ENTROPY BOUNDS FOR GRAMMAR-BASED TREE COMPRESSIONS

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Abstract. The definition of $k$th-order empirical entropy of strings is extended to node-labelled binary trees. A suitable binary encoding of tree straight-line programs (that have been used for grammar-based tree compression before) is shown to yield binary tree encodings of size bounded by the $k$th-order empirical entropy plus some lower order terms. This generalizes recent results for grammar-based string compression to grammar-based tree compression.

Keywords. Grammar-based compression, binary trees, empirical entropy, lossless compression

1. Introduction

Grammar-based string compression. The idea of grammar-based compression is based on the fact that in many cases a word $w$ can be succinctly represented by a context-free grammar that produces exactly $w$. Such a grammar is called a straight-line program (SLP) for $w$. In the best case, one gets an SLP of size $O(\log n)$ for a word of length $n$, where the size of an SLP is the total length of all right-hand sides of the rules of the grammar. A grammar-based compressor is an algorithm that produces for a given word $w$ an SLP $G_w$ for $w$, where, of course, $G_w$ should be smaller than $w$. Grammar-based compressors can be found at many places in the literature. Probably the best known example is the classical LZ78-compressor of Lempel and Ziv [27]. Indeed, it is straightforward to transform the LZ78-representation of a word $w$ into an SLP for $w$. Other well-known grammar-based compressors are Bisection [18], Sequitur [24], and Repair [19], just to mention a few.

Recently, several upper bounds on the compression performance of grammar-based compressors in terms of higher order empirical entropy have been shown. For this, the choice of a concrete binary encoding $B(G)$ of an SLP $G$ is crucial. Kieffer and Yang [17] came up with such a binary encoding $B$ and proved that under certain assumptions on the grammar-based compressor $w \mapsto G_w$, the combined compressor $w \mapsto B(G_w)$ yields a universal code with respect to the family of finite-state information sources over finite alphabets. Concretely, it is needed that the size of the SLP $G_w$ is bounded by $O(|w|/\log \sigma |w|)$ where $\sigma$ is the size of the underlying alphabet and $\hat{\sigma} = \max\{2, \sigma\}$. This upper bound is met by all grammar-based compressors that only produce so-called irreducible SLPs [17], which is the case for e.g. LZ78, Bisection, and Repair after a small modification of the latter. In their recent paper [25], Navarro and Ochoa used the binary encoding $B(G_w)$ in order to prove for every word $w$ over an alphabet of size $\sigma$ the upper bound $|B(G_w)| \leq |w|H_k(w) + o(|w| \log \hat{\sigma})$ for every $k \in o(\log \sigma |w|)$. Here, $H_k(w)$ is the

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empirical $k^{th}$-order entropy of $w$, and the grammar-based compressor $w \mapsto G_w$ must satisfy the upper bound $|G_w| \leq O(|w|/\log_\sigma |w|)$. Similar but weaker upper bounds for different binary SLP-encodings have been shown in \cite{12, 23}.

**Grammar-based tree compression.** Grammar-based compression has been generalized from strings to trees by means of linear context-free tree grammars generating exactly one tree \cite{3}. Such grammars are also known as tree straight-line programs, TSLPs for short, see \cite{21} for a survey. TSLPs can be seen as a proper generalization of SLPs and DAGs (directed acyclic graphs, which are a widely used compact representation of trees). Whereas DAGs only have the ability to share repeated subtrees of a tree, TSLPs can also share repeated tree patterns with a hole (so-called contexts). In \cite{9}, the authors presented a linear time algorithm that computes for a given binary tree $t$ of size $n$ and with $\sigma$ node labels a TSLP $G_t$ of size $O(n/\log_\sigma n)$; an alternative algorithm with the same asymptotic size bound can be found in \cite{10}. TSLPs have been also extended to so-called forest straight-line programs (FSLPs) which allow to compress unranked node-labelled trees \cite{13}. FSLPs are very similar to top DAGs \cite{2} and also meet the size bound $O(n/\log_\sigma n)$ for unranked trees of size $n$ with $\sigma$ node labels. The reader should notice that the $O(n/\log_\sigma n)$-bound cannot be achieved by DAGs: the smallest DAG for an unlabelled binary tree of size $n$ may still contain $n$ edges.

**Entropy bounds for grammar-based tree compressors.** In this paper we first consider binary node-labelled trees: every node has a label from a finite set $\Sigma$ of size $\sigma$ and every non-leaf node has a left and a right child. For binary unlabelled trees the results of Kieffer and Yang on universal grammar-based compressors have been extended to trees in \cite{15, 26}. Whereas the universal tree encoder from \cite{26} is based on DAGs (and needs a certain assumption on the average DAG size with respect to the input distribution), the encoder from \cite{15} uses TSLPs of size $O(n/\log_\sigma n)$. For this, a binary encoding of TSLPs similar to the one for SLPs from \cite{17} is proposed. In this paper we extend the binary TSLP-encoding from \cite{15} to node-labelled binary trees and prove an upper bound similar to the one from \cite{25} for strings. To do this, we first have to come up with a reasonable higher order entropy for binary node-labelled trees (we just speak of binary trees in the following). Several notions of tree entropy can be found in the literature, but all are tailored towards unranked trees and do not yield nontrivial results for binary trees.

- The $k^{th}$-order label entropy from \cite{6} is based on the empirical probability that a node $v$ is labelled with a certain symbol conditioned on the $k$ first labels from the parent node of $v$ to the root of the tree.
- The tree entropy from \cite{16} is the $0^{th}$ order entropy of the node degrees.
- Recently, two combinations of the two previous entropy measures were proposed in \cite{11}. The first combination is based on the empirical probability that a node $v$ is labelled with a certain symbol conditioned on (i) the $k$ first labels from the parent node of $v$ to the root and (ii) the node degree of $v$. The second combination uses the empirical probability that a node $v$ has a certain degree conditioned on (i) the $k$ first labels from the parent node of $v$ to the root and (ii) the node label of $v$.

Tree entropy \cite{16} is not useful in the context of binary trees, since a binary tree with $n$ leaves has $n-1$ nodes of degree 2, which shows that the tree entropy divided by the number of nodes $(2n-1)$ converges to 1 when $n$ increases. On the other
hand, the $k^{th}$-order label entropy is not useful for unlabelled trees. For the special case of unlabelled binary trees, also the combinations of $[11]$ do not lead to useful entropy measures.

Our first contribution is the definition of a reasonable entropy measure for binary trees that can be also used for the unlabelled case. For this we define the $k$-history of a node $v$ in a binary tree $t$ by taking the last $k$ edges on the unique path from the root to $v$. For each edge $(v_1, v_2)$ traversed on this path we write down the node label of $v_1$ and a 0 (resp., 1) if $v_2$ is a left (resp., right) child of $v_1$. Thus, the $k$-history of a node is a word of length $2k$ that alternatingly consists of symbols from $\Sigma$ and directions that are encoded by 0 or 1. For nodes at depth smaller than $k$ we pad the history with 0’s and a default node label $\square \in \Sigma$ in order to get length exactly $k$. \footnote{This is an ad hoc decision to make the definitions easier. Alternatively, one could allow histories of length shorter than $k$; this would not change our results.}

For each $k$-history $h$ we then consider the joint probability distribution $P_h^t$ of the node degree (either 0 or 2) and the node label, conditioned on the history $h$. Thus, $P_h^t(a,i)$ is the probability that a randomly chosen node among the nodes with history $h$ is labelled with the symbol $a$ and has $i \in \{0,2\}$ children. The $k^{th}$-order empirical entropy of $t$, $H_k(t)$ for short, is then the sum of the entropies of these distributions $P_h^t$ (the sum is taken over all histories $h$) weighted with the number of nodes with history $h$. This definition is similar to the definition of the $k^{th}$ order empirical entropy of a string (see Section 6).

Our main result states that

\begin{equation}
|B(G_t)| \leq H_k(t) + \mathcal{O}(kn \log \hat{\sigma}/\log_2 n) + \mathcal{O}(n \log \log_2 n/\log_2 n) + \sigma,
\end{equation}

where $t$ is a binary tree with $n$ leaves, the grammar-based compressor $t \mapsto G_t$ produces TSLPs of size $\mathcal{O}(n/\log n)$ for binary trees of size $n$, and $B$ is the binary TSLP-encoding from [15]. If $k \leq o(\log_2 n)$ then this bound can be simplified to $|B(G_t)| \leq H_k(t) + o(n \log \hat{\sigma})$. The assumption $k \leq o(\log_2 n)$ can be also found in [25]. In fact, Gagie argued in [8] that $k^{th}$-order empirical entropy for strings stops being a reasonable complexity measure for almost all strings of length $n$ over alphabets of size $\sigma$ when $k \geq \log_2 n$.

In the final section of the paper we present a simple extension of our entropy notion to node-labelled unranked trees. In an unranked tree the number of children of a node is arbitrary. Unranked trees are important in the area of XML, where the hierarchical structure of a document is represented by a node-labelled unranked tree. For such a tree $t$ we define the $k^{th}$-order empirical entropy as the $k^{th}$-order empirical entropy of the first-child next-sibling (fcns for short) encoding of $t$. The fcns-encoding of $t$ is a binary tree which contains all nodes of $t$. If a node $v$ of $t$ has the first (i.e., left-most) child $v_1$ and the right sibling $v_2$ then $v_1$ (resp., $v_2$) is the left (resp., right) child of $v$ in the fcns-encoding of $t$. If $v$ has no child or no right sibling then one adds dummy leaves to the fcns encoding in order to obtain a full binary tree. Our choice of defining the $k^{th}$-order empirical entropy of an unranked tree via the fcns-encoding is motivated by the fact that in XML document trees the label of a node $v$ usually depends on the labels of the ancestors and the labels of the left siblings of $v$. This information is contained in the history of $v$ in the fcns-encoding.

We present experimental results with real XML document trees showing that in these cases the $k^{th}$-order empirical entropy is indeed very small compared to
the worst case bit size. An unranked tree with \(n\) nodes and \(\sigma\) node labels can be
encoded with \(2n + \log_2(\sigma)n\) bits [14]. Up to low order terms, this is optimal. Table 1
shows the values of the \(k^{th}\)-order empirical entropy (for \(k = 1, 2, 4, 8\)) divided by
\(2n + \log_2(\sigma)n\) for several real XML trees (that were also used in other experiments
for XML compression). For \(k = 4\), these quotients never exceed 20% and for \(k = 8\)
all quotients are bounded by 13.5%.

Our experimental results combined with our entropy bound [11] for grammar-
based compression are in accordance with the fact that grammar-
based tree com-
pressors yield excellent compression ratios for XML document trees, see e.g. [22].
Some of the XML documents from our experiments were also used in [22], where
the performance of TreeRePair (currently the best grammar-based tree compressor
from a practical point of view) on XML document trees was tested. It is interesting
to note that those XML trees, where our \(k\)-th order empirical entropy is large (in
particular, Treebank) are indeed those XML trees with the worst compression ratio
for TreeRePair in [22].

2. Preliminaries

In this section, we introduce some basic definitions concerning information theory
(Section 2.1) and binary trees (Section 2.2). The latter are our key formalism for
the compression of binary trees.

With \(\mathbb{N}\) we denote the natural numbers including 0. We use the standard \(O\)-
notation. If \(b > 0\) is a constant, then we just write \(O(\log n)\) for \(O(\log_b n)\). We make
the convention that \(0 \cdot \log(0) = 0\). For the unit interval \(\{r \in \mathbb{R} \mid 0 \leq r \leq 1\}\) we
write \([0, 1]\).

Let \(w = a_1a_2 \cdots a_l \in \Gamma^*\) be a word over an alphabet \(\Gamma\). With \(|w| = l\) we denote
the length of \(w\). The empty word is denoted by \(\varepsilon\). For \(a \in \Gamma\) we denote with
\(|w|_a = |\{i \mid 1 \leq i \leq l, a_i = a\}|\) the number of occurrences of \(a\) in \(w\).

2.1. Empirical distributions and empirical entropy. Let \(A\) be a finite set. A
probability distribution on \(A\) is a mapping \(p : A \to [0, 1]\) such that \(\sum_{a \in A} p(a) = 1\).
For a probability distribution \(p\) on \(A\) we define its Shannon entropy

\[
H(p) = \sum_{a \in A} -p(a) \log_2 p(a) = \sum_{a \in A} p(a) \log_2 (1/p(a)) .
\]

We have \(0 \leq H(p) \leq \log_2 |A|\). A well-known generalization of Shannon’s inequality
states that for every probability distribution \(p\) on \(A\) and any mapping \(q : A \to [0, 1]\)
such that \(\sum_{a \in A} q(a) \leq 1\) we have

\[
H(p) = \sum_{a \in A} -p(a) \log_2 p(a) \leq \sum_{a \in A} -p(a) \log_2 q(a) ;
\]

see [1] for a proof. Shannon’s inequality is the special case where \(q\) is a probability-
distribution as well. The Kullback-Leibler divergence between two probability
distributions \(p, q\) on \(A\) (see [5] Section 2-3) is defined as

\[
D(p \parallel q) = \sum_{a \in A} p(a) \cdot \log_2 (p(a)/q(a)) .
\]

It is known that \(D(p \parallel q) \geq 0\) for all \(p, q\) (this follows from Shannon’s inequality)
and \(D(p \parallel q) = 0\) if and only if \(p = q\).
Let $\pi = (a_1, a_2, \ldots, a_n)$ be a tuple of elements that are from some (not necessarily finite) set $S$. The empirical distribution $p_\pi : \{a_1, a_2, \ldots, a_n\} \to [0, 1]$ of $\pi$ is defined by

$$p_\pi(a) = \frac{|\{i \mid 1 \leq i \leq n, a_i = a\}|}{n}.$$  

We use this (and the following) definition also for words over some alphabet by identifying a word $w = a_1a_2 \cdots a_n$ with the tuple $(a_1, a_2, \ldots, a_n)$. The unnormalized empirical entropy of $\pi$ is

$$H(\pi) = n \cdot H(p_\pi) = -\sum_{i=1}^{n} \log_2 p_\pi(a_i).$$  

From [2] it follows that for a tuple $\pi = (a_1, a_2, \ldots, a_n)$ with $a_1, \ldots, a_n \in S$ and real numbers $q(a) \geq 0$ ($a \in S$) with $\sum_{a \in \{a_1, \ldots, a_n\}} q(a) \leq 1$ we have

$$\sum_{i=1}^{n} -\log_2 p_\pi(a_i) \leq \sum_{i=1}^{n} -\log_2 q(a_i).$$

2.2. Trees, tree processes, and tree entropy.

2.2.1. Trees and contexts. Let $\Sigma$ denote a finite non-empty alphabet of size $|\Sigma| = \sigma$. Later, we will need a fixed distinguished symbol from $\Sigma$ that we will denote with $\Box \in \Sigma$. We will also need the value $\hat{\sigma} = \max\{2, \sigma\}$. With $T(\Sigma)$ we denote the set of labelled binary trees over the alphabet $\Sigma$. Formally, it is inductively defined as the smallest set of terms over $\Sigma$ such that (i) $\Sigma \subseteq T(\Sigma)$ and (ii) if $t_1, t_2 \in T(\Sigma)$ and $a \in \Sigma$, then $a(t_1, t_2) \in T(\Sigma)$.

With $|t|$ we denote the number of leaves of $t$, which can be inductively defined by $|a| = 1$ and $|a(t_1, t_2)| = |t_1| + |t_2|$ for $a \in \Sigma$ and $t_1, t_2 \in T(\Sigma)$. Note that $2|t| - 1$ is the number of occurrences of symbols from $\Sigma$ in $t$. Let $T_n(\Sigma) = \{t \in T(\Sigma) \mid |t| = n\}$ for $n \geq 1$. We have $|T_n(\Sigma)| = \sigma^{2n-1}C_{n-1}$, where $C_k$ is the $k^{\text{th}}$ Catalan number. These numbers satisfy the following well-known asymptotic estimate

$$C_k \sim \frac{4^k}{\sqrt{\pi}k^2}.$$  

see e.g. [7]. In fact, we have $C_k \leq 4^k$ for all $k \geq 0$ and hence $|T_n(\Sigma)| \leq (2\sigma)^{2n}$.

A context is a labelled binary tree $c$, where exactly one leaf is labelled with the special symbol $x \notin \Sigma$ (called the parameter); all other nodes are labelled with symbols from $\Sigma$. Formally, the set of contexts $C(\Sigma)$ is the smallest set such that (i) $x \in C(\Sigma)$ and (ii) if $a \in \Sigma$, $c \in C(\Sigma)$ and $t \in T(\Sigma)$ then also $a(c, t), a(t, c) \in C(\Sigma)$.

For a tree or context $t \in T(\Sigma) \cup C(\Sigma)$ and a context $c \in C(\Sigma)$, we denote by $c[t]$ the tree or context which results from $c$ by replacing the unique occurrence of the parameter $x$ by $t$. For example $c = f(a, x)$ and $t = g(a, b)$ yields $c[t] = f(a, g(a, b))$ (with $\Sigma = \{a, b, f, g\}$). For a context $c$ we define $|c|$ inductively by $|x| = 0$ and $|a(c, t)| = |a(t, c)| = |t| + |c|$ for $c \in C(\Sigma)$ and $t \in T(\Sigma)$. In other words, $|c|$ is the number of leaves of $c$, where the unique occurrence of the parameter $x$ is not counted. Note that $|c| = |c[a]| - 1$, where $a \in \Sigma$ is arbitrary. We define $C_n(\Sigma) = \{c \in C(\Sigma) \mid |c| = n\}$ for $n \in \mathbb{N}$. Since the set $\Sigma$ will not change in this paper, we use the abbreviations $T$, $T_n$, $C$, and $C_n$ for $T(\Sigma)$, $T_n(\Sigma)$, $C(\Sigma)$, and $C_n(\Sigma)$, respectively.

Occasionally, we will consider a binary tree or context as a graph with nodes and edges in the usual way, where each node is labelled with a symbol from $\Sigma$ (or $x$ in
the case of a context). Note that $t \in T \cup C$ has $2n - 1$ nodes in total: $n$ leaves and $n - 1$ internal nodes.

It is convenient to define a node $v$ of $s \in T \cup C$ as a bit string that describes the path from the root to the node ($0$ means left, $1$ means right). Formally, we define the node set $V(s) \subseteq \{0, 1\}^*$ of $s \in T \cup C$ by

- $V(a) = \{\varepsilon\}$ for every $a \in \Sigma$,
- $V(x) = \emptyset$ and
- $V(a(s_0, s_1)) = \{iw \mid i \in \{0, 1\}, w \in V(s_i)\} \cup \{\varepsilon\}$ for every $a \in \Sigma$.

Note that for a context $c \in C$, the set $V(c)$ does not contain the unique node in $c$ labelled with the parameter $x$. We use this definition due to better readability of the paper since we mostly need the set of nodes without the parameter node. Also, it is still possible to uniquely determine from $V(c)$ the path to the parameter $x$ due to the following properties: For a tree $t \in T$ we have $w0 \in V(t)$ if and only if $w1 \in V(t)$ for all $w \in \{0, 1\}^*$ since each node has zero or two children. The only context $c$ which fulfills this property is $c = x$, i.e. the parameter node is the only node of $c$ and $V(c) = \emptyset$. For all other contexts $c \in C$ this property is violated since there exists a unique $w \in \{0, 1\}^*$ such that $w0 \in V(c)$ (respectively, $w1 \in V(c)$) and $w1 \notin V(c)$ (respectively, $w0 \notin V(c)$). In this case the parameter node is $w1$ (respectively, $w0$). Alternatively, the parameter node of a context $c$ is the single node in the set $V(c[a]) \setminus V(c)$ for a symbol $a \in \Sigma$. We denote this node with $\omega(c) \in \{0, 1\}^*$. In other words: $V(c[a]) \setminus V(c) = \{\omega(c)\}$.

**Example 1.** Consider the tree $t = a(b(b(a, b), a), a(b, a))$ with $\Sigma = \{a, b\}$ depicted on the left of Figure 1. We have $V(t) = \{\varepsilon, 0, 1, 00, 01, 10, 11, 000, 001\}$. For the context $c = a(b(b(a, b), x), a(b, a))$ depicted on the right of Figure 1, we have $t = c[a]$ and $\omega(c) = 01$.

Consider a tree or context $s$ and let $v \in V(s)$. The leaves of $s$ are those strings in $V(s)$ that are maximal with respect to the prefix relation. The length $|v|$ is the depth of the node $v$ in $s$ and the depth of $s$ is the maximal depth of a node in $V(s)$.

Let $\lambda_s : V(s) \to \Sigma \times \{0, 2\}$ denote the function mapping a node $v$ to a pair $(a, i)$ where $a \in \Sigma$ is the label of $v$ and $i \in \{0, 2\}$ is the number of children of $v$. We can define this function inductively as follows:

- $\lambda_s(\varepsilon) = (a, 0)$,
- $\lambda_s(s) = (a, 2)$ for $s = a(s_0, s_1)$,
- $\lambda_s(iw) = \lambda_s(w)$ for $s = a(s_0, s_1)$ and $iw \in V(s)$.

Note that in the last case, if $s$ is a context, we cannot have $s_1 = x$ because we must have $w \in V(s_i)$. If $s$ is clear from the context then we will omit the subscript $s$ in $\lambda_s(v)$.
We define the set of histories as
\[ \mathcal{L} = (\Sigma \{0, 1\})^* = \{a_1 i_1 \cdots a_n i_n \mid n \geq 0, a_k \in \Sigma, i_k \in \{0, 1\} \text{ for all } 1 \leq k \leq n\}. \]

For an integer \( k \geq 1 \), let \( \mathcal{L}_k = \{v \in \mathcal{L} \mid |v| = 2k\} \) and let \( \ell_k : \mathcal{L} \to \mathcal{L}_k \) denote the partial function mapping a history \( z \in \mathcal{L} \) with \(|z| \geq 2k\) to the suffix of \( z \) of length \( 2k \), i.e., \( \ell_k(a_1 i_1 \cdots a_n i_n) = a_{n-k+1} i_{n-k+1} \cdots a_n i_n \).

For a tree \( t \) and a node \( v \in V(t) \) (resp., a context \( c \) and a node \( v \in V(c) \cup \{\omega(c)\} \)), we inductively define its history \( h(v) \in \mathcal{L} \) by (i) \( h(\varepsilon) = \varepsilon \) and (ii) \( h(wi) = h(w)ai \) for \( i \in \{0, 1\} \) and \( wi \in V(t) \) (resp., \( wi \in V(c) \cup \{\omega(c)\} \)). Here, \( a \) is the symbol that labels the node \( w \), i.e., \( \lambda(w) = (a, 2) \). That is, in order to obtain \( h(v) \), while walking downwards in the tree from the root node to the node \( v \), we alternately concatenate symbols from \( \Sigma \) with binary numbers in \( \{0, 1\} \) such that the symbol from \( \Sigma \) corresponds to the label of the current node and the binary number 0 (resp., 1) states that we move on to the left (resp. right) child node. Note that the symbol that labels \( v \) is not part of the history of \( v \). The \( k \)-history of a tree node \( v \in V(t) \) is \( h_k(v) = \ell_k((\Box 0)^k h(v)) \in \mathcal{L}_k \), i.e., the suffix of length \( 2k \) of the word \( (\Box 0)^k h(v) \), where \( \Box \) is a fixed dummy symbol in \( \Sigma \). The choice is arbitrary. This means that if \(|v| \geq k\) then \( h_k(v) \) describes the last \( k \) directions and node labels along the path from the root to node \( v \). If \(|v| < k\), we pad the history of \( v \) with \( \Box \)’s and zeros such that \( h_k(v) \in \mathcal{L}_k \). For \( z \in \mathcal{L}_k \) we denote with \( V_z(t) = \{v \in V(t) \mid h_k(v) = z\} \) the set of nodes in \( t \) with \( k \)-history \( z \).

A tree encoder is an injective mapping \( E : \mathcal{T} \to \{0, 1\}^* \) such that the range \( E(\mathcal{T}) \) is prefix-free, i.e., there do not exist \( t, t' \in \mathcal{T} \) with \( t \neq t' \) such that \( E(t) \) is a prefix of \( E(t') \).

2.2.2. Tree processes. A tree process is an infinite tuple \( \mathcal{P} = (P_z)_{z \in \mathcal{L}} \) where every \( P_z \) is a probability distribution on \( \Sigma \times \{0, 2\} \). With \( \mathcal{P} \) we associate the function \( \text{Prob}_\mathcal{P} : \mathcal{T} \cup \mathcal{C} \to [0, 1] \) with
\[
\text{Prob}_\mathcal{P}(s) = \prod_{v \in V(s)} P_{h(v)}(\lambda_s(v)).
\]

We are mainly interested in this definition for the case that \( s \) is a tree, but for technical reasons we also have to allow contexts. Note that if \( c \) is a context, then the parameter node of \( c \) is not in \( V(c) \) and therefore does not contribute to \( \text{Prob}_\mathcal{P}(c) \).

A tree process can be used to randomly construct a tree from \( \mathcal{T} \) as follows: In a top-down way we determine for every tree node its label (from \( \Sigma \)) and its number of children, where this decision depends on the history of the tree node. We start at the root node, whose history is the empty word \( \varepsilon \). If we have reached a tree node \( v \) with history \( z \in \mathcal{L} \) then we use the probability distribution \( P_z \) to randomly choose a pair \((a, i) \in \Sigma \times \{0, 2\} \). We assign the label \( a \in \Sigma \) to \( v \). If \( i = 0 \) then \( v \) becomes a leaf, otherwise the process continues at the two children \( v0 \) and \( v1 \) (whose history is well-defined). Note that in this way we may produce infinite trees with non-zero probability (e.g., if \( P_z(a, 2) = 1 \) for some \( a \in \Sigma \)). Therefore, we only obtain an inequality instead of an equality in the following lemma (recall that \( \mathcal{T} \) only contains finite trees).

Lemma 1. Let \( \mathcal{P} \) be a tree process. Then \( \sum_{t \in \mathcal{T}} \text{Prob}_\mathcal{P}(t) \leq 1 \).

Proof. Define the set of trees \( \mathcal{T}'_n \) inductively by \( \mathcal{T}'_1 = \mathcal{T}_1 \) and \( \mathcal{T}'_{n+1} = \mathcal{T}'_n \cup \{a(t_1, t_2) \mid a \in \Sigma, t_1, t_2 \in \mathcal{T}'_n\} \). We have \( \mathcal{T}'_n \subseteq \mathcal{T}'_{n+1} \) and \( \mathcal{T} = \bigcup_{n \geq 1} \mathcal{T}'_n \). It then suffices to show
that \(\sum_{t \in T'} \operatorname{Prob}_P(t) \leq 1\) for every \(n \geq 1\). This follows easily from the definition of \(\operatorname{Prob}_P(t)\) and the inductive definition of \(T_n'\).

\[ \square \]

**Lemma 2.** Let \(P\) be a tree process. For every \(n \geq 1\) we have \(\sum_{c \in C_n} \operatorname{Prob}_P(c) \leq n + 1\).

**Proof.** As a first step we represent the probability of each context \(c \in C\) as a sum of probabilities of trees. So we fix a context \(c \in C\) for the first part of the proof. Recall that \(\omega(c)\) (the parameter node of \(c\)) does not contribute to the probability of the context \(c\), which is the reason why in general no tree \(t\) exists such that \(\operatorname{Prob}_P(c) = \operatorname{Prob}_P(t)\). For example the tree \(c[a]\) has probability \(\operatorname{Prob}_P(c) \cdot P_{h(\omega(c))}(a, 0)\). Therefore, instead of using one tree, we need to consider the set \(c[T] = \{c[t] | t \in T\}\) of all trees that arise from \(c\) by replacing the parameter by an arbitrary tree. Unfortunately, the total probability \(\sum_{t \in c[T]} \operatorname{Prob}_P(t)\) can still be strictly smaller than \(\operatorname{Prob}_P(c)\) since there might be infinite trees with positive probability with respect to \(P\). To get rid of that problem, we fix an element \(a \in \Sigma\) and modify \(P\) to a tree process \(P' = (P'_z)_{z \in \mathcal{L}}\) such that (i) \(P'_z = P_z\) for \(|z| \leq 2n\) and (ii) \(P'_z(a, 0) = 1\) and \(P'_z(a', i) = 0\) for every \((a', i) \in \Sigma \times \{0, 2\} \setminus \{(a, 0)\}\) and \(|z| > 2n\). The tree process \(P'\) is created such that all nodes \(v\) of depth \(|v| \leq n\) contribute the probability \(P_{h(v)}(\lambda(v))\) as before and all nodes of depth \(n + 1\) in a tree are \(a\)-labelled leaves with probability 1. Note first that for each context \(c \in C\) and each node \(v \in V(c)\) we have \(|v| \leq n\) and thus \(P'_{h(v)}(\lambda(v)) = P_{h(v)}(\lambda(v))\). Secondly, all trees of depth larger than \(n + 1\) have probability 0 with respect to \(P'\) (including infinite trees). Hence, we get \(\sum_{t \in T} \operatorname{Prob}_{P'}(t) = 1\). We obtain

\[
\sum_{t \in c[T]} \operatorname{Prob}_{P'}(t) = \sum_{t \in c[T]} \prod_{v \in V(t)} P'_{h(v)}(\lambda(v))
\]

\[
= \sum_{t \in c[T]} \left( \prod_{v \in V(c)} P'_{h(v)}(\lambda(v)) \prod_{v \in V(t) \setminus V(c)} P'_{h(v)}(\lambda(v)) \right)
\]

\[
= \operatorname{Prob}_P(c) \cdot \sum_{t \in c[T]} \prod_{v \in V(t) \setminus V(c)} P'_{h(v)}(\lambda(v))
\]

We claim that (a) equals 1. To see this, consider the tree process \(P'' = (P''_z)_{z \in \mathcal{L}}\) with \(P''_z = P'_{h(\omega(c))}z\). It is still true that only finite trees have non-zero probability and thus \(\sum_{t \in T} \operatorname{Prob}_{P''}(t) = 1\). We have

\[
(a) = \sum_{t \in T} \prod_{v \in V(t)} P'_{h(\omega(c))h(v)}(\lambda(v)) = \sum_{t \in T} \prod_{v \in V(t)} P''_{h(v)}(\lambda(v))
\]

\[
= \sum_{t \in T} \operatorname{Prob}_{P''}(t) = 1.
\]

It follows that \(\operatorname{Prob}_P(c) = \sum_{t \in c[T]} \operatorname{Prob}_{P'}(t)\). In the second part of the proof it remains to bound \(\sum_{c \in C_n} \operatorname{Prob}_P(c) = \sum_{c \in C_n} \sum_{t \in c[T]} \operatorname{Prob}_{P'}(t)\). The key point here is that for each tree \(t \in T\) there are at most \(n + 1\) different contexts \(c \in C\) such that \(t \in c[T]\). Note that for a tree \(t\), the number of different contexts \(c \in C\) such that \(t \in c[T]\) is exactly the number of nodes \(v \in V(t)\) such that replacing the subtree rooted at \(v\) by the parameter \(x\) yields a context of size \(n\). This is the same as the
number of subtrees of $t$ with $|t| - n$ leaves. Since different subtrees in $t$ of equal size do not share nodes, we can bound the number of subtrees with $|t| - n$ leaves by $|t|/(|t| - n)$. We can assume that $|t| > n$ since otherwise there is no context $c \in C_n$ such that $t \in c[T]$. So we have $|t| = n + k$ for some $k > 0$ and the number of subtrees of $t$ with $|t| - n$ leaves is at most $(n + k)/k = n/k + 1 \leq n + 1$. We get

$$\sum_{c \in \mathcal{C}_n} \sum_{t \in [T]} \text{Prob}_P(t) \leq (n + 1) \sum_{t \in [T]} \text{Prob}_P(t) = n + 1.$$ 

This concludes the proof of the lemma.

A $k$th-order tree process is a tree process $P = (P_z)_{z \in \mathcal{L}}$ such that $P_z = P_{z'}$ if $|z| = |z'|$, which is encoded with $2 \log_2 |z|$ symbols. Thus, the probability distribution that is chosen for a certain tree node depends only on the $2k$ last symbols of the history of the node (where histories are padded with $\emptyset$ on the left to reach length $2k$ for the fixed symbol $\emptyset \in \Sigma$). We will identify the $k$th-order tree process $P = (P_z)_{z \in \mathcal{L}}$ with the finite tuple $(P_z)_{z \in \mathcal{L}_k}$; it contains all information about $P$. Note that for a $k$th-order tree process $P$ we can compute $\text{Prob}_P(s)$ for a tree or context $s$ as

$$\text{Prob}_P(s) = \prod_{z \in \mathcal{L}_k} \prod_{v \in V_z(s)} P_z(\lambda(v)),$$

where the empty product (which arises in case $V_z(s) = \emptyset$) is 1.

2.2.3. Higher-order entropy of a tree. We define the $k$th-order (unnormalized) empirical entropy $H_k(t)$ of a tree $t \in \mathcal{T}_n$ as follows: For $z \in \mathcal{L}$ let $m_z^t = |V_z(t)|$ be the number of nodes of $t$ with history $z$ and for $\tilde{a} \in \Sigma \times \{0, 2\}$ let $m_{\tilde{a}, z}^t = |\{v \in V_z(t) \mid \lambda(v) = \tilde{a}\}|$. We then define the empirical $k$th-order tree process $P^t = (P_z^t)_{z \in \mathcal{L}_k}$ by

$$P^t_{z} (\tilde{a}) = m_{z, \tilde{a}}^t / m_z^t,$$

for all $\tilde{a} \in \Sigma \times \{0, 2\}$ and all $z \in \mathcal{L}_k$ with $m_z^t > 0$. If $m_z^t = 0$, then we can define $P_z^t$ as an arbitrary distribution. Then

$$H_k(t) = \sum_{z \in \mathcal{L}_k} m_z^t H(P_z^t).$$

Note that $0 \leq H_k(t) \leq (2n - 1) \log_2 (2\sigma) = (2n - 1)(1 + \log_2 \sigma)$ since $0 \leq H(P_z^t) \leq \log_2 (2\sigma)$ and $\sum_{z \in \mathcal{L}_k} m_z^t = 2n - 1$. This upper bound on the entropy matches the information theoretic bound for the worst-case output length of any tree encoder on $T_n$. Using the asymptotic bound [6] for the Catalan numbers, one sees that for any tree encoder there must exist a tree $t \in \mathcal{T}_n$ which is encoded with $2 \log_2 (2\sigma)n - o(n) = 2(\log_2 \sigma + 1)n - o(n)$ bits. The $k$th-order empirical entropy $H_k(t)$ is a lower bound on the coding length of a tree encoder that encodes for each node the relevant information (the label of the node and the binary information whether the node is a leaf or internal) depending on the $k$-history of the node.

Example 2. Let $t$ denote the binary tree $t = a(b(a,b,a),a(b,a))$ as depicted on the left of Figure [4]. In order to compute the first order empirical entropy $H_1(t)$ of $t$, we have to consider $k$-histories of $t$ with $k = 1$: Let $\emptyset = a$. We find $V_{a0}(t) = \{\varepsilon, 0, 10\}$, $V_{a1}(t) = \{00, 000\}$, $V_{b1}(t) = \{1, 11\}$ and $V_{b0}(t) = \{01, 001\}$. Thus, we have $m_{a0}^t = 3$ and $m_{b1}^t = m_{a0}^t = m_{b0}^t = 2$. Next, for each $k$-history $z$, we consider $\lambda(v)$ for $v \in V_z(t)$: For $z = a0$, we have $\lambda(\varepsilon) = (a, 2)$, $\lambda(0) = (b, 2)$ and $\lambda(10) = (b, 0)$. Hence, $m_{a0,(a,2)}^t = m_{a0,(b,0)}^t = m_{a0,(b,2)}^t = 1$ and $H(P_{a0}^t) = \log(3)$. 
Analogously, we find $H(P_n^0) = H(P_n^1) = H(P_n^u) = 1/2 \log(2) + 1/2 \log(2) = 1$. Altogether, this yields $H_1(t) = 3 \cdot \log(3) + 2 \cdot 1 + 2 \cdot 1 = 9.3$ which is roughly $9.3$.

One can define $H_k(t)$ alternatively in the following way: Take a $k$-history $z \in \mathcal{L}_k$ and enumerate the set $V_z(t)$ in an arbitrary way as $v_1, v_2, \ldots, v_j$. Define the string $w(t, z) = \lambda(v_1)\lambda(v_2) \cdots \lambda(v_j) \in (\Sigma \times \{0, 2\})^*$. We have

$$H_k(t) = \sum_{z \in \mathcal{L}_k} H(w(t, z)),$$

where the empirical entropy $H(w(t, z))$ is defined according to (3).

The following lemma and its proof are very similar to a corresponding statement for the $k^{th}$-order empirical entropy of strings, see [3].

**Theorem 1.** Let $t \in \mathcal{T}$. For every $k^{th}$-order tree process $\mathcal{P} = (P_z)_{z \in \mathcal{L}_k}$ with $\text{Prob}_\mathcal{P}(t) > 0$ we have

$$H_k(t) \leq -\log_2 \text{Prob}_\mathcal{P}(t)$$

with equality if and only if $P^t_z = P_z$ for all $z \in \mathcal{L}_k$ with $m^t_z > 0$.

**Proof.** We have

$$-\log_2 \text{Prob}_\mathcal{P}(t) = \sum_{z \in \mathcal{L}_k} \sum_{v \in V_z(t)} \log_2(1/P_z(\lambda(v)))$$

$$= \sum_{z \in \mathcal{L}_k} \sum_{a \in \Sigma \times \{0, 2\}} m^t_{z,a} \log_2(1/P_z(\tilde{a}))$$

$$= \sum_{z \in \mathcal{L}_k} m^t_z \sum_{a \in \Sigma \times \{0, 2\}} P^t_z(\tilde{a}) \cdot (\log_2(P^t_z(\tilde{a})/P_z(\tilde{a})) + \log_2(1/P_z(\tilde{a})))$$

$$\geq H_k(t)$$

with equality in the last line if and only if $P^t_z = P_z$ for all $z \in \mathcal{L}_k$ with $m^t_z > 0$. □

3. **Tree straight-line programs and compression of binary trees**

We now introduce tree straight-line programs and use them for the compression of binary trees.

3.1. **General tree straight-line programs.** Let $V$ be a finite ranked alphabet, where each symbol $A \in V$ has an associated rank 0 or 1. The elements of $V$ are called *nonterminals*. We assume that $V$ contains at least one element of rank 0 and that $V$ is disjoint from the set $\Sigma \cup \{x\}$, which are the labels used for binary trees and contexts. We use $V_0$ (resp., $V_1$) for the set of nonterminals of rank 0 (resp., of rank 1). The idea is that nonterminals from $V_0$ (resp., $V_1$) derive to trees from $\mathcal{T}$ (resp., contexts from $\mathcal{C}$). We denote by $\mathcal{T}_V(\Sigma)$ the set of trees over $\Sigma \cup V$, i.e., each node in a tree $t \in \mathcal{T}_V(\Sigma)$ is labelled with a symbol from $\Sigma \cup V$ and the number of children of a node corresponds to the rank of its label. With $\mathcal{C}_V(\Sigma)$ we denote the corresponding set of all contexts, i.e., the set of trees over $\Sigma \cup \{x\} \cup V$, where the parameter symbol $x$ occurs exactly once and at a leaf position. Formally, we define $\mathcal{T}_V(\Sigma)$ and $\mathcal{C}_V(\Sigma)$ as the smallest sets with the following conditions, where $\mathcal{C}_V(\Sigma)$ here and in the rest of the paper we use the abbreviations $\mathcal{T}_V$ for $\mathcal{T}_V(\Sigma)$ and $\mathcal{C}_V$ for $\mathcal{C}_V(\Sigma)$:
We also allow the TSLP:

\[ T \in C \]

If \( \rho \in \mathcal{G}(A) \) for some \( A \in \mathcal{T}_V \), then we set \( \rho(t) = \rho(A) \) for every \( t \in \mathcal{C}_V \). Furthermore, the binary relation \( \{ (A, B) \in V \times V \mid B \text{ occurs in } r(A) \} \) has to be acyclic. These conditions ensure that exactly one tree is derived from the start nonterminal \( A_0 \) by using the rewrite rules \( A \rightarrow r(A) \) for \( A \in V \). To define this formally, we define \( \text{val}_G(t) \in T \) for \( t \in \mathcal{T}_V \) and \( \text{val}_G(t) \in C \) for \( t \in \mathcal{C}_V \) inductively by the following rules:

1. \( \text{val}_G(a) = a \) for \( a \in \Sigma \) and \( \text{val}_G(x) = x \).
2. \( \text{val}_G(a(t_1, t_2)) = a(\text{val}_G(t_1), \text{val}_G(t_2)) \) for \( a \in \Sigma \) and \( t_1, t_2 \in \mathcal{T}_V \) or \( t_1 \in \mathcal{T}_V \) and \( t_2 \in \mathcal{C}_V \) since there is at most one parameter in \( a(t_1, t_2) \).
3. \( \text{val}_G(A) = \text{val}_G(r(A)) \) for \( A \in \mathcal{V}_0 \).
4. \( \text{val}_G(A(s)) = \text{val}_G(r(A))[\text{val}_G(s)] \) for \( A \in \mathcal{V}_1 \), \( s \in \mathcal{T}_V \) or \( \mathcal{C}_V \) (note that \( \text{val}_G(r(A)) \) is a context, so we can build \( c[\text{val}_G(s)] \)).

The tree defined by \( G \) is \( \text{val}(G) = \text{val}_G(A_0) \) is \( T \).

**Example 3.** Let \( \Sigma = \{ a, b \} \) and \( G = \{ (A_0, A_1, A_2), A_0, r \} \) be a TSLP with \( A_0, A_1 \in \mathcal{V}_0, A_2 \in \mathcal{V}_1 \) and

\[ r(A_0) = a(A_1, A_2(b)), r(A_1) = A_2(A_2(b)), r(A_2) = b(x, a). \]

We get \( \text{val}_G(A_2) = b(x, a), \text{val}_G(A_1) = b(b(b, a), a) \) and \( \text{val}(G) = \text{val}_G(A_0) = a(b(b(b, a), a), b(b, a)) \).

### 3.2. Tree straight-line programs in normal form

In this section, we will use TSLPs in a certain normal form, which we introduce first.

A TSLP \( G = (V, A_0, r) \) is in normal form if the following conditions hold:

1. \( V = \{ A_0, A_1, \ldots, A_{m-1} \} \) for some \( m \in \mathbb{N} \), \( m \geq 1 \).
2. For every \( A_i \in \mathcal{V}_0 \), the right-hand side \( r(A_i) \) is a term of the form \( A_j(\alpha) \), where \( A_j \in \mathcal{V}_1 \) and \( \alpha \in \mathcal{V}_0 \) or \( \mathcal{V}_1 \).
3. For every \( A_i \in \mathcal{V}_1 \) the right-hand side \( r(A_i) \) is a term of the form \( A_j(A_k(\alpha)), a(\alpha, x), \) or \( a(\alpha, x) \), where \( A_j, A_k \in \mathcal{V}_1 \), \( a \in \Sigma \) and \( \alpha \in \mathcal{V}_0 \) or \( \mathcal{V}_1 \).
4. For every \( A_i \in \mathcal{V} \) define the word \( \rho(A_i) \in (V \cup \Sigma)^* \) as follows:

\[
\rho(A_i) = \begin{cases} 
A_j(\alpha) & \text{if } r(A_i) = A_j(\alpha) \\
A_jA_k & \text{if } r(A_i) = A_j(A_k(\alpha)) \\
AA & \text{if } r(A_i) = a(\alpha, x) \text{ or } a(\alpha, x) 
\end{cases}
\]

Let \( \rho_G = \rho(A_0) \rho(A_1) \cdots \rho(A_{m-1}) \in (\Sigma \cup \{A_1, A_2, \ldots, A_{m-1}\})^* \). Then we require that \( \rho_G \) is of the form \( \rho_G = A_1u_1A_2u_2 \cdots A_{m-1}u_{m-1} \) with \( u_i \in (\Sigma \cup \{A_1, A_2, \ldots, A_i\})^* \).

5. \( \text{val}_G(A_i) \neq \text{val}_G(A_j) \) for \( i \neq j \)

We also allow the TSLP \( G_a = \{ (A_0), A_0, a \} \) for every \( a \in \Sigma \) in order to get the singleton tree \( a \). In this case, we set \( \rho_G = \rho(A_0) = a \).

Let \( G = (V, A_0, r) \) be a TSLP in normal form with \( V = \{ A_0, A_1, \ldots, A_{m-1} \} \) for the further definitions. We define the size of \( G \) as \( |G| = |V| = m \). Thus \( 2|G| \) is the length of \( \rho_G \). Let \( \omega_G \) be the word obtained from \( \rho_G \) by removing for every \( 1 \leq i \leq m-1 \)
Let $\alpha T s$ subtree of $T$ be a node from $\rho_G$. Thus, if $\rho_G = A_1 u_1 A_2 u_2 \cdots A_{m-1} u_{m-1}$ with $u_i \in (\Sigma \cup \{A_1, A_2, \ldots, A_l\})^*$, then $\omega_G = u_1 u_2 \cdots u_{m-1}$. Note that $|\omega_G| = |\rho_G| - m + 1 = m + 1$. The entropy $H(\mathcal{G})$ of the normal form TSLP $\mathcal{G}$ is defined as the empirical unnormalized entropy (see (3)) of the word $\omega_G$ (see also (3)):

$$H(\mathcal{G}) = H(\omega_G).$$

**Example 4.** Let $\Sigma = \{a, b\}$ and $\mathcal{G} = (\{A_0, A_1, A_2, A_3, A_4\}, A_0, r)$ be the normal form TSLP with $A_0, A_2, A_3 \in V_0$, $A_1, A_4 \in V_1$ and

$$r(A_0) = A_1(A_2), \quad r(A_1) = a(x, A_3), \quad r(A_2) = A_4(A_3),
$$

$$r(A_3) = A_4(b), \quad r(A_4) = b(x, a).$$

We have $\text{val}(\mathcal{G}) = a(b(b(a, a), a), b(b, a))$, $\rho_G = A_1 A_2 A_3 A_4 A_3 A_4 b b a a (u_1 = u_3 = \varepsilon, u_2 = a, u_4 = A_3 A_4 b b a)$, $|\mathcal{G}| = 10$ and $\omega_G = a A_3 A_4 b b a$.

The derivation tree $T_G$ of $\mathcal{G}$ is a binary tree with node labels from $V \cup \Sigma$. The root is labelled with $A_0$. Nodes labelled with a symbol from $\Sigma$ are the leaves of $T_G$. A node $v$ that is labelled with a nonterminal $A_i$ has $|\rho(A_i)| = 2$ many children. If $\rho(A_i) = \alpha \beta$ with $\alpha, \beta \in V \cup \Sigma$, then the left child of $v$ is labelled with $\alpha$ and the right child is labelled with $\beta$. For every node $u$ of $T_G$ we define the tree or context $s_u = \text{val}_2(\alpha)$ where $\alpha \in V \cup \Sigma$ is the label of $u$. If $\alpha \in V_0 \cup \Sigma$ then $s_u \in T$ and if $\alpha \in V_1$ then $s_u \in C$. An initial subtree of the derivation tree $T_G$ is a tree that can be obtained from $T_G$ as follows: Take a subset $U$ of the nodes of $T_G$ and remove from $T_G$ all proper descendants of nodes from $U$, i.e., all nodes that are located strictly below a node from $U$.

**Example 5.** Let $\mathcal{G}$ be the normal form TSLP from Example 4. The derivation tree $T_G$ is shown in Figure 2 on the left; an initial subtree $T'$ of it is shown on the right.

**Lemma 3.** Let $\mathcal{G}$ be a TSLP in normal form with $t = \text{val}(\mathcal{G})$. Let $T'$ be an initial subtree of $T_G$ and let $v_1, \ldots, v_l$ be the sequence of all leaves of $T'$ (in left-to-right order). Then $2|t| \geq \sum_{i=1}^l |s_{v_i}|$.

**Proof.** Let $u$ be a node of $T_G$ and let $T_u$ be the subtree of $T_G$ rooted in $u$. Then, the nodes of $s_u$ are in an one-to-one correspondence with the leaves of $T_u$, that is, if $s_u \in T$, we have $2|s_u| - 1 = |T_u|$ and if $s_u \in C$, we have $2|s_u| = |T_u|$ (recall that $|T_u|$ is the number of leaves of $T_u$). Thus, $2|s_u| - 1 \leq |T_u|$. Since $T'$ is an initial subtree of $T_G$ we get $2|t| - 1 = 2|\text{val}(\mathcal{G})| - 1 = |T_G| = \sum_{i=1}^l |T_{v_i}| \geq \sum_{i=1}^l (2|s_{v_i}| - 1)$.
Since $|s_i| \geq 1$ we get $2|t| \geq \sum_{i=1}^l 2|s_i| - l + 1 \geq \sum_{i=1}^l |s_i| + 1$ and the statement follows. \hfill \Box

A grammar-based tree compressor is an algorithm $\psi$ that produces for a given tree $t \in T$ a TSLP $G_t$ in normal form. It is not hard to show that every TSLP can be transformed with a linear size increase into a normal form TSLP that derives the same tree. For example, the TSLP from Example 3 is transformed into the normal form TSLP described in Example 4. We will not use this fact, since all we need is the following theorem from [5] (recall that $\hat{\sigma} = \max\{2, \sigma\}$):

**Theorem 2.** There exists a grammar-based compressor $\psi$ (working in linear time) with $\max_{i \in \tau_n} |G_i| \leq O(n/\log_2 n)$.

3.3. Binary coding of TSLPs in normal form. In this section we fix a binary encoding for normal form TSLPs. This encoding is similar to the one for SLPs 17 and DAGS 20. Let $G = (V, A_0, r)$ be a TSLP in normal form with $m = |V| = |G|$ nonterminals. We define the type $\text{type}(A_i) \in \{0, 1, 2, 3\}$ of a nonterminal $A_i \in V$ as follows:

\[
\text{type}(A_i) = \begin{cases} 
0 & \text{if } \rho(A_i) \in V_1(A_0 \cup \Sigma) \\
1 & \text{if } \rho(A_i) \in V_1 V_1 \\
2 & \text{if } r(A_i) = a(\alpha, x) \text{ for some } \alpha \in V_0 \cup \Sigma \text{ and } a \in \Sigma \\
3 & \text{if } r(A_i) = a(x, \alpha) \text{ for some } \alpha \in V_0 \cup \Sigma \text{ and } a \in \Sigma 
\end{cases}
\]

We define the binary word $B(G) = w_0 w_1 w_2 w_3 w_4$, where the words $w_i \in \{0, 1\}^+$, $0 \leq i \leq 4$, are defined as follows:

- $w_0 = 0^{m-1}1$
- $w_1 = a_0 b_0 a_1 b_1 \cdots a_{m-1} b_{m-1}$, where $a_j b_j$ is the 2-bit binary encoding of type$(A_j)$. Note that $|w_1| = 2m$.
- Let $\rho_G = A_1 v_1 A_2 v_2 \cdots A_{m-1} v_{m-1}$ with $u_i \in (\Sigma \cup \{A_1, A_2, \ldots, A_i\})^*$. Then $w_2 = 10^{w_1} 10^{w_2} \cdots 10^{w_{m-1}}$. Note that $|w_2| = m$.
- For $1 \leq i \leq m - 1$ let $k_i = |\rho_G|_{A_i} \geq 1$ be the number of occurrences of the nonterminal $A_i$ in the word $\rho_G$. Moreover, fix a total ordering on $\Sigma$. For $1 \leq i \leq \sigma$, let $a_i$ denote the $i^{th}$ symbol in $\Sigma$ according to this ordering and let $l_i = |\rho_G|_{A_i} \geq 0$ be the number of occurrences of the symbol $a_i$ in the word $\rho_G$. Then $w_3 = 0^{k_1 - 1} 10^{k_2 - 1} \cdots 0^{k_{m-1} - 1} 10^{l_1} 10^{l_2} \cdots 10^{l_{m-1}}$. Note that $|w_3| = m + \sigma$.
- The word $w_4$ encodes the word $\omega_G$ using the well-known enumerative encoding [4]. Every nonterminal $A_i$, $1 \leq i \leq m - 1$, has $\eta(A_i) := k_i - 1$ occurrences in $\omega_G$. Every symbol $a_i \in \Sigma$, $1 \leq i \leq \sigma$, has $\eta(a_i) = l_i$ occurrences in $\omega_G$. Let $S$ be the set of words over the alphabet $\Sigma \cup \{A_1, \ldots, A_{m-1}\}$ with $\eta(a_i)$ occurrences of $a_i \in \Sigma (1 \leq i \leq \sigma)$ and $\eta(A_i)$ occurrences of $A_i (1 \leq i \leq m - 1)$. Hence,

\[
|S| = \frac{(m + 1)!}{\prod_{i=1}^{\sigma} \eta(a_i)! \prod_{i=1}^{m-1} \eta(A_i)!}.
\]

Let $v_0, v_1, \ldots, v_{|S| - 1}$ be the lexicographic enumeration of the words from $S$ with respect to the alphabet order $a_1, a_2, \ldots, a_\sigma, A_1, A_2, \ldots, A_{m-1}$. Then $w_4$ is the binary encoding of the unique index $i$ such that $\omega_G = v_i$, where $|w_4| = \lceil \log_2 |S| \rceil$ (leading zeros are added to the binary encoding of $i$ to obtain the length $\lfloor \log_2 |S| \rfloor$).
Example 6. Consider the normal from TSLP \( G \) from Example 4. We have \( w_0 = 00001, w_1 = 0011000011, w_2 = 11011000000 \) and \( w_3 = 110101001001 \). To compute \( w_4 \), note first that there are \(|S| = 180\) words with two occurrences of \( a \) and \( b \) and one occurrence of \( A_3 \) and \( A_4 \). It follows that \(|w_4| = \lceil \log_2(180) \rceil = 8\). Furthermore, with the canonical ordering on \( \Sigma = \{a,b\} \), the order of the alphabet is \( a, b, A_3, A_4 \). The word \( \omega_G = aA_3A_4bba \) is the lexicographically largest element in \( S \) starting with \( aA_3 \). There are 12 words in \( S \) starting with \( A_4 \), so there are 12 words in \( S \) starting with \( a \), which are lexicographically larger than \( \omega_G \). Moreover, there are 60 words in \( S \) starting with \( b \), and 30 words in \( S \) starting with \( A_3 \), respectively, \( A_4 \). Hence, \( \omega_G = w_4 = 110101001001 \) and thus \( w_4 = 001011111 \).

The following lemma generalizes a result from [15]:

Lemma 4. The set of code words \( B(G) \), where \( G \) ranges over all TSLPs in normal form, is a prefix code.

Proof. Let \( B(G) = w_0w_1w_2w_3w_4 \) with \( w_i \) defined as above. We show how to recover the TSLP \( G \), given the alphabet \( \Sigma \) and the ordering on \( \Sigma \). From \( w_0 \) we can determine \( m = |V| \) and the factors \( w_1, w_2, \) and \( w_3 \) of \( B(G) \). Hence, we can determine the type of every nonterminal from \( w_1 \). The types allow to compute \( G \) from the word \( \rho_G \). Hence, it remains to determine \( \rho_G \). To compute \( \rho_G \) from \( w_2 \), one only needs \( \rho_G \). For this, one determines the frequencies \( \eta(A_1), \ldots, \eta(A_{m-1}), \eta(a_1), \ldots, \eta(a_{|\Sigma|}) \) of the symbols in \( \omega_G \) from \( w_3 \). Using these frequencies one computes the size \(|S| \) from \( G \) and the length \( |\log_2 |S|| \) of \( w_4 \). From \( w_4 \), one can finally compute \( \omega_G \). □

Note that \(|B(G)| \leq 5|G| + \sigma + |w_4| \). By using the well-known bound on the code length of enumerative encoding [5, Theorem 11.1.3], we get:

Lemma 5. For the length of the binary coding \( B(G) \) we have: \(|B(G)| \leq O(|G|) + \sigma + H(G)\).

4. Entropy bounds for binary encoded TSLPs

For this section we fix a grammar-based tree compressor \( \psi : t \mapsto G_t \) such that \( \max_{t \in \mathcal{T}_n} |G_t| = O(n/\log_2 n) \). We allow that the alphabet size \( \sigma \) grows with \( n \), i.e., \( \sigma = \sigma(n) \) is a function in the tree size \( n \) such that \( 1 \leq \sigma(n) \leq 2n - 1 \) (a binary tree \( t \in \mathcal{T}_n \) has \( 2n - 1 \) nodes). Let \( \gamma > 0 \) be a concrete constant such that \(|G_t| \leq \gamma n/\log_2 n \) for every tree \( t \in \mathcal{T}_n \) and \( n \) large enough. We then consider the tree encoder \( E_\psi : T \rightarrow \{0,1\}^* \) defined by \( E_\psi(t) = B(G_t) \).

Lemma 6. Let \( t \in \mathcal{T}_n \) with \( n \geq 2 \) and let \( \mathcal{P} = (P_w)_{w \in \mathcal{L}_k} \) be a \( k \)-th order tree process with \( P(t) > 0 \). We have

\[
H(G_t) \leq -\log_2 \text{Prob}_P(t) + O\left(\frac{kn \log \sigma}{\log_2 n}\right) + O\left(\frac{n \log \log_2 n}{\log_2 n}\right).
\]

Proof. Let \( m = |G_t| = |V| \) be the size of \( G_t \). Let \( T = T_{G_t} \) be the derivation tree of \( G_t \). We define an initial subtree \( T' \) as follows: If \( v_1 \) and \( v_2 \) are non-leaf nodes of \( T \) that are labelled with the same nonterminal and \( v_1 \) comes before \( v_2 \) in preorder, then we remove from \( T \) all proper descendants of \( v_2 \). Thus, for every \( A_i \in V \) there is exactly one non-leaf node in \( T' \) that is labelled with \( A_i \). For the TSLP from Example 4 the tree \( T' \) is shown in Figure 2 on the right.

Note that \( T' \) has \( m \) non-leaf nodes and \( m + 1 \) leaves. Let \( v_1, v_2, \ldots, v_{m+1} \) be the sequence of all leaves of \( T' \) (w.l.o.g. in preorder) and let \( \alpha_i \in \Sigma \cup \{A_1, \ldots, A_{m-1}\} \)
be the label of \( v_i \). Let \( \overline{\pi} = (\alpha_1, \alpha_2, \ldots, \alpha_{m+1}) \). Then \( |\overline{\omega_{\alpha}}_1|_a = |\overline{\pi}|_a \) for every \( \alpha \in \Sigma \cup \{A_1, \ldots, A_{m-1}\} \). Hence, \( p_{\overline{\pi}} \) and \( p_{\overline{\omega_{\alpha}}_1} \) are the same empirical distributions. For the TSLP from Example 3 we get \( \overline{\pi} = (a, b, a, b, A_1, A_3) \). Let \( s_i = \text{val}_{\alpha}(a_i) \in T \cup (\mathcal{C} \setminus \{x\}) \). Since \( \text{val}_{\alpha}(A_i) \neq \text{val}_{\alpha}(A_j) \) for all \( i \neq j \) (\( G_i \) is in normal form) and \( \text{val}_{\alpha}(A_i) \notin \Sigma \) for all \( i \) (this holds for every normal form TSLP that produces a tree of size at least two), the tuple \( \overline{\pi} = (s_1, s_2, \ldots, s_{m+1}) \) satisfies \( p_{\text{val}_a}(a_i) = p_{\overline{\pi}}(s_i) \) for all \( 1 \leq i \leq m + 1 \).

We define from \( \mathcal{P} \) for every \( z \in \mathcal{L}_k \) a modified tree process \( \mathcal{P}_z = (P_{z,u})_{u \in \mathcal{L}} \) by setting \( P_{z,u}(\tilde{a}) = P_{t_k(z,w)}(\tilde{a}) \) for all \( \tilde{a} \in \Sigma \times \{0, 2\} \). Note that the \( k^{th} \)-order tree process \( \mathcal{P} \) is obtained for \( z = (\square 0)^k \) for the fixed padding symbol \( \square \in \Sigma \). We define a mapping \( \tau : T \cup \mathcal{C} \to [0, 1] \) by

\[
\tau(s) = \max_{z \in \mathcal{L}_k} \text{Prob}_{\mathcal{P}_z}(s)
\]

for every \( s \in T \cup \mathcal{C} \). Thus, \( \tau \) maximizes the values of the function \( \text{Prob}_\mathcal{P} \) associated with the \( k^{th} \)-order tree process \( \mathcal{P} = (P_{u})_{u \in \mathcal{L}_k} \) by choosing an optimal \( k \)-history for the nodes of \( s \) whose history is of length smaller than \( 2k \). We show that \( \tau \) satisfies

\[
(7) \quad \tau(t) \leq \prod_{i=1}^{m+1} \tau(s_i).
\]

In order to prove (7), first note that by definition of the tree/context \( s_u \), for each node \( u \) of the derivation tree \( T \), the tree/context \( s_u \) corresponds to a subtree/subcontext of the binary tree \( t \). We define a function \( \chi \) which maps a node \( u \) of the derivation tree \( T \) to a node \( \chi(u) \in V(t) \subseteq \{0, 1\}^* \). Intuitively, \( \chi(u) \) is the root of the subtree/subcontext of \( t \) which corresponds to \( s_u \). Formally, \( \chi \) is defined inductively as follows: For the root node \( u \) of \( T \), we set \( \chi(u) = \varepsilon \). Furthermore, let \( u \) be a non-leaf node of \( T \) which is labelled with the non-terminal \( A_i \) and for which \( \chi(u) \) has been defined. Let \( u_1 \) be the left child and \( u_2 \) be the right child of \( u \) in \( T \). We define \( \chi(u_1) = \chi(u) \). The node \( \chi(u_2) \) is defined as follows:

(i) If \( r(A_i) = A_j(\alpha) \) with \( A_j \in V_1 \) and \( \alpha \in V \cup \Sigma \), then we set \( \chi(u_2) = \chi(u)\omega(s_{u_1}) \).

(ii) If \( r(A_i) = a(\alpha, x) \) (respectively, \( r(A_i) = a(x, \alpha) \)) for \( \alpha \in \Sigma \) and \( \alpha \in \Sigma \cup V \), then we define \( \chi(u_2) = \chi(u)0 \) (respectively, \( \chi(u_2) = \chi(u)1 \)).

This yields a well-defined function \( \chi \) mapping a node \( u \) of \( T \) to a node \( \chi(u) \in V(t) \).

Let us define \( V_u = \chi(u)V(s_u) \subseteq V(t) \). The definition of these sets implies that if two nodes \( u \) and \( v \) of \( T \) are not in an ancestor-descendant relationship, then \( V_u \cap V_v = \emptyset \). In particular, the nodes \( v_1, \ldots, v_l \) are leaves of the initial subtree \( T' \) and thus not in an ancestor-descendant relationship. Hence, the sets \( V_i := V_{v_i} \) are
disjoint subsets of $V(t)$. We can now show (7):

$$\tau(t) = \max_{z \in \mathcal{L}_k} \text{Prob}_{P_z}(t)$$

$$= \max_{z \in \mathcal{L}_k} \prod_{v \in V(t)} P_{\ell_k(zh(v))}(\lambda(v))$$

$$\leq \max_{z \in \mathcal{L}_k} \prod_{i=1}^{m+1} \prod_{v \in V_i} P_{\ell_k(zh(v))}(\lambda(v)) \quad \text{(since $P_{\ell_k(zh(v))}(\lambda(v)) \leq 1$ for all $v \in V(t)$)}$$

$$\leq \prod_{i=1}^{m+1} \max_{z \in \mathcal{L}_k} \prod_{v \in V_i} P_{\ell_k(zh(v))}(\lambda(v))$$

$$\leq \prod_{i=1}^{m+1} \max_{z \in \mathcal{L}_k} \prod_{v \in V(s_i)} P_{\ell_k(zh(v))}(\lambda(v)) \quad \text{(since $|\chi(v_i)|v \geq |v|$ for $v \in V(s_i)$)}$$

$$= \prod_{i=1}^{m+1} \tau(s_i).$$

Next, we define the function $\xi : \mathcal{T} \cup \mathcal{C} \setminus \{x\} \to [0, 1]$ as follows:

$$\xi(s) = \begin{cases} 2^{-(k+1)} \sigma^{-k} \tau(s) & \text{if } s \in \mathcal{T} \\ \frac{6}{\pi^2} 2^{-(k+1)} \sigma^{-k} \frac{\tau(s)}{|s|^2(|s|+1)} & \text{if } s \in \mathcal{C} \setminus \{x\}. \end{cases}$$

We get

$$\sum_{s \in \mathcal{T} \cup \mathcal{C} \setminus \{x\}} \xi(s) = 2^{-(k+1)} \sigma^{-k} \sum_{s \in \mathcal{T}} \tau(s) + \frac{6}{\pi^2} 2^{-(k+1)} \sigma^{-k} \sum_{s \in \mathcal{C} \setminus \{x\}} \frac{\tau(s)}{|s|^2(|s|+1)}$$

$$= 2^{-(k+1)} \sigma^{-k} \sum_{z \in \mathcal{L}_k} \max_{s \in \mathcal{T}} \text{Prob}_{P_z}(s) +$$

$$+ \frac{6}{\pi^2} 2^{-(k+1)} \sigma^{-k} \sum_{r \geq 1} \frac{1}{r^2(r+1)} \sum_{s \in \mathcal{C}_r} \max_{s \in \mathcal{L}_k} \text{Prob}_{P_z}(s)$$

$$\leq 2^{-(k+1)} \sigma^{-k} \sum_{z \in \mathcal{L}_k} \sum_{s \in \mathcal{T}} \text{Prob}_{P_z}(s) +$$

$$+ \frac{6}{\pi^2} 2^{-(k+1)} \sigma^{-k} \sum_{r \geq 1} \sum_{s \in \mathcal{C}_r} \frac{1}{r^2(r+1)} \sum_{s \in \mathcal{L}_k} \text{Prob}_{P_z}(s)$$

$$\leq \frac{1}{2} + \frac{6}{\pi^2} 2^{-(k+1)} \sigma^{-k} \sum_{r \geq 1} \sum_{s \in \mathcal{L}_k} \frac{1}{r^2} = 1$$

where the inequality in the last line follows from Lemmas 1 and 2 and from $|\mathcal{L}_k| = 2^k \sigma^k$, and the equality in the last line follows from the well-known fact that $\sum_{r \geq 1} r^{-2} = \pi^2/6$. In particular, we have $\sum_{s \in \{s_1, \ldots, s_{m+1}\}} \xi(s) \leq 1$. Thus, with Shannon’s inequality [1], we obtain:

$$H(\mathcal{G}_t) = H(\omega_t) = \sum_{i=1}^{m+1} -\log_2 p_{\omega_t}(a_i) = \sum_{i=1}^{m+1} -\log_2 P(s_i) \leq \sum_{i=1}^{m+1} -\log_2 \xi(s_i).$$
We define the set $\mathcal{I}_0 = \{ i \in \{1, \ldots, m+1 \} | s_i \in T \}$ and $\mathcal{I}_1 = \{ i \in \{1, \ldots, m+1 \} | s_i \in C \}$ and obtain

$$H(\mathcal{G}_t) \leq \sum_{i \in \mathcal{I}_0} -\log_2 \xi(s_i) + \sum_{i \in \mathcal{I}_1} -\log_2 \xi(s_i)$$

and thus

$$H(\mathcal{G}_t) \leq \sum_{i \in \mathcal{I}_0} -\log_2 \left( 2^{-|s_i|} \right) + \sum_{i \in \mathcal{I}_1} -\log_2 \left( \frac{6}{\pi^2} \frac{2^{-|s_i|}}{|s_i|^2} \right)$$

by definition of $\xi$. Using logarithmic identities, we get

$$H(\mathcal{G}_t) \leq |\mathcal{I}_0| (k+1) + |\mathcal{I}_0| k \log_2 \sigma - \log_2 \left( \prod_{i \in \mathcal{I}_0} \tau(s_i) \right) +$$

$$\log_2 \left( \frac{\pi^2}{6} \right) |\mathcal{I}_1| + |\mathcal{I}_1| (k+1) + |\mathcal{I}_1| k \log_2 \sigma - \log_2 \left( \prod_{i \in \mathcal{I}_1} \tau(s_i) \right) +$$

$$\sum_{i \in \mathcal{I}_1} \log_2 |s_i|^2 (|s_i| + 1).$$

Using $|\mathcal{I}_0| + |\mathcal{I}_1| = m + 1 \leq 2|\mathcal{G}_t|$, $\log_2 (\pi^2/6) |\mathcal{I}_1| \leq |\mathcal{I}_1| \leq 2|\mathcal{G}_t|$ and $|s_i| + 1 \leq 2|s_i|$, we obtain

$$H(\mathcal{G}_t) \leq 2(k+3)|\mathcal{G}_t| + 2k|\mathcal{G}_t| \log_2(\sigma) - \log_2 \left( \prod_{i=1}^{m+1} \tau(s_i) \right) + \sum_{i=1}^{m+1} \log_2 2|s_i|^3.$$ 

Equation (7) and $\tau(t) \geq \text{Prob}_P(t)$ yield

$$H(\mathcal{G}_t) \leq 2(k+3)|\mathcal{G}_t| + 2k|\mathcal{G}_t| \log_2(\sigma) - \log_2 (\tau(t)) + 3 \sum_{i=1}^{m+1} \log_2 |s_i|$$

$$\leq - \log_2 (\text{Prob}_P(t)) + O(k|\mathcal{G}_t| \log \sigma + \sum_{i=1}^{m+1} \log_2 |s_i|).$$

Let us bound the sum $\sum_{i=1}^{m+1} \log_2 |s_i|$: Using Jensen’s inequality and Lemma 3 (which yields $\sum_{i=1}^{m+1} |s_i| \leq 2n$), we get

$$\sum_{i=1}^{m+1} \log_2 |s_i| \leq (m+1) \log_2 \left( \frac{\sum_{i=1}^{m+1} |s_i|}{m+1} \right)$$

$$\leq (m+1) \log_2 \left( \frac{2n}{m+1} \right)$$

$$\leq 2|\mathcal{G}_t| \log_2 \left( \frac{2n}{|\mathcal{G}_t|} \right)$$

and thus

$$H(\mathcal{G}_t) \leq - \log_2 (\text{Prob}_P(t)) + O \left(k|\mathcal{G}_t| \log \sigma + |\mathcal{G}_t| \log_2 \left( \frac{n}{|\mathcal{G}_t|} \right) \right).$$

For every $n \geq 1$, the function $\varphi : (0, \infty) \to \mathbb{R}$ with $\varphi(x) = x \log_2 \left( \frac{n}{x} \right)$ is monotonically increasing for $x \in (0, \frac{n}{e}]$ ($e$ is Euler’s number). If $n \geq \sigma^{-ex}$, i.e., $\log_\sigma n \geq ex$
then $|G_t| \leq \gamma \cdot n / \log_{\sigma} n \leq n/e$ (if $n$ is large enough). With (8) we get
\[
|G_t| \log_2 \left( \frac{n}{|G_t|} \right) \leq \gamma n \log_2 \left( \frac{1}{\log_{\sigma} n} \right) \leq O \left( \frac{n \log \log_{\sigma} n}{\log_{\sigma} n} \right).
\]
and thus
\[
H(G_t) \leq - \log_2 \text{Prob}_P(t) + O \left( \frac{kn \log \hat{\sigma}}{\log_{\sigma} n} \right) + O \left( \frac{n \log \log_{\sigma} n}{\log_{\sigma} n} \right),
\]
which proves the lemma in case $n \geq \hat{\sigma}^{\gamma e}$. Now assume that $n < \hat{\sigma}^{\gamma e}$. We must have $|G_t| \geq \hat{\sigma}/2$ (every right-hand side of a normal form TSLP contains at most two symbols from $\Sigma$). Hence we get
\[
\log_2 \left( \frac{n}{|G_t|} \right) < \log_2 \left( \frac{2\hat{\sigma}^{\gamma e}}{\sigma} \right) \leq O(\log \hat{\sigma})
\]
and (8) simplifies to
\[
H(G_t) \leq - \log_2 \left( \text{Prob}_P(t) \right) + O(k|G_t| \log \hat{\sigma}).
\]
Again we obtain the bound from the lemma. \hfill \Box

**Theorem 3.** For every $t \in T_n$ and every $k \geq 0$ we have
\[
|E_\psi(t)| \leq H_k(t) + O \left( \frac{kn \log \hat{\sigma}}{\log_{\sigma} n} \right) + O \left( \frac{n \log \log_{\sigma} n}{\log_{\sigma} n} \right) + \sigma.
\]

**Proof.** Let $\mathcal{P} = (P_w)_{w \in \{0,1\}^*}$ be a $k^{th}$-order tree process with $P(t) > 0$. Lemmas 5 and 6 yield
\[
|E_\psi(t)| \leq O(|G_t|) + H(G_t) + \sigma
\]
\[
\leq O(|G_t|) - \log_2 \text{Prob}_P(t) + O \left( \frac{kn \log \hat{\sigma}}{\log_{\sigma} n} \right) + O \left( \frac{n \log \log_{\sigma} n}{\log_{\sigma} n} \right) + \sigma
\]
\[
= - \log_2 \text{Prob}_P(t) + O \left( \frac{kn \log \hat{\sigma}}{\log_{\sigma} n} \right) + O \left( \frac{n \log \log_{\sigma} n}{\log_{\sigma} n} \right) + \sigma,
\]
where the last equality uses the bound $|G_t| \in O(n/\log_{\sigma} n)$. Finally, by taking for $\mathcal{P}$ be the empirical $k^{th}$-order tree process $\mathcal{P}^t$, we get
\[
|E_\psi(t)| \leq H_k(t) + O \left( \frac{kn \log \hat{\sigma}}{\log_{\sigma} n} \right) + O \left( \frac{n \log \log_{\sigma} n}{\log_{\sigma} n} \right) + \sigma
\]
from Theorem 1. \hfill \Box

5. **Extension to unranked tree**

So far, we have only considered binary trees. In this section, we consider $\Sigma$-labelled unranked ordered trees, where “ordered” means that the children of a node are totally ordered, and “unranked” means that the number of children of a node (also called its degree) can be any natural number. Let us denote by $\mathcal{U}$ the set of all such trees. For technical reasons we also define forests which are ordered sequences of trees from $\mathcal{U}$. The set of forests is denoted with $\mathcal{F}$. The sets $\mathcal{U}$ and $\mathcal{F}$ can be inductively defined as the smallest sets of strings over the alphabet $\Sigma \cup \{(,\})$ such that the following conditions hold:

- $\varepsilon \in \mathcal{F}$ (this is the empty forest),
- if $a \in \Sigma$ and $f \in \mathcal{F}$ then $a(f) \in \mathcal{U}$,
- if $t \in \mathcal{U}$ and $f \in \mathcal{F}$ then $tf \in \mathcal{F}$.
The singleton tree $a()$ (which is obtained by taking $f = \varepsilon$ in the second point) is usually written as $a$. Note that $\mathcal{U} \subseteq \mathcal{F}$ and that $\mathcal{F} = \mathcal{U}^*$. The size $|f|$ of $f \in \mathcal{F}$ is the number of occurrences of $\Sigma$-labels in $f$; formally: $|\varepsilon| = 0$, $|a(f)| = 1 + |f|$ and $|tf| = |t| + |f|$ for $a \in \Sigma$, $t \in \mathcal{U}$, and $f \in \mathcal{F}$.

The first-child/next-sibling encoding transforms a forest $f \in \mathcal{F}$ into a binary tree $\text{fcns}(f) \in \mathcal{T}$. It is defined inductively as follows (recall that $\Box \in \Sigma$ is a fixed distinguished symbol in $\Sigma$):

- $\text{fcns}(\varepsilon) = \Box$
- $\text{fcns}(a(f)g) = a(\text{fcns}(f), \text{fcns}(g))$ for $f, g \in \mathcal{F}$ and $a \in \Sigma$.

Thus, the left (resp., right) child of a node in $\text{fcns}(f)$ is the first child (resp., right sibling) of the node in $f$ or a $\Box$-labelled leaf if it does not exist.

**Example 7.** If $f = a(bc)d(e)$ then
\[
\text{fcns}(f) = \text{fcns}(a(bc)d(e)) = a(\text{fcns}(bc), \text{fcns}(d(e)) = a(b(\Box, \text{fcns}(c)), d(\text{fcns}(e), \Box)) = a(b(\Box, c(\Box, \Box)), d(e(\Box, \Box), \Box)),
\]
see also Figure 3.

Note that if $t \in \mathcal{U}$, $|t| = n$ then $\text{fcns}(t)$ is a binary tree with $n$ internal nodes. Hence we have $|\text{fcns}(t)| = n + 1$ (which is the number of leaves of $\text{fcns}(t)$). We define the $k^{th}$-order empirical entropy of an unranked tree $t \in \mathcal{U}$ as $H_k(t) = H_k(\text{fcns}(t))$.

The above definition of the $k^{th}$-order empirical entropy of an unranked tree has a practical motivation. Unranked trees occur for instance in the context of XML, where the hierarchical structure of a document is represented as an unranked node labelled tree. In this setting, the label of a node quite often depends on (i) the labels of the ancestor nodes and (ii) the labels of the (left) siblings. This dependence is captured by our definition of the $k^{th}$-order empirical entropy.

We also confirmed this intuition by experimental data, shown in Table 1. We computed for 21 real XML document trees\footnote{All data are available from http://xmlcompbench.sourceforge.net/Dataset.html} the $k^{th}$-order empirical entropy and divided the value by the worst case bit length $2n + \log_2(\sigma)n$, where $n$ is the number of nodes and $\sigma$ is the number of node labels. As can be seen from Table 1 these quotients are indeed quite small.

6. Discussion of our definition of $k^{th}$-order empirical entropy

Our definition of $k^{th}$-order empirical entropy does not capture all regularities that can be exploited in grammar-based compression. Take for instance a complete unlabelled binary tree $t_n$ of height $n$ (all paths from the root to a leaf have length
This tree has $2^n$ leaves and is very well compressible: its minimal DAG has only $n + 1$ nodes, hence there also exists a TSLP of size $n + 1$ for $t_n$. But for every fixed $k$ the $k^{th}$-order empirical entropy of $t_n$ divided by $n$ converges to 2 (the trivial upper bound) for $n \to \infty$. If $n \gg k$ then for every $k$-history $z$ the number of leaves with $k$-history $z$ is roughly the same as the number of internal nodes with $k$-history $z$. Hence, although $t_n$ is highly compressible with TSLPs (and even DAGs), its $k^{th}$-order empirical entropy is close to the maximal value. In the rest of this section we show that the same phenomenon occurs for the empirical entropy of strings as well.

The $k^{th}$ order empirical entropy of a string is defined as follows (see e.g. [8]). Let $\Sigma$ denote a finite alphabet and let $w \in \Sigma^*$. For a non-empty string $\alpha \in \Sigma^*$, define $w(\alpha) \in \Sigma^*$ as the string whose $i^{th}$ character is the character in $w$ immediately following the $i^{th}$ occurrence of the string $\alpha$ in $w$. Thus, if $\alpha$ is not a suffix of $w$, the length of $w(\alpha)$ is equal to the number of occurrences of the string $\alpha$ in $w$. In case $\alpha$ is a suffix of $w$, $|w(\alpha)|$ is the number of occurrences of $\alpha$ in $w$ minus one. Recall the definition of the unnormalized empirical entropy $H(w)$ of a string $w \in \Sigma^*$ (or tuple) from Section 2.1. For an integer $k \geq 1$, the $k^{th}$-order (unnormalized) empirical entropy of a string $w \in \Sigma^*$ is defined as

$$H_k(w) = \sum_{\alpha \in \Sigma^k} H(w(\alpha)),$$

where we set $H(\varepsilon) = 0$.

A straight-line program (SLP) for a string $w$ is a context-free grammar that produces only the string $w$. The size of an SLP is the sum of the lengths of the right-hand sides of the context-free grammar, see e.g. [20] for details. We prove that for each $n \geq 1$ there exists a string of length $2^{n+1} - 1$, which is highly compressible with SLPs, but whose $k^{th}$-order empirical entropy takes maximal values.

| XML document | $n$ | $\sigma$ | $w := (2 + \log_2 \sigma)n$ | $H_1/w$ | $H_2/w$ | $H_4/w$ | $H_8/w$ |
|--------------|----|---------|------------------------------|---------|---------|---------|---------|
| Baseball     | 28  | 306     | $212,961.9447$              | 2.9818% | 1.2547% | 0.6739% | 0.6662% |
| DBLP         | 332 | 130     | $23,755,697.8193$            | 10.9775%| 8.7407% | 8.2134% | 6.7270% |
| DCSD-Normal  | 2  | 495     | $3,134,658.5046$             | 8.8952% | 2.3753% | 2.3753% | 2.3750% |
| EnWikiQuote  | 262 | 955     | $1,711,288.1304$             | 0.2506% | 0.2495% | 0.2492% | 0.2483% |
| EnWikiNew     | 404 | 652     | $534,379.7451$               | 2.2034% | 0.9450% | 0.8132% | 0.8092% |
| EXI-Array     | 55  | 453     | $124,193.9713$               | 0.0484% | 0.0268% | 0.0139% | 0.0098% |
| EXI-Invoice   | 15  | 075     | $49,845.0890$                | 0.0464% | 0.0268% | 0.0139% | 0.0098% |
| EXI-Telecomp  | 177 | 935     | $123,379.9713$               | 0.0484% | 0.0268% | 0.0139% | 0.0098% |
| EXI-Telecomp  | 2  | 495     | $3,134,658.5046$             | 8.8952% | 2.3753% | 2.3753% | 2.3750% |
| EXI-Telecomp  | 495 | 652     | $1,711,288.1304$             | 0.2506% | 0.2495% | 0.2492% | 0.2483% |

Table 1. Experimental results for XML tree structures, where $n$ denotes the number of nodes and $\sigma$ denotes the number of node labels.
Theorem 4. There exists a family of string \( S_n \) \((n \geq 1)\) over a binary alphabet with the following properties:

- \( |S_n| = 2^{n+1} - 1 \),
- there exists an SLP of size \( 3n \) for \( S_n \), and
- \( H_k(S_n) \geq 2^{n-k} \) for all \( 1 \leq k < n \).

Proof. We inductively define a string \( S_n \in \{a,b\}^* \) for \( n \geq 1 \) as follows: We set (i) \( S_1 = baa \) and (ii) \( S_n = bS_{n-1}S_{n-1} \). We have \( |S_n| = 2^{n+1} - 1 \). The string \( S_n \) corresponds to the preorder traversal of the perfect binary tree of size \( 2^n \), whose internal nodes are labelled with the character \( b \) and whose leaves are labelled with the character \( a \). The recursive definition of \( S_n \) implies that there is an SLP of size \( 3n \) for \( S_n \).

It remains to show that \( H_k(S_n) \geq 2^{n-k} \) for \( 1 \leq k < n \). In order to prove the lower bound, we start with estimating the \( H(S_n) \). Recall that \( |w|x \) denotes the number of occurrences of a character \( x \) in a string \( w \), as defined in Section 2. We have \( |S_n|a = 2^n \) and \( |S_n|b = 2^n - 1 \), which yields

\[
H(S_n) = \sum_{x \in \{a,b\}} |S_n|x \log_2 \left( \frac{|S_n|x}{|S_n|} \right) = 2^n \log_2 \left( \frac{2^{n+1} - 1}{2^n} \right) + (2^n - 1) \log_2 \left( \frac{2^{n+1} - 1}{2^n - 1} \right) + \frac{1}{2^n} \log_2 \left( \frac{2^{n+1} - 1}{2^n - 1} \right).
\]

Let \( g(x) = x/(2x - 1) \log_2 ((2x - 1)/x) + (x - 1)/(2x - 1) \log_2 ((2x - 1)/(x - 1)) \) with \( x \in [2, \infty) \). Since \( |S_n| = 2^{n+1} - 1 \) we have \( H(S_n) = g(2^n) |S_n| \). Computing the derivative of \( g \), we obtain \( g'(x) = (2x - 1)^{-2} \log_2(x/(x - 1)) \). As \( g'(x) > 0 \) for \( x \in [2, \infty) \), we find that \( g \) is monotonically increasing in \( x \). Thus, we have \( g(2^n) \geq g(2) \) and hence \( H(S_n) \geq (\log_2(3) - 2/3) |S_n| > 0.9 |S_n| \). In particular, \( H(S_n)|S_n| - 1 = g(2^n) \) converges to 1 for \( n \to \infty \), that is, for large values of \( n \), \( H(S_n) \) is close to the maximal value.

Let \( 1 \leq k < n \) and let \( 1 \leq m \leq n \). By construction of \( S_n \), the last character of \( S_n \) is \( a \). Therefore, the length of the string \( S_n(b^m) \) equals the number of occurrences of the string \( b^m \) in \( S_n \). In order to lower-bound the \( k \)th-order empirical entropy of \( S_n \), we first show inductively in \( n \), that \( |S_n(b^m)| = 2^{n-m+1} - 1 \) for \( 1 \leq m \leq n \). For the base case, let \( n = 1 \). We have \( S_1 = baa \) and thus, \( |S_1(b)| = 1 \). For the induction step, let \( n > 1 \). By definition of \( S_n \), we have \( S_n = bS_{n-1}S_{n-1} \). By the induction hypothesis, we have \( |S_{n-1}(b^m)| = 2^{n-m} - 1 \) for \( 1 \leq m \leq n - 1 \). Moreover, \( b^m \) does not occur in \( S_{n-1} \) (which follows by induction), i.e., \( |S_{n-1}(b^n)| = 0 = 2^{n-n} - 1 \). By construction, the last character of the string \( S_{n-1} \) is \( a \). Thus, for all \( 1 \leq m \leq n \) we have \( |S_{n-1}S_{n-1}(b^m)| = 2|S_{n-1}(b^m)| = 2^{n-m+1} - 2 \). Hence, as the string \( b^m \) with \( 1 \leq m \leq n \) occurs additionally as a prefix of the string \( S_n = bS_{n-1}S_{n-1} \), the number of occurrences of \( b^m \) in \( S_n \) in total is \( |S_n(b^m)| = 2^{n-m+1} - 1 \) for every \( 1 \leq m \leq n \). This proves the claim.

Next, we count the number of occurrences of \( b^m \) in \( S_n \), which are followed by the character \( a \), that is, we count \( |S_n(b^m)|a \). We show inductively in \( n \), that \( |S_n(b^m)|a = 2^{n-m} \). For the base case, let \( n = 1 \). As \( S_1 = baa \), we have \( |S_1(b)|a = 1 \). For the induction step, let \( n > 1 \). By the induction hypothesis, we have \( |S_{n-1}(b^m)|a = 2^{n-1-m} \) for \( 1 \leq m \leq n - 1 \). As \( b^m \) is not a suffix of \( S_{n-1} \), we obtain \( |S_{n-1}S_{n-1}(b^m)|a = 2^{n-m} \) for \( 1 \leq m \leq n - 1 \). Moreover, from the construction of \( S_n \), we find that the prefix \( b^n \) of \( S_n \), which is the only occurrence of \( b^n \) in
$S_n$, is followed by the character $a$. Thus, $|S_n(b^m)|_a = 2^{n-m}$ for $1 \leq m \leq n$, which proves the claim.

As $|S_n(b^m)|_a = 2^{n-m}$, we have $|S_n(b^m)|_a = 2^{n-m} - 1$. Thus, we obtain the following lower bound for the $k$th-order empirical entropy of $S_n$ for all $1 \leq k < n$.

\[
H_k(S_n) = \sum_{a \in \{a, b\}^k} H(S_n(a)) \\
\geq \sum_{x \in \{a, b\}} |S_n(b^k)|_x \log_2 \left( \frac{|S_n(b^k)|_x}{|S_n(b^k)|} \right) \\
= 2^{n-k} \log_2 \left( \frac{2^{n-k+1} - 1}{2^{n-k}} \right) + (2^{n-k} - 1) \log_2 \left( \frac{2^{n-k+1} - 1}{2^{n-k} - 1} \right)
\]

with $g : [2, \infty) \to \mathbb{R}$ defined as above. Note that $n-k \geq 1$ as $k < n$ by assumption. Analogously as in the first case, we get $H_k(S_n) \geq 0.9(2^{n-k+1} - 1) \geq 2^{n-k}$. This proves the claim. \qed

References

[1] Janos Aczél. On Shannon’s inequality, optimal coding, and characterizations of Shannon’s and Renyi’s entropies. Technical Report Research Report AA-73-05, University of Waterloo, 1973. https://cs.uwaterloo.ca/research/tr/1973/CS-73-05.pdf

[2] Philip Bille, Inge Li Gørtz, Gad M. Landau, and Oren Weimann. Tree compression with top trees. Information and Computation, 243:166–177, 2015.

[3] Giorgio Busatto, Markus Lohrey, and Sebastian Maneth. Efficient memory representation of XML document trees. Information Systems, 33(4–5):456–474, 2008.

[4] Thomas M. Cover. Enumerative source encoding. IEEE Transactions on Information Theory, 19(1):73–77, 1973.

[5] Thomas M. Cover and Joy A. Thomas. Elements of Information Theory (2. ed.). Wiley, 2006.

[6] Paolo Ferragina, Fabrizio Luccio, Giovanni Manzini, and S. Muthukrishnan. Compressing and indexing labeled trees, with applications. Journal of the ACM, 57(1):4:1–4:33, 2009.

[7] Philippe Flajolet and Robert Sedgewick. Analytic Combinatorics. Cambridge University Press, 2009.

[8] Travis Gagie. Large alphabets and incompressibility. Information Processing Letters, 99(6):246–251, 2006.

[9] Moses Ganardi, Danny Hucke, Artur Jez, Markus Lohrey, and Eric Noeth. Constructing small tree grammars and small circuits for formulas. Journal of Computer and System Sciences, 86:136–158, 2017.

[10] Moses Ganardi and Markus Lohrey. A universal tree balancing theorem. ACM Transaction on Computation Theory, 11(1):1:1–1:25, October 2018.

[11] Michal Ganczorz. Entropy bounds for grammar compression. CoRR, abs/1804.08547, 2018.

[12] Michal Ganczorz. Using statistical encoding to achieve tree succinctness never seen before. CoRR, abs/1807.06359, 2018.

[13] Adrià Gascón, Markus Lohrey, Sebastian Maneth, Carl Philipp Reh, and Kurt Sieber. Grammar-based compression of unranked trees. In Proceedings of the 13th International Computer Science Symposium in Russia, CSR 2018, volume 10846 of Lecture Notes in Computer Science, pages 118–131. Springer, 2018.

[14] Richard F. Geary, Rajeev Raman, and Venkatesh Raman. Succinct ordinal trees with level-ancestor queries. ACM Transactions on Algorithms, 2(4):510–534, 2006.

[15] Danny Hucke and Markus Lohrey. Universal tree source coding using grammar-based compression. In Proceedings of the 2017 IEEE International Symposium on Information Theory, ISIT 2017, pages 1753–1757. IEEE Computer Society Press, 2017.

[16] Jesper Jansson, Kunihiko Sadakane, and Wing-Kin Sung. Ultra-succinct representation of ordered trees with applications. Journal of Computer and System Sciences, 78(2):619–631, 2012.
[17] 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.

[18] John C. Kieffer, En-Hui Yang, Gregory J. Nelson, and Pamela C. Cosman. Universal lossless compression via multilevel pattern matching. *IEEE Transactions on Information Theory*, 46(4):1227–1245, 2000.

[19] N. Jesper Larsson and Alistair Moffat. Offline dictionary-based compression. In *Proceedings of the 1999 Data Compression Conference (DCC 1999)*, pages 296–305. IEEE Computer Society Press, 1999.

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

[21] Markus Lohrey. Grammar-based tree compression. In *Proceedings of the 19th International Conference on Developments in Language Theory, DLT 2015*, volume 9168 of *Lecture Notes in Computer Science*, pages 46–57. Springer, 2015.

[22] Markus Lohrey, Sebastian Maneth, and Roy Mennicke. XML tree structure compression using RePair. *Information Systems*, 38(8):1150–1167, 2013.

[23] Gonzalo Navarro and Luís M. S. Russo. Re-pair achieves high-order entropy. In *Proceedings of Data Compression Conference (DCC 2008)*, page 537. IEEE Computer Society, 2008.

[24] Craig G. Nevill-Manning and Ian H. Witten. Identifying hierarchical structure in sequences: A linear-time algorithm. *J. Artif. Intell. Res. (JAIR)*, 7:67–82, 1997.

[25] Carlos Ochoa and Gonzalo Navarro. RePair and all irreducible grammars are upper bounded by high-order empirical entropy. *IEEE Transactions on Information Theory*, 2018. to appear.

[26] Jie Zhang, En-Hui Yang, and John C. Kieffer. A universal grammar-based code for lossless compression of binary trees. *IEEE Transactions on Information Theory*, 60(3):1373–1386, 2014.

[27] Jacob Ziv and Abraham Lempel. Compression of individual sequences via variable-rate coding. *IEEE Transactions on Information Theory*, 24(5):530–536, 1978.

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