Counting Irreducible
Double Occurrence Words

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Abstract

A double occurrence word w over a finite alphabet Σ is a word in which each alphabet letter appears exactly twice. Such words arise naturally in the study of topology, graph theory, and combinatorics. Recently, double occurrence words have been used for studying DNA recombination events. We develop formulas for counting and enumerating several elementary classes of double occurrence words such as palindromic, irreducible, and strongly-irreducible words.

1 Introduction

A *double occurrence* word w of size n is a word containing n distinct letters in any order which appear exactly twice, i.e., the *length* of w is $2n$. There are three common pictorial representations of double occurrence words: self-intersecting closed curves in $\mathbb{R}^3$, chord diagrams, and linked diagrams as depicted in Figure 1.

Topologically, a double occurrence word with n distinct letters can be interpreted as a closed curve traversing n fixed points in $\mathbb{R}^3$ twice. Such a curve (also called an assembly graph [2]) is self-intersecting and may contain over and under crossings when projected into the plane. Each curve of this type can be characterized through the double occurrence word corresponding to a path following the direction of the curve in relation to a fixed *base point*. Self-intersecting closed curves are closely related to Gauss words, knot diagrams, and their shadows [3, 7].

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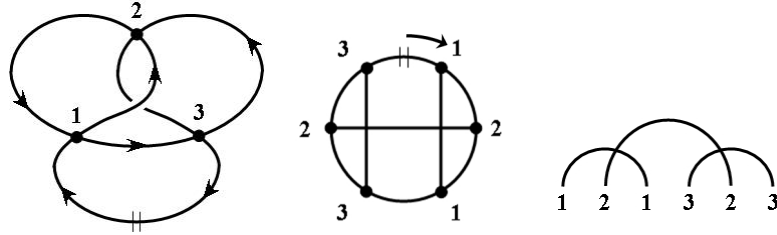†University of South Florida, `tmuche@mail.usf.edu`

Figure 1: Self-intersecting closed curve (left), chord diagram (center), and linked diagram (right) representations of the double occurrence word 121323. Base points, indicating the starting point for reading the word, are marked by ‖.

Chord diagrams are defined in the following way. Start with a circle and place n distinctly labeled chords with distinct endpoints in any arrangement (possibly crossing) around the circle. Label the endpoints of each chord with the chord label. Fix a *base point* on the circle between any two chord endpoints on the circle. The resulting diagram is called a *chord diagram*. Each chord diagram has an associated double occurrence word formed by reading the labels of the endpoints, from the base point back to base point, clockwise around the circle. See [6, 8] for more information on chord diagrams.

A *linked* (or *linearized chord* [16]) *diagram* is a pairing of $2n$ distinct ordered points. Graphically, the ordered points are positioned on a line and their pairing is illustrated by an arc connecting them. Such a diagram can be specified by listing the pairs defined by the n arcs. See [17, 18, 15]. A linked diagram can be obtained from a chord diagram by cutting the outer circle at the base point. Conversely, if we arrange the points of the link diagram in a circle and mark a base point between the first and last point, the corresponding representation is a chord diagram.

Since double occurrence words naturally arise in a variety of contexts, insight into their combinatorial structure enriches several fields simultaneously. In this paper, we explore several classifications of double occurrence words based on separating larger double occurrence words into smaller double occurrence words. Further, we count and enumerate members of these

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classes.

Some of these formulas have been derived in completely different contexts using a variety of approaches. Moreover none of the papers we came across seemed to contain a compilation of the known formulas. In this paper we give a unified approach to deriving these formulas and provide a new formula, giving what appears to be an unobserved integer sequence.

We note that applications of double occurrence words extend to other disciplines. In 2.2, we observe that certain double occurrence words are related to particular Feynman diagrams in physics, and in Section 4 we establish a connection between double occurrence words and DNA recombination events.

2   Preliminaries

2.1   Types of Equivalences

For convenience, we let $\Sigma = \{1, 2, \ldots, n\}$ and relabel each double occurrence word such that when i appears for the first time in the word, it is preceded by $1, 2, \ldots, i-1$. Double occurrence words labeled by this convention are said to be in *ascending order*. Two double occurrence words are said to be *equivalent* if they are equal after being relabeled in ascending order. If two double occurrence words are not equivalent, they are said to be *distinct*. Throughout this paper, we shall assume that all double occurrence words are in ascending order unless stated otherwise.

For example, 122313 is a double occurrence word in ascending order. Its *reverse* with the same letters is 313221, which is not in ascending order. By relabeling 313221 in asscending order we obtain 121332. In this example 122313 is distinct from its reverse 121332. However it is easily checked that 123312 is equivalent to its reverse which motivates the following classification.

Definition 2.1 A double occurrence word is *palindromic* (or *symmetric*) if it is equivalent to its reverse. A double occurrence word that is palindromic is called a *palindrome*.

In all three interpretations of double occurrence words (topological, graph theoretic, and linked diagrams), the reverse word induces a diagram,

isomorphic to the original, with the orientation reversed. In the topological sense, the orientation refers to the orientation of the closed curve. While the reverse of a linked diagram may be interpreted as reading the diagram right-to-left rather than left-to-right. Finally, the reverse chord diagram may be achieved by reading the letters of the circle in a counter-clockwise fashion rather than clockwise.

If we wish to count the non-isomorphic diagrams generated from double occurrence words, we observe that each diagram can have exactly two orientations. Thus, no more than two distinct double occurrence words can correspond to the same diagram with regard to a starting base point.

If a diagram corresponds to a palindrome, only one distinct double occurrence word is associated with the diagram. Therefore we may count the number of non-isomorphic diagrams with regard to a base point as

$$\text{Total Diagrams } = (\text{\# of Palindromes}) + \frac{1}{2}(\text{\# of Non-Palindromes})$$

$$= \frac{(\text{\# of D.O. Words}) + (\text{\# of Palindromes})}{2}. \qquad (*)$$

We will make use of this formula extensively throughout Section 3 to count the number of distinct diagrams corresponding to double occurrence words with each separation property.

It should be noted that omitting the base point in the closed curve or chord diagram makes it possible for more than two double occurrence words to be associated with the same diagram. For instance, rotating the base point around the circle in Figure 1 would lead to 121323, 213231, and 132312 which is 121323, 123132, and 123213 in ascending order, respectively. We do not consider isomorphisms of this type in this paper.

2.2   Types of Separations

As mentioned in the introduction, double occurrence words regularly appear in various fields of mathematics. Unfortunately as a result, there are several different, and sometimes conflicting, definitions used to express identical properties. We shall make note of these discrepancies in notation as they come up.

Jacques Touchard was one of the first researchers to comprehensively consider the counting of double occurrence words. In his paper [17], he

classified several types of linked diagrams and enumerated the number of diagrams containing a fixed number of crossings. He introduced the classification of "unique systems" and "proper unique systems" which coincide with the following two definitions for irreducible and strongly-irreducible words.

Definition 2.2 If a double occurrence word w can be written as a product $w = uv$ of two non-empty double occurrence words u, v, then w is called *reducible*; otherwise, it is called *irreducible*.

The number of irreducible double occurrence words has a close connection with the number of non-isomorphic unlabeled connected Feynman diagrams (also called *irreducible Feynman diagrams* [14]) arising in a simplified model of quantum electrodynamics [4, 9].

This definition for irreducibility agrees with [1] and [2] yet conflicts with [15] where "irreducible" is used for our notion of strongly-irreducible as defined below.

Definition 2.3 A non-empty double occurrence word is *strongly-irreducible* if it does not contain a proper sub-word that is also a double occurrence word.

The double occurrence word 12213434 is reducible because it can be written as the product of the two double occurrence words 1221 and 3434, but 12344123 is irreducible. However, since 44 is a proper sub-word of 12344123 it is not strongly-irreducible. The word 12132434 is strongly-irreducible. By definition, strongly-irreducible words are also irreducible, so 12132434 is irreducible as well. In particular 11 is strongly-irreducible.

Strongly-irreducible double occurrence words are also called *connected* words [8]. This terminology is motivated by the *circle graph* associated with a chord diagram. The circle graph is formed by representing the chords as vertices and the intersection of those chords as edges in the graph. In the topological convention, a circle graph is also called an *interlinking graph* [3]. Without too many difficulties it can be proven that a double occurrence word is strongly-irreducible if and only if the circle graph of the corresponding chord diagram, or interlinking graph of the corresponding closed curve, is connected.

Lemma 2.4 Every double occurrence word contains a strongly-irreducible sub-word.

Proof. If a double occurrence word w is strongly-irreducible, then w itself is a strongly-irreducible sub-word of w. Double occurrence words which are not strongly-irreducible, by definition, contain a proper sub-word w_1 which is a double occurrence word and is either strongly-irreducible or not. If the sub-word is not strongly-irreducible we check the reducibility of its proper sub-word w_2. Since w has finite length, we must reach a double occurrence word w_i, which is a strongly-irreducible proper sub-word of w_{i-1}, through finite recursion. Since w_i must be a proper sub-word of w, this completes the proof. $\square$

3 Counting

It is well known [2, 8, 15, 18] and straightforward to show that the total number of double occurrence words is $(2n-1)!!$. Formula $(*)$ motivates us to enumerate the number of double occurrence words which correspond to palindromes.

3.1 Palindromes

Theorem 3.1 *The number L_n of palindromic double occurrence words of length $2n$, is given by*

$$L_n = \sum_{k=0}^{\lfloor n/2 \rfloor} \frac{n!}{(n-2k)!\, k!} \quad \text{for } n \geq 1.$$

Proof. Observe that $L_1 = 1$ since there is a unique one letter palindrome, and $L_2 = 3$ because 1122, 1212, and 1221 are all the two letter palindromes.

If a double occurrence word w of size $n \geq 2$ is a palindrome beginning and ending with 1, then the word formed by removing both 1s is also a palindrome. Hence there are L_{n-1} palindromes with n letters that start and end with 1.

Now consider a word w of size $n \geq 3$ where the second symbol 1 is at the position $j \neq 2n$. Note that there are $2n - 2$ possible positions for j. Then the word w is a palindrome if and only if w contains the same symbol

s at the positions $2n$ and $n-j+1$. Removing symbols 1 and s from w, and relabeling the resulting word accordingly, produces a palindrome of length $n-2$. Hence there are L_{n-2} palindromes that have a symbol 1 at the jth position for $2 \leq j \leq 2n-1$.

According to the above argument,

$$L_n = L_{n-1} + (2n-2)L_{n-2} \text{ for } n \geq 3, \quad L_1 = 1 \text{ and } L_2 = 3$$

is a recurrence relation for L_n. It is known [11] that the closed formula for this recursive relations is as stated. □

This formula is expressed without proof in a comment by Ross Drewe in $A047974$ of the OEIS [11] in 2008, but this may not be the original source. Similar results, such as the number of palindromic chord diagrams without a base point, were known in 2000 [16]. The above proof reprinted here is found in [2].

3.2   Irreducibles

Though Touchard introduced the classification of irreducible words in 1952, there seems to be little continuation of his efforts. In 2000, Martin and Kearney [9] expressed the number of irreducible words in the broader context of solutions to generating functions. Here, we address the count and construction of both the irreducible double occurrence words and irreducible palindromes directly.

Lemma 3.2 *The number of irreducible double occurrence words I_n with length $2n$ satisfies the recurrence formula $I_1 = 1$ and*

$$I_n = (2n-1)!! - \sum_{k=1}^{n-1} I_{n-k} \, (2k-1)!! \quad for \ n \geq 2.$$

Proof. We shall count the number of irreducible double occurrence words by subtracting the number of reducible double occurrence words from the total number of double occurrence words of length $2n$ and show that each reducible word may be written as the product of an irreducible word and a non-empty double occurrence word.

Without loss of generality, let $w = uv$ be a reducible double occurrence word of length $2n$ such that u is also an irreducible double occurrence word.

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Note that every proper prefix of an irreducible word is not necessarily a double occurrence word. If the length of v is $2k$, for some $1 \leq k \leq n - 1$, then the length of u is $2(n - k)$. By construction, u is irreducible and is counted among I_{n-k} and v is counted among the $(2k - 1)!!$ possible double occurrence words of length $2k$.

Summing over the possible symbols in v yields the desired count. Since u is irreducible and v is non-empty, this ensures that each reducible double occurrence word w is counted exactly once. $\qquad\square$

Theorem 3.3 *The number of irreducible palindromes J_n with length $2n$ satisfies the recurrence formula $J_1 = 1$ and*

$$J_n = L_n - \sum_{k=1}^{\lfloor n/2 \rfloor} (2k - 1)!! \, J_{n-2k} \quad for \ n \geq 2.$$

where L_n is the total number of palindromes with length $2n$.

Proof. Similar to the above argument, we first count the reducible palindromes and subtract them from the total number of palindromic words.

Suppose w is a reducible double occurrence word with length $2n$. Then w can be written as $w = uvu'$ where u is an arbitrary double occurrence word with length $2k$ ($1 \leq k \leq \lfloor n/2 \rfloor$), u' is the double occurrence word corresponding to u by reversing the orientation, and v is an irreducible palindrome with length $2(n - 2k)$. $\qquad\square$

Though the number of irreducible double occurrence words appears in the OEIS (A000698), we note that the number of irreducible palindromes is the only sequence discussed in this paper which is not currently listed in the OEIS [11]. See Table 1, Table 2, and Table 3 for the number of irreducibles, strong-irreducibles, and the number of non-isomorphic diagrams as defined according to (∗), respectively.

3.3 Strong-Irreducibles

The classification of strongly-irreducible double occurrence words was introduced in [18] and the first counting of the strong-irreducibles was done by Stein in [15]. Stein was the first to count both the strongly-irreducible double occurrence words and the strongly-irreducible palindromes, but his counting methods and recursive formulas were simplified in [10] and later

by Klazar in [8]. In Theorem 3.5, we present a proof similar to [8] expressed in terms of language theory.

Using language theory to count double occurrence words led directly to a characterization of the strongly-irreducible double occurrence words, which we express in Lemma 3.4, and Theorem 3.5 follows as a natural consequence.

Lemma 3.4 *Every strongly-irreducible double occurrence word w in ascending order may be written in a unique form as $w = 1u_1v_11v_2u_2$ where $1u_11u_2$ and v_1v_2 are both strongly-irreducible.*

Proof. Let w be strongly-irreducible. Every double occurrence word w in ascending order must be of the form $w = 1p_11p_2$. Delete both 1's. Then we have a double occurrence word $p_1p_2 = u_1xu_2$ where x is the first strongly-irreducible double occurrence word of smallest positive length. Thus u_1 and u_2 are uniquely defined. Note that u_1 and u_2 may be empty words.

Let v_1 be the prefix of x which is a suffix of p_1 and let v_2 be the suffix of x which is the prefix of p_2. This means that $x = v_1v_2$. Neither v_1 nor v_2 is empty as it would imply that x is a sub-word of either p_1 or p_2 which would constitute a proper sub-word of w. Since w is taken to be strongly-irreducible, this cannot be.

We show that $1u_11u_2$ is strongly-irreducible. Suppose not. Then there exists a non-empty double occurrence sub-word z in either u_1 or u_2 which implies that w contains z and is not strongly-irreducible. This is a contradiction. Hence $1u_11u_2$ and v_1v_2 are strongly-irreducible. $\square$

Theorem 3.5 *The number of strongly-irreducible double occurrence words S_n with length $2n$ satisfies the recurrence formula*

$$S_n = (n-1)\sum_{k=1}^{n-1} S_k S_{n-k},$$

where $S_1 = 1$ and $n \geq 2$.

Proof. Note that the only strongly-irreducible double occurrence word of length 2 is 11, i.e., $S_1 = 1$.

Let u and v be strongly-irreducible double occurrence words such that the length of v is $2k$, the length of u is $2(n-k)$, $u = 1u_11u_2$, and $v = v_1v_2$.

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Since the length of v is $2k$, there are $2k-1$ ways to write $v = v_1 v_2$ with v_1, v_2 not empty. By Lemma 3.4, each strongly-irreducible double occurrence word w of length $2n$ can be uniquely represented as $w = 1u_1v_11v_2u_2$. Hence there are $2k-1$ possibilities for such w's to be formed from each u and v.

Since there are S_{n-k} choices for u and S_k choices for v the total counting for S_n when $n \geq 2$ is given by

$$S_n = \sum_{k=1}^{n-1}(2k-1)S_kS_{n-k} = (n-1)\sum_{k=1}^{n-1}S_kS_{n-k}. \qquad \square$$

For completeness, we state Klazar's counting formula of the strongly-irreducible palindromes. See [8] for the proof.

Theorem 3.6 *Let S_n and T_n be the number of strongly-irreducible double occurrence words and strongly-irreducible palindromes of length $2n$, respectively. Then*

$$T_n = \sum_{i=1}^{n-2}T_iT_{n-i} + \sum_{i=1}^{\lfloor n/2 \rfloor}(2n - 4i - 1)S_iT_{n-2i}$$

for $n \geq 2$ where $T_0 = -1$ and $T_1 = 1$.

Theorem 3.5 and Theorem 3.6 correspond to the sequences A000699 and A004300 listed in the OEIS. For the first few values of these sequences, see Table 1 and Table 2.

4   Connection with DNA recombination

Several species of ciliates, such as *Oxytricha* and *Stylonychia*, undergo massive genome rearrangement during sexual reproduction. These massively occurring recombination processes make them ideal model organisms to study gene rearrangements. See [5] and references therein for details of the descriptions below.

There are two types of nuclei, a micronucleus and a macronucleus, in these species. Micronuclear genes contain both coding and non-coding segments which are reassembled to macronuclear genes during sexual reproduction. The coding segments, called *macronuclear destined sequences* or *MDSs*, are part of the final unscrambled gene. The individual MDSs within

Figure 2: Scrambled Actin I micronuclear gene in *Oxytricha nova* [13].

Figure 3: Unscrambled Actin I macronuclear gene in *Oxytricha nova* [13].

a micronuclear gene may be separated by non-coding segments, called *internal eliminated sequences* or *IESs*, which are excised during the recombination process.

In relation to an unscrambled macronuclear gene (Fig. 3), a scrambled micronuclear gene (Fig. 2) may have permuted or inverted MDS segments separated by IESs. Formation of the macronuclear genes in these ciliates thus requires any combination of the following three events: unscrambling of segment order, DNA inversion, and IES removal.

Since the IESs are removed in the unscrambled gene, it is only necessary to record the order and direction of the MDSs in the scrambled gene. A *micronuclear arrangement* (cf. [5]) is a sequence of permuted and inverted MDSs. In particular, each micronuclear arrangement α with k MDSs has a corresponding permutation $\sigma_\alpha : [k] \to [k]$ and a signing function $\epsilon_\alpha : [k] \to \{-1, +1\}$ which uniquely defines the arrangement. A sign of -1 indicates that an MDS is inverted with respect to the gene sequence in the macronuclear gene while a sign of $+1$ indicates a regular orientation.

For example, the micronuclear arrangement of the Actin I gene in Figure 2 is

$$M_3^{+1} M_4^{+1} M_6^{+1} M_5^{+1} M_7^{+1} M_9^{+1} M_2^{-1} M_1^{+1} M_8^{+1}$$

or more commonly denoted

$$M_3 M_4 M_6 M_5 M_7 M_9 \overline{M}_2 M_1 M_8$$

where $\overline{M}_2$ indicates that MDS$_2$ is inverted in the scrambled micronuclear gene.

Proposition 4.1 *Let A_n be the number of micronuclear arrangements of n MDSs. Then*

$$A_n = 2^n n! = (2n)!!.$$

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Proof. Each micronuclear arrangement α with n MDSs is uniquely defined by its corresponding permutation σ_α and signing function ϵ_α. Since each MDS may be signed in one of two ways, there are 2^n ways to sign the $n!$ permutations of all arrangements of α with n MDSs. $\qquad\square$

The exact process by which the scrambled micronuclear gene recombines into an unscrambled macronuclear gene is unknown. However it is theorized [12] that short sequences of nucleotides, called *pointers*, found at the beginning and end of each MDS, guide the recombination process. In fact, each MDS is characterized by its pointers in the following sense.

Each MDS is labeled according to its order in the unscrambled macronuclear gene. The pointers flanking the MDSs correspond to the order of the MDSs such that the pointer sequence at the end of the ith MDS coincides with the pointer sequence at the beginning of the $(i+1)$th MDS. IESs are excised and their coding is not necessary. Since the pointers at the beginning and end of the whole gene do not align with any other pointers, we omit them. Mathematically, this translates to the following.

Let $\mathcal{A}_n$ be the set of all micronuclear arrangements with n MDSs and $\mathcal{K}_n$ be the set of all double occurrence words with length $2n$. Then $\varrho : \mathcal{A}_n \to \mathcal{K}_{n-1}$ is a homomorphism which translates a micronuclear arrangement to the ordered sequence of pointers which describes it, i.e.,

1. $\varrho(M_1^{-1}) \mapsto (1)$ and $\varrho(M_1^{+1}) \mapsto (1)$

2. $\varrho(M_i^{-1}) \mapsto (i)(i-1)$

3. $\varrho(M_i^{+1}) \mapsto (i-1)(i)$

4. $\varrho(M_n^{-1}) \mapsto (n-1)$ and $\varrho(M_n^{+1}) \mapsto (n-1)$.

For the micronuclear arrangement $\alpha = M_2^{-1} M_4^{+1} M_1^{+1} M_5^{-1} M_3^{+1}$,

$$\varrho(\alpha) = (2)(1)(3)(4)(1)(4)(2)(3)$$

which corresponds to the double occurrence word 12342413 in ascending order. Therefore each scrambled micronuclear gene corresponds to a micronuclear arrangement which, in turn, has an associated double occurrence word.

A double occurrence word is called *realizable* if it has a corresponding micronuclear arrangement. The shortest double occurrence word which is

not realizable is 11233244. For further information on realizable double occurrence words see [2].

5   Conclusions

Double occurrence words are studied in topology, graph theory, and combinatorics by way of self-intersecting closed curves in $\mathbb{R}^3$, chord graphs and linked diagrams, respectively. Their applications extend beyond abstraction to other disciplines such as physics and genetics. We considered the counting and enumeration of several reducibility classes of double occurrence words which directly led to a new characterization of strongly-irreducible double occurrence words. Further, all but one of the enumerated sequences are listed in the OEIS [11], which suggests both the relevance of the previously listed enumerations and the novelty of the unlisted irreducible palindrome count. It should be noted that all the counting arguments present in this paper followed a similar theme: separate the classes of double occurrence words into palindromes and non-palindromes and describe the construction of large double occurrence words from smaller double occurrence words. We believe that the counting techniques presented here could be used to enumerate new classes of double occurrence words as they arise in future research.

6   Acknowledgments

Symbols	All	Irreducible	Strongly Irreducible
1	1	1	1
2	3	2	1
3	15	10	4
4	105	74	27
5	945	706	248
6	10395	8162	2830
7	135135	110410	38232
8	2027025	1708394	593859
9	34459425	29752066	10401712
10	654729075	576037442	202601898
11	13749310575	12277827850	4342263000
12	316234143225	285764591114	101551822350
OEIS	A001147 (K_n)	A000698 (I_n)	A000699 (S_n)

Table 1: All Double Occurrence Words.

Symbols	All	Irreducible	Strongly Irreducible
1	1	1	1
2	3	2	1
3	7	6	2
4	25	20	7
5	81	72	22
6	331	290	96
7	1303	1198	380
8	5937	5452	1853
9	26785	25176	8510
10	133651	125874	44940
11	669351	637926	229836
12	3609673	3448708	1296410
OEIS	A047974 (L_n)	—— (J_n)	A004300 (T_n)

Table 2: Palindromic Double Occurrence Words.

Symbols	All	Irreducible	Strongly Irreducible
1	1	1	1
2	3	2	1
3	11	8	3
4	65	47	17
5	513	389	135
6	5363	4226	1463
OEIS	A001147 (K_n) A047974 (L_n)	A000698 (I_n) —— (J_n)	A000699 (S_n) A004300 (T_n)

Table 3: Non-isomorphic diagrams in ($*$) are obtained by summing all words with the palindromes of each class and halving the total. These sequences do not appear in the OEIS [11], but can be built from listed sequences.

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