Theoretical Analysis of Byte-Pair Encoding

László Kozma and Johannes Voderholzer

Institut für Informatik, Freie Universität Berlin, Germany

Abstract

Byte-Pair Encoding (BPE) is a widely used method for subword tokenization, with origins in grammar-based text compression. It is employed in a variety of language processing tasks such as machine translation or large language model (LLM) pretraining, to create a token dictionary of a prescribed size. Most evaluations of BPE to date are empirical, and the reasons for its good practical performance are not well understood.

In this paper we focus on the optimization problem underlying BPE: finding a *pair encoding* that achieves optimal compression utility. We show that this problem is APX-complete, indicating that it is unlikely to admit a polynomial-time approximation scheme. This answers, in a stronger form, a question recently raised by Zouhar et al. [ZMG+23].

On the positive side, we show that BPE approximates the compression utility of the optimal pair encoding to a worst-case factor between 0.333 and 0.625. Our results aim to explain the ongoing success of BPE and are, to our knowledge, the first rigorous guarantees on its compression utility that hold for all inputs.

1. Introduction

A common step in the modern NLP application pipeline is tokenization: given an input text, the task is to partition it into *tokens*, i.e., frequently occurring consecutive groups of symbols. The main goal is to identify semantically meaningful units (words or subwords) in order to facilitate higher level tasks (e.g., translation or text generation) [MAS+21, AFT+23]. As this goal is difficult to directly optimize for, tokenization is usually solved heuristically, or formulated as a different but closely related task: *data compression*. Indeed, the dictionary-encoding of tokens reduces text length; the amount of compression is easy to measure, and was found to be a good predictor of the quality of tokenization for downstream tasks, e.g., for translation accuracy [Gal19]. It is thus natural to study tokenization with the proxy optimization goal of *compression utility*.

Byte-Pair Encoding (BPE), introduced by Gage in 1994 [Gag94], is a commonly used heuristic for tokenization. It proceeds by repeatedly identifying the *most frequently occurring* pair of symbols and replacing all occurrences of this pair with a new symbol, thereby shortening the text. The new symbols, together with the pairs they replace, are stored in a lookup-table, which allows the reconstruction of the original text. In typical applications, the number of new symbols (and thus the size of the lookup-table) is fixed upfront, and the goal is to achieve the best compression within this budget. The symbols of the resulting (shortened) text correspond to the tokens of the input. Figure 1 shows an example of the encoding of a text by BPE.

$$\texttt{aabaaaba} \rightarrow \texttt{XbXaba} \rightarrow \texttt{YXaba} \rightarrow \texttt{Zaba}$$
$$\texttt{aabaaaba} \rightarrow \texttt{aXaaXa} \rightarrow \texttt{YaYa} \rightarrow \texttt{ZZ}$$

Figure 1: Input $s = \texttt{aabaaaba}$ encoded by BPE merge sequence ($\texttt{aa} \rightarrow \texttt{X}$, $\texttt{Xb} \rightarrow \texttt{Y}$, $\texttt{YX} \rightarrow \texttt{Z}$) (above). An optimal encoding by the merge sequence ($\texttt{ab} \rightarrow \texttt{X}$, $\texttt{aX} \rightarrow \texttt{Y}$, $\texttt{Ya} \rightarrow \texttt{Z}$) (below).

BPE has become a de-facto standard in NLP applications, widely employed in machine translation [Sen15, XZG+21, DGMH+19, Gal19, GVBS23] and in the preprocessing stage of training large language models [BMR+20, LLSZ21, TLI+23, RWC+19, LSFA+23, WGC+23][1]. Besides its effectiveness, the popularity of BPE is likely due to its simplicity and computational efficiency, when compared with more sophisticated or linguistically motivated methods (e.g., see [BD20, SRZ+24]). A careful implementation of BPE has a total runtime that is linear in the input length, for an arbitrary number of replacement rounds. In addition, a BPE-encoded representation can support efficient random access and pattern-matching on the original text, which is important in some applications [SKF+99].

Given the popularity and good empirical performance of BPE, there is a surprising lack of rigorous guarantees for the quality of its output. In this paper we study the problem of compressing a text (a string s over some alphabet Σ) by successive encoding of pairs (strings of length two). Adopting the framework of approximation algorithms [WS11] we study how well BPE, as a natural greedy heuristic, approximates this problem. Our optimization goal is to maximize *compression utility*, i.e., the reduction in text length, within k pair-encoding rounds, where s and k are given as the input (we precisely define this problem – *optimal pair encoding* – later in this section).

The problem formulation we use closely resembles the one recently introduced by Zouhar et al. [ZMG+23] for the same task. This abstract setting presents a challenging algorithm design problem of independent interest and allows a clean theoretical analysis of BPE. Note however, that we necessarily ignore some practical aspects and optimizations of BPE-variants (e.g., special treatment of whitespace and punctuation or language-specific rules [RWC+19, AFT+23]).

An algorithm $\mathcal{A}$ for optimal pair encoding has *approximation ratio* $\alpha \leq 1$, if the compression utility of $\mathcal{A}$ is at least α times the optimum for all inputs (s, k). The greedy step of BPE is locally optimal, and thus, for $k = 1$ it achieves optimal compression. For $k > 1$, however, simple examples show that BPE may not achieve optimal compression (see Figure 1).

As our main complexity-result, we show that optimal pair encoding is *APX-complete*. This means (informally) that no polynomial-time algorithm can approximate it to a factor arbitrarily close to 1, unless P=NP. On the positive side, we show that BPE achieves an approximation ratio α, with $0.333 < \alpha \leq 0.625$. We note that previously no constant-approximation guarantee was known for BPE or other algorithms. The question of whether optimal pair encoding is NP-complete was raised recently by Zouhar et al. [ZMG+23]; our result settles this question in a stronger form.

Before precisely stating our results, we review some further related work and give a formal definition of the problem and the algorithms that we study.

Related work. BPE has its origins in text compression, in particular, the class of *grammar-based* compression methods or *macro schemes*, e.g., see [SS82, KY00, CLL+05, Loh12] for surveys. (The encoding obtained by BPE can be seen as a restricted kind of context-free grammar or string straight-line program.) A compression method closely related to BPE is Re-Pair [LM00]. Re-Pair differs from BPE in that its number of replacement rounds k is not fixed; instead, it performs

---

[1]See also https://github.com/google/sentencepiece and
https://github.com/openai/tiktoken.

replacements as long as they achieve a saving (i.e., as long as some pair appears in at least two disjoint copies). Re-Pair is widely used, e.g., in bioinformatics, and several variants and practical improvements of it have been proposed [KVOB24, GJ17, GIM+19, FTN+19].

The central question of grammar-based compression is to find a minimal grammar that generates a given text. This task is known to be NP-hard, as well as hard to approximate [SS82, CLL+05] (by some constant factor). The best known approximation ratio for the grammar-based compression of an input of length n is $O(\log n)$ [Ryt03, Jeż14]. The approximation ratio of Re-Pair is $O((n/\log n)^{2/3})$ and $\Omega(\log n/\log\log n)$ [CLL+05, BHH+20]. Note that these results relate the size of the obtained grammar to that of the minimal grammar, where the latter can be of a more general kind than what Re-Pair (or BPE) can produce.

Navarro and Russo [NR08] show a different kind of theoretical guarantee for Re-Pair, namely that its cost approximates the order-t entropy of the input, for a certain range of t and alphabet size. Furuya et al. [FTN+19] bound the gap between runs of Re-Pair with different tie-breaking. These results use a different cost measure (compressed length versus reduction, which will be discussed in deail later) and are not directly comparable to ours; nevertheless, a construction from [FTN+19] is also useful in our context, as shown below.

Closest to our work is the recent paper of Zouhar et al. [ZMG+23], which initiated the formal study of BPE and optimal pair encoding that we also largely follow in this paper, apart from small notational differences and a more general problem formulation. Using the theory of submodular functions, they relate the approximation ratio of BPE to a certain parameter (total backward curvature) that depends on the unknown optimum. Zouhar et al. also observe an empirical bound on this quantity, however, without giving any worst-case guarantees.

Problem definition. We consider strings (sequences of symbols) over some alphabet Σ and denote concatenation of strings a and b by $a \cdot b$, omitting the $\cdot$ when clear from context. We denote the *length* of a string s by $|s|$, the i-th symbol of s by $s[i]$, and the substring $s[i] \cdot s[i+1] \cdots s[j]$ by $s[i:j]$. We thus have $s = s[1:|s|]$.

A *replacement rule* is a function $\mathsf{replace}_{x \to y}$ that transforms a string s by replacing *all* occurrences of the string x in s with the string y. Formally, $\mathsf{replace}_{x \to y}(s) = s$ if s does not contain x, and otherwise $\mathsf{replace}_{x \to y}(s) = s[1:i] \cdot y \cdot \mathsf{replace}_{x \to y}(s[i+|x|+1:|s|])$, where i is the smallest index for which $s[i+1:i+|x|] = x$.

A sequence of replacement rules $\mathcal{R} = (\mathcal{R}_1, \ldots, \mathcal{R}_k)$ with $\mathcal{R}_i = \mathsf{replace}_{a_i b_i \to c_i}$, where a_i, b_i, c_i are symbols, is called a *merge sequence* of length k. Denoting $s' = (\mathcal{R}_k \circ \cdots \circ \mathcal{R}_1)(s)$, where $\circ$ is the function composition, we refer to $|s'|$ as the *compressed length*, and $|s| - |s'|$ as the *utility* of $\mathcal{R}$ for s. In words, s' is obtained from s by applying the sequence of replacement rules $\mathcal{R}_1, \ldots, \mathcal{R}_k$. We refer to the i-th step, i.e., the application of $\mathcal{R}_i$ as the i-th *merge*. We sometimes use the term *full merge* to emphasize that no copies of $a_i b_i$ remain after the operation.

Given the resulting encoded (compressed) string s', we can recover s by applying the sequence of reverse transformations $\mathcal{R}' = (\mathcal{R}'_k, \ldots, \mathcal{R}'_1)$ to s', with $\mathcal{R}'_i = \mathsf{replace}_{c_i \to a_i b_i}$. Notice that the symbols c_i, for all $i \in [k]$, can be assumed w.l.o.g., to be new, i.e., not appearing in s or in $(\mathcal{R}_j \circ \cdots \circ \mathcal{R}_1)(s)$ for $j < i$. Indeed, if c_i already appears in the string, then the replacement $a_i b_i \to c_i$ may not be unambiguously reversible.

We can now formulate our main optimization problems. Given a string s and an integer $k > 0$, find a merge sequence $\mathcal{R}$ of length k, of maximal utility for s (or equivalently, of minimal compressed length). We denote this optimal utility as $\mathsf{OPT}^m(s, k)$, and call the task of computing it the **optimal merge sequence (OMS) problem**.[2] Note that maximizing compression utility and minimizing compressed length are equivalent for exact computation, but not necessarily for approximability.

---

[2]Apart from slightly different notation that is more convenient for our arguments, the OMS problem is identical to the problem defined by Zouhar et al. [ZMG+23].

$$\texttt{abcd} \,|\, \texttt{bc} \,|\, \texttt{bcda} \,|\, \texttt{cd} \,|\, \texttt{cdab} \,|\, \texttt{da} \,|\, \texttt{dabc} \,|\, \texttt{ab} \;\rightarrow\; \texttt{XY} \,|\, \texttt{Z} \,|\, \texttt{ZT} \,|\, \texttt{Y} \,|\, \texttt{YX} \,|\, \texttt{T} \,|\, \texttt{TZ} \,|\, \texttt{X}$$
$$\texttt{abcd} \,|\, \texttt{bc} \,|\, \texttt{bcda} \,|\, \texttt{cd} \,|\, \texttt{cdab} \,|\, \texttt{da} \,|\, \texttt{dabc} \,|\, \texttt{ab} \;\rightarrow\; \texttt{XZ} \,|\, \texttt{Y} \,|\, \texttt{YT} \,|\, \texttt{Z} \,|\, \texttt{ZX} \,|\, \texttt{T} \,|\, \texttt{dXc} \,|\, \texttt{X}$$

Figure 2: Input $s = \texttt{abcd} \,|\, \texttt{bc} \,|\, \texttt{bcda} \,|\, \texttt{cd} \,|\, \texttt{cdab} \,|\, \texttt{da} \,|\, \texttt{dabc} \,|\, \texttt{ab}$, where $|$ denotes a distinct symbol for each occurrence. An optimal OPE encoding of s (above) with utility $\mathsf{OPT}(s, 4) = 12$. An optimal OMS encoding of s (below) with utility $\mathsf{OPT}^m(s, 4) = 11$. The OMS solution is obtained via the merge sequence ($\texttt{ab} \rightarrow \texttt{X}$, $\texttt{bc} \rightarrow \texttt{Y}$, $\texttt{cd} \rightarrow \texttt{Z}$, $\texttt{da} \rightarrow \texttt{T}$).

We also define a more general optimization problem where we do not require to replace *every occurrence* of a pair. Formally, a *partial replacement rule* $\mathcal{R}_i^* = \mathsf{replace}_{a_i b_i \rightarrow c_i}^*$ can be any function that satisfies $\mathsf{replace}_{c_i \rightarrow a_i b_i}(\mathsf{replace}_{a_i b_i \rightarrow c_i}^*(s)) = s$ for all s. In words, $\mathcal{R}_i^*$ replaces *some* occurrences of $a_i b_i$ with c_i. A sequence of partial replacement functions $\mathcal{R}^* = (\mathcal{R}_1^*, \ldots, \mathcal{R}_k^*)$ is a *partial merge sequence*. Denoting $s' = (\mathcal{R}_k^* \circ \cdots \circ \mathcal{R}_1^*)(s)$, we define utility and compressed length of $\mathcal{R}^*$ analogously to merge sequences. Notice that s can be recovered from s' identically to the case of merge sequences.

The **optimal pair encoding (OPE) problem** asks, given a string s and an integer $k > 0$, to find a partial merge sequence $\mathcal{R}^*$ of length k, of maximal utility for s. We denote this optimal utility as $\mathsf{OPT}(s, k)$.

While the OMS problem is perhaps more natural, OPE is more general, and as shown in Figure 2, it can indeed be stronger (i.e., it is sometimes worth not merging every occurrence of a pair). Most of our results in this paper apply to both problems.

Byte-pair encoding (BPE). BPE solves both the OPE and OMS problem as follows. Starting with the input string s, it performs k *locally optimal* full merge steps, always choosing a pair whose replacement maximizes compression utility.

Formally, for input (s, k), we output $\mathcal{R} = (\mathcal{R}_1, \ldots, \mathcal{R}_k)$, where $\mathcal{R}_i = \mathsf{replace}_{a_i b_i \rightarrow c_i}$. Denoting $s^{(0)} = s$, and $s^{(i)} = \mathcal{R}_i(s^{(i-1)})$ for $i \in [k]$, each c_i is a new symbol, i.e., not occurring in $s^{(j)}$ with $j < i$, and for $i = 1, \ldots, k$, the pair $a_i b_i$ is chosen so that $|\mathcal{R}_i(s^{(i-1)})|$ is minimal.

With careful data structuring, identifying $a_i b_i$ and performing $\mathcal{R}_i$ can be done in linear total time over all k merge steps, e.g., see [SKF+99]. In this paper, we ignore such implementation details and focus on the total utility of BPE, i.e., $|s| - |s'|$, where $s' = s^{(k)}$. We denote this quantity as $\mathsf{BPE}(s, k)$. Note that clearly $\mathsf{BPE}(s, k) \leq \mathsf{OPT}^m(s, k) \leq \mathsf{OPT}(s, k)$.

We remark that a number of choices allow for small variation in the definition of BPE (and partly of OPT^m): (1) when choosing a pair to replace, in case of a tie in utility, we pick the pair that appears first; (2) the utility of a chosen pair equals its number of occurrences, except for the case of overlapping pairs (e.g., the pair $\texttt{aa}$ appears twice in $\texttt{aaa}$, but only one of its copies can be replaced) – one could also decide based on the number of occurrences; and (3) in case of such overlapping pairs, we do the replacements left-to-right, e.g., $\texttt{aaa} \rightarrow \texttt{Xa}$, whereas $\texttt{aaa} \rightarrow \texttt{aX}$ would also be a valid choice.

Overall, the effect of these design decisions appears negligible. Our results hold regardless of the tie-breaking strategy for (1). As for (2) and (3), the implementation we chose appears better motivated than the alternatives, but our results can easily be adapted to the other variants; see also [LM00, ZMG+23] for discussion.

Our results. As defined, OPE and OMS are natural string compression problems (maximizing compression utility), and BPE is a straightforward greedy heuristic for both. Surprisingly, no worst-case guarantee is known for BPE or for any other algorithm solving OPE or OMS.

Zouhar et al. [ZMG+23] formulated the OMS problem (under slightly different terminology), and raised the question whether its exact decision problem is NP-hard. Our first result, shown in §2 answers this question in a stronger form. We show that both OMS and OPE are in fact APX-complete, ruling out the existence of a *polynomial time approximation scheme* (PTAS), unless P=NP.

Theorem 1.1. *OPE and OMS are APX-complete.*

The fact that the number k of merge-steps is part of the input is crucial; for fixed values of k a polynomial-time exact algorithm is easy to derive. The APX-hardness also holds for the problem of minimizing compressed length, as well as for some other variants of the problem, as discussed in §2.

As for BPE, we analyze its approximation ratio for compression utility, showing in §3:

Theorem 1.2. *BPE approximates OPE with a ratio of α, where $0.333 < \alpha \le 0.625$.*

Closing this gap is an intriguing open question. Note that the result also implies an approximation of OMS with the same or better ratio, as well as that OPT and OPT^m are within a constant factor of each other. Unlike the hardness result, this guarantee does not transfer to the dual optimization problem of minimizing compressed length. In particular, we show in §4 that BPE cannot achieve a constant approximation for this measure.

Theorem 1.3. *The approximation ratio of BPE for compression length in OPE or OMS is $\Omega(n)$.*

While our main focus is on the BPE algorithm, we find the OPE optimization problem of independent interest. We give in §5 a simple algorithm we call EvenOdd, that achieves an approximation ratio of 0.5. We stress that despite this guarantee, on most inputs BPE likely behaves better than EvenOdd, which should be seen as a proof of concept.

Theorem 1.4. *EvenOdd is a 0.5-approximation for OPE.*

The following four sections are dedicated to the proofs of Theorems 1.1–1.4. In §6 we conclude with a list of open questions.

2. Hardness of Approximation

In this section we show that the optimal merge sequence (OMS) problem is APX-complete, proving part of Theorem 1.1. The APX-completeness of OPE is based on similar ideas and is completed in Appendix A. As we show in §3, both OPE and OMS are in APX (i.e., admit a constant-factor approximation), it just remains therefore to show APX-hardness. We do so via an L-reduction (linear reduction, see [PY91]) from maximum cut in cubic graphs.

In maximum cut, given an undirected graph $G = (V, E)$, the task is to partition the vertex set V into two parts, such as to maximize the number of edges between the two parts. Maximum cut is NP-complete [Kar72], and its optimization version is APX-complete [PY91] even when restricted to input graphs in which every vertex has degree exactly three [AK00].

Our reduction is from such (cubic, undirected, unweighted) instances $G = (V, E)$ of maximum cut. Assume $V = \{v_1, \ldots, v_n\}$ and associate a symbol ℓ_i to each vertex $v_i \in V$. We construct a string s by concatenating, for each edge $\{v_i, v_j\} \in E$ in arbitrary order, a string s_{ij}, with $i < j$. Then, we append for each vertex $v_i \in V$ four copies of a string s_i. Finally, we append $20n$ copies of a

padding string s_0. These strings are defined as follows, with product signs indicating concatenation:

$$
\begin{aligned}
s_{ij} &= \#\ell_i\#\#\ell_j\# \,|\, \#\ell_j\#\#\ell_i\# \,|, \\
s_i &= \ell_i\# \,|\, \#\ell_i \,|\, \ell_i\#\ell_i \,|, \\
s_0 &= \#\# \,|, \\
s &= \prod_{\substack{\{v_i,v_j\}\in E \\ i<j}} s_{ij} \cdot \prod_{v_i\in V} s_i s_i s_i s_i \cdot \prod_{t=1}^{20n} s_0.
\end{aligned}
$$

Here, $\#$ is a single fixed symbol, and $|$ denotes a distinct symbol for each occurrence. Setting $k = n+1$, we take (s,k) to be the resulting OMS instance. Notice that the construction takes polynomial time.

We first show that G has a cut of size at least c if and only if $\mathsf{OPT}^m(s,k) \geq 34n + c$, i.e., if there is a merge sequence of length k, of at least the given utility for s. This claim already implies the NP-hardness of the problem and sets the stage for our hardness of approximation proof.

($\Rightarrow$) Consider a cut of G, i.e., a partitioning $(S, V \setminus S)$ of V with c edges across the cut. We construct a merge sequence of length k (recall that a *merge* replaces every occurrence of a pair with a new symbol). We first merge $\#\ell_i$ for every $v_i \in S$, and $\ell_i\#$ for every $v_i \in V \setminus S$. Notice that each merge step achieves utility 14 (6 from the s_{ij} corresponding to the three edges incident to v_i, and 8 from the s_i strings), for a total of $14n$. Then, we merge $\#\#$, which achieves utility $c + 20n$. To see this, notice that, after the first n merges, one of the two $\#\#$ pairs remains in a string s_{ij} exactly if the corresponding edge $\{v_i, v_j\}$ is in the cut, and otherwise no such pair remains in s_{ij}. The term $20n$ is from the padding string s_0. This adds up to a utility of $34n + c$ as required.

($\Leftarrow$) Consider a merge sequence $\mathcal{R}$ of length k, of utility $34n + c$ for s. We call the merge sequence *well-formed* if it includes merging the pair $\#\#$ and for each $v_i \in V$, exactly one of the pairs $\ell_i\#$ and $\#\ell_i$. We show that it is sufficient to consider well-formed merge sequences.

Claim 2.1. *If $\mathcal{R}$ is not well-formed, then we can find (in polynomial time) a well-formed merge sequence $\mathcal{R}'$ of the same length that achieves strictly greater utility on s.*

Proof. Observe that any new symbol introduced in a merge encodes a substring of s. Since pairs other than $\#\#$ occur at most 14 times in s, a string different from $\#\#$ can also occur at most this many times. Thus, any merge other than $\#\#$ can have utility at most 14.

Recall that *any* well-formed merge sequence has utility at least $34n$, by the earlier correspondence to an arbitrary cut, possibly of size zero. So, if $\mathcal{R}$ does not merge $\#\#$, then its total utility is at most $14(n+1) < 34n$ and we can replace $\mathcal{R}$ by an arbitrary well-formed merge sequence of larger utility. Assume therefore that $\#\#$ is merged by $\mathcal{R}$.

If $\mathcal{R}$ is not well-formed, then there are t indices (for some $t > 0$) $i_1, \ldots, i_t \in [n]$ such that none of the two pairs $\ell_{i_j}\#$, $\#\ell_{i_j}$ are merged by $\mathcal{R}$, for all $j \in [t]$. Instead, there are exactly t "bad" merges, which can be of the types listed below. We show that removing the t bad pairs from $\mathcal{R}$ and adding the missing pairs $\ell_{i_j}\#$, for all $j \in [t]$, we obtain a merge sequence $\mathcal{R}'$ of larger utility on s.

As $\mathcal{R}'$ is well-formed, each newly added pair contributes a utility of at least 11. This is because the pair appears once in each of the three relevant strings s_{ij}, in copies that do not overlap with $\#\#$, and thus contribute to the gain. An additional utility of 8 comes from the four copies of s_i. As we add the pairs to the end of the merge sequence, they do not affect the utilities of other merges.

To finish the proof, we argue that the "bad" merges that we removed from $\mathcal{R}$ had a gain of at most 10 each; as the remaining merges are unaffected, we obtain an overall increase in utility of at least one for each bad merge. Bad merges that deviate from a well-formed merge sequence can be of the following types:

6

1. A merge involving the symbol $|$: this yields a utility of one, by construction.

2. A merge involving a new symbol (not part of the original s): such a merge corresponds to a substring of s of length at least three. Of all such substrings, those involving $|$ occur at most once, $\#\ell_i\#$ occurs 6 times, $\#\#\ell_i$ and $\ell_i\#\#$ occur 3 times, and $\ell_i\#\ell_i$ occurs 4 times, for all i; there are no further cases (longer substrings also cannot occur more than 6 times). Thus any such merge can yield utility of at most 6.

3. A merge of $\ell_i\#$ after $\#\ell_i$ has already been merged, or a merge of $\#\ell_i$ after $\ell_i\#$ has already been merged: this yields utility at most 10. To see this, observe that for all such pairs, initially there are 6 copies in s_{ij} strings and 8 copies in s_i strings. Of the latter, at least 4 have been destroyed, yielding the claim. □

Suppose now that $\mathcal{R}$ is well-formed (otherwise, transform it according to Claim 2.1). Using $\mathcal{R}$, compute a cut $(S, V \setminus S)$ of G by letting S be the set of vertices $v_i \in V$ where merge $\#\ell_i$ is in $\mathcal{R}$.

Consider the string s_{ij} for an edge $\{v_i, v_j\}$. Notice that we can achieve a total utility of 5 for this string, if and only if one of v_i and v_j was placed in S and the other was not, i.e., if the edge contributes to the constructed cut. (This is possible either if we merge $\#\#$ last, or if we merge $\#\#$ between the two merges corresponding to v_i and v_j.) Otherwise, both $\#\ell_i$ and $\#\ell_j$, or both $\ell_i\#$ and $\ell_j\#$ are merged, and a utility of at most 4 is achievable for s_{ij}, as both $\#\#$ pairs overlap with the two other pairs.

Of the total utility of at least $34n + c$ we obtain $20n$ in the s_0-strings, $8n$ in the s_i-strings, with $6n + c$ remaining for the s_{ij}-strings corresponding to the $3n/2$ edges of G. By the above calculations these can contribute exactly $4 \cdot 3n/2 = 6n$ plus the size of the constructed cut, which must therefore be at least c. This concludes the reduction for NP-hardness.

We next turn the argument into an L-reduction [PY91], thus showing the APX-hardness of OMS. Let OPT^c denote the maximum cut size for graph G, and let $\mathsf{OPT}^m = \mathsf{OPT}^m(s, k)$ be the maximum utility for the OMS instance resulting from the above reduction. It remains to show that there exist positive constants α and β (independent of the input G) so that, for all sufficiently large G:

1. $\mathsf{OPT}^m \leq \alpha \cdot \mathsf{OPT}^c$, and

2. for every feasible solution of the OMS instance (s, k) of utility u we can obtain, in polynomial time, a cut of G of size c, with $|\mathsf{OPT}^c - c| \leq \beta \cdot |\mathsf{OPT}^m - u|$.

Part 1. is immediate: $|s| = 121 \cdot n$ (using that G is cubic), which is an upper bound on OPT^m; on the other hand, from the well-known lower bound on the maximum cut we have $\mathsf{OPT}^c \geq 3n/4$, implying the inequality for $\alpha = 162$.

For Part 2., consider a merge sequence $\mathcal{R}$ of utility u for (s, k). If $\mathcal{R}$ is not well-formed, we use the transformation of Claim 2.1 to obtain a well-formed merge sequence $\mathcal{R}'$ for (s, k) of utility $u' > u$. Otherwise let $u' = u$ and $\mathcal{R}' = \mathcal{R}$. Now, as $\mathcal{R}'$ is well-formed, we interpret it as a cut of size c in G, where, by the earlier reduction, $c = u' - 34n$. Moreover, by applying this argument to the optimal OMS solution, we obtain a cut of size $\mathsf{OPT}^m - 34n$. As we have shown earlier that $\mathsf{OPT}^m \geq 34n + c'$ for every cut c', our cut must be maximal and $\mathsf{OPT}^c = \mathsf{OPT}^m - 34n$. We thus have $|\mathsf{OPT}^c - c| = |\mathsf{OPT}^m - u'| \leq |\mathsf{OPT}^m - u|$, proving the inequality for $\beta = 1$.

This completes the APX-hardness of OMS. In Appendix A we extend the argument to show the APX-hardness of the OPE problem.

Two small remarks are in order. First, we note that the APX-hardness also applies for the compressed length minimization version of OMS (and OPE); in the above hard instance the input length is $|s| = 121n$, and $\mathsf{OPT}^m(s, k) \geq 34n$. Thus, a $(1 + \varepsilon)$-approximation for $|s'| = |s| - \mathsf{OPT}^m(s, k)$ would also yield a $(1 - \varepsilon')$-approximation for OPT^m, with $\varepsilon' = ((121 - 34)/34)\varepsilon \leq 2.6\,\varepsilon$.

Second, we can define restricted forms of the OMS (and OPE) problems where it is only allowed to merge pairs of original input symbols, and not pairs involving new symbols. (Equivalently, all resulting tokens would be of length at most two; note that the BPE solution does not necessarily conform to this restriction.) Since in the above reduction all merges involve only input symbols, our APX-hardness results immediately transfer to these restricted variants.

3. Approximation ratio of Byte-Pair Encoding

In this section we study the approximation ratio of BPE for the OPE problem, showing constant upper and lower bounds for this ratio, proving Theorem 1.2.

Upper bound. Consider the string $s = \texttt{abaacaaba}\,|\,\texttt{aca}$, with a merge sequence of length $k = 4$. Suppose BPE first performs the merge $\texttt{aa} \to \texttt{X}$, resulting in the string $\texttt{abXcXba}\,|\,\texttt{aca}$. As now each pair occurs at most once, subsequent merges can only shorten the string by 1, for a total utility of 5. Consider now the alternative merge sequence ($\texttt{ac} \to \texttt{X}$, $\texttt{Xa} \to \texttt{Y}$, $\texttt{ab} \to \texttt{Z}$, $\texttt{Za} \to \texttt{T}$) resulting in $\texttt{TYT}\,|\,\texttt{Y}$, with utility 8, and a ratio of $5/8 = 0.625$.

To enforce that BPE merges $\texttt{aa}$ first, we can concatenate t copies of $s{\cdot}\#$, and a final $\texttt{aa}$. The utility of BPE is now (without relying on favorable tie-breaking) $5t + 1$, whereas the alternative merge sequence yields $8t$, for a ratio arbitrarily close to 0.625. Notice that while we claimed the result for OPE, the upper bound (more strongly) applies to OMS (i.e., for the ratio $\mathsf{BPE}(s, k)/\mathsf{OPT}^m(s, k)$), as the alternative encoding above is given by a full merge sequence.

Lower bound. We show our lower bound (more strongly) for OPE. Consider an optimal (possibly partial) merge sequence $\mathcal{R}^* = (\mathcal{R}_1^*, \ldots, \mathcal{R}_k^*)$, where $\mathcal{R}_i^* = \mathsf{replace}^*_{a_i b_i \to c_i}$ for $i \in [k]$. Let s' be the string resulting from applying $\mathcal{R}^*$ to input s. Recall that $\mathsf{OPT}(s, k) = |s| - |s'|$.

In order to relate $\mathsf{BPE}(s, k)$ and $\mathsf{OPT}(s, k)$, we first introduce a simpler quantity that upper bounds both.

For a string s of length n, a set of t indices $\{i_1, \ldots, i_t\} \subseteq [n-1]$ is a *pair packing*, if the pairs starting at the given indices of s do not overlap and are all equal as strings. Formally, $|i_j - i_k| \geq 2$ for $j, k \in [t]$, and $s[i_1 : i_1 + 1] = \cdots = s[i_t : i_t + 1]$. A *$k$-packing* is the union of k pair packings where no element appears in more than one of the pair packings. We refer to a largest possible k-packing as the *optimal k-packing* and denote its size by $P_k(s)$. We remark that $P_k(s)$ can be computed in polynomial time, but this is not needed in our current study.

Lemma 3.1. *For s' obtained from s by applying an arbitrary (partial) merge sequence $\mathcal{R}^*$ of length k, we have $|s| - |s'| \leq P_k(s)$.*

Proof. We create a k-packing from s and $\mathcal{R}^*$, of size $|s| - |s'|$. To do this, it will be useful to map every occurrence of a symbol during the application of $\mathcal{R}^*$, to the substring of s which is encoded by the symbol. For a string c let $\mathsf{decode}(c, 0) = c$, and for $i \in [k]$ let $\mathsf{decode}(c, i) = \mathsf{decode}(\mathsf{replace}_{c_i \to a_i b_i}(c), i - 1)$. Observe that every occurrence of c_i after the application of $\mathcal{R}_i^*$ encodes a unique copy of $\mathsf{decode}(c_i, i)$ in s, these copies do not overlap, and $\mathsf{decode}(c_i, i) = \mathsf{decode}(a_i, i - 1) \cdot \mathsf{decode}(b_i, i - 1)$.

We *charge* each replacement $a_i b_i \to c_i$, i.e., each unit of the compression utility, in the order of their application in $\mathcal{R}^*$, to a certain index of s. More precisely, charge the replacement $a_i b_i \to c_i$ to the index in s of the last symbol of $\mathsf{decode}(a_i, i - 1)$ in the location encoded by the current copy of a_i. Intuitively, we charge the merging of a pair to the location in s where the "gluing" happens.

Observe that this index cannot be charged again in any step, since after replacement $a_i b_i \to c_i$, it points to a symbol "inside" $\mathsf{decode}(c_i, i)$, that is not the last one, and future merges cannot cause it to become a last symbol. The indices charged due to $\mathcal{R}_i^*$ are at pairwise distance at least 2, for

all $i \in [k]$ (as otherwise two copies of $\mathsf{decode}(c_i, i)$ would overlap in s), and the pairs starting at the charged indices are equal as strings, as all consist of the last symbol of $\mathsf{decode}(a_i, i-1)$ and first symbol of $\mathsf{decode}(b_i, i-1)$. It follows that the set of indices charged during the entire process is a k-packing, thus, the total utility $|s| - |s'|$ is at most the size $P_k(s)$ of the optimal k-packing. $\qquad\square$

Notice that as a corollary of Lemma 3.1 we have $\mathsf{OPT}(s, k) \leq P_k(s)$.

In the remainder of the section we *lower bound* the BPE utility in terms of the quantity we defined, which, together with Lemma 3.1 will immediately imply the claimed upper bound on the approximation ratio of BPE.

Lemma 3.2. *For all strings s and $k \geq 0$ we have $\mathsf{BPE}(s, k) \geq P_k(s)/3$.*

Proof. As before, $s^{(0)} = s$ and let $s^{(k)} = s'$ denote the encoding obtained by BPE, with $s^{(i)}$ resulting from $s^{(i-1)}$ (for $i \in [k]$) by a greedy merge step, as described in the definition of BPE.

Let $a_i b_i$ be the pair merged by BPE when going from $s^{(i-1)}$ to $s^{(i)}$, for $i \in [k]$, and let $\mathcal{B}$ be a k-packing derived from the BPE merge sequence according to the process in Lemma 3.1. Let $\mathcal{B}_1 \cup \cdots \cup \mathcal{B}_k$ be the partitioning of $\mathcal{B}$ into the k pair packings corresponding to the k merge steps of BPE. (When BPE does a replacement $a_i b_i \to c_i$ in $s^{(i-1)}$, then the corresponding entry in $\mathcal{B}_i$ is the index of the last symbol of the substring in s encoded by a_i.) Note that $|\mathcal{B}| = \mathsf{BPE}(s, k)$.

Let $\mathcal{P}$ be an optimal k-packing partitioned into k pair packings $\mathcal{P}_1 \cup \cdots \cup \mathcal{P}_k$, where $\mathcal{P}_i$ contains starting indices of the pair $x_i y_i$ in s for $i \in [k]$. Note that $|\mathcal{P}| = P_k(s)$. Also note that pairs $x_i y_i$, $x_j y_j$ from different pair packings are not necessarily distinct, and the same holds for pairs $a_i b_i$, $a_j b_j$ from different steps of BPE.

We iterate i from 1 to k, relating for each i the number of entries in $\mathcal{B}_i$ and the number of entries in $\mathcal{P}_i$. In each step we delete at most $3|\mathcal{B}_i|$ elements from $\mathcal{P}$. The set $\mathcal{B}$ is not modified during the process. In the end, $\mathcal{P}$ will be empty, implying the claim.

We maintain two invariants:
$\mathbf{I_1}$: After step i, the sets $\mathcal{P}_j$ for $j \leq i$ are empty.
$\mathbf{I_2}$: After step i, no index $x \in \mathcal{P}$ is a neighbor of an index $y \in \mathcal{B}_j$, for $j \leq i$.
Two indices x and y are neighbors if $|x - y| = 1$.

Intuitively, $\mathbf{I_1}$ ensures that all elements of $\mathcal{P}$ are accounted for, and $\mathbf{I_2}$ ensures that pairs $s[x : x+1]$ corresponding to $x \in \mathcal{P}$ can still be merged by BPE, as the two symbols forming the pair did not take part in merges yet. Initially both invariants are trivially true.

Consider step i. For all elements $x \in \mathcal{B}_i$, delete x and its neighbors $x - 1$ and $x + 1$ from $\mathcal{P}$. Note that we delete at most $3|\mathcal{B}_i|$ elements in this way. Also note that this establishes $\mathbf{I_2}$ for the current step. It remains to verify $\mathbf{I_1}$. We distinguish two cases.

Case 1. If $a_i b_i = x_\ell y_\ell$, for some $i \leq \ell \leq k$, then swap $x_i y_i$ with $x_\ell y_\ell$ and $\mathcal{P}_i$ with $\mathcal{P}_\ell$ (this is only necessary if $\ell \neq i$; also note that the swap does not affect $\mathbf{I_1}$, $\mathbf{I_2}$). Now, if $\mathcal{P}_i$ is nonempty (after the deletions and swap), then take any element $x \in \mathcal{P}_i$. Notice that BPE could have also merged $s[x : x+1]$ in the i-th step, in addition to the pairs indexed by $\mathcal{B}_i$. This is because the pair equals $a_i b_i$, it does not neighbor to any pair merged by BPE in the present or past rounds (by $\mathbf{I_2}$), and the pair itself was not merged before, as otherwise x would have been deleted. This contradicts the definition of BPE, showing $\mathcal{P}_i = \emptyset$, and hence, $\mathbf{I_1}$.

Case 2. If $a_i b_i \neq x_\ell y_\ell$ for $i \leq \ell \leq k$. Notice that in this case, $\mathcal{P} \cap \mathcal{B}_i = \emptyset$ even before the deletion (by $\mathbf{I_1}$), thus we could have only deleted the neighbors of $\mathcal{B}_i$ from $\mathcal{P}$ in the i-th step. If, before the deletion, $|\mathcal{P}_i| > |\mathcal{B}_i|$, then BPE could have merged, instead of the pairs $a_i b_i$ indexed by $\mathcal{B}_i$, the pairs $x_i y_i$ indexed by $\mathcal{P}_i$, contradicting the definition of BPE. This is because pairs $s[x : x + 1]$ for $x \in \mathcal{P}_i$ do not neighbor to any pair merged by BPE in the present or past rounds (by $\mathbf{I_2}$), and were

9

not merged before (as otherwise x would have been deleted). Moreover, as $\mathcal{P}_i$ forms a pair packing, the pairs indexed by $\mathcal{P}_i$ are not neighboring each other and could thus have been merged in one round of BPE.

Thus, $|\mathcal{P}_i| \leq |\mathcal{B}_i|$ and $\mathcal{P} \cap \mathcal{B}_i = \emptyset$ (before the deletion). As we cannot delete entries of $\mathcal{B}_i$ from $\mathcal{P}$, we instead use our remaining budget of $|\mathcal{B}_i|$ deletions to delete the entries of $\mathcal{P}_i$, establishing $\mathbf{I_1}$.

After the k-th step, $\mathbf{I_1}$ implies that $\mathcal{P}$ is empty, proving the lemma. $\qquad\square$

4. Lower bound for compressed length

In this section we show that for the dual optimization problem of OPE of minimizing compressed length (instead of maximizing compression utility), the approximation ratio of BPE is *unbounded*, and in fact, linear in the input size. This proves Theorem 1.3.

The construction is essentially the same as the example used in [FTN$^+$19, Thm. 3] to prove a different property of Re-Pair.

Consider the string

$$s = \prod_{i=1}^{t} x_i \mathtt{aa} y_i \cdot \prod_{i=1}^{t} |\, x_i \mathtt{a} \cdot \prod_{i=1}^{t} |\, \mathtt{a} y_i,$$

where $t > 2$, each occurrence of $|$ is a distinct symbol, and $\mathtt{a}$, x_i, y_i are symbols for $i \in [t]$.

If we merge every occurrence of $x_i \mathtt{a}$ and $\mathtt{a} y_i$, the resulting string has length $2t + 2t + 2t = 6t$ after $2t$ steps. So after $2t + (6t - 1) = 8t - 1$ total steps, we have reduced s to a single symbol.

On the other hand, BPE will always start with $\mathtt{aa}$, since it occurs t times, while every other pair occurs at most twice. After merging $\mathtt{aa}$, no pair occurs more than once in the string, so every subsequent step has a utility of one. After merging $\mathtt{aa}$, the length of the string is $3t + 3t + 3t = 9t$. So after $8t - 1$ total steps, the resulting string will be of length $9t - (8t - 2) = t + 2$. Since $|s| = 10t$, it holds that $t + 2 = \frac{|s|}{10} + 2 \in \Omega(|s|)$.

Notice that since all merges were full, the approximation lower bound also holds for the OMS problem (in the compression length version).

5. Approximating Optimal Pair Encoding

In this section we give a simple algorithm that achieves a 0.5-approximation for the OPE problem, proving Theorem 1.4.

For a pair xy, let $\mathsf{freq}_{xy}(s)$ denote the number of occurrences of xy in s. Note that we allow overlaps, e.g., $\mathsf{freq}_{\mathtt{aa}}(\mathtt{aaa}) = 2$. Let $F_k(s)$ denote the total number of occurrences of the k most frequent pairs in s (breaking ties arbitrarily, as this does not affect the total value). Let $x_1 y_1, \ldots, x_k y_k$ be such a set of most frequent pairs, and let $I = \{i_1, \ldots, i_N\}$, where $N = F_k(s)$, denote the set of indices where they occur, i.e., $s[i_j : i_j + 1] \in \{x_i y_i \mid i \in [k]\}$ for all $j \in [N]$.

We can efficiently compute a set $I = \{i_1, \ldots, i_N\}$ by enumerating all pairs occurring in s and taking the indices of the k most frequent of them. Assume that $i_1, \ldots, i_N$ are sorted increasingly. We then sparsify I, by removing neighboring indices. More precisely, for each index of the form $i_{2\ell}$, remove $i_{2\ell}$ if $i_{2\ell} = i_{2\ell-1} + 1$ or $i_{2\ell} = i_{2\ell+1} - 1$. Let I' denote the indices in I remaining after this process. Observe that I' has at least $N/2$ elements. As there are no neighboring indices in I', the occurrences of pairs in s indexed by I' do not overlap, can therefore be merged simultaneously. Notice that only k distinct pairs appear, so we obtain a valid OPE solution of utility $|I'|$. We call this the EvenOdd algorithm.

Since $|I'| \geq F_k(s)/2$, and clearly, $F_k(s) \geq P_k(s) \geq \mathsf{OPT}(s, k)$, the theorem follows.

$$\begin{array}{c}
\texttt{abcd}\,|\,\texttt{bc}\,|\,\texttt{bcda}\,|\,\texttt{cd}\,|\,\texttt{cdab}\,|\,\texttt{da}\,|\,\texttt{dabc}\,|\,\texttt{ab} \;\rightarrow\; \texttt{XY}\,|\,\texttt{Z}\,|\,\texttt{bYa}\,|\,\texttt{Y}\,|\,\texttt{YX}\,|\,\texttt{T}\,|\,\texttt{dXc}\,|\,\texttt{X}\\[-2pt]
{\scriptstyle\uparrow\,\uparrow\quad\uparrow\quad\ \ \uparrow\quad\ \ \uparrow\quad\ \ \uparrow\,\uparrow\quad\ \uparrow\quad\ \ \uparrow\quad\ \ \uparrow}
\end{array}$$

$$\begin{array}{c}
\texttt{abcd}\,|\,\texttt{bc}\,|\,\texttt{bcda}\,|\,\texttt{cd}\,|\,\texttt{cdab}\,|\,\texttt{da}\,|\,\texttt{dabc}\,|\,\texttt{ab} \;\rightarrow\; \texttt{XY}\,|\,\texttt{Z}\,|\,\texttt{ZT}\,|\,\texttt{Y}\,|\,\texttt{YX}\,|\,\texttt{T}\,|\,\texttt{TZ}\,|\,\texttt{X}\\[-2pt]
{\scriptstyle\uparrow\!\!\nwarrow\!\uparrow\quad\uparrow\quad\ \uparrow\!\!\nwarrow\!\uparrow\quad\ \uparrow\quad\ \uparrow\!\!\nwarrow\!\uparrow\quad\ \uparrow\quad\ \uparrow\!\!\nwarrow\!\uparrow\quad\ \uparrow}
\end{array}$$

Figure 3: Encoding $s = \texttt{abcd}\,|\,\texttt{bc}\,|\,\texttt{bcda}\,|\,\texttt{cd}\,|\,\texttt{cdab}\,|\,\texttt{da}\,|\,\texttt{dabc}\,|\,\texttt{ab}$, where $|$ denotes a distinct symbol for each occurrence. The BPE encoding (above) with utility $\mathsf{BPE}(s,4) = 10$ via the merge sequence ($\texttt{ab} \to \texttt{X}$, $\texttt{cd} \to \texttt{Y}$, $\texttt{bc} \to \texttt{Z}$, $\texttt{da} \to \texttt{T}$). Arrows show the k-packing solution derived from the BPE merge sequence. The EvenOdd encoding (below) with $k = 4$ and utility 12. Arrows show the indices of most frequent pairs, with crossed ones removed.

On some inputs, EvenOdd can have larger utility than BPE. Indeed, consider the earlier example $s = \texttt{abcd}\,|\,\texttt{bc}\,|\,\texttt{bcda}\,|\,\texttt{cd}\,|\,\texttt{cdab}\,|\,\texttt{da}\,|\,\texttt{dabc}\,|\,\texttt{ab}$. With $k = 4$ merge rounds, BPE achieves utility 10 due to the unfavorable tie-breaking, but as seen earlier, the maximum utility of *any* OMS algorithm (regardless of tie-breaking) is at most 11. EvenOdd takes the most frequent 4 pairs $\{\texttt{ab}, \texttt{bc}, \texttt{cd}, \texttt{da}\}$ with 16 occurrences in s. After sparsification, 12 non-neighboring pairs remain and are merged, matching the OPE optimum utility of 12 on this instance; see Figure 3.

We remark that the EvenOdd algorithm only merges input symbols (and not newly introduced symbols), and thus, the decoded string of each symbol is of length at most two. Note that, instead of removing even-ranked indices, we could, in polynomial time, find the minimal set of indices whose removal makes the remainder non-overlapping (by a simple greedy strategy). In the worst case, however, no algorithm in this class can improve the approximation ratio 0.5.

Indeed, consider an input string s consisting of $2n$ identical symbols, followed by $2(k-1)$ pairwise distinct symbols. Setting $k = \log_2 n + 1$, the optimal pair encoding of s will collapse the first $2n$ symbols to one, with utility $2n - 1$. An algorithm that can only merge input pairs can achieve a maximum utility of n on the first part of the string (in one merge), and an additional $k - 1$ on the last part, yielding an approximation ratio of $(n + \log_2 n)/(2n - 1) = 0.5 + o(1)$. In this example, the optimal encoding coincides with the one found by BPE, also showing a factor $2 - o(1)$ gap between BPE and input-symbol-only algorithms, to the advantage of the former.

6. Conclusion and open questions

In this paper we studied the complexity of optimal pair encoding: the task of compressing a string by replacing pairs with new symbols, such as to maximize the overall reduction in length. We showed that the problem is APX-complete and that BPE, a popular greedy heuristic, achieves a constant-factor approximation for this task. Our work can be seen as an initial theoretical investigation with a number of open questions remaining. We list those we find the most interesting.

Finding the best approximation ratio for the OPE or OMS problems, by BPE or by other polynomial-time algorithms, i.e., closing the gaps between our bounds in Theorem 1.2, resp., Theorems 1.1 and 1.4 are the central remaining questions. In particular: is there an efficient algorithm for OPE with approximation ratio above 0.5? Note that analyzing natural greedy strategies for some other string problems turned out to be very difficult. For instance, the famous *greedy superstring conjecture* concerns a very intuitive string merging process, with worst-case approximation ratio conjectured to be 2 but only proven to be at most 3, e.g., see [BJL+94].

Our hardness result (Theorem 1.1) relies on an alphabet whose size increases with the input. The complexity of both problems with a fixed alphabet remains open. In particular, an initial alphabet of size two may make the problem tractable. It is likely that stronger guarantees for BPE can also

be shown in this case.

While the APX-hardness (Theorem 1.1) extends to the compression length, the approximation guarantee (Theorem 1.2) does not, as implied by Theorem 1.3. The polynomial-time approximability of compression length (for OPE or OMS by any algorithm, with or without restrictions on the alphabet) is left open. In fact, as we lack a constant-factor approximation for this problem, we can only claim its APX-hardness, not APX-completeness.

A. APX-hardness of OPE

In §2 we showed that the OMS problem is APX-complete. We now show the same for the the more general OPE problem (where partial merges are also allowed).

We follow the exact same reduction as in §2, just adding a necessary extra step in the proof. Recall that given a cubic, undirected, unweighted graph G, we construct a string s and an integer k. We now take (s, k) to be an OPE instance. We claim that G has a cut of size at least c if and only if $\mathsf{OPT}(s, k) \geq 34n + c$, where n is the number of vertices in G.

The forward direction is identical to the proof in §2, as the constructed OMS merge sequence also serves as a partial merge sequence for OPE.

For the reverse direction, consider a partial merge sequence $\mathcal{R}^*$ of length $k = n + 1$, of utility $34n + c$ for s. Claim 2.1 showed that a merge sequence $\mathcal{R}$ that is not *well-formed* can be transformed into a well-formed one, while increasing its utility. We now extend the argument to a partial merge sequence $\mathcal{R}^*$. We show that we can transform $\mathcal{R}^*$ into a *full merge sequence* (with no partial merges) that is well-formed, and the remainder of the proof in §2 can go through unchanged.

Claim A.1. *If $\mathcal{R}^*$ is a partial merge sequence, then we can find (in polynomial time) a well-formed (full) merge sequence $\mathcal{R}$ of the same length that achieves greater or equal utility on s.*

Proof. As pairs other than $\#\#$ occur at most 14 times in s, we assume $\mathcal{R}^*$ (at least partially) merges $\#\#$, for otherwise the total utility would be at most $14(n + 1) < 34n$, and any well-formed merge sequence $\mathcal{R}$ would have larger utility.

Substrings of s containing $|$ occur at most once, and substrings of length 3 occur at most 6 times; it follows that any (partial) merge involving $|$ or a newly created symbol has utility at most 6. Suppose there are t such partial merges in $\mathcal{R}^*$. Remove them from $\mathcal{R}^*$, and notice that all remaining merges in $\mathcal{R}^*$ can only involve pairs of the form $\#\#$, $\ell_i\#$, and $\#\ell_i$. Add to the end of $\mathcal{R}^*$, t full merges for pairs $\ell_i\#$, where no other merge involves ℓ_i. (As there are $n + 1$ merges initially in $\mathcal{R}^*$, and n symbols ℓ_i, there must be t such pairs.) Each added merge has utility at least 8 (2 from each copy of s_i), so the total utility of $\mathcal{R}^*$ has increased.

We now only have merges of the form $\#\#$, $\ell_i\#$, $\#\ell_i$ in $\mathcal{R}^*$, but some may be partial, and for some ℓ_i, we may not have any of the two merges. If there are duplicate merges in $\mathcal{R}^*$, i.e., more than one merge of the same pair, then we extend the first such merge to also perform the replacements of the other merges of the same pair. After this, we can remove the later duplicate merges (as they no longer have any utility), and replace them by some full merge $\ell_j\#$ where no other merge involves ℓ_j.

We then move $\#\#$ to be the last merge in $\mathcal{R}^*$. Notice that a partial merge sequence where all merges involve only input symbols (as the case here) can be freely re-arranged without changing utility. After we have moved $\#\#$ to the end of $\mathcal{R}^*$, we can turn it into a full merge, as this can only increase the utility of $\mathcal{R}^*$.

We next fix the cases where both pairs $\#\ell_i$ and $\ell_i\#$ are (partially) merged in $\mathcal{R}^*$, for some i. Suppose $\#\ell_i$ appears first (the other case is symmetric). We remove, one by one, all the replacements of $\ell_i\#$. In each copy of s_i there can be two such replacements. The one in $\ell_i\#\ell_i$ can be compensated by an additional replacement of $\#\ell_i$, but the other one cannot, so we account for it as a loss. In total, there are at most 4 such losses in s_i strings. In s_{ij} (or s_{ji}) strings there can be overall at most 6 replacements of $\ell_i\#$, which we account as a loss. The total loss due to removing $\ell_i\#$ is thus at most 10. Now we add instead of $\ell_i\#$ in $\mathcal{R}^*$, a new merge $\ell_q\#$, where no other merge involves ℓ_q. This new merge has utility at least 8 from the s_q strings, without affecting other merges. In each of the 3 strings $s_{qq'}$ or $s_{q'q}$, where q' is a vertex such that (q, q') is an edge in G, we can find one copy of $\ell_q\#$ that does not overlap with $\#\#$ (or with any other pair that we merge), and we add these replacements to the partial merge. We thus get a utility of at least 11,

13

compensating the loss of 10. After doing this for each pair, we end up with $\mathcal{R}^*$ containing, for each i, exactly one of the merges $\#\ell_i$ and $\ell_i\#$.

Finally, we proceed inductively through $\mathcal{R}^*$ from the end to the beginning and turn each merge into a full merge. Suppose we are at the i-th merge step and for all $j > i$, the j-th merge is full. Suppose the i-th merge is for $\#\ell_q$ (the case $\ell_q\#$ is entirely symmetric, and thus omitted). We turn $\#\ell_q$ into a full merge. Within a copy of s_q, this can only increase utility, as $\#\ell_q$ does not overlap with any other merged pair. Within some $s_{qq'}$ or $s_{q'q}$, a new replacement of $\#\ell_q$ may only interfere with a later $\#\#$ merge, but in this case we just exchange one replacement by another, leaving the total utility unchanged.

At the end of the process all merges are full and we have turned $\mathcal{R}^*$ into a well-formed merge sequence that we call $\mathcal{R}$. $\qquad\square$

References

[AFT+23]   Mehdi Ali, Michael Fromm, Klaudia Thellmann, Richard Rutmann, Max Lübbering, Johannes Leveling, Katrin Klug, Jan Ebert, Niclas Doll, Jasper Schulze Buschhoff, et al. Tokenizer choice for LLM training: Negligible or crucial? *arXiv preprint arXiv:2310.08754*, 2023.

[AK00]   Paola Alimonti and Viggo Kann. Some APX-completeness results for cubic graphs. *Theor. Comput. Sci.*, 237(1-2):123–134, 2000.

[BD20]   Kaj Bostrom and Greg Durrett. Byte pair encoding is suboptimal for language model pretraining. In *Findings of the Association for Computational Linguistics: EMNLP 2020*, pages 4617–4624, 2020.

[BHH+20]   Hideo Bannai, Momoko Hirayama, Danny Hucke, Shunsuke Inenaga, Artur Jeż, Markus Lohrey, and Carl Philipp Reh. The smallest grammar problem revisited. *IEEE Transactions on Information Theory*, 67(1):317–328, 2020.

[BJL+94]   Avrim Blum, Tao Jiang, Ming Li, John Tromp, and Mihalis Yannakakis. Linear approximation of shortest superstrings. *J. ACM*, 41(4):630–647, July 1994.

[BMR+20]   Tom B. Brown, Benjamin Mann, Nick Ryder, Melanie Subbiah, Jared Kaplan, Prafulla Dhariwal, Arvind Neelakantan, Pranav Shyam, Girish Sastry, Amanda Askell, Sandhini Agarwal, Ariel Herbert-Voss, Gretchen Krueger, Tom Henighan, Rewon Child, Aditya Ramesh, Daniel M. Ziegler, Jeffrey Wu, Clemens Winter, Christopher Hesse, Mark Chen, Eric Sigler, Mateusz Litwin, Scott Gray, Benjamin Chess, Jack Clark, Christopher Berner, Sam McCandlish, Alec Radford, Ilya Sutskever, and Dario Amodei. Language models are few-shot learners. In *Advances in Neural Information Processing Systems 33: Annual Conference on Neural Information Processing Systems 2020, NeurIPS 2020, December 6-12, 2020, virtual*, 2020.

[CLL+05]   Moses Charikar, Eric Lehman, Ding Liu, Rina Panigrahy, Manoj Prabhakaran, Amit Sahai, and Abhi Shelat. The smallest grammar problem. *IEEE Trans. Inf. Theory*, 51(7):2554–2576, 2005.

[DGMH+19]   Miguel Domingo, Mercedes García-Martínez, Alexandre Helle, Francisco Casacuberta, and Manuel Herranz. How much does tokenization affect neural machine translation? In *International Conference on Computational Linguistics and Intelligent Text Processing*, pages 545–554. Springer, 2019.

[FTN+19]   Isamu Furuya, Takuya Takagi, Yuto Nakashima, Shunsuke Inenaga, Hideo Bannai, and Takuya Kida. MR-RePair: Grammar compression based on maximal repeats. In Ali Bilgin, Michael W. Marcellin, Joan Serra-Sagristà, and James A. Storer, editors, *Data Compression Conference, DCC 2019, Snowbird, UT, USA, March 26-29, 2019*, pages 508–517. IEEE, 2019.

[Gag94]   Philip Gage. A new algorithm for data compression. *The C Users Journal*, 12(2):23–38, 1994.

[Gal19]   Matthias Gallé. Investigating the effectiveness of BPE: The power of shorter sequences. In *Proceedings of the 2019 conference on empirical methods in natural language processing and the 9th international joint conference on natural language processing (EMNLP-IJCNLP)*, pages 1375–1381, 2019.

[GIM+19]   Travis Gagie, Tomohiro I, Giovanni Manzini, Gonzalo Navarro, Hiroshi Sakamoto, and Yoshimasa Takabatake. Rpair: rescaling RePair with rsync. In *International Symposium on String Processing and Information Retrieval*, pages 35–44. Springer, 2019.

[GJ17]   Michał Gańczorz and Artur Jeż. Improvements on Re-Pair grammar compressor. In *2017 Data Compression Conference (DCC)*, pages 181–190. IEEE, 2017.

[GVBS23]   Ximena Gutierrez-Vasques, Christian Bentz, and Tanja Samardžić. Languages through the looking glass of BPE compression. *Computational Linguistics*, 49(4):943–1001, 2023.

[Jeż14]   Artur Jeż. A really simple approximation of smallest grammar. In *Symposium on Combinatorial Pattern Matching*, pages 182–191. Springer, 2014.

[Kar72]   Richard M. Karp. Reducibility among combinatorial problems. In Raymond E. Miller and James W. Thatcher, editors, *Proceedings of a symposium on the Complexity of Computer Computations, held March 20-22, 1972, at the IBM Thomas J. Watson Research Center, Yorktown Heights, New York, USA*, The IBM Research Symposia Series, pages 85–103. Plenum Press, New York, 1972.

[KVOB24]   Justin Kim, Rahul Varki, Marco Oliva, and Christina Boucher. Recursive RePair: Increasing the scalability of repair by decreasing memory usage. *bioRxiv*, pages 2024–07, 2024.

[KY00]   John C Kieffer and En-Hui Yang. Grammar-based codes: A new class of universal lossless source codes. *IEEE Transactions on Information Theory*, 46(3):737–754, 2000.

[LLSZ21]   Zhuang Liu, Wayne Lin, Ya Shi, and Jun Zhao. A robustly optimized bert pre-training approach with post-training. In *China National Conference on Chinese Computational Linguistics*, pages 471–484. Springer, 2021.

[LM00]   N Jesper Larsson and Alistair Moffat. Off-line dictionary-based compression. *Proceedings of the IEEE*, 88(11):1722–1732, 2000.

[Loh12]   Markus Lohrey. Algorithmics on slp-compressed strings: A survey. *Groups-Complexity-Cryptology*, 4(2):241–299, 2012.

[LSFA+23]   Teven Le Scao, Angela Fan, Christopher Akiki, Ellie Pavlick, Suzana Ilić, Daniel Hesslow, Roman Castagné, Alexandra Sasha Luccioni, François Yvon, Matthias Gallé, et al. Bloom: A 176b-parameter open-access multilingual language model. 2023.

[MAS+21]   Sabrina J Mielke, Zaid Alyafeai, Elizabeth Salesky, Colin Raffel, Manan Dey, Matthias Gallé, Arun Raja, Chenglei Si, Wilson Y Lee, Benoît Sagot, et al. Between words and characters: A brief history of open-vocabulary modeling and tokenization in nlp. *arXiv preprint arXiv:2112.10508*, 2021.

[NR08]   Gonzalo Navarro and Luís Russo. Re-pair achieves high-order entropy. In *Proceedings of the Data Compression Conference*, page 537, 2008.

[PY91]   Christos H. Papadimitriou and Mihalis Yannakakis. Optimization, approximation, and complexity classes. *J. Comput. Syst. Sci.*, 43(3):425–440, 1991.

[RWC+19]   Alec Radford, Jeffrey Wu, Rewon Child, David Luan, Dario Amodei, Ilya Sutskever, et al. Language models are unsupervised multitask learners. *OpenAI blog*, 1(8):9, 2019.

[Ryt03]   Wojciech Rytter. Application of Lempel–Ziv factorization to the approximation of grammar-based compression. *Theoretical Computer Science*, 302(1-3):211–222, 2003.

[Sen15]   Rico Sennrich. Neural machine translation of rare words with subword units. *arXiv preprint arXiv:1508.07909*, 2015.

[SKF+99]   Yusuke Shibata, Takuya Kida, Shuichi Fukamachi, Masayuki Takeda, Ayumi Shinohara, Takeshi Shinohara, and Setsuo Arikawa. Byte pair encoding: A text compression scheme that accelerates pattern matching. *Technical Report DOI-TR-161, Department of Informatics, Kyushu University*, 1999.

[SRZ+24]   Craig W Schmidt, Varshini Reddy, Haoran Zhang, Alec Alameddine, Omri Uzan, Yuval Pinter, and Chris Tanner. Tokenization is more than compression. *arXiv preprint arXiv:2402.18376*, 2024.

[SS82]   James A Storer and Thomas G Szymanski. Data compression via textual substitution. *Journal of the ACM (JACM)*, 29(4):928–951, 1982.

[TLI+23]   Hugo Touvron, Thibaut Lavril, Gautier Izacard, Xavier Martinet, Marie-Anne Lachaux, Timothée Lacroix, Baptiste Rozière, Naman Goyal, Eric Hambro, Faisal Azhar, et al. Llama: Open and efficient foundation language models. *arXiv preprint arXiv:2302.13971*, 2023.

[WGC+23]   Jiayang Wu, Wensheng Gan, Zefeng Chen, Shicheng Wan, and S Yu Philip. Multimodal large language models: A survey. In *2023 IEEE International Conference on Big Data (BigData)*, pages 2247–2256. IEEE, 2023.

[WS11]   David P. Williamson and David B. Shmoys. *The Design of Approximation Algorithms*. Cambridge University Press, 2011.

[XZG⁺21]   Jingjing Xu, Hao Zhou, Chun Gan, Zaixiang Zheng, and Lei Li. Vocabulary learning via optimal transport for neural machine translation. In *Proceedings of the 59th Annual Meeting of the Association for Computational Linguistics and the 11th International Joint Conference on Natural Language Processing (Volume 1: Long Papers)*, pages 7361–7373, 2021.

[ZMG⁺23]   Vilém Zouhar, Clara Meister, Juan Luis Gastaldi, Li Du, Tim Vieira, Mrinmaya Sachan, and Ryan Cotterell. A formal perspective on byte-pair encoding. *arXiv preprint arXiv:2306.16837*, 2023.