Data Compression and Entropy Estimates by Non-sequential Recursive Pair Substitution

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We argue that Non-sequential Recursive Pair Substitution (NSRPS) as suggested by Jiménez-Montaño and Ebeling can indeed be used as a basis for an optimal data compression algorithm. In particular, we prove for Markov sequences that NSRPS together with suitable codings of the substitutions and of the substitute series does not lead to a code length increase, in the limit of infinite sequence length. When applied to written English, NSRPS gives entropy estimates which are very close to those obtained by other methods. Using ca. 135 GB of input data from the project Gutenberg, we estimate the effective entropy to be \( \approx 1.82 \) bit/character. Extrapolating to infinitely long input, the true value of the entropy is estimated as \( \approx 0.8 \) bit/character.

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I. INTRODUCTION

The discovery that the amount of information in a message (or in any other structure) can be objectively measured was certainly one of the major scientific achievements of the 20th century. On the theoretical side, this quantity – the information theoretic entropy – is of interest mainly because of its close relationship to thermodynamic entropy, its importance for chaotic systems, and its role in Bayesian inference (maximum entropy principle). Practically, estimating the entropy of a message (text document, picture, piece of music, etc.) is important because it measures its compressibility, i.e. the optimal achievement for any possible compression algorithm. In the following, we shall always deal with sequences \( s_0, s_1, \ldots \) built from the characters of a finite alphabet \( A = \{a_0, \ldots, a_{m-1}\} \) of size \( m \). In the simplest case the alphabet consists just of 2 characters, in which case the maximum entropy is 1 bit per character.

Indeed, information entropy as introduced by Shannon is a probabilistic concept. It requires a measure (probability distribution) to be defined on the set of all possible sequences. In particular, the probability for \( s_t \) to be given by \( a_k \), given all characters \( s_0, s_1, \ldots, s_{t-1} \), is given by

\[
p_t(k|k', k'', \ldots) = \text{prob}(s_t = a_k \mid s_{t-1} = a_{k'}, s_{t-2} = a_{k''}, \ldots).
\]

In case of a stationary measure with finite range correlations, \( p_t(k|k', k'', \ldots) \) becomes independent of \( t \) for \( t \to \infty \). Then Shannon’s famous formula,

\[
h = \lim_{i \to \infty} h^{(i)}(2)
\]

with

\[
h^{(i)} = - \sum_{k_1 \ldots k_i} p(k_1 \ldots k_i) \log_2 p(k_1 | k_2 \ldots k_i), \quad (3)
\]
gives the average information per character. The generalization to non-stationary measures is straightforward but will not be discussed here.

In contrast to this approach are attempts to define the exact information content of a single finite sequence. Theoretically, the basic concept here is the algorithmic complexity \( AC \) (or algorithmic randomness) \( \boxed{3} \). For any given universal computer \( U \), the AC of a sequence \( S \) relative to \( U \) is given by the length of the shortest program which, when input to \( U \), prints \( S \) and then makes \( U \) to stop, so that the next sequence can be read. If \( S \) is randomly drawn from a stationary ensemble with entropy \( h \), then one can show that the AC per character tends towards \( h \), for almost all \( S \) and all \( U \), as the length of \( S \) tends towards infinity \( \boxed{4} \). Thus, except for rare sequences which do not contribute to averages, \( h \) sets the limit for the compressibility.

Practically, the usefulness of AC is limited by the fact that there cannot exist any algorithm which finds for each \( S \) its shortest code (such an algorithm could be used to solve Turing’s halting problem, which is known to be impossible \( \boxed{4} \)). But one can give algorithms which are often quite efficient. Huffman, arithmetic, and Lempel-Ziv coding are just three well known examples \( \boxed{4} \). Any such algorithm can be used to give an upper bound to \( h \) (modulo fluctuations from the finite sequence length) while, inversely, knowledge of \( h \) sets a lower limit to the average code length possible with these codes.

A data compression scheme is called optimal, if it does not do much worse than the best possible for typical random strings. More precisely, let \( \{S\} \) be a set of sequences with entropy \( h(S) \), and let the code string \( C(S) \) be built from an alphabet of \( m_C \) characters. Then we call the coding scheme \( C : S \to C(S) \) optimal, if

\[
\frac{\text{length}[C(S)]}{\text{length}[S]} \to \frac{h}{\log_2 m_C} \quad \text{for } \text{length}[S] \to \infty \quad (4)
\]

and for nearly all \( S \). While Huffman coding is not optimal, arithmetic and Lempel-Ziv codings are \( \boxed{\boxed{4}} \).

In several papers, Jiménez-Montaño, Ebeling, and others \( \boxed{\boxed{4}} \) have suggested coding schemes by non-sequential recursive pair substitution (NSRPS) \( \boxed{\boxed{4}} \). Call the original sequence \( S_0 \). We count the numbers \( n_{jk} \) of non-overlapping successive pairs of characters in \( S_0 \)
where $s_t = a_j$ and $s_{t+1} = a_k$, and find their maximum, $n_{\text{max}} = \max_{j,k \leq m} n_{jk}$. The corresponding index pair is $(j_0, k_0)$. Then we introduce a new character by concatenation

$$a_m = (a_{j_0} a_{k_0})$$

and form the sequence $S_1$ by replacing everywhere the pair $a_{j_0} a_{k_0}$ by $a_m$. For the special case of $j_0 = k_0$, any string of $2r + 1$ characters $a_{j_0}$ is replaced by $r$ characters $a_m$, followed by one $a_{j_0}$.

This is then repeated recursively: The sequence $S_{i+1}$ is obtained from $S_i$ by replacing the most frequent pair $a_{j_i} a_{k_i}$ by a new character $a_{m_i}$. The procedure stops if one can argue that further replacements would not possibly be of any use. Typically this will happen if the code length consisting of both a description of $S_{i+1}$ and a description of the pair $(j_i, k_i)$ is definitely longer than a description of $S_i$, for the present and all subsequent $i$.

Thus one sees that efficient encodings (which must also be uniquely decodable!) of the sequences $S_i$ and of the type of substituted pairs become crucial for the analysis of NSRPS. Unfortunately, the “codings” given in [3, 4] are neither efficient nor uniquely decodable [1]. Thus their “complexities” have no direct relationship to $h$ or to algorithmic complexity (in contrast to their claim), and it is not clear from their work whether NSRPS can be made into an optimal coding scheme at all.

It is the purpose of the present paper to give at least partial answers to this. More precisely, we shall only be concerned with the limit of infinitely long strings, where the information encoded in the pairs $(j_i, k_i)$ can be neglected in comparison with the information stored in $S_i$, at least for any finite $i$. We will first show analytically that a coding scheme for $S_i$ exists which satisfies a necessary condition for optimality (Sec.2). We then apply this to written English (Sec.3), where we shall also compare our estimates of $h$ to those obtained with other methods.

II. NSRPS FOR MARKOV SEQUENCES

Let us for the moment assume that $S_0$ is binary (the two characters are “0” and “1”), and that it is completely random, i.e. identically and independently distributed (iid) with the same probability for each character. Thus $p(0|\ldots) = p(1|\ldots) = 1/2$, and $h = 1$ bit. The length of $S_0$ is $N_0$, thus the total average information stored in $S_0$ is $N_0$ bits.

No coding scheme can reduce the length of $C(S_0)$ to less than $N_0$ bits on average. Indeed, all schemes will have $\text{length}[C(S_0)] > N_0$ bits (strict inequality!), unless the “coding” is a verbatim copy. For a coding scheme to be optimal, a necessary (but not sufficient) condition is that

$$\text{length}[C(S_0)]/N_0 \to 1 \text{ bit}$$

for $N_0 \to \infty$, i.e. the overhead in the code must be less than extensive in the sequence length. This is what we want to show here, together with its generalization to arbitrary (first order) Markov sequences.

For this, we need two lemmata:

**Lemma 1:** For any Markov sequence $S_0$ (not necessarily binary, and not necessarily iid) built from $m$ letters, the sequence $S_1$ is again Markov.

**Lemma 2:** If a word $w = (k, k', k'', \ldots)$ appears several times in $S_0$, and if one of these instances is substituted in $S_i$ by a string of characters not straddling its boundaries, then all other instances of $w$ in $S_0$ are also substituted in $S_i$ by the same string.

**Lemma 1** tells us that NSRPS might make the structure of $S_i$ more complex than that of $S_0$, but not much so. Being a Markov chain, its entropy can be estimated if the transition probabilities $p(k|k_1)$ are known. Thus estimating the entropy of $S_1$ reduces to estimating di-block entropies $h^{(2)}$, which is straightforward (at least in the limit $N_0 \to \infty$).

**Lemma 2** tells us that there cannot be any ambiguity in $S_i$. In particular, it cannot happen that more information is needed to specify $S_i$ than there is needed to specify $S_0$, since the mapping $S_0 \to S_i$ is bijective, once the substitution rules are fixed.

The proofs of the lemmata are easy. Let us denote by $p_j(\ldots)$ the probability distributions after $j$ pair substitutions. For lemma 1 we just have to show that $p_1(k|k', k'')$ is independent of $k''$ for each pair $(k, k')$, provided the same holds also for $p_0$. This follows basically from the fact that any substitution makes the sequence shorter. But the detailed proof is somewhat tedious, because $p_1(k|k', k'') \neq p_0(k|k', k'')$, even if all $k$’s are less than $m$, $k \neq k_0$, $k'' \neq j_0$, and neither $(k, k')$ nor $(k', k'')$ are equal to the pair $(j_0, k_0)$. In that case, $(N_0 - n_{\text{max}})p_1(k|k', k'') = N_0 p_0(k|k', k'')$, and independence of $k''$ follows immediately. All other cases have to be dealt with similarly. For instance, if either $(k, k')$ or $(k', k'')$ is the pair $(j_0, k_0)$, then $p_1(k|k', k'') = 0$. Else, if $k'' = m \neq k, k'$, then $p_1(k|k', k'' = N_0/(N_0 - n_{\text{max}})p_0(k|k', j_0, k_0) = N_0/(N_0 - n_{\text{max}})p_0(k|k')$. We leave the other cases as exercises to the reader.

For proving **Lemma 2** we proceed indirectly. We assume that there is a word in $S_0$ which is encoded differently in different locations. Let us assume that this difference happened for the first time after $i$ substitutions. Since only one type of pair is exchanged in each step, this means that a substitution is skipped in one of the locations, at this step. But this is impossible, since all possible substitutions are made at each step.

From the two lemmata we obtain immediately our central

**Theorem:** If $S_0$ is drawn from a (first order) Markov process with length $N_0$ and entropy $h_0 = -\sum_{k,k'} p_0(k|k') \log_2 p_0(k|k')$, then every $S_i$ is also Markovian in the limit $N_0 \to \infty$, with entropy

$$h_i = h^{(2)} = -\sum_{k,k'} p_i(k|k') \log_2 p_i(k|k')$$

and with length $N_i$ satisfying $N_i/N_0 = h_0/h_i$. 

Thus the total amount of information needed to specify $S_i$ is the same as that for $S_0$ for infinitely long sequences. Since the overhead needed to specify the pairs $(j_i, k_i)$ can be neglected in this limit, we see that we do not lose code length efficiency by pair substitution, provided we take pair probabilities correctly into account during the coding. The actual encoding can be done by means of an arithmetic code based on the probabilities $p_i(k|k')$, but we shall not work out the details. It is enough to know that the code length then becomes equal to the information (both measured in bits), for $N_0 \to \infty$.

Let us see in detail how all this works for completely random iid binary sequences. The original sequence $S_0 = 001010011101001101011 \ldots$ has $p_0(00) = p_0(01) = p_0(10) = p_0(11) = 1/4$ and therefore $h_i = 1$ bit. Thus we can, without loss of generality, assume that the new character is $2 = (01)$, so that $S_1 = 02202111202121 \ldots$. The 3 characters are now equiprobable, $p_1(0) = p_1(1) = p_1(2) = 1/3$, but they are not independent since of course $p_1(01) = 0$. Indeed, one finds $p_1(00) = p_1(02) = p_1(11) = p_1(21) = 1/6, p_1(10) = p_1(12) = p_1(20) = p_1(22) = 1/12$. The order-2 entropy of $S_1$ is easily calculated as $h_i^{(2)} = 4/3 \log_2 2$. On the other hand, since $N_0/4$ pairs have been replaced by single characters, the length of $S_1$ is $N_1 = 3N_0/4$. Thus, if $S_1$ is Markov, then the total information needed to specify it is $N_1 h_i^{(2)} = N_0$ bits, the same as for $S_0$. If it were not Markov, its information would be smaller. But this cannot be, because the map $S_0 \to S_1$ was invertible. Thus $S_1$ must indeed be Markov, as can also be checked explicitly.

In the next step, we can either replace $(21) \to 3$ or $(02) \to 3$, since both have the same probability. If we do the former, the sequence becomes $S_2 = 02203112033 \ldots$. Now the letters are no longer equiprobable, $p_2(1) = p_2(2) = p_2(3) = 1/5, p_2(0) = 2/5$. Calculating $N_2$, $p_2(kk')$, and $h_i^{(2)}$ is straightforward, and one finds again $N_2 h_i^{(2)} = N_0$ bits. Thus one concludes that $S_2$ must also be Markov. For the next few steps one can still verify

\[ N_i h_i^{(2)} = \ldots N_0 \text{ bits,} \]

by hand, but this becomes increasingly tedious as $i$ increases.

Thus we have verified Eq. (8) by extensive simulations, where we found that it is exact, within the expected fluctuations, up to several thousand substitutions (Fig.1). The distribution of the probabilities $p_i(k)$ becomes very wide for large $i$, i.e. the sequences $S_i$ are far from uniform for large $i$, but they are Markov and their entropies $h_i^{(2)}$ are exactly (within the expected systematic finite sample corrections \[\text{[1]}\]) equal to $N_0/N_i$ bits. Notice that if we would encode the last $S_i$ without taking the correlations into account (as seems suggested in \[\text{[1]}\]), then the code length for it would be larger and the coding scheme would not be optimal.

We have also made some simulations where we started with non-trivial Markov processes for $S_0$, or even with non-Markov sequences with known entropy. The latter were generated by creating initially a binary iid sequence with $p(0) \neq p(1)$, and then using this as an input configuration for a few iterations of the bijective cellular automaton R150 (in Wolfram’s notation \[\text{[4]}\]).

From these simulations it seems that $N_i h_i^{(2)}$ always tends towards $N_0$. Also, the probability distributions $p_i(k)$ seem to tend (very slowly, see Fig.2) to the same scaling limit as for iid and uniform $S_0$. This suggests that indeed $S_j$ tends to a Markov process for arbitrary
$S_0$. In this case an optimal coding would be obtained if one would use, e.g., an arithmetic code to encode $S_i$ by using approximate values of the observed $p_i(k|k')$ for large $i$.

Thus we have given strong (but still incomplete) arguments that NSRPS combined with efficient coding of $S_i$ gives indeed an optimal coding scheme. In practice, it would of course be extremely inefficient in terms of speed, and thus of no practical relevance. But it could well be that it might lead to more stringent entropy estimates than other methods. To test this we shall now turn to one of the most complex and interesting system, written natural language.

### III. THE ENTROPY OF WRITTEN ENGLISH

The data used for the application of NSRPS to entropy estimation of written English consisted of ca. 150 MB of text taken from the Project Gutenberg homepage \[10\]. It includes mainly English and American novels from the 19th and early 20th century (Austen, Dickens, Galsworthy, Melville, Stevenson, etc.), but also some technical reports (e.g. Darwin, historical and sociological texts, etc.), Shakespearean collected works, the King James Bible, and some novels translated from French and Russian (Verne, Tolstoy, Dostoevsky, etc.).

From these texts we removed first editorial and legal remarks added by the editors of Project Gutenberg. We also removed end-of-line, end-of-page, and carriage return characters. All runs of consecutive blanks were replaced by a single blank. Finally, we also removed all characters not in the 7-bit ASCII alphabet (ca. 4200 in total). These cleaned texts were then concatenated to form one big input string of 148,214,028 characters.

Entropies were estimated both from this string (which still contained upper and lower case letters, numbers, all kinds of brackets and interpunctuation marks, 95 different characters in total), and from a version with reduced alphabet. In the latter, we changed all letters to upper case; all brackets to either ( or ); the symbols $, #, &, *, %, @ to one single symbol; colons, exclamation and question marks to points; quotation marks to apostrophes; and semicolons to commas. This reduced alphabet had then 46 letters (including, of course, the blank “”).

The most frequent pair of letters in English is “e”.

After replacing it by a new “letter”, the next pair to substitute is “en”, then “e”, “et”, “th”, etc. Very soon also longer strings are substituted, e.g. after 92 steps appears the first two-word combination, “of the”. As long as the number of new symbols is still small, it is easy to estimate the pair probabilities, and from this an upper bound $h_i = h(2) N_i / N_0$ on the entropy. This becomes more and more difficult as the alphabet size increases, as the sampling becomes insufficient even with our very long input file, and we can no longer approximate the $p_i(k, k')$ by the observed relative frequencies. As long as the number of different subsequent pairs is much smaller than the sequence length (i.e., most pairs are observed many times), we can still get reliable estimates of $h_i$ by using the leading correction term discussed in \[12\] \[13\]. But finally, when many pairs are seen only once in the entire text, we have to stop since any estimate of $h_i(2)$ becomes unreliable.

We went up to 6000 substitutions. The longest substrings substituted by a single new symbol had length 13 in the original (95 letter) alphabet, and length 16 in the reduced (46 letter) one (the latter was “would have been”). The entropies $h$ per (original) character are plotted in Fig.3. We see that they are very similar for both alphabets. We find $h \approx 1.8$ bits/character after 6000 substitutions. This number is very close to the value obtained from most other methods (with the exception of \[14\], where $\approx 1.5$ bits/character were obtained), if one uses $10 – 100$ MB of input text \[15\] \[17\]. This is surprising in view of two facts. First of all, the methods applied in \[15\] \[17\] are very different, and one might have thought a priori that they are able to use different structures of the language to achieve high compression rates. Apparently they do not.

Secondly, it is clear that $h \approx 1.8$ bits/character is not a realistic estimate of the true entropy of written English. Even though we can not, with our present text lengths and our computational resources, go to much larger alphabet sizes (i.e. to more substitutions), it is clear from Fig.3 that both curves would continue to decrease. Let us denote by $i$ the number of substitutions. Then one empirical fit to both curves in Fig.3 are given by

$$\hat{h}_i = h + \frac{c}{(i + i_0)^\alpha}, \quad (9)$$

Such a fit to the 46 letter data, with $h = 0.7$, $i_0 = 34$, $c = 4.99$, and $\alpha = 0.1745$, is also shown in Fig.3. One should
of course not take it too serious in view of the very slow convergence with $i$ and the very long extrapolation, but it suggests that the true entropy of written English is $0.7 \pm 0.2$ bits/character.

This estimate is somewhat lower than estimate of \cite{10} and the extrapolations given in \cite{17}. It is comparable with that of \cite{18} and with Shannon’s original estimate \cite{2}. It seems definitely to exclude the possibility $h = 0$ which was proposed in \cite{20,22}.

IV. CONCLUSIONS

We have shown how a strategy of non-sequential replacements of pairs of characters can yield efficient data compression and entropy estimates. A similar strategy was first proposed by Jiménez-Montaño and others, but details and the actual coding done in the present paper are quite different from those proposed in \cite{6,7,13}. Indeed, this strategy was never used in \cite{6,7,13} for actual codings, and it was also not used for realistic entropy estimates.

Compared to conventional sequential codes (such as Lempel-Ziv or arithmetic codes \cite{5}, just to mention two), the present method would be much slower. Instead of a single pass through the data as in sequential coding schemes, we had gone up to 6000 times through the data file, in order to achieve a high compression rate. We could do of course with much less passes, if we would be content with compression rates comparable to those of commercial packages such as “zip” or “compress”. For written English these achieve typically compression factors $\approx 2.6$, i.e. ca. 3 bits/character. As seen from Fig.1, this can be achieved by NSRPS very easily with very few passes, but even then the overhead and the computational complexity of NSRPS is much too high to make it a practical alternative.

NSRPS can be seen as a greedy and extremely simple version of off-line textual substitution \cite{21}. In combination with other sophisticated techniques, similar substitutions can give excellent results \cite{4}. But without these techniques, it is in general believed that only much more sophisticated versions of off-line textual substitution are advantageous in this case \cite{21}. Again this is presumably true as far as practical coding schemes are concerned. But things seem to be different if one is interested in entropy estimation. Here the present method is much simpler (even though computationally more demanding) than the tree-based coding algorithms \cite{13,7} that had given the best results up to now. Without extrapolation, it gives the same (upper bound) estimates as these methods. But it seems that it allows a more reliable extrapolation to infinite text length and infinite substitution depth, and thus a more reliable estimate of the true asymptotic entropy.

From the mathematical point of view, we should however stress that we have only partial results. While we have proven that the Markov structure is a fixed point of the substitution, we have not proven that it is attractive. We thus cannot prove that the present strategy is indeed universally optimal, although we believe that our numerical results strongly support this conjecture. A rigorous proof would of course be extremely welcome.

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