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INTRODUCTION

- 1.1 WHY COMPACT DATA STRUCTURES?
- 1.2 SOMETHING TO EXPLAIN WHAT WE HAVE DONE
- 1.3 STRUCTURE OF THE THESIS

Entropy, in essence, represents the minimal quantity of bits required to unequivocally distinguish an object within a set. Consequently, it serves as a foundational metric for the space utilization in compressed data representations. The ultimate aim of compressed data structures is to occupy space nearly equivalent to the entropy required for object identification, while simultaneously enabling efficient querying operations. This pursuit lies at the core of optimizing data compression techniques: achieving a balance between storage efficiency and query responsiveness.

WORST CASE ENTROPY

In its simplest form, entropy can be seen as the minimum number of bits required by identifiers (*codes*, see Section 2.2), when each element of a set U has a unique code of identical length. This is called the *worst case entropy* of U and it's denoted by $H_{wc}(U)$. The worst case entropy of a set U is given by the formula:

$$H_{wc}(U) = \log |U| \tag{1}$$

where |U| is the number of elements in U.

Remark 2.1. If we used codes of length $l < H_{wc}(U)$, we would have only $2^l \le 2^{H_{wc}(U)} = |U|$ possible codes, which is not enough to uniquely identify all elements in U.

The reason behind the attribute *worst case* is that if all codes are of the same length, then this length must be at least $\lceil \log |U| \rceil$ bits to be able to uniquely identify all elements in U. If they all have different lengths, the longest code must be at least $\lceil \log |U| \rceil$ bits long.

Example 2.2 (Worst-case entropy of \mathcal{T}_n). Let \mathcal{T}_n denote the set of all general ordinal trees [5] with n nodes. In this scenario, each node can have an arbitrary number of children, and their order is distinguished. With n nodes, the number of possible ordinal trees is the (n-1)-th Catalan number, given by:

$$|\mathcal{T}_{n}| = \frac{1}{n} \binom{2n-2}{n-1} \tag{2}$$

Using Stirling's approximation, we can estimate the worst-case entropy of \mathfrak{T}_n as:

$$|\mathfrak{T}_n| = \frac{(2n-2)!}{n!(n-1)!} = \frac{(2n-2)^{2n-2}e^ne^{n-1}}{e^{2n-2}n^n(n-1)^{n-1}\sqrt{\pi n}} \left(1 + O\left(\frac{1}{n}\right)\right)$$

This simplifies to $\frac{4^n}{n^{3/2}} \cdot \Theta(1)$, hence

$$H_{wc}(\mathfrak{T}_n) = \log |\mathfrak{T}_n| = 2n - \Theta(\log n)$$
(3)

Thus, we have determined the minimum number of bits required to uniquely identify (encode) a general ordinal tree with n nodes.

2.1 ENTROPY

Let's introduce the concept of entropy as a measure of uncertainty of a random variable. A deeper explanation can be found in [19, 25, 8]

Definition 2.3 (Entropy of a Random Variable). Let X be a random variable taking values in a finite alphabet X with the probabilistic distribution $P_X(x) = Pr\{X = x\}$ ($x \in X$). Then, the entropy of X is defined as

$$H(X) = H(P_X) \stackrel{\text{def}}{=} E_{P_X} \{ -\log P_X(x) \} = -\sum_{x \in X} P_X(x) \log P_X(x)$$
 (1)

This is also known as Shannon entropy, named after Claude Shannon, who introduced it in his seminal work [31]

Where E_P denotes the expectation with respect to the probability distribution P. The log is taken to the base 2 and the entropy is expressed in bits. It is then clear that the entropy of a discrete random variable will always be nonnegative¹.

Example 2.4 (Toss of a fair coin). Let X be a random variable representing the outcome of a toss of a fair coin. The probability distribution of X is $P_X(0) = P_X(1) = \frac{1}{2}$. The entropy of X is

$$H(X) = -\frac{1}{2}\log\frac{1}{2} - \frac{1}{2}\log\frac{1}{2} = 1$$
 (2)

This means that the toss of a fair coin has an entropy of 1 bit.

Remark 2.5. Due to historical reasons, we are abusing the notation and using H(X) to denote the entropy of the random variable X. It's important to note that this is not a function of the random variable: it's a functional of the distribution of X. It does not depend on the actual values taken by the random variable, but only on the probabilities of these values.

The concept of entropy, introduced in definition 2.3, helps us quantify the randomness or uncertainty associated with a random variable. It essentially reflects the average amount of information needed to identify a specific value drawn from that variable. Intuitively, we can think of entropy as the average number of digits required to express a sampled value.

¹ The entropy is null if and only if X = c, where c is a costant with probability one

2.1.1 Properties

In the previous section 2.1, we have introduced the entropy of a single random variable X. What if we have two random variables X and Y? How can we measure the uncertainty of the pair (X,Y)? This is where the concept of joint entropy comes into play. The idea is to consider (X,Y) as a single vector-valued random variable and compute its entropy. This is the joint entropy of X and Y.

Definition 2.6 (Joint Entropy). Let (X,Y) be a pair of discrete random variables (X,Y) with a joint distribution $P_{XY}(x,y) = Pr\{X = x,Y = y\}$. The joint entropy of (X,Y) is defined as

$$H(X,Y) = H(P_{XY}) = -\sum_{x \in \mathcal{X}} \sum_{y \in \mathcal{Y}} P_{XY}(x,y) \log P_{XY}(x,y)$$
(3)

Which we can be extended to the joint entropy of n random variables $(X_1, X_2, ..., X_n)$ as $H(X_1, ..., X_n)$.

We also define the conditional entropy of a random variable given another as the expected value of the entropies of the conditional distributions, averaged over the conditioning random variable. Given two random variables X and Y, we can define W(y|x), with $x \in \mathcal{X}$ and $y \in \mathcal{Y}$, as the conditional probability of Y given X. The set W of those conditional probabilities is called *channel* with *input alphabet* \mathcal{X} and *output alphabet* \mathcal{Y} .

Definition 2.7 (Conditional Entropy). Let (X,Y) be a pair of discrete random variables with a joint distribution $P_{XY}(x,y) = Pr\{X = x, Y = y\}$. The conditional entropy of Y given X is defined as

$$H(Y|X) = H(W|P_X) \stackrel{\text{def}}{=} \sum_{x} P_X(x)H(Y|x)$$
(4)

$$= \sum_{\mathbf{x} \in \mathcal{X}} P_{\mathbf{X}}(\mathbf{x}) \left\{ -\sum_{\mathbf{y} \in \mathcal{Y}} W(\mathbf{y}|\mathbf{x}) \log W(\mathbf{y}|\mathbf{x}) \right\}$$
 (5)

$$= -\sum_{\mathbf{x} \in \mathcal{X}} \sum_{\mathbf{y} \in \mathcal{Y}} P_{\mathbf{X}\mathbf{Y}}(\mathbf{x}, \mathbf{y}) \log W(\mathbf{y}|\mathbf{x})$$
 (6)

$$= \mathsf{E}_{\mathsf{P}_{\mathsf{X}\mathsf{Y}}} \{ -\log W(\mathsf{Y}|\mathsf{X}) \} \tag{7}$$

Since entropy is always nonnegative, conditional entropy is likewise nonnegative; it has value zero if and only if Y can be entirely determined from X with certainty, meaning there exists a function f(X) such that Y = f(X) with probability one.

The connection between joint entropy and conditional is more evident when considering that the entropy of two random variables equals the entropy of one of them plus the conditional entropy of the other. This connection is formally proven in the following theorem. **Theorem 2.8** (Chain Rule). Let (X,Y) be a pair of discrete random variables with a joint distribution $P_{XY}(x,y)$. Then, the joint entropy of (X,Y) can be expressed as

This is also known as additivity of entropy.

$$H(X,Y) = H(X) + H(Y|X)$$
(8)

Proof. From the definition of conditional entropy (2.7), we have

$$\begin{split} H(X,Y) &= -\sum_{x,y} P_{XY}(x,y) \log W(y|x) \\ &= -\sum_{x,y} P_{XY}(x,y) \log \frac{P_{XY}(x,y)}{P_{X}(x)} \\ &= -\sum_{x,y} P_{XY}(x,y) \log P_{XY}(x,y) + \sum_{x,y} P_{X}(x) \log P_{X}(x) \\ &= H(XY) + H(X) \end{split}$$

Where we used the relation

$$W(y|x) = \frac{P_{XY}(x,y)}{P_X(x)}$$
(9)

When
$$P_X(x) \neq 0$$
.

Corollary 2.9.

$$H(X,Y|Z) = H(X|Z) + H(Y|X,Z)$$
 (10)

Proof. The proof is analogous to the proof of the chain rule. \Box

Corollary 2.10.

$$H(X_1, X_2, ..., X_n) = H(X_1) + H(X_2|X_1) + H(X_3|X_1, X_2)$$

$$+ ... + H(X_n|X_1, X_2, ..., X_{n-1})$$
(11)

Proof. We can apply the two-variable chain rule in repetition obtain the result. \Box

2.1.2 Mutual Information

Given two random variables X and Y, the mutual information between them quantifies the reduction in uncertainty about one variable due to the knowledge of the other. It is defined as the difference between the entropy and the conditional entropy. Figure 1 illustrates the concept of mutual information between two random variables.

Definition 2.11 (Mutual Information). Let (X,Y) be a pair of discrete random variables with a joint distribution $P_{XY}(x,y)$. The mutual information between X and Y is defined as

$$I(X;Y) = H(X) - H(X|Y)$$
 (12)

Using the chain rule (2.8), we can rewrite it as

$$\begin{split} I(X;Y) &= H(X) - H(X|Y) \\ &= H(X) + H(Y) - H(X,Y) \\ &= -\sum_{x} P_{X}(x) \log P_{X}(x) - \sum_{y} P_{Y}(y) \log P_{Y}(y) \end{split} \tag{13}$$

$$+\sum_{x,y} P_{XY}(x,y) \log P_{XY}(x,y) \tag{14}$$

$$= \sum_{x,y} P_{XY}(x,y) \log \frac{P_{XY}(x,y)}{P_{X}(x)P_{Y}(y)}$$
 (15)

$$= E_{P_{XY}} \left\{ log \frac{P_{XY}(x,y)}{P_X(x)P_Y(y)} \right\}$$
 (16)

It follows immediately that the mutual information is symmetric, I(X;Y) = I(Y;X).

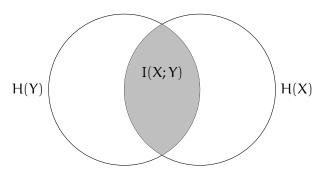


Figure 1: Mutual information between two random variables X and Y.

2.1.3 Fano's inequality

Information theory serves as a cornerstone for understanding fundamental limits in data compression. It not only allows us to prove the existence of encoders (Section 2.2) achieving demonstrably good performance, but also establishes a theoretical barrier against surpassing this performance. The following theorem, known as Fano's inequality, provides a lower bound on the probability of error in guessing a random variable X to it's conditional entropy H(X|Y), where Y is another random variable².

Theorem 2.12 (Fano's Inequality). Let X and Y be two discrete random variables with X taking values in some discrete alphabet X, we have

$$H(X|Y) \leqslant Pr\{X \neq Y\} \log(|\mathcal{X}| - 1) + h(Pr\{X \neq Y\}) \tag{17}$$

where $h(p) = -p \log p - (1-p) \log (1-p)$ is the binary entropy function.

² We have seen in 2.7 that the conditional entropy of X given Y is zero if and only if X is a deterministic function of Y. Hence, we can estimate X from Y with zero error if and only if H(X|Y) = 0.

Proof. Let Z be a random variable defined as follows:

$$Z = \begin{cases} 1 & \text{if } X \neq Y \\ 0 & \text{if } X = Y \end{cases}$$
 (18)

We can then write

$$\begin{split} H(X|Y) &= H(X|Y) + H(Z|XY) = H(XZ|Y) \\ &= H(X|YZ) + H(Z|Y) \\ &\leqslant H(X|YZ) + H(Z) \end{split} \tag{19}$$

The last inequality follows from the fact that conditioning reduces entropy. We can then write

$$H(Z) = h(Pr\{X \neq Y\}) \tag{20}$$

Since $\forall y \in \mathcal{Y}$, we can write

$$H(X|Y = y, Z = 0) = 0$$
 (21)

and

$$H(X|Y=y,Z=1) \leqslant \log(|\mathcal{X}|-1) \tag{22}$$

Combining these results, we have

$$H(X|YZ) \leqslant \Pr\{X \neq Y\} \log(|\mathcal{X}| - 1) \tag{23}$$

From equations 19, 20 and 23, we have Fano's inequality. \Box

TODO: Add some conclusion to the section

2.2 SOURCE AND CODE

TODO: Some introduction about the source and coding, maybe with some very simple example like the morse code that uses a single dot to represent the most common symbol.

2.2.1 *Codes*

A source characterized by a random process generates symbols from a specific alphabet at each time step. The objective is to transform this output sequence into a more concise representation. This data reduction technique, known as *source coding* or *data compression*, utilizes a code to represent the original symbols more efficiently. The device that performs this transformation is termed an *encoder*, and the process itself is referred to as *encoding*. [19]

Definition 2.13 (Source Code). A source code for a random variable X is a mapping from the set of possible outcomes of X, called \mathfrak{X} , to \mathfrak{D}^* , the set of all finite-length strings of symbols from a \mathfrak{D} -ary alphabet. Let C(X) denote the codeword assigned to x and let l(x) denote length of C(x)

Definition 2.14 (Expected length). The expected length L(C) of a source code C for a random variable X with probability mass function $P_X(x)$ is defined as

$$L(C) = \sum_{x \in \mathcal{X}} P_X(x) l(x)$$
 (1)

where l(x) is the length of the codeword assigned to x.

Let's assume from now for simplicity that the \mathcal{D} -ary alphabet is $\mathcal{D} = \{0, 1, ..., D-1\}$.

Example 2.15. Let's consider a source code for a random variable X with $\mathcal{X} = \{a,b,c,d\}$ and $P_X(a) = 0.5$, $P_X(b) = 0.25$, $P_X(c) = 0.125$ and $P_X(d) = 0.125$. The code is defined as

$$C(a) = 0$$

C(b) = 10

C(c) = 110

C(d) = 111

The entropy of X is

$$H(X) = 0.5 \log 2 + 0.25 \log 4 + 0.125 \log 8 + 0.125 \log 8 = 1.75 \text{ bits}$$

The expected length of this code is also 1.75:

$$L(C) = 0.5 \cdot 1 + 0.25 \cdot 2 + 0.125 \cdot 3 + 0.125 \cdot 3 = 1.75 \ bits$$

In this example we have seen a code that is optimal in the sense that the expected length of the code is equal to the entropy of the random variable.

Example 2.16 (Morse Code). TODO from [8]

Definition 2.17 (Nonsingular Code). A code is nonsingular if every element of the range of X maps to a different element of \mathbb{D}^* . Thus:

$$x \neq y \Rightarrow C(x) \neq C(y) \tag{2}$$

While a single unique code can represent a single value from our source X without ambiguity, our real goal is often to transmit sequences of these values. In such scenarios, we could ensure the receiver can decode the sequence by inserting a special symbol, like a "comma," between each codeword. However, this approach wastes the special symbol's potential. To overcome this inefficiency, especially when dealing with sequences of symbols from X, we can leverage the concept of self-punctuating or instantaneous codes. These codes possess a special property: the structure of the code itself inherently indicates the end of each codeword, eliminating the need for a separate punctuation symbol. The following definitions formalize this concept. [8]

Definition 2.18 (Extension of a Code). The extension C^* of a code C is the mapping from finite-length sequences of symbols from X to finite-length strings of symbols from the D-ary alphabet defined by

$$C^*(x_1x_2...x_n) = C(x_1)C(x_2)...C(x_n)$$
(3)

where $C(x_1)C(x_2)...C(x_n)$ denotes the concatenation of the codewords assigned to $x_1, x_2, ..., x_n$.

Example 2.19. If $C(x_1) = 0$ and $C(x_2) = 110$, then $C^*(x_1x_2) = 0110$.

Definition 2.20 (Unique Decodability). *A code* C *is uniquely decodable if its extension is nonsingular*

Thus, any encoded string in a uniquely decodable code has only one possibile source string that could have generated it.

Definition 2.21 (Prefix Code). A code is a prefix code if no codeword is a prefix of any other codeword.

Also called instantaneous code

Imagine receiving a string of coded symbols. An *instantaneous code* allows us to decode each symbol as soon as we reach the end of its corresponding codeword. We don't need to wait and see what comes next. Because the code itself tells us where each codeword ends, it's like the code "punctuates itself" with invisible commas separating the symbols. This let us decode the entire message by simply reading the string and adding commas between the codewords without needing to see any further symbols. Consider the example 2.15 seen a the beginning of this section, where the binary string 01011111010 is decoded as 0,10,111,110,10 because the code used naturally separates the symbols. [8]. Figure 2 shows the relationship between different types of codes.

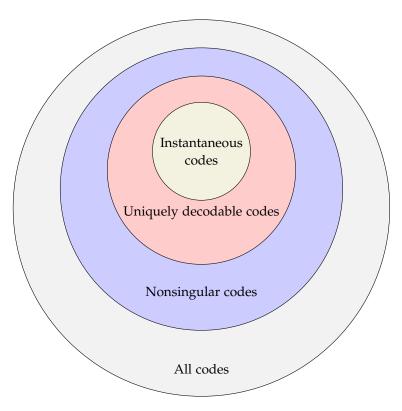


Figure 2: Relationship between different types of codes

2.2.2 Kraft's Inequality

We would like to construct instantaneous codes that are optimal in the sense that the expected length of the code is equal to the entropy of the random variable. However, we can't assign short codewords to all symbols and hope to be still prefix-free. Kraft's inequality provides a necessary and sufficient condition for the existence of a prefix code with given codeword lengths.

Let's denote the size of the source and code alphabets with $J=|\mathfrak{X}|$ and $K=|\mathfrak{D}|$, respectively. Different proofs of the following theorem can be found in [8, 19], here we report the one from [19], however the one proposed in [8] is also very interesting, based on the concept of a source tree.

Theorem 2.22 (Kraft's Inequality). The codeword length l(x), $x \in \mathcal{X}$, of any separable code C must satisfy the inequality

$$\sum_{\mathbf{x} \in \mathcal{X}} \mathsf{K}^{-\mathsf{l}(\mathbf{x})} \leqslant 1 \tag{4}$$

Proof. Consider the left hand side of the inequality 4 and consider its n-th power

$$\left(\sum_{\mathbf{x}\in\mathcal{X}} \mathsf{K}^{-\mathsf{l}(\mathbf{x})}\right)^{\mathsf{n}} = \sum_{\mathbf{x}_1\in\mathcal{X}} \sum_{\mathbf{x}_2\in\mathcal{X}} \dots \sum_{\mathbf{x}_n\in\mathcal{X}} \mathsf{K}^{-\mathsf{l}(\mathbf{x}_1)} \mathsf{K}^{-\mathsf{l}(\mathbf{x}_2)} \dots \mathsf{K}^{-\mathsf{l}(\mathbf{x}_n)}$$

$$= \sum_{\mathbf{x}^n\in\mathcal{X}^{\setminus}} \mathsf{K}^{-\mathsf{l}(\mathbf{x}^n)}$$
(5)

Where $l(x^n) = l(x_1) + l(x_2) + ... + l(x_n)$ is the length of the concatenation of the codewords assigned to $x_1, x_2, ..., x_n$. If we consider the all the extended codewords of length m we have

$$\sum_{\mathbf{x}^{\mathbf{n}} \in \mathcal{X}^{\setminus}} K^{-l(\mathbf{x}^{\mathbf{n}})} = \sum_{m=1}^{nl_{m} a \mathbf{x}} A(m) K^{-m}$$
(6)

where $A(\mathfrak{m})$ is the number source sequences of length \mathfrak{n} whose codewords have length \mathfrak{m} and $l_{\mathfrak{max}}$ is the maximum length of the codewords in the code. Since the code is separable, we have that $A(\mathfrak{m}) \leqslant K^{\mathfrak{m}}$ and therefore each term of the sum is less than or equal to 1. Hence

$$\left(\sum_{\mathbf{x}\in\mathcal{X}}\mathsf{K}^{-\mathsf{l}(\mathbf{x})}\right)^{\mathsf{n}}\leqslant\mathsf{nl}_{\mathsf{max}}\tag{7}$$

That is

$$\sum_{x \in \mathcal{X}} K^{-l(x)} \leqslant (n l_{max})^{1/n} \tag{8}$$

Taking the limit as n goes to infinity and using the fact that $(nl_{max})^{1/n} = e^{1/n \log(nl_{max})} \to 1$ we have that

$$\sum_{x \in \mathcal{X}} K^{-l(x)} \leqslant 1 \tag{9}$$

That concludes the proof.

2.2.3 Source Coding Theorem

Some introduction from [8, 31, 1, 19]

Theorem 2.23 (Source Coding Theorem). TODO from [8, 19]

Proof. TODO from
$$[8, 19]$$

2.3 EMPIRICAL ENTROPY

Before digging into the concept of empirical entropy, let's begin with the notion of binary entropy. Consider an alphabet \mathcal{U} , where $\mathcal{U}=\{0,1\}$. Let's assume it emits symbols with probabilities \mathfrak{p}_0 and $\mathfrak{p}_1=1-\mathfrak{p}_0$. The entropy of this source can be calculated using the formula:

$$H(p_0) = -p_0 \log_2 p_0 - (1 - p_0) \log_2 (1 - p_0)$$

We can extend this concept to scenarios where the elements are no longer individual bits, but sequences of these bits emitted by the source. Initially, let's assume the source is *memoryless* (or *zero-order*), meaning the probability of emitting a symbol doesn't depend on previously emitted symbols. In this case, we can consider chunks of n bits as our elements. Our alphabet becomes $\Sigma = \{0,1\}^n$, and the Shannon Entropy of two independent symbols $x,y \in \Sigma$ will be the sum of their entropies. Thus, if the source emits symbols from an alphabet $\Sigma = [0,\sigma]$ where each symbol has a probability p_s , the entropy of the source becomes:

$$H(p_1, \dots, p_{\sigma}) = -\sum_{s=1}^{\sigma} p_s \log p_s = \sum_{s=1}^{\sigma} p_s \log \frac{1}{p_s}$$

Remark 2.24. If all symbols have a probability of $p_s = 1$, then the entropy is 0, and all other probabilities are 0. If all symbols have the same probability $\frac{1}{\sigma}$, then the entropy is $\log \sigma$. So given a sequence of n elements from an alphabet Σ , belonging to $U = \Sigma^n$, its entropy is straightforwardly $n\mathcal{H}(p_1, \ldots, p_\sigma)$

2.3.1 Bit Sequences

Let's consider a bit sequence, B[1, n], which we aim to compress without access to an explicit model of a known bit source. Instead, we only have access to B. Although lacking a precise model, we may reasonably anticipate that B exhibits a bias towards either more 0s or more 1s. Hence, we might attempt to compress B based on this characteristic. Specifically, we say that B is generated by a zero-order source emitting 0s and 1s. Assuming m represents the count of 1s in B, it's reasonable to posit that the source emits 1s with a probability of p = m/n. This leads us to the concept of zero-order empirical entropy:

Definition 2.25 (Zero-order empirical entropy). Given a bit sequence B[1,n] with m 1s and n-m 0s, the zero-order empirical entropy of B is defined as:

$$\mathcal{H}_0(B) = \mathcal{H}\left(\frac{m}{n}\right) = \frac{m}{n}\log\frac{n}{m} + \frac{n-m}{n}\log\frac{n}{n-m}$$
 (1)

The concept of zero-order empirical entropy carries significant weight: it indicates that if we attempt to compress B using a fixed code C(1) for 1s and C(0) for 0s, then it's impossible to compress B to fewer than $\mathcal{H}_0(B)$ bits per symbol. Otherwise, we would have $m|C(1)|+(n-m)|C(0)|< n\mathcal{H}_0(B)$, which violates the lower bound established by Shannon entropy.

CONNECTION WITH WORST CASE ENTROPY TBD if to add this paragraph, from [25] 2.3.1

2.3.2 Entropy of a Text

The zero-order empirical entropy of a string S[1,n], where each symbol s occurs n_s times in S, is similarly determined by the Shannon entropy of its observed probabilities:

Definition 2.26 (Zero-order empirical entropy of a text). Given a text S[1,n] with n_s occurrences of symbol s, the zero-order empirical entropy of S is defined as:

$$\mathcal{H}_0(S) = \mathcal{H}\left(\frac{n_1}{n}, \dots, \frac{n_\sigma}{n}\right) = \sum_{s=1}^\sigma \frac{n_s}{n} \log \frac{n}{n_s}$$
 (2)

Example 2.27. TODO: Classic example on finding the zero-order empirical entropy of a word like abracadabra or banana

However, this definition falls short because in most natural languages, symbol choices aren't independent. For example, in English text, the sequence "don'" is almost always followed by "t". Higher-order entropy (section 2.4) is a more accurate measure of the entropy of a text, as it considers the probability of a symbol given the preceding symbols

2.4 HIGHER ORDER ENTROPY

TODO: A bit of introduction

Definition 2.28 (Redundacy). *TODO: Give a formal definition of redundacy: informally is a measure of the distance between the source's entropy and the compression ration, and can thereby be seen as a measure of how fast the algorithm reaches the entropy of the source.*

While using measures like 2.28 are certainly intriguing, their actual usability is questionable due to the inherent challenge of determining the entropy of the source generating the string we aim to compress. To address this issue, an alternative empirical approach is the concept of the *k-th order empirical entropy* of a string S, denoted as $\mathcal{H}_k(S)$. In statistical coding (Section 2.6), we will see a scenario where k=0, relying on symbol frequencies within the string. Now, with $\mathcal{H}_k(S)$, our objective is to extend the entropy concept by examining the frequencies of k-grams in string S. This requires analyzing subsequences of symbols with a length of k, thereby capturing the *compositional structure* of S. [10]

Let S be a string over the alphabet $\Sigma = {\sigma_1, ..., \sigma_n}$. Denote with n_ω the number of occurrences of the k-gram ω in S. ³

Definition 2.29 (k-th Order Empirical Entropy). *The* k-th order empirical entropy *of a string* S *is defined as*

$$\mathcal{H}_{k}(S) = \frac{1}{|S|} \sum_{\omega \in \Sigma^{k}} \left(\sum_{i=1}^{h} n_{\omega \sigma_{i}} \log \left(\frac{n_{\omega}}{n_{\omega \sigma_{i}}} \right) \right) \tag{1}$$

where |S| is the length of the string S.

When considering a sequence S[1, n] we can compute the *empirical k-th entropy* of S by considering the frequencies of symbols depending on the k preceding symbols.

$$\mathcal{H}_{k}(S) = \sum_{\omega \in \Sigma^{k}} \frac{|S_{\omega}|}{n} \cdot \mathcal{H}_{l}(S_{\omega})$$
 (2)

where S_{ω} is a string formed by collecting the symbol that follows each occurrence of the k-gram $\omega = \sigma_1 \dots \sigma_k$ in S.

Example 2.30. TODO: add here a numerical example where the first order empirical entropy is much less then the zero order empirical entropy.

Extending the concept of zero-order empirical entropy, $n\mathcal{H}_k(S)$ serves as a lower bound for the minimum number of bits attainable by any

³ We will use the notation $\omega \in \Sigma^k$ to denote a k-gram, i.e., a subsequence of k symbols in the string S.

encoding of S, under the condition that the encoding of each symbol may rely on itself and the k symbols preceding it in S. Consistently, any compressor that surpasses this threshold would also have the capability to compress symbols originating from the related kth-order source to a level lower than its Shannon entropy.

Remark 2.31. As k grows large (up to k = n - 1, and often sooner), the k-th order empirical entropy of S reaches null, given that each k-gram appears only once. This renders our model ineffective as a lower bound for compressors. Even before reaching the k value where $\mathcal{H}_k(S) = 0$, compressors face practical difficulties in achieving the target of $n\mathcal{H}_k(S)$ bits, particularly for high k values. This is due to the necessity of storing the set of σ^{k+1} probabilities or codes, adding complexity to compression. Likewise, adaptive compressors must incorporate σ^{k+1} escape symbols into the compressed file, further complicating the process. In theory, it is commonly assumed that S can be compressed up to $n\mathcal{H}_k(S) + o(n)$ bits for any $k+1 \leq \alpha \log \sigma n$ and any constant $0 < \alpha < 1$. In such cases, storing σ^{k+1} numbers within the range [1,n] (such as the frequencies of the k-grams) requires $\sigma^{k+1} \log n \leq n^{\alpha} \log n = o(n)$ bits. [25]

Definition 2.32 (Coarsely Optimal Compression Algorithm). A compression algorithm is coarsely optimal if, for every value of k, there exists a function $f_k(n)$ that tends to zero as the length of the sequence n approaches infinity, such that for all sequences S of increasing length, the compression ratio achieved by the algorithm remains within $\mathcal{H}_k(S) + f_k(|S|)$.

The *Lempel-Ziv* algorithm (LZ78) serves as an example of a coarsely optimal compression technique, as outlined by Plotnik et al. in [27]. This algorithm relies on the idea of dictionary-based compression. However, as highlighted by Manzini and Korařaju [22], the notion of coarse optimality doesn't necessarily guarantee the effectiveness of an algorithm. Even when the entropy of the string is extremely low, the algorithm might still perform inadequately due to the presence of the supplementary term $f_k(|S|)$.

FURTHER COMMENTS ON LZ77 AND LZ78 TBD if to include this section, but I think it's not relevant for the thesis. If included, it should discuss very briefly the LZ77 and LZ78 algorithms, and the differences between them. [10]. And then prove two lemmas: one about the compression ration achieved by LZ78 and the other about LZ77 not being coarsely optimal. [10], end of chapter 13.

2.5 INTEGER CODING

Most important references for this section: [10, 29, 25]

TODO: Introduce the following problem: given $S = \{x_1, x_2, ..., x_n\}$, where $x_i \in \mathbb{N}$, we want to represent the integers of S as a sequence of bits that are self-delimiting. The goal is to minimize the space occupancy of the representation [10]. Add here some examples of where this problem appears in practice [32]

The central concern in this section revolves around formulating an efficient binary representation method for an indefinite sequence of integers. Our objective is to minimize bit usage while ensuring that the encoding remains prefix-free. In simpler terms, we aim to devise a binary format where the codes for individual integers can be concatenated without ambiguity, allowing the decoder to reliably identify the start and end of each integer's representation within the bit stream and thus restore it to its original uncompressed state.

2.5.1 Unary Code

TODO: Introduction to unary code, from [10, 29]

Theorem 2.33. The unary code of a positive integer x takes x bits, and thus it is optimal for the distribution $P(x) = 2^{-x}$. [10]

Theorem 2.34. Given a set of S integers, of maximum value M, the fixed-length binary code represents each of them in $\lceil \log_2(M) \rceil$ bits and is optimal for the distribution P(x) = 1/M. [10]

2.5.2 Elias Codes: γ and δ

TODO: Introduction and explanation of Elias codes, from [10, 9]

Theorem 2.35. The γ code of a positive integer x takes $2\lceil \log_2(x+1)\rceil - 1$ bits, and thus it is optimal for the distribution $P(x) = 1/x^2$. This is within a factor of two from the bit length $|B(x)| = \lceil \log_2(x) \rceil$ of the fixed-length binary code. [10]

TODO: Talk a bit about the inefficiency of the γ code [10]

Theorem 2.36. The δ code of a positive integer x takes $1 + \log_2 x + 2\log_2 \log_2 x$ bits, and thus it is optimal for the distribution $P(x) = 1/x(|\log x|^2)$. This is within a factor of 1 + o(1) from the bit length $|B(x)| = \lceil \log_2(x) \rceil$ of the fixed-length binary code. [10]

2.5.3 Rice Code

TODO: Just a brief mention on why we use it when values are concentrated around a certain range [10, 29] and on how it works.

2.5.4 Elias-Fano Code

TBD if to include this section or not. If included, it should be a brief mention of the Elias-Fano code and its use in integer compression [10].

2.6 STATISTICAL CODING

TODO: Introduction to statistical coding, from [19] and [10]

2.6.1 Huffman Coding

Sources for this section: Chapter 4 of [29], chapter 12 of [10], 3.8 from [19], 5.6/7/8 of [8], 2.6 of [25] and the original paper [20]

TODO: Introduction of the type of source and the situation we are in.

TODO: Talk about construction, encoding and decoding, canonical Huffman codes [30], and the optimality of Huffman codes. [10, 29].

Example 2.37. TODO: Classic example of Huffman coding with for example $\mathcal{X} = \{a, b, c, d, e\}$ and P(a) = 0.25, P(b) = 0.25, P(c) = 0.2, P(d) = 0.15, P(e) = 0.15. Do a nice tree and show the encoding of each symbol.

There a are a few other theorems and lemmas that can be included in this section, TBD if to include them.

Theorem 2.38. Let H be the entropy of a source emitting the symbols of an alphabet Σ , hence $H = \sum_{\sigma \in \Sigma} P(\sigma) \log_2 \left(\frac{1}{P(\sigma)}\right)$. Then, the average length of the Huffman code is $L \leq H < L + 1$.

Proof. TODO: from [10], page 215.

TODO and TBD: There are a lot of comments that can be done after this theorem. Still to decide what to include.

2.6.2 *Arithmetic Coding*

TODO: Do a brief introduction to Arithmetic Coding, explaining the idea behind it (Elias Code from 1960s) and the main differences with Huffman Coding. Section 12.2 from [10], section 4.2 fron [19], chapter 5 from [29].

Example 2.39. TODO: Begin with an example to underline this differences

Decoding Process

TODO: Talk about the compression algorithm and make an example of encoding a sequence of symbols. Add a pseudo code of the algorithm.

Decoding Process

TODO: Talk about the decompression algorithm and make an example of decoding a sequence of symbols. Add a pseudo code of the algorithm.

Efficiency of Arithmetic Coding

Theorem 2.40. The number of bits emitted by arithmetic coding for a sequence S of n symbols is at most 2 + nH, where H is the empirical entropy of the sequence S.

Proof. TODO: from [10], page 228-229. □

NOTE: this theorem requires a lemma and corollary to be proven first.

FURTER COMMENTS ON ARITHMETIC CODING TBD if to include this section. If so, it should show some other techniques such as range coding and prediction by partial matching.

3.1 BITVECTORS

Consider the following problem [10]: imagine a dictionary $\mathcal D$ containing n strings from an alphabet Σ . We can merge all strings in $\mathcal D$ into a single string T[1, m], without any separators between them, where m is the total length of the dictionary. The task is to handle the following queries:

- Access_string(i): retrieve the i-th string in \mathfrak{D} .
- Which_string(x): find the starting position of the string in T, including the character T[x].

The conventional solution involves employing an array of pointers A[1,n] to the strings in \mathbb{D} , represented by their offsets in T[1,m], requiring $\Theta(n \log n)$ bits. Consequently, Access_string(i) simply returns A[i], while Which_string(x) involves locating the predecessor of x in A. The first operation is instantaneous, whereas the second one necessitates $O(\log n)$ time using binary search.

We can address the problem by employing a compressed representation of the offsets in A via a binary array B[1,m] of m bits, where B[i] = 1 if and only if i is the starting position of a string in T. In this case then $Access_string(i)$ searches for the i-th 1 in B, while $Which_string(x)$ counts the number of 1s in the prefix B[1,x].

In modern literature this two operations are well known as *rank* and *select* queries, respectively.

Definition 3.1 (Rank and Select). *Given* B[1,n] *a binary array of* n *bits (a bitvector), we define the following operations:*

- The rank of an index i in B relative to a bit b is the number of occurrences of b in the prefix B[1, i]. We denote it as $\operatorname{rank}_1(i) = \sum_{j=1}^i B[j]$. Similarly we can compute $\operatorname{rank}_0(i) = i \operatorname{rank}_1(i)$ in constant time.
- The **select** of the i-th occurrence of a bit b in B is the index of the i-th occurrence of b in B. We denote it as $select_b(i)$. Opposite to rank, we can't derive select of 0 from select of 1 in constant time.

Example 3.2. *TODO: Maybe add a simple example of a bitvector and show how to compute rank and select.*

In the following sections, our aim is to built structures of size o(n) bits that can be added on top either the bit array or the compressed representation of B to facilitate rank and select operations.

TBD: Do I talk also about how to compress the bitvector to $n\mathcal{H}_0(B)$ + o(n) bits with those extra o(n) to support rank and select operations still in O(1) time? There is also the compressed solution via Elias Fano, when the numbers of 1s in B is much smaller than n, where I can achieve $n\mathcal{H}_0(B) + O(m)$ bits of space occupancy. This approach poses a much lower overhead over the entropy. It supports Select in constant time, while access and Rank in $O(\log \frac{n}{m})$ [25, 10]. On a further note, in [13] Ferragina and Venturini achieved higher order compression for general strings, supporting access in constant time (so adding rank and select for bitvectors are natural extensions), do I talk about this as well?

3.1.1 Rank

TODO:

- Explain the tree level succinct data structure supporting the rank operation as in RRR [28]
- Proof of the space occupancy in bits of the structure. [10]
- Explain how to answer rank queries upon this data structure [10, 25]

Theorem 3.3. The space occupancy of the Rank data structure is o(m) bits, and thus it is asymptotically sublinear in the size of the binary array B[1, m]. The Rank algorithm takes constant time in the worst case, and accesses the array B only in read-mode

TBD: Do I talk about [18]?

Example 3.4. TODO: numeric small example to show how to answer rank queries.

3.1.2 *Select*

TODO:

- Explain how to the implementation of the Select operation mainly follows the three-level design of the Rank data structure, with the algorithmic twist that here the binary array B is not split into big and small blocks of fixed length, but the splitting is driven by the number of bits set to 1. [10, 25]
- Talk about the space occupancy in bits of the structure. [10, 25]

Theorem 3.5. The space occupancy of the $Select_1$ data structure is o(m) bits, and thus it is asymptotically sublinear in the size of the binary array B[1,m]. The $Select_1$ algorithm takes constant time in the worst case, and accesses the array B only in read-mode. The same time and space bounds hold for the $Select_0$ algorithm. [10]

3.2 WAVELET TREES

TODO: Improve this introduction, just a draft.

Wavelet trees, introduced in 2003 by Grossi, Gupta, and Vitter [15] are a self indexing data structure: meaning they can answer rank and select queries, while still allowing to access the text. This combination makes them particularly useful for compressed full-text indexes like the FM-index [12]. In such indexes, wavelet trees are employed to efficiently answer rank queries during the search process.

TBD if to add: Upon closer examination, one can recognize that the wavelet tree is a slight extension of an older (1988) data structure by Chazelle [7], commonly used in Computational Geometry. This structure represents points on a two-dimensional grid, undergoing a reshuffling process to sort them by one coordinate and then by the other. Kärkkäinen (1999) [21] was the first to apply this structure to text indexing, although the concept and usage differed from Grossi et al.'s proposal four years later.

Wavelet Trees can be seen in different ways: (i) as sequence representation, (ii) as a permutation of elements, and (iii) as grid point representation. Since 2003, these perspectives and their interconnections have proven valuable across diverse problem domains, extending beyond text indexing and computational geometry, where the structure originated [26, 17, 11].

An introduction to the problem

Consider a sequence S[1, n] as a generalization of bitvectors whose elements S[i] are drawn from an alphabet Σ^1 . The problem is to support the following queries:

- Access(i): return the i-th element of S.
- Rank(c,i): return the number of occurrences of character c in the prefix S[1,i].
- Select(c,i): return the position of the i-th occurrence of character c in S.

However, dealing with sequences is much more complex than dealing with bitvectors (as we have seen in Section 3.1) TODO: further expand this concept: show an attemp to solve this problem with a

¹ The size of the alphabet varies depending on the application. For example, in DNA sequences, the alphabet is $\Sigma = \{A, C, G, T\}$ (in Chapter 4 we will focus more on this specific case), while in other case it could be of millions of characters, such as in natural language processing.

naive approach, and see its shortcomings. The problem will be space occupancy, since if we use the solution for bitvectors, then the total space occupancy will be $n\sigma + o(n\sigma)$ bits, which is way too much. [25]

From now on, let $S[1,n] = s_1 s_2 \dots s_n$ be a sequence of length n over an alphabet Σ that for simplicity we write as $\Sigma = \{1, \dots, \sigma\}$. In this way, the string can be represented using $n\lceil \log \sigma \rceil = n \log \sigma + o(n)$ bits in plain form.

3.2.1 Structure

In the beginning of this section we showed that storing one bitvector per symbol is not space-efficient. The wavelet tree is a data structure that solves this problem by using a recursive hierarchical partitioning of the alphabet. Consider the subset $[a,b] \subset [1,\ldots,\sigma]$, then a wavelet tree over [a,b] is a balanced binary tree with b-a+1 leaves². The root node ν_{root} is associated with the whole sequence S[1,n], and stores a bitmap $B_{\nu_{root}}[1,n]$ defined as follows: $B_{\nu_{root}}[i]=0$ if $S[i] \leq (\alpha+b)/2$ and $B_{\nu_{root}}[i]=1$ otherwise. The tree is then recursively built by associating the subsequence $S_0[1,n_0]$ of elements in $[a,\ldots,\lfloor(\alpha+b)/2\rfloor]$ to the left child of ν , and the subsequence $S_1[1,n_1]$ of elements in $[\lfloor(\alpha+b)/2\rfloor+1,\ldots,b]$ to the right child of ν . This process is repeated until the leaves are reached. In this way the left child of the root node, is a wavelet tree for $S_0[1,n_0]$ over the alphabet $[a,\ldots,\lfloor(\alpha+b)/2\rfloor]$, and the right child is a wavelet tree for $S_1[1,n_1]$ over the alphabet $[\lfloor(\alpha+b)/2\rfloor+1,\ldots,b]$. [26]

Example 3.6. TODO: Add an example of a wavelet tree for a sequence with small alphabet.

Remark 3.7. The wavelet tree described has σ leaves and $\sigma-1$ internal nodes, and the height of the tree is $\lceil \log \sigma \rceil$. The space occupancy of each level it's exactly $\mathfrak n$ bits, while we have at most $\mathfrak n$ bits for the last level. The total number of bits stored by the wavelet tree in then upper bounded by $\mathfrak n \lceil \log \sigma \rceil$ bits. [26]. This however is not sufficient, if we want to also store the topology of the tree, we need to add extra $O(\sigma \log \mathfrak n)$ bits.

Tracking symbols

We have seen how the wavelet tree serves as a representation for a string S, but more than that it is a succinct data structure for the string. Thus, it takes space asymptotically close to the plain representation of the string and allows us to access the i-th symbol of the string in $O(\log \sigma)$ time. In algorithm 1 we show how extract the i-th symbol of the string S using a wavelet tree T, this operation is called Access.

² if a = b then the tree is just a leaf

Algorithm 1 Answering Access queries on a wavelet tree

```
Require: Sequence S (as a wavelet tree T), position i
Ensure: The i-th symbol of S, i.e the output of Access(S,i)
   [a, b] \leftarrow [1, \sigma]
  while a \neq b do
       if access(v.B, i) = 0 then
                                                      \triangleright i-th bit of the bitmap of \nu
           i \leftarrow rank_0(v.B, i)
                                              \triangleright move to the left child of node \nu
           v \leftarrow v.left
           b \leftarrow |(a+b)/2|
       else
           i \leftarrow rank_1(v.B, i)
           v \leftarrow v.right
                                            \triangleright move to the right child of node \nu
           a \leftarrow |(a+b)/2| + 1
       end if
   end while
   return a
```

In order to find S[i], we first look at the bitmap associated with the root node of the wavelet tree, and depending on the value of the ith bit of the bitmap, we move to the left or right child of the root node and continue recursively. However, the problem is to determine where our i has been mapped to: if we move to the left child, then we need to find the i-th o in the bitmap of the left child, and if we move to the right child, then we need to find the i-th 1 in the bitmap of the right child. This is done by the $rank_0$ and $rank_1$ functions, respectively. We continue this process until we reach a leaf node, and then we return the value of the leaf node.

Example 3.8. TODO and TBD: add a figure with the wavelet tree and the process of finding the i-th symbol of the string.

In addition to retrieving the i-th symbol of the string, we might also need to perform the inverse operation. That is, given a symbol's position at a leaf node, we aim to determine the position of the symbol in the string. This operation is referred to as Select and is outlined in Algorithm ??..

TODO: add the select algorithm and explain the process of finding the position of a symbol in the string. The references are Navarro's [26, 25]

TODO: Show how to generalize the rank and select operations to the wavelet tree. So with a query $rank_c(S,i)$, instead of moving from the root toward the leaf corresponding to S[i], we move toward the leaf of c. The idea is similar for select. [25] 6.2.2

TODO: Add some pratical consideration about using constant-time rank and select on the bitvectors. [25] 6.2

TBD if to add: Reducing redundancy

TODO: In 3.7 we mentioned that storing the topology of the wavelet tree requires $O(\sigma \log n)$ bits. This may be critical for large alphabets, and in this section we will show that this term can be removed by slightly altering the balanced wavelet tree shape. [24, 23].

3.2.2 Construction

TODO: Explain how to build a wavelet tree in $O(n \log n)$ time (and also talk about space occupancy), the procedure is well described in [25] 6.2.3.

Algorithm 2 Building a wavelet tree

Require: Sequence S[1, n] over alphabet $\Sigma = \{1, ..., \sigma\}$

Ensure: Wavelet tree T for S

TODO: add the algorithm to build the wavelet tree

3.3 COMPRESSED WAVELET TREES

TODO: An introduction on why we need to compress wavelet trees. From [25] 6.2.4

3.3.1 Entropy Coding

Compressing the bitvectors, from [26] 3.1 and [25] 6.2.4

3.3.2 Huffman-Shaped Wavelet Trees

TODO: An alternative to obtain nearly zero-order compressed space while using plain bitvectors is to give a Huffman shape to the wavelet tree, instead of using a balanced tree of height $\log \sigma$. From [25] 6.2.4, [26] 3.2

3.3.3 Higher Order Entropy Coding

TODO: In 3.3 from [26] there is a good explanation on how to compress the bitvectors using higher-order entropy coding. It references papers as [16]. There is also section 5 from [11] that gives a more technical explanation

SUBSET WAVELET TREES

4.1 INTRODUCTION: DEGENERATE STRINGS

Brief introduction to degenerate strings [14, 4]

4.2 STRUCTURE OF THE SUBSET WAVELET TREE

TODO: Describe the structure of the subset wavelet tree, from [3]

4.3 SUBSET-RANK AND SUBSET-SELECT

TODO: Describe the problem of subset-rank and subset-select, from [3]. Add pseudocode for the algorithms.

4.4 TBD WHAT TO DO FROM HERE

In [3] they compare 5 methods that supports rank and rank-pairs queries on small alphabet sequences (they need it to answer those queries on the sequences stored at the nodes of the subset wavelet tree). The methods are

- Wavelet Trees
 - Wavelet Trees with un-compressed bitvectors
 - Wavelet Trees with compressed bitvectors (RRR [28])
- Scanning Rank
- Sequence Splitting
- Generalized RRR

TBD: Do I have to talk about them? They developed this methods to support fast membership queries on de Bruijn graphs (Do I care about this in the thesis?). Further more, the danish in [6] say that:

we show that any structure supporting either subset-rank or subset-select must use at least $N\log\sigma-o(N\log\sigma)$ bits in the worst case (Theorem 2). By plugging a standard rank-select data structure into Theorem 1 we, in many cases, match this bound to within lower order terms, while simultaneously matching the query time of the fastest known rank-select data structures (see below). Note that any lower

bound for rank-select queries also holds for subset rank-select queries since any string is also a degenerate string. All our results hold on a word RAM with logarithmic word-size. Finally, we provide implementations of the reductions and compare them to the implementations of the Subset Wavelet Tree provided in [3], and the implementations of the reductions provided in [2]. Our most compact structure matches the space of their most compact structure while answering queries twice as fast. We also provide a structure using vector processing features that matches the space of the most compact structure while improving query time by a factor four to seven, remaining competitive with the fast structures for queries.

Of course it remains the open problem stated in [3]:

The main open problem we leave is to find a tighter analysis of the space required by subset wavelet trees when entropy compression is applied to their node sequences. In particular, can the size of the resulting structure be related in some way to the entropy of the subset sequence

So a part of this chapter will focus on trying to answer this question. It's TBD how to structure all this and what to keep and what to leave out.

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