient guided generation for large language models. *CoRR*, abs/2307.09702, 2023. doi: 10.48550/ARXIV.2307.09702. URL https://doi.org/10.48550/arXiv.2307.09702.
- Thomas Wolf, Lysandre Debut, Victor Sanh, Julien Chaumond, Clement Delangue, Anthony Moi, Pierric Cistac, Tim Rault, Remi Louf, Morgan Funtowicz, Joe Davison, Sam Shleifer, Patrick von Platen, Clara Ma, Yacine Jernite, Julien Plu, Canwen Xu, Teven Le Scao, Sylvain Gugger, Mariama Drame, Quentin Lhoest, and Alexander Rush. State-of-the-art natural language processing. In *Proceedings of the Conference on Empirical Methods in Natural Language Processing: System Demonstrations*, 2020. doi: 10.18653/v1/2020.emnlp-demos.6. URL https: //aclanthology.org/2020.emnlp-demos.6.

A THE SIZE OF THE COVERING

We now set about to bound the worst-case size of the covering function. To do so, we introduce additional definitions that characterize the different growth factors.

We define the κ 's **fertility** as

$$F \stackrel{\text{def}}{=} \max_{\delta \in \Delta^*} \max_{\sigma \in \Sigma^*} |\{\delta' \in \Delta \colon \sigma = \kappa(\delta \cdot \delta')\}| \le |\Delta|$$
(28)

Example 4. The BPE tokenizer has $F_{BPE} = 1$ because it is multiplicative, and its tokens represent distinct substrings. More formally,

$$F_{\text{BPE}} = \max_{\boldsymbol{\delta} \in \Delta^*} \max_{\boldsymbol{\sigma} \in \Sigma^*} \left| \left\{ \delta' \in \Delta : \boldsymbol{\sigma} = \kappa(\boldsymbol{\delta} \cdot \delta') \right\} \right| \qquad [def of fertility]$$
(29)

$$= \max_{\delta \in \Delta^*} \max_{\sigma \in \Sigma^*} |\{\delta' \in \Delta : \sigma = \kappa(\delta) \cdot \kappa(\delta')\}| \qquad [def multiplicativity]$$
(30)

$$= |\{\delta' \in \Delta \colon \boldsymbol{\sigma}' = \kappa(\delta')\}$$
 [def function] (31)

$$= 1 \qquad [distinctness] \qquad (32)$$

Additionally, we define a κ 's **munch** as follows.

$$M \stackrel{\text{def}}{=} \max_{\delta \in \Delta^*} \max_{\delta \in \Delta} |\kappa(\delta \cdot \delta)| - |\kappa(\delta)|$$
(33)

In words, the munch measures the length of the largest number of characters that can be introduced by adding one more token to any given context.

Example 5. The munch of a multiplicative κ , such as BPE, is $\max_{\delta \in \Delta} |\kappa(\delta)|$. Put in words, it is the length of the longest detokenization. The munch for GPT-2 is surprisingly long (128), as they are common in, for example, markdown syntax.

Proposition 3. Let *F* and *M* be the fertility and munch of κ . Then, for all $\sigma \in \Sigma^*$, $|\mathcal{C}(\sigma)| \leq C(|\sigma|)$ (34)

where

$$C(n) \stackrel{\text{def}}{=} \begin{cases} 0 & \text{if } n < 0\\ 1 & \text{if } n = 0\\ F \sum_{j=n-M}^{n-1} C(j) & \text{otherwise} \end{cases}$$
(35)

Proof. The base cases $N \leq 0$ are straightforward. Consider the case of a string of length $N \geq 0$. *Inductive hypothesis*: Suppose for all strings σ' with $|\sigma'| < N$, $|\mathcal{C}(\sigma')| \leq C(|\sigma'|)$.

Let σ be an arbitrary string with length N > 0.

$$|\mathcal{C}(\sigma_1 \cdots \sigma_N)| \tag{36}$$

$$= \left| \left\{ \delta \cdot \delta \in \Delta^{+} : \kappa(\delta) \prec \sigma_{1} \cdots \sigma_{N} \preceq \kappa(\delta \cdot \delta) \right\} \right|$$

$$(37)$$

$$= \left| \bigcup_{j=0}^{N} \underbrace{\left\{ \boldsymbol{\delta} \cdot \boldsymbol{\delta} \in \Delta^{+} : \kappa(\boldsymbol{\delta}) = \sigma_{1} \cdots \sigma_{j}, \sigma_{1} \cdots \sigma_{N} \preceq \kappa(\boldsymbol{\delta} \cdot \boldsymbol{\delta}) \right\}}_{=\emptyset \text{ if } N - (j+1) > M \text{ or } N = j+1} \right|$$
(38)

$$\leq \sum_{\substack{j=N-M\\N}}^{N-1} \left| \underbrace{\{\delta \in \Delta^* \colon \kappa(\delta) = \sigma_1 \cdots \sigma_j\}}_{\subseteq \mathcal{C}(\sigma_1 \cdots \sigma_j)} \right| \cdot \underbrace{|\{\delta \in \Delta \colon \delta \in \Delta^*, \sigma_1 \cdots \sigma_N \preceq \kappa(\delta \cdot \delta)\}|}_{\leq F}$$
(39)

$$\leq F \cdot \sum_{j=N-M}^{N} \underbrace{|\mathcal{C}(\sigma_1 \cdots \sigma_j)|}_{\text{inductive hypothesis}}$$
(40)

$$\leq F \cdot \sum_{N=N}^{N} C(j) \tag{41}$$

$$j=N-M$$

$$= C(N) \tag{42}$$

Thus, the proposition holds true by the principle of induction.

Corollary 2. Let $N = |\sigma|$. Consider the following cases:

- When M = N and F = 1, C(N) = 2^N.
 When M = N and F ≥ 0, C(N) = F(1 + F)^N.
 Otherwise, C(N) = F^NFib(N, M) where Fib(N, M) is Nth Mth-order Fibonacci number.¹⁹

In all cases, $C_M^F(N) < \infty$.

In the proposition below, we show that the covering can easily be exponential in size:

Proposition 4.

$$|\mathcal{C}(\boldsymbol{\sigma})| \in \Omega(2^{|\boldsymbol{\sigma}|}) \tag{43}$$

Proof. We prove the proposition by constructing an example that achieves the lower bound.

- Let $\Sigma = \{a\}, \Delta = \begin{cases} a & aa \\ 1, & 2 \end{cases}$.
- Let κ be multiplicative, and define $\kappa \binom{a}{1} \stackrel{\text{def}}{=} a, \kappa \binom{aa}{2} \stackrel{\text{def}}{=} aa.$
- Let σ be an arbitrary string from Σ^* . Let $N = |\sigma|$.

Then, $|\mathcal{E}(\sigma)|$ equals the number of nonnegative integer solutions (n, m) to 1m + 2n = N. This is because we can build the a^N using a sequence of $\frac{1}{2}$ or $\frac{aa}{2}$, but each $\frac{1}{4}$ accounts for 1 a and each $\frac{aa}{2}$ accounts for 2. So if n is the number of token 1 and m is the number of token 2, we must have that 1 m + 2 n = N. The number of solutions grows like $\Omega(2^N)$. Lastly, because $\mathcal{C}(\boldsymbol{\sigma}) \supseteq \mathcal{E}(\boldsymbol{\sigma})$, we have that $|\mathcal{C}(\boldsymbol{\sigma})| \in \Omega(2^{|\boldsymbol{\sigma}|})$. Thus, the proposition holds.

 $^{^{19}}M^{\text{th}}$ -order Fibonacci numbers are a variation of the well-known Fibonacci (i.e., M = 2) that sums the previous M numbers in the sequence instead of the previous two.

B BUNDLED BEAM SUMMING IMPLEMENTATION

Upon implementing this scheme, we observed that it is possible to efficiently reason about all the next tokens that extend a given token sequence in the cover in bulk. The key idea is to group the token sequences that fall into the same bucket in prune_top_K_buckets into a Bundle (see below) that represents them compactly. In particular, we can use a probability trie to efficiently filter out the next tokens that disagree with the next character. This improves the per-iteration cost of that filter as it can via the data structure, as it does the organizational work ahead of time in bulk. We can regard the probability trie as a local language model that generates the next token character-by-character according to the probability assigned to it by $\vec{p}_{\Delta}(\cdot | \delta)$. Each bundle can be unbundled (see method unbundle) into the respective tuples that the enumerate_cover algorithm maintains. The algorithms are otherwise equivalent.

```
73 def beam(\sigma_1 \cdots \sigma_N):
     if N = 0: return [Bundle(1, \varepsilon, \varepsilon, build_trie(\varepsilon))]
74
    candidates = []
75
     for bundle in beam(\sigma_1 \cdots \sigma_{N-1}):
76
       filtered_bundle = bundle.filter(\sigma_N)
77
       if filtered_bundle is not None:
78
          candidates.append(filtered_bundle)
79
       for extended_bundle in bundle.extend():
80
          candidates.append(extended_bundle.filter(\sigma_N))
81
     # Keep top-K bundles according to their prefix probability
82
     return top<sub>K</sub>(candidates, key=lambda bundle: -bundle.p)
83
```

Each bundle is an instance of the following class with four member variables: the prefix probability p, token string δ , character string σ , and a reference to a local probability trie *trie*. The trie provides the character-level probabilities of the distribution over possible next tokens: $p_{\Delta}(\cdot | \delta)$. The trie is also augmented with a special symbol EOT to denote the end of this next token.²⁰

```
<sup>84</sup> class Bundle(p, \delta, \sigma, trie):
85
        def filter(\sigma'):
86
             if trie.p(\sigma' \mid \sigma) = 0: return # no tokens give prefix \sigma \cdot \sigma' prob
87
             return Bundle(p \cdot trie(\sigma' \mid \sigma), \delta, \sigma \cdot \sigma', trie)
88
89
        def extend():
90
             Z = trie.p(EOT \mid \boldsymbol{\sigma})
91
             if Z>0: # emit tokens that decode to \sigma
92
                 \begin{array}{l} \text{for } (\delta',p') \text{ in } trie.tokens[\boldsymbol{\sigma}]:\\ \text{ yield } \text{Bundle}(\frac{p}{Z}\cdot p', \ \boldsymbol{\delta}\cdot\delta', \ \varepsilon, \ \text{build\_trie}(\boldsymbol{\delta}\cdot\delta')) \end{array}
93
94
```

The code below builds the probability trie from the possible next tokens. It figures out the character strings associated with those next tokens and puts them into the trie with the respective probabilities.²¹

The probability trie has the following functionality:

• trie.tokens $[\sigma']$ stores the set of tokens that decode to σ' along with their respective.

²⁰This is completely analogous to how EOS marks the end of a string.

²¹Note that EOS is handled as an indivisible symbol in the probability trie, whereas other strings are predicted one character at a time in the trie.

• trie. $p(\sigma' \mid \sigma)$ returns the probability of the character σ' given σ , it is equal to

$$trie.p(\sigma' \mid \boldsymbol{\sigma}) \propto \sum_{\delta' \in \Delta} p_{\Delta}(\delta' \mid \boldsymbol{\delta}) \begin{cases} \mathbbm{1}\{\kappa(\boldsymbol{\delta} \cdot \delta') = \boldsymbol{\sigma}\} & \text{if } \sigma' = \text{EOT} \\ \mathbbm{1}\{\kappa(\boldsymbol{\delta} \cdot \delta') \succeq \boldsymbol{\sigma} \cdot \sigma'\} & \text{otherwise} \end{cases}$$
(44)

We note that the trie implicitly depends on the token string δ used in its creation.

To aid in understanding (and testing) how the bundled algorithm relates to the original algorithm, we give the following methods.

```
102 class Bundle(p, \delta, \sigma, trie):
103
       def unbundle():
104
105
           agenda = [\sigma]
           while agenda:
106
              \sigma' = agenda.pop()
107
              Z = trie.p(\text{EOT} | \boldsymbol{\sigma})
108
              if Z > 0:
109
                  for (\delta', p') \in trie.tokens[\sigma']:
110
                     yield (p \cdot p', \kappa(\boldsymbol{\delta} \cdot \boldsymbol{\delta}'), \boldsymbol{\delta} \cdot \boldsymbol{\delta}')
111
              for \sigma'' in trie.p(\cdot \mid \sigma'):
112
                  if \sigma'' \neq EOT:
113
                     agenda.append(\sigma' \cdot \sigma'')
114
115 def unbundle_beam(beam):
       return [item for bundle in beam for item in bundle.unbundle()]
116
```

We note that unbundle_beam(σ)) gives precisely the same set of elements as the unbundled algorithm (i.e., enumerate_cover(σ)) run on the same string σ and the bucket-based pruning scheme with parameter K (up to reordering).

To compute the next-character probability, we use the following algorithm:

```
117 def next_character_probability(\screwtar):
      \overline{p} = \{ \sigma' : 0 \text{ for } \sigma' \in \Sigma \cup \{ \text{EOS} \} \}
118
119
        for bundle in beam(\sigma):
           for \sigma' \in \Sigma:
120
               \overline{p}(\sigma') += bundle.p · bundle.trie.p(\sigma' | bundle.\sigma)
121
           for ext_bundle in bundle.extend():
122
               for \sigma' \in \Sigma:
123
                  \overline{p}(\sigma') = \text{ext\_bundle.} p \cdot \text{ext\_bundle.} trie.p(\sigma' | \text{ext\_bundle.} \sigma)
124
        Z = sum(\overline{p}.values())
125
        return {\sigma': \overline{p}(\sigma')/Z for \sigma' \in \Sigma}
126
```