Subword Tokenization Meets Formal Language Theory

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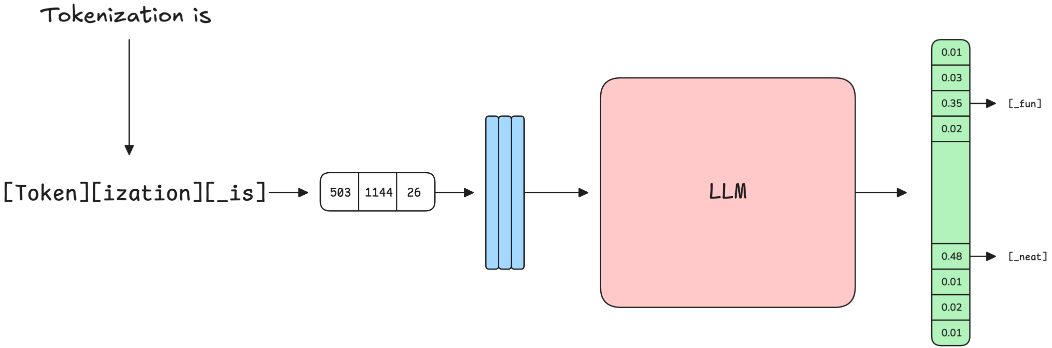
Neural Language Modeling



- There is a mismatch between what the user inputs and what the model processes!

Subword Tokenization

- People read and write *text*
- Language models operate on *tokens*
- Tokens are produced by a subword tokenizer
  - Minor surface variations: `[un][_comfort][_able]` vs `[un][comfort][able_]`
- Many competing goals:
  - Alignment with text/linguistic features
  - Coverage of all possible input text
  - Sequence compression
  - Parameter counts
- This is basically the "steering wheel" of LLMs

Tokenizers Are Pretty Brittle

- This is ok in academic datasets, where data is fairly clean
- Not so true in real life, where users make tons of mistakes

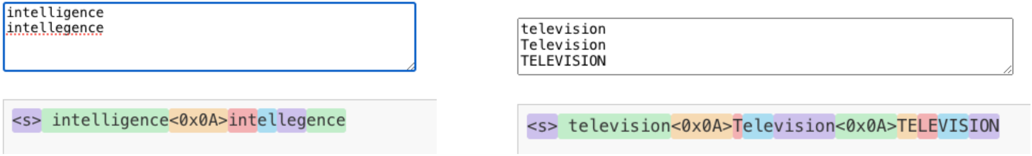


Figure: https://huggingface.co/meta-llama

Tokenizers Are Pretty Brittle

Tokenization is at the heart of much weirdness of LLMs. Do not brush it off.

- Why can't LLM spell words? **Tokenization**.
- Why can't LLM do super simple string processing tasks like reversing a string? **Tokenization**.
- Why is LLM worse at non-English languages (e.g. Japanese)? **Tokenization**.
- Why is LLM bad at simple arithmetic? **Tokenization**.
- Why did GPT-2 have more than necessary trouble coding in Python? **Tokenization**.
- Why did my LLM abruptly halt when it sees the string "<|endoftext|>"? **Tokenization**.
- What is this weird warning I get about a "trailing whitespace"? **Tokenization**.
- Why the LLM break if I ask it about "SolidGoldMagikarp"? **Tokenization**.
- Why should I prefer to use YAML over JSON with LLMs? **Tokenization**.
- Why is LLM not actually end-to-end language modeling? **Tokenization**.
- What is the real root of suffering? **Tokenization**.

Figure: https://twitter.com/karpathy/status/1759996551378940395

Origins of Tokenization

- Word-level
- Character-level
- Morpheme-level
- Needed something with total coverage, but finite vocabulary
  - Subwords are an intermediate granularity between words and characters
  - Subword vocabularies contain all characters, so any input can be represented

- Weird trivia: only 2 years between BPE and Transformers

MaxMatch (WordPiece) Encoding

- Given a subword vocabulary, greedily find the longest matching token
- The subword vocabulary construction is not really relevant

Step							
0.	b	a	n	a	n	a	s
1.	b	a	n	a	n	a	s
2.	b	a	n	a	n	a	s
3.	b	a	n	a	n	a	s

Figure: MaxMatch encoding of bananas with $\Gamma = \{\texttt{a}, \texttt{b}, \texttt{n}, \texttt{s}, \texttt{ba}, \texttt{na}, \texttt{ban}, \texttt{bana}\}$.

Byte-Pair Encoding

- Two stages: training and inference

Algorithm 2: BPE Training
Input: Corpus C over alphabet Σ, Target merge size k
Output: Vocabulary Γ, Merge list μ

$\Gamma = \Sigma,\ \ \mu = \langle\,\rangle$ ▷ *The initial vocabulary and merge list, respectively.*
for $i \in 1 \ldots k$ **do**
  $(a, b) = \arg\max_{(a,b)\in\Gamma^2} \textsc{Count}(C, a{\sqcup}b)$ ▷ *The most frequent cooccuring pair in C.*
  $\textsc{Append}(\mu, (a, b))$ ▷ *Add merge information to μ (which is ordered by priority).*
  $\textsc{Append}(\Gamma, ab)$ ▷ *Update the token vocabulary.*
  $\textsc{Apply}(C, (a, b))$ ▷ *Merge all instances of $a{\sqcup}b$ to ab in C.*
return (Γ, μ)

Byte-Pair Encoding

Algorithm 3: BPE Tokenization

Input: BPE Tokenizer $\mathcal{B} = (\Gamma, \mu)$, String $w \in \Sigma^+$

Output: Tokenized sequence $t \in \Gamma^+$

$t \leftarrow w$ ▷ *The initial character sequence, interpreted as tokens.*

$\psi \leftarrow \langle (t_i, t_{i+1}) \mid (t_i, t_{i+1}) \in \mu \rangle$ ▷ *The set of all current possible merges.*

while $\psi \neq \emptyset$ **do**

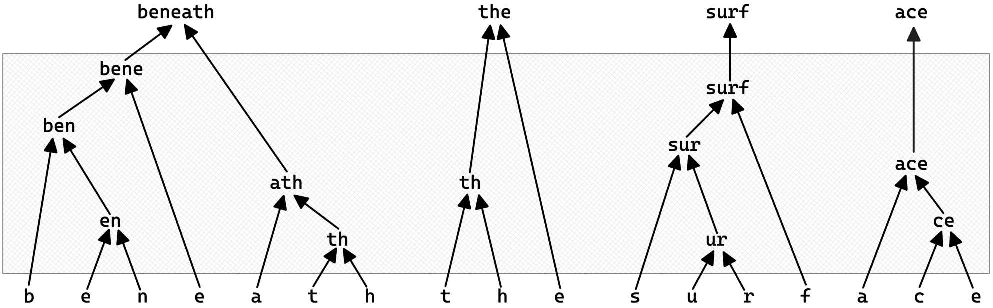
  $(a, b) \leftarrow \arg\max_{\mu} \psi$ ▷ *The highest priority merge according to the ordering in μ.*

  $t \leftarrow \textsc{Apply}(t, (a, b))$ ▷ *Apply the merge and update t.*

  $\psi \leftarrow \langle (t_i, t_{i+1}) \mid (t_i, t_{i+1}) \in \mu \rangle$ ▷ *The new list of possible merges.*

return t

Byte-Pair Encoding

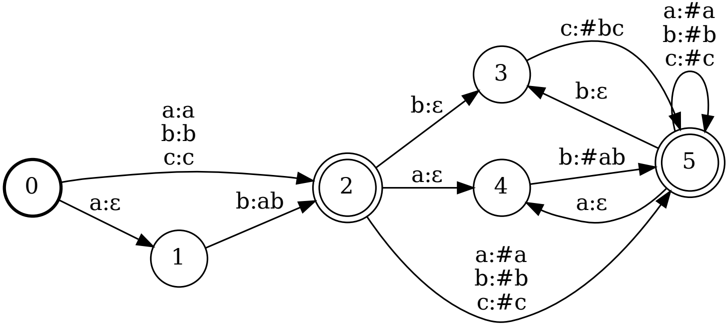


Usage in Modern NLP

- All major GPT-style models use BPE
  - SentencePiece
  - TikToken
  - HuggingFace
- BERT uses MaxMatch
- Vocabulary sizes over 200k
- Multi-lingual
- Pre-tokenization

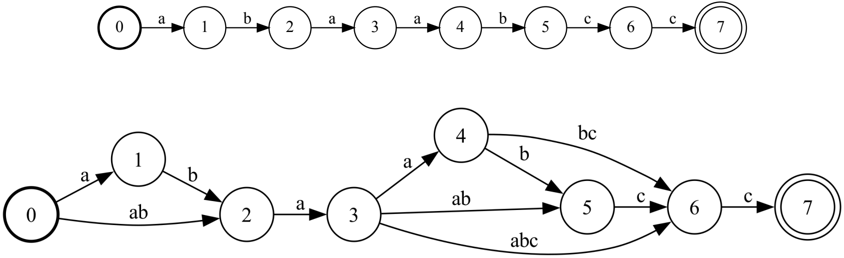
The Subword Lexicon Transducer

- Convert sequences of characters (text) into sequences of subwords



The Subword Lattice

- Encode the input as an automaton
- Compose with the subword transducer
- Project to output labels
- $\textsc{Min}(\textsc{Proj}(\mathcal{A} \circ \mathcal{T}))$



An Aside: Sampling Tokenizations

- So far, we have considered tokenizers to be unweighted/bijective
  - What if they were weighted (e.g., stochastic tokenizers)?
- During training:
  - Acts as data augmentation
  - Adds robustness to the model
  - Makes it more likely all tokens are trained well
- During inference:
  - Acts as self-ensemble
  - Can be used for importance sampling (marginalization)

An Aside: Sampling Tokenizations

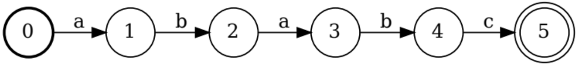
Inputs: Word $w \in \Sigma^{+}$, (Ordered) Merges μ
Output: Tokenized sequence $t \in \mathcal{V}^{+}$

$\varphi \leftarrow \langle (w_i, w_{i+1}) | (w_i, w_{i+1}) \in \mu \ \wedge \text{RAND}() > p \rangle$
for $\varphi \neq \emptyset$ **do**
  $(x, y) \leftarrow \arg\max_{\mu} \varphi$ ▷ Ordered by μ
  $w \leftarrow \text{REPLACE}((x, y) \rightarrow xy, w)$
  $\varphi \leftarrow \langle (w_i, w_{i+1}) | \ (w_i, w_{i+1}) \in \mu \ \wedge \text{RAND}() > p \rangle$
return w

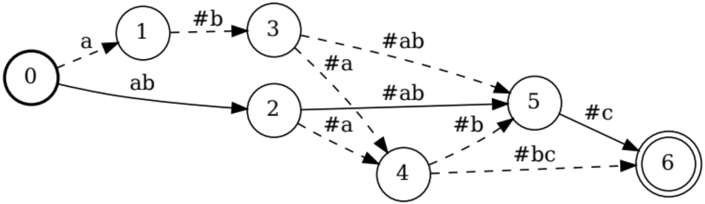
Algorithm 1: BPE Inference (with dropout)

BPE-Dropout $p = 0.1$	
to ken ization	97.77%
to ke n ization	1.89%
to k en ization	0.25%
to ken iz ation	0.04%
t oken ization	0.03%
to k en iz ation	0.01%
to ke n iz ation	0.01%
to ken i z ation	$<$ 0.01%

An Aside: Sampling Tokenizations



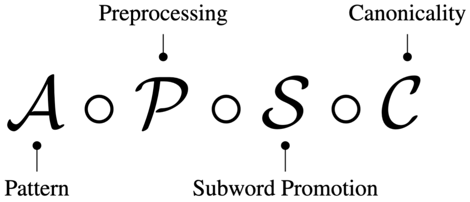
(a) An automaton $\mathcal{A}$ representing ababc.



(c) A lattice, $\mathcal{A} \circ \mathcal{T}$, of all possible tokenizations of ababc.

Constrained Generation

- Language models can output *any text*
- Sometimes we want it to output only a specified format
  - Strings that match a regex
  - JSON
  - Syntactically correct code
- What if we could attach a regex to the end of a model?
  - We can do it with a modular FST pipeline



Locally Masked Constrained Generation

- Standard autoregressive distribution is:
  - $p(t_i \mid c_l) = \text{SOFTMAX}(l)_i$
  - $p(t) = p(t_1 \mid \text{<s>}) \prod_{i=1}^{|t|-1} p(t_{i+1} \mid \text{<s>} t_1 t_2 \ldots t_i)$
- Define a constraint mask:

$$m_i = \begin{cases} 1 & v_i \in \Gamma \text{ can satisfy the constraint} \\ -\infty & \text{otherwise.} \end{cases}$$

  - Constraint satisfication comes from the tokenization lattice
  - "Is there a path from the current state to a final state after reading this token?"
- Replace with a *masked* distribution:
  - $p'(t_i \mid c_l) = \text{SOFTMAX}(l \odot m)_i$
  - $p'(t) = p'(t_1 \mid \text{<s>}) \prod_{i=1}^{|t|-1} p'(t_{i+1} \mid \text{<s>} t_1 t_2 \ldots t_i)$

Three Problems With Constrained Generation

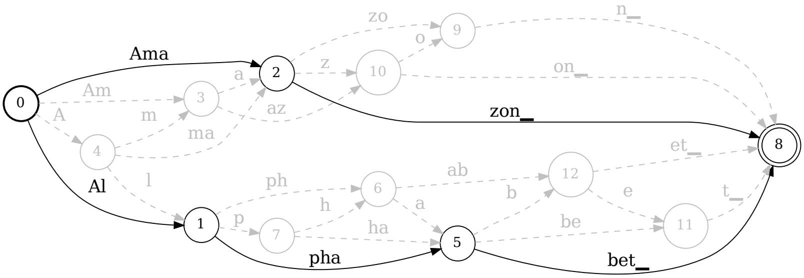
- Mismatch between regex (character level) and LLMs (subword level)
    - Solved by the subword lexicon transducer
    - Promotes character patterns to subword patterns
- Warped distribution
    - Missing a normalization factor for $p(\mathcal{A})$
    - Solved by importance sampling
- Allows *any* matching tokenization
    - Throws away canonical tokenization inductive bias

Importance Sampling and Marginalization

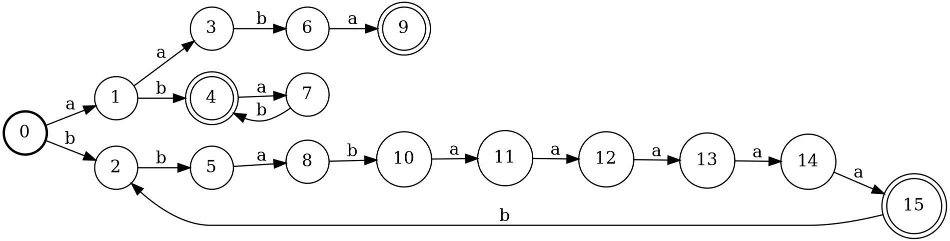
- Constrained generation needs a normalization factor:
  - $p'(t) = p(t)/z$
  - $z = \sum_{t \in \mathcal{A}} p(t)$
- Difficult to compute (exponentially many tokenizations)
- Difficult to sample with rejection sampling
- Importance Sampling:
  - Pick a proxy distribution q with the desired support
  - q should be easy to sample from
  - Compute $\mathbb{E}_{t \sim q}\left[\frac{p(t)}{q(t)}\right] \approx \frac{1}{N} \sum_t \frac{p(t)}{q(t)}$
- p' can serve as our proxy distribution

Tokenization-Aware Constrained Generation

- Constrained generation allows *any* matching tokenization
- Models are trained on *canonical* tokenizations
- During generation, models don't know they are being constrained
  - Can accidentally generate poor tokenizations
  - `[_r][a][ce][car]` vs `[_race][car]`
  - Bad downstream performance



An Example With MaxMatch



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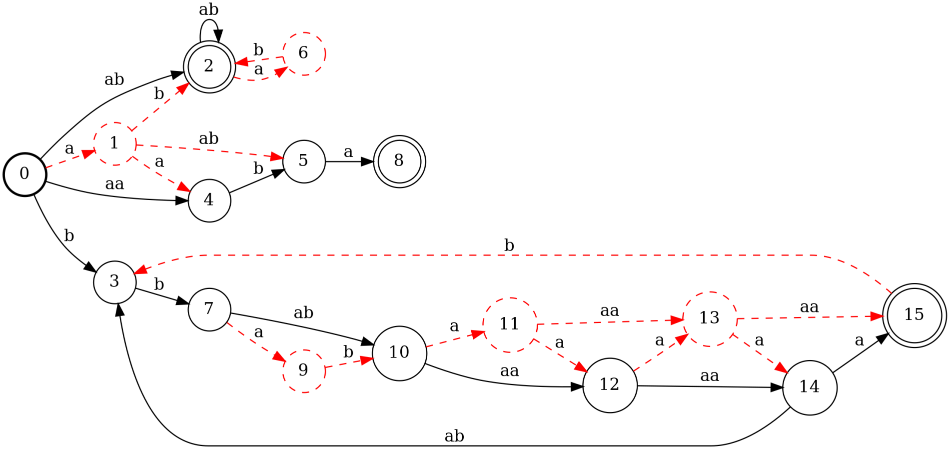
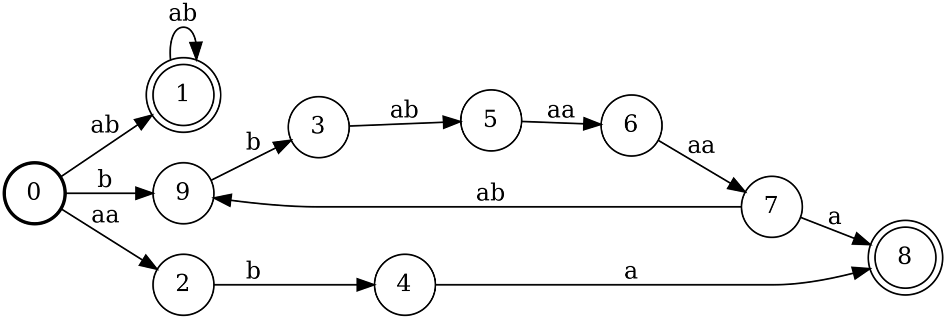
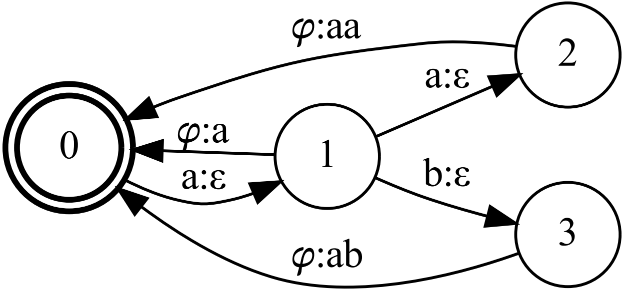


An Example With MaxMatch



The MaxMatch Lexicon Transducer



Is Byte-Pair Encoding Regular?

- Doesn’t process in left-to-right order ✕
  - Merges can happen in random places in the string
- Requires a notion of "priority" ✕
  - Some merges take precedence over others
- Recent result showed you only need a constant-lookahead window to tokenize in a streaming manner ✓
  - Berglund & van der Merwe, 2023

An Algorithm for BPE Promotion

- Berglund, et al. 2024 give an algorithm for BPE promotion
- For each merge, iteratively check triplets of states to see if they match, then modify the states/arcs
- Runs in polynomial time and space

BPE As Finite-State Transduction

Algorithm 5: Iterative BPE

Input: Word $w \in \Sigma^+$, BPE Tokenizer $\mathcal{B} = (\Gamma, \mu)$

Output: Tokenized sequence $t \in \Gamma^+$

```
for (a, b) ∈ μ do
    w ← APPLY((a, b), w)
return w
```

- We construct transducers that act as merges
- Everything is done via finite-state automata composition

BPE Merge Gadgets

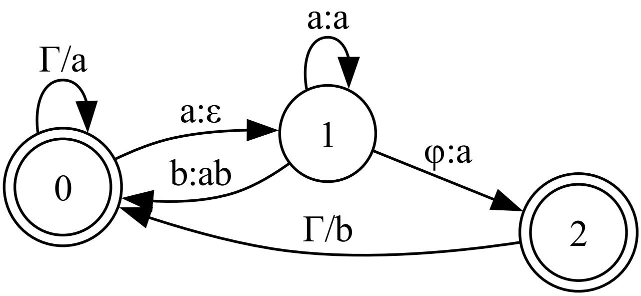
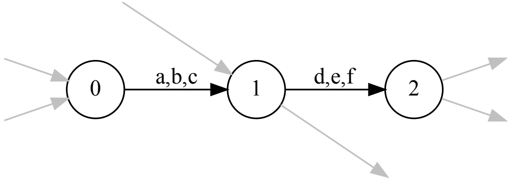
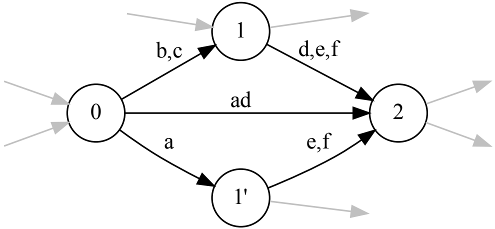


Figure: Merge gadget for the merge $(a, b) \to ab$.

BPE Merge Gadgets





BPE Transduction

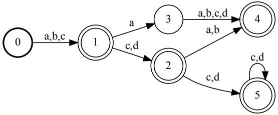


Figure: An automaton $\mathcal{A}$.

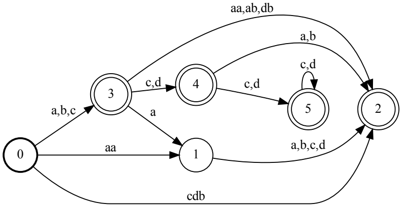


Figure: $\textsc{Min}(\textsc{Proj}(\mathcal{A} \circ \mathcal{T}))$

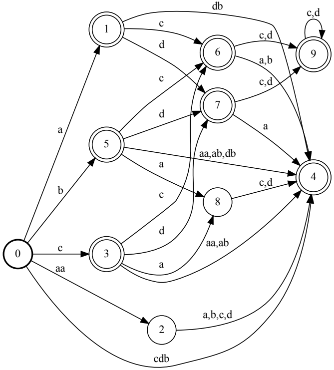
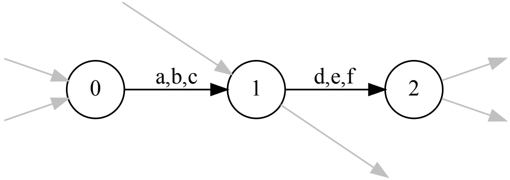


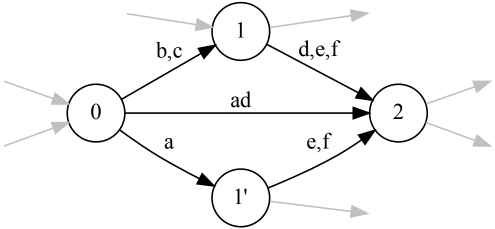
Figure: $\textsc{Min}(\textsc{Proj}(\mathcal{A} \circ G_{(a,a)} \circ G_{(a,b)} \circ G_{(d,b)} \circ G_{(c,db)}))$

BPE Transduction Complexity

- Naive analysis: $O(3^{|\mu|}|\mathcal{A}||\mu|)$
  - Prohibitively expensive even for small vocabularies
  - Gemma3 has 260k tokens in the vocabulary
- We prove the complexity is actually polynomial

BPE Transduction





A Very Brief Proof Sketch

- Merges act on triplets of states
  - Merge $(a, b) \in \mu$
  - $x, y, z \in \mathcal{A}$, s.t. $\delta(x, a) = y$ and $\delta(y, b) = z$
- Merges "split" state y into y', y''.
  - We call these *derived* triplets from the triplet x, Y, z (y, y', y'', etc $\in Y$)
- An issue is if more than one state in a derived subset can be split during a merge
  - A merge $(c, d) \in \mu$ that matches (x, y', z) and $(x, y'', z) \in Y$
  - Or (x', y, z) and (x'', y, z)
  - If so, we get exponential blowup
- We prove this cannot happen
  - Each derived triplet can only add one new *distinct* state per merge
- This bounds the runtime size at $Poly(|A|, |\mu|)$
  - And therefore also the automaton size

An Alternative Promotion Procedure

- Full composition is very slow
  - $\textsc{Min}(\textsc{Proj}(\mathcal{A} \circ G_{\mu_1} \circ G_{\mu_2} \circ \cdots \circ G_{\mu_k}))$ is inherently serial
  - We are usually minimizing between each composition
  - In practice, most merges are unnecessary
- What if we had a "canonical filter"?
  - $\mathcal{A}_{\text{BPE}} = \textsc{Min}(\textsc{Proj}(\Sigma^* \circ G_{\mu_1} \circ G_{\mu_2} \circ \cdots \circ G_{\mu_k}))$
  - Accepts *all* canonical BPE sequences
  - Slow to construct, but can be reused
  - Combine with $\textsc{Min}(\textsc{Proj}(\mathcal{A} \circ \mathcal{T}))$, which is fast to construct

$$\textsc{Min}(\textsc{Proj}(\mathcal{A} \circ G_{\mu_1} \circ G_{\mu_2} \circ \cdots \circ G_{\mu_k})) \equiv \textsc{Min}(\textsc{Proj}(\mathcal{A} \circ \mathcal{T})) \circ \mathcal{A}_{\text{BPE}}$$

An Alternative Promotion Procedure (Speedup)

Vocabulary Size	Full Composition (Equation 4)	Preconstructed $\mathcal{A}_{\text{BPE}}$ (Equation 5)	Speedup
4k	16.09s	0.19s	85x
8k	43.39s	0.24s	181x
16k	103.37s	0.38s	272x
32k	228.57s	0.45s	514x

Figure: Full composition vs preconstructed BPE filter composition on an edit-distance automaton with 2k states.

A Speedup From Canonicalization

```
{
    "alias": "[a-z]{1,5}",
    "description": "[A-Z][a-z][0-9][\w\s,.!?]{1,3}",
    "type": "(Bug|Dark|Dragon|Electric|Fairy|Fighting|Fire|Flying|Ghost|Grass|Ground|Ice|Normal|Poison|Psychic|Rock|
        Steel|Stellar|Water)",
    "height_m": [0-9]{1,2}\.[0-9]{1},
    "weight_kg": [0-9]{1,3}\.[0-9]{1},
    "evolution_stage": "(Basic|Stage 1|Stage 2)",
    "legendary": "(true|false)",
    "abilities": [
        "(Overgrow|Blaze|Torrent|Shield Dust|Intimidate|Levitate|Pressure|Static)"(, "(Overgrow|Blaze|Torrent|Shield
            Dust|Intimidate|Levitate|Pressure|Static)"){0,6}
    ]
}
```

Model	Canonical	Skip Rate	Rel. Time
LLAMA2-7B	no	24.5%	-
	yes	77.9%	-15.7%
LLAMA2-13B	no	26.5%	-
	yes	78.9%	-21.0%

What Comes with Proving Things Are Regular?

- Pros:
  - Tokenizer equivalence testing
  - Tokenizer minimization
  - Hook into all transducer machinery

- Cons:
  - Some linguistic features are not regular
    - Reduplication
    - 드르렁드르렁
  - These can't be perfectly captured by existing tokenizers

Pretokenizer Issues

```
"normalizer": {
  "type": "Sequence",
  "normalizers": [
    {
      "type": "Prepend",
      "prepend": "__"
    },
    {
      "type": "Replace",
      "pattern": {
        "String": " "
      },
      "content": "__"
    }
  ]
},
"pre_tokenizer": null,
```

```
pat_str = "|".join(
    [
        r"""[^\r\n\p{L}\p{N}]?[\p{Lu}\p{Lt}\p{Lm}\p{Lo}\p{M}]*[\p{Ll}
        r"""[^\r\n\p{L}\p{N}]?[\p{Lu}\p{Lt}\p{Lm}\p{Lo}\p{M}]+[\p{Ll}
        r"""\p{N}{1,3}""",
        r""" ?[^\s\p{L}\p{N}]+[\r\n/]*""",
        r"""\s*[\r\n]+""",
        r"""\s+(?!\S)""",
        r"""\s+""",
    ]
)
```

Unreachable Tokens

```
token id  decoded to token        re-encoded     strings for re-encoded
  3413    " I'"                [357, 6]        [' I', "'"]
  3914    '\n//'               [198, 393]      ['\n', '//']
 24091    '\r\n//'             [370, 393]      ['\r\n', '//']
 48235    '\n///'              [198, 5991]     ['\n', '///']
 63100    '\n\n//'             [279, 393]      ['\n\n', '//']
 65447    '\n//\n//'           [198, 5754]     ['\n', '//\n//']
125141    '\r\n\r\n//'             [1414, 393]     ['\r\n\r\n', '//']
175653    '\n\n\n//'           [2499, 393]     ['\n\n\n', '//']
```

Figure: https://tokencontributions.substack.com/p/unreachable-tokens-in-gpt-4o

Future Work

- Runtime/space-complexity analysis for CFG
- Tokenization algorithms with better properties
  - Runtime
  - Space-complexity for composition
  - Output compression
- Interaction with non-regular pretokenization
  - This precludes end-to-end finite-state pipelines
- Constrained Generation with Diffusion Language Models
  - These don’t generate text from left-to-right, so automata might not be a good choice

Links

Merge with us

The Token ##ization Discord

Figure: Slides + Reading List

Figure: My Personal Site