Enumeration of Self-orthogonal Latin Squares

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Abstract

In this report we consider the problem of enumerating self-orthogonal Latin squares (SOLS) of small orders. We present enumeration tables of unequal SOLS, idempotent SOLS, isomorphism classes of SOLS and isotopy classes of SOLS. The isotopy classes are enumerated by an (almost) exhaustive computerised tree search which generates a representative from each isotopy class, whereafter the autotopism groups of these representatives are used together with results from abstract algebra in order to enumerate unequal SOLS, idempotent SOLS and isomorphism classes of SOLS. Finally, the results are validated by using an alternative computerised search-tree method for all four classes of SOLS.

Keywords: Latin square, Self-orthogonal Latin square, Enumeration, Isomorphism classes, Isotopy classes.

AMS Classification: 05A15, 05B15.

1 Introduction

During the time the work presented in this report was done, we were unaware of a publication by Graham and Roberts [8] concerning the enumeration of self-orthogonal Latin squares (SOLS) of orders $1 \le n \le 9$. We only became aware of the paper after we have completed the writing of this report. Although most of our results were found in the Graham and Roberts paper, the results were obtained independently and by utilising different methods and validation techniques. A section of this report does, however, contain new results, and this section have been written up and submitted as a research paper [4]. The results obtained in this report verifies the correctness of the results found by Graham and Roberts, as explained in [4]. It should also be noted that the classes of SOLS defined in this report borrows their names from the Latin square literature (names such as isomorphism and isotopism), but for the purpose of classifying SOLS they are defined differently for SOLS than for Latin squares in general. Since we never refer to these classes of Latin squares in general, there should be no confusion as to the definitions of these classes. In [4], however, different names are given to these classes in order to avoid ambiguity.

Given a set of n distinct symbols, a Latin square of order n is an $n \times n$ array containing each symbol exactly once in every row and every column. In this paper we denote the entry in row i and column j of a Latin square L by L(i,j) and take the n symbols from the set $\mathbb{Z}_n = \{0,\ldots,n-1\}$. We also use \mathbb{Z}_n as index set for the rows and columns of a Latin square. The transpose of a Latin square L, denoted by L^T , is a Latin square for which $L^T(i,j) = L(j,i)$. Two Latin squares L and L' are said to be orthogonal if each ordered pair (L(i,j), L'(i,j)) is unique among all such pairs for all i and j. If a Latin square L is orthogonal to its transpose, then L is said to be a self-orthogonal Latin square (SOLS). The existence of a SOLS is guaranteed for every order $n \in \mathbb{N}$, except for $n \neq 2, 3, 6$ [3]. For orders 2 and 3 this fact is easily verifiable by exhaustive enumeration, and it is well known that there exists no pair of mutually orthogonal Latin squares (MOLS)

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of order 6 [20]. Notable existence and construction results for SOLS appear in Mendelsohn [16], Hedayat [9, 10] and Brayton et al. [3].

The purpose of this report is to count the number of different types of SOLS with the aid of a computer and to present the results in tabular form. More specifically, we count the number of unequal SOLS, the number of idempotent SOLS, the number of isomorphism classes of SOLS and the number of isotopy classes of SOLS of orders $4 \le n \le 9$. In Section 2 our general approach towards the enumeration of SOLS is discussed in some detail, followed by the enumeration of the isotopy and isomorphism classes in Sections 3 and 4 respectively, and the enumeration of unequal and idempotent SOLS in Section 5. Finally the results are reported in tabular form in Section 6, together with the description of a number of methods used to validate those numerical results. The paper closes with a summary of the work presented and possibilities for future work in Section 7.

2 Our general approach towards enumerating SOLS

We employ an exhaustive depth-first search tree approach with backtracking to enumerate SOLS, enabling us to build up a repository of SOLS in addition to enumerating them. We incorporate various pruning rules in order to limit the size of the tree and hence render the approach tractable.

A universal in a Latin square L is a list of n entries taken from L, all containing the same element. The enumeration of SOLS is performed by branching on the inclusion of all possible universals of a specific symbol, one at a time, within a given partially completed square, provided that the inclusion of a universal does not destroy the property of self-orthogonality. This process is repeated on every level of the tree for another symbol until either a completed SOLS is found or the inclusion of no further universal is possible.

To maintain self-orthogonality a list of all ordered pairs of symbols is kept, adding the pair $(L(i,j), L^T(i,j))$ to the list once the entry L(i,j) assumes a value during the search process, while avoiding the inclusion of universals which result in listing an ordered pair twice. A transversal in a Latin square L is a list of n entries taken from L such that no two entries appear in the same row or column of L and no two entries contain the same symbol. Another way of maintaining self-orthogonality is to note that each universal in L corresponds to a transversal in L^T . When an attempt is thus made to include a universal in the square a test may be performed in L^T to ensure that the corresponding elements form at least a partial transversal.

For clarity the pseudocode for an implementation of the method described above, using recursion, is given in Algorithm 1. All enumeration methods described in this paper were implemented in Wolfram's MATHE-MATICA 6.0 [21] on an Intel(R) Core(TM) 2 Duo processor with 3.25 GB of RAM, except where otherwise stated, and the trivial cases of SOLS of orders n=2,3 are omitted. All computing times are reported in the format dd:hh:mm:ss.x where dd represents the number of days, hh the number of hours, mm the number of minutes, ss the number of seconds and x the number of tenths of a second.

Algorithm 1 Recursion

Input: A partially completed SOLS S of order n, a set S of completed SOLS and a current element e. **Output:** The set S with addition of all possible completions of S to SOLS of order n.

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1: U \leftarrow the set of all possible universals of element e.

2: if U = \emptyset and S is a SOLS then

3: \mathbb{S} \leftarrow \mathbb{S} \cup \{S\}.

4: else

5: for all u_i \in U do

6: S' \leftarrow u_i inserted into corresponding entries in S.

7: \mathbb{S} \leftarrow \text{Recursion}(S', \mathbb{S}, e+1)

8: end for

9: end if

10: Return \mathbb{S}
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3 Enumeration of the isotopy classes

Two SOLS \boldsymbol{L} and \boldsymbol{L}' are isotopic if two permutations performed on \boldsymbol{L} or \boldsymbol{L}^T , one on the rows and columns, and one on the symbol set, results in \boldsymbol{L}' . An isotopism is an element of the group $S_n \times S_n \times S_2$ acting on a SOLS, where S_n is the symmetric group of order n. We denote an isotopism by $\boldsymbol{p}=(p_r,p_s,p_t)$, where $p_r \in S_n$ is the permutation applied to the rows and columns, $p_s \in S_n$ is the permutation applied to the symbol set and $p_t \in S_2$ permutes the roles of the rows and columns of \boldsymbol{L} (i.e. it incorporates matrix transposition). Two different approaches to the enumeration of the isotopy classes were implemented and both utilise the search-tree approach described in Section 2. The first approach completes a set of partially completed SOLS in such a way that the generation of a SOLS from each isotopy class is guaranteed. This method requires a certain degree of isotopy testing on the final set of generated SOLS. The second approach completes an initially empty array by iteratively inserting universals for the symbols $0, 1, \ldots, n-1$ while ensuring that after each universal is inserted the resulting partially completed SOLS cannot be transformed via an isotopism into a lexicographically smaller partially completed SOLS, a method generally referred to as orderly generation [7, 14, 18]. This method therefore ensures that a single class-representative from each isotopy class is generated, and no isotopy testing is required.

3.1 Enumeration based on the notion of a skeleton

The diagonal of a SOLS is necessarily a transversal,¹ and the diagonal and any row of a SOLS share a common element, called the *root* of the row. Upon the exclusion of the root L(j, j), the diagonal and row j form the permutation

$$\begin{pmatrix} L(0,0) & L(1,1) & \dots & L(j-1,j-1) & L(j+1,j+1) & \dots & L(n-1,n-1) \\ L(j,0) & L(j,1) & \dots & L(j,j-1) & L(j,j+1) & \dots & L(j,n-1) \end{pmatrix}$$

whose cycle structure² is called the *diagonal cycle structure* of row j and is denoted by $\delta(\boldsymbol{L},j)$. The diagonal cycle structure for column j is defined similarly and is denoted by $\delta(\boldsymbol{L}^T,j)$. For example, the diagonal cycle structures $\delta(\boldsymbol{S},i)=x_2^3$ and $\delta(\boldsymbol{S}^T,i)=x_3^2$ for $i=0,\ldots,6$, result for the SOLS

$$S_7 = \left[\begin{array}{c} 0 \ 2 \ 1 \ 4 \ 3 \ 6 \ 5 \ 3 \ 1 \ 6 \ 0 \ 5 \ 4 \ 2 \ 4 \ 5 \ 2 \ 6 \ 0 \ 1 \ 3 \ 5 \ 6 \ 4 \ 3 \ 2 \ 0 \ 1 \ 6 \ 3 \ 5 \ 1 \ 4 \ 2 \ 0 \ 1 \ 0 \ 3 \ 2 \ 6 \ 5 \ 4 \ 2 \ 4 \ 0 \ 5 \ 1 \ 3 \ 6 \ \end{array} \right]$$

of order 7. Note that the diagonal cycle structure of any row or column of a SOLS is invariant under an isotopism. The *cycle structure representative* of a diagonal cycle structure $\delta(\boldsymbol{L},j)$ is the lexicographically smallest permutation that assumes $\delta(\boldsymbol{L},j)$ as its cycle structure. For instance, the cycle structure representative of x_2x_4 is $\binom{123456}{214563}$.

A SOLS L is idempotent if L(i, i) = i for all $i \in \mathbb{Z}_n$. Our first enumeration approach for non-isotopic SOLS is based on the notion of a SOLS skeleton. An $n \times n$ skeleton is a partially completed SOLS of order n in which the first row is a cycle structure representative, its diagonal is a transversal in natural order and the only other non-empty entries occur in the first column, which is complete. Since a skeleton is a partially completed SOLS, its first row and column are both derangements with respect to the diagonal, and the

¹Since each entry on the diagonal of a SOLS forms a pair $(L(i,i), L^T(i,i))$ and since $L(i,i) = L^T(i,i)$, it follows that if any symbol appears more than once on the diagonal, the property of orthogonality is destroyed. Therefore the main diagonal of a SOLS is necessarily a transversal, implying that $L(i,j) \neq L(j,i)$ for $i \neq j$.

²We used the standard notation $x_1^{\alpha_1} x_2^{\alpha_2} \dots x_n^{\alpha_n}$ to denote the cycle structure of a permutation of order n, where α_i denotes the number of cycles of length i (see [1, p. 442]).

first row and column are derangements with respect to one another³ and contain no 2-cycles with respect to each other. These requirements are necessary so as to maintain the property of self-orthogonality when completing a skeleton to form a SOLS. If a SOLS \boldsymbol{L} contains a skeleton (*i.e.* if the first row, the first column and the main diagonal of \boldsymbol{L} form a skeleton), this skeleton is denoted by $\langle \boldsymbol{L} \rangle$. Also, any SOLS that contains a skeleton is idempotent. For instance, the skeleton of \boldsymbol{S}_7 is

$$\langle \boldsymbol{S}_7
angle = \left[egin{array}{cccc} 0 & 2 & 1 & 4 & 3 & 6 & 5 \ 3 & 1 & & & & \ 4 & 2 & & & & \ 5 & & 3 & & & \ 6 & & 4 & & & \ 1 & & & 5 & & \ 2 & & & & 6 \end{array}
ight].$$

A SOLS L is induced by a skeleton K if it is isotopic to a SOLS L' for which $\langle L' \rangle = K$. If it may be shown that any SOLS is induced by at least one skeleton, then an exhaustive list of skeletons may be presented as starting conditions to the enumeration method described in Section 2.

Theorem 3.1 Every SOLS is induced by at least one skeleton.

Proof: The proof is constructive in the sense that we demonstrate an isotopism from any SOLS L to a SOLS L' such that L' contains a skeleton. The first step is to permute all the rows and columns of a SOLS L except the first row and column, such that each cycle in the diagonal cycle structure of the first row has the form

$$\left(\begin{array}{cccc} p_1 & p_2 & \dots & p_{k-1} & p_k \\ p_2 & p_3 & \dots & p_k & p_1 \end{array}\right),\,$$

and that the cycles occur in order of non-decreasing length. Hence the first row has the form of a cycle structure representative. If the symbols are renamed such that the diagonal is in natural order, the first row is a cycle structure representative, and the resulting SOLS contains a skeleton. \Box

A cycle structure $a = x_1^{\alpha_1} x_2^{\alpha_2} \dots x_n^{\alpha_n}$ is lexicographically smaller than a cycle structure $b = x_1^{\beta_1} x_2^{\beta_2} \dots x_n^{\beta_n}$, denoted by $a \prec b$, if $\alpha_i > \beta_i$ for some i and $\alpha_j = \beta_j$ for all $1 \leq j < i$. Our approach is to construct a list of all $n \times n$ skeletons in increasing lexicographic order according to the diagonal cycle structure of the first row. However, not all of these skeletons need be considered, since some will be incapable of producing new SOLS when used as a starting point for the enumeration method described in Section 2.

Consider a permutation on the row, column and diagonal of a skeleton \mathcal{K} , which is equivalent to a permutation on the rows and columns of a SOLS with skeleton \mathcal{K} . In order for the resulting row, column and diagonal to form a skeleton, an appropriate change in symbols has to be performed in order for the diagonal to be in natural order. If this change in symbols causes the row to form a cycle structure representative, then the resulting skeleton \mathcal{K}' is isotopic to \mathcal{K} . If this change in symbols causes the column to form a cycle structure representative, then the row and column may be swapped and the resulting skeleton \mathcal{K}' is again isotopic to \mathcal{K} . This implies that a SOLS with skeleton \mathcal{K} is isotopic to at least one SOLS with skeleton \mathcal{K}' . Thus only non-isotopic skeletons are considered, and this is done by exhaustively considering all isotopes of a skeleton, grouping them together in an isotopism class and repeating the process for a skeleton not yet assigned to a class. One skeleton from each class may then be selected as a starting point for the enumeration method of Section 2. For illustrative purposes all non-isotopic skeletons of orders n=4,5 and 6 are given in Table 3.1. The non-isotopic skeletons of orders n=7,8 and 9 may be found in [12].

A small section of the search tree for n=7 is shown in Figure 3.1. It shows three branches for three different universals of the element 4 (after universals for the elements 1, 2 and 3 have already been inserted), how the insertion of two of them destroy the property of self-orthogonality (as underlined) and how one is eventually completed to a SOLS. For this latter branch there is, after the insertion of the universal for the element 4,

³The first row and column are derangements with respect to one another if they have no fixed point other than the element they have in common when viewed as a permutation.

$$\begin{bmatrix} 0 & 2 & 3 & 1 \\ 3 & 1 \\ 1 & 2 \\ 2 & 3 \\ n & = 4 \end{bmatrix} \quad \begin{bmatrix} 0 & 2 & 1 & 4 & 3 \\ 3 & 1 \\ 4 & 2 \\ 2 & 3 \\ 1 & 4 \end{bmatrix} \quad \begin{bmatrix} 0 & 2 & 1 & 4 & 5 & 3 \\ 3 & 1 \\ 4 & 2 \\ 5 & 3 \\ 2 & 4 \\ 1 & 5 \end{bmatrix} \begin{bmatrix} 0 & 2 & 3 & 4 & 5 & 1 \\ 3 & 1 \\ 1 & 2 \\ 5 & 3 \\ 2 & 4 \\ 4 & 5 \end{bmatrix} \begin{bmatrix} 0 & 2 & 3 & 4 & 5 & 1 \\ 3 & 1 \\ 4 & 2 \\ 5 & 3 \\ 1 & 4 \\ 5 \end{bmatrix} \begin{bmatrix} 0 & 2 & 3 & 4 & 5 & 1 \\ 3 & 1 \\ 4 & 2 \\ 5 & 3 \\ 1 & 4 \\ 4 & 5 \end{bmatrix} \begin{bmatrix} 0 & 2 & 3 & 4 & 5 & 1 \\ 3 & 1 \\ 4 & 2 \\ 5 & 3 \\ 1 & 4 \\ 4 & 5 \end{bmatrix}$$

Table 3.1: All non-isotopic skeletons of orders n = 4, 5 and 6.

only one possible universal for the element 5 and similarly for the element 6. Note that the universals are inserted in the order $1, 2, \ldots, n-1$, while the universal for the element 0 is uniquely defined once all other universals are inserted. Since the only appearance of the element 0 in a skeleton is in the top-left corner, the element 0 initially has, above all other elements, the largest number of possible universals, and is thus not inserted until the very end.

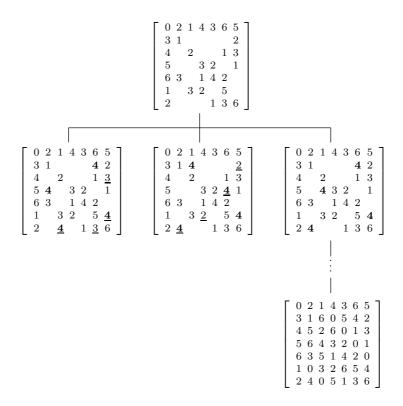


Figure 3.1: A small section of the search tree for n = 7.

Theorem 3.1 guarantees that no SOLS are omitted during the search, but it does not guarantee that the SOLS eventually enumerated will all be non-isotopic (in pairs). Also, if two skeletons are non-isotopic it does not necessarily mean the SOLS generated from them are non-isotopic. An isotopy test therefore has to be performed on the set of enumerated SOLS so as to rid the set of redundant SOLS.

An efficient method for discarding a few redundant SOLS stems from the realisation that if all skeletons for which the first row has the cycle structure x_2x_4 have been completed to SOLS, any SOLS \boldsymbol{L} found at a later stage for which $\delta(\boldsymbol{L},j) = x_2x_4$ or $\delta(\boldsymbol{L}^T,j) = x_2x_4$ for any j is isotopic to some SOLS already enumerated. This implies that if, for any enumerated SOLS \boldsymbol{L} , $\delta(\boldsymbol{L},j) \prec \delta(\boldsymbol{L},0)$ or $\delta(\boldsymbol{L}^T,j) \prec \delta(\boldsymbol{L},0)$ for any j, \boldsymbol{L} may be discarded from the set. The above-mentioned method is useful, but it still does not guarantee that all SOLS in the remaining set are non-isotopic.

Consider two idempotent SOLS L and L' for which we want to test for an isotopism. Since both are

idempotent, any change of symbols in \boldsymbol{L} must be followed by a unique permutation on the rows and columns of \boldsymbol{L} in order for the resulting square to be idempotent. Hence an appropriate isotopy test consists of only finding the specific change of symbols in \boldsymbol{L} which will result in \boldsymbol{L}' . Consider a permutation on the symbol set of \boldsymbol{L} such that a is replaced by α and b by β , and suppose a, b, c and d form the subsquare in \boldsymbol{L} shown in Figure 3.2 (a), where a and b lie on the diagonal of \boldsymbol{L} . Similarly, let α , β , γ and δ form the subsquare in \boldsymbol{L}' shown in Figure 3.2 (b), where α and β lie on the diagonal of \boldsymbol{L}' . It is easy to see that these subsquares remain intact during any isotopism from \boldsymbol{L} to \boldsymbol{L}' , and thus that if a is replaced by α and b by β , then c must be replaced by γ and d by δ . If we initially apply a change in name on two symbols, it will immediately imply a change in name on two more symbols, eventually causing a chain reaction resulting in either a partially completed permutation or a contradiction. This process may be repeated until either a complete permutation on the symbol set is found, thus implying an isotopism from \boldsymbol{L} to \boldsymbol{L}' , or until all possibilities result in contradictions, implying that \boldsymbol{L} and \boldsymbol{L}' are non-isotopic.



Figure 3.2: Two subsquares of a SOLS.

We denote the number of non-isotopic skeletons of order n by $\kappa(n)$ and the number of SOLS of order n generated from the $\kappa(n)$ skeletons by $\Gamma(n)$. The number of isotopy classes of SOLS of order n, found by applying the methods described above to the SOLS generated from the skeletons, is denoted by $\Psi(n)$. The results for the enumeration of skeletons and the isotopy classes are given in Table 3.2 together with the required computing times. The depth-first tree search used to enumerate $\Gamma(9)$ was achieved by means of 15 computers running in parallel. Two computers were as previously mentioned in Section 2, two were Intel(R) Pentium(R) D processors with 1.024 GB of RAM each, one was an Intel(R) Pentium IV processor with 512 MB of RAM and the remainder were Intel(R) Core(TM) 2 Duo processors with 1.024 GB of RAM each.

| | Skeleton generation | | Depth-first Tree Search | | Final isotopy testing | | |
|----------------|---------------------|---------|-------------------------|---------------|-----------------------|-----------|--|
| \overline{n} | $\kappa(n)$ | Time | $\Gamma(n)$ | Time | $\Psi(n)$ | Time | |
| 4 | 1 | 0.0 | 1 | 0.0 | 1 | _ | |
| 5 | 1 | 0.0 | 1 | 0.0 | 1 | | |
| 6 | 4 | 0.1 | 0 | 0.1 | 0 | _ | |
| 7 | 20 | 0.8 | 8 | 3.5 | 4 | 1.3 | |
| 8 | 78 | 14.6 | 12 | 9:25.2 | 4 | 2.2 | |
| 9 | 595 | 11:57.7 | 1561 | 19:20:11:00.5 | 175 | 2:55:35.1 | |

Table 3.2: The number, $\Psi(n)$, of isotopy classes of SOLS of order n together with the required computing times.

A complete set of all $\Psi(n)$ isotopy class representatives of SOLS of order n appear in the appendix for all $4 \le n \le 9$.

3.2 An alternative enumeration approach

Our second approach is to initialise with an empty array and use the search-tree approach described in Section 2 together with a number of additional pruning rules in order to generate a single class representative from each isotopy class.

The (3,2,1)-conjugate of a SOLS \boldsymbol{L} for which $\boldsymbol{L}(i,j)=k$, denoted by $\boldsymbol{L}_{(3,2,1)}$, is a Latin square for which $\boldsymbol{L}_{(3,2,1)}(k,j)=i$. Note that if \boldsymbol{L} is idempotent, then so is $\boldsymbol{L}_{(3,2,1)}$. Given a set of n distinct symbols, a $k\times n$

row-scattered Latin rectangle (RSLR) for $k \le n$ is a Latin square of order n with n-k of its rows removed, in other words a Latin squares with n-k empty rows and k complete rows. A RSLR \mathbf{R} is idempotent if $\mathbf{R}(i,i)=i$ for every row i that is not empty. The (1,3,2)-conjugate of \mathbf{R} , denoted by $\mathbf{R}_{(1,3,2)}$, is the RSLR resulting from the replacement of each row by its inverse permutation. Two RSLRs \mathbf{R} and \mathbf{R}' are pseudo-isotopic if two permutations performed on \mathbf{R} or $\mathbf{R}_{(1,3,2)}$, one on the columns and symbol set and one on the rows, results in \mathbf{R}' . It may be noted that a permutation applied to the rows of an RSLR permutes the compelete rows as well as the empty rows.

Given a $k \times n$ RSLR \mathbf{R} and a $k \times n$ RSLR \mathbf{R}' , let $\ell \leq k$ be the smallest index for which row ℓ of either \mathbf{R} or \mathbf{R}' is empty. Then \mathbf{R} is lexicographically smaller than \mathbf{R}' if the rows indexed by $0, 1, \ldots, i-1$ for some index $i < \ell$ are equal for both \mathbf{R} and \mathbf{R}' , and row i in \mathbf{R} is lexicographically smaller (in a permutation sense) than row i in \mathbf{R}' . If all rows indexed by $i < \ell$ are equal, then the lexicographic order of \mathbf{R} and \mathbf{R}' is undecided. The lexicographically smallest SOLS in a single isotopy class is defined to be the isotopy class leader of that class

It may be noted that each universal in a SOLS L corresponds to the row in $L_{(3,2,1)}$ indexed by its symbol and that an isotopism performed on L corresponds to a pseudo-isotopism performed on $L_{(3,2,1)}$. Also, after universals for the symbols $0,1,\ldots,k-1$ have been inserted into an empty $n\times n$ array, the (3,2,1)-conjugate of the partially completed SOLS is a $k\times n$ RSLR. If there exists no pseudo-isotopism which transforms this RSLR into a lexicographically smaller RSLR, we henceforth refer to such a RSLR as a candidate with respect to SOLS isotopy class leadership. Our approach is to branch on a partially completed SOLS only if the (3,2,1)-conjugate is a candidate, and in this way a single representative from each isotopy class of SOLS is generated.

Consider any non-empty row of a $k \times n$ RSLR \mathbf{R} as a permutation

$$r = \begin{pmatrix} 0 & 1 & \dots & n-1 \\ r(0) & r(1) & \dots & r(n-1) \end{pmatrix},$$

where r(i) represents the *i*-th entry in the row, and let

$$p = \begin{pmatrix} 0 & 1 & \dots & n-1 \\ p(0) & p(1) & \dots & p(n-1) \end{pmatrix}.$$

It is easy to see that if p is applied to the columns of \mathbf{R} , then r is replaced by $r \circ p^{-1}$. Similarly, if p is applied to the symbol set of \mathbf{R} , then r is replaced by $p \circ r$. Hence, if p is applied to the columns and the symbol set of \mathbf{R} , then r is replaced by $p \circ r \circ p^{-1}$, known as a conjugate permutation of r, which, according to [2, p. 80, Lemma 3.13], necessarily has the same cycle structure as r. In fact, for any two permutations p_1 and p_2 with the same cycle structure there always exists a permutation q such that $q \circ p_1 \circ q^{-1} = p_2$. Since a permutation and its inverse have the same cycle structure, the non-empty rows of $\mathbf{R}_{(1,3,2)}$ and \mathbf{R} also exhibit the same cycle structure. Hence the cycle structures of the non-empty rows of a RSLR are invariant under a pseudo-isotopism.

Since the diagonal of a SOLS L is a transversal and $L(i,j) \neq L(j,i)$, the cycle structure of the rows of $L_{(3,2,1)}$ must contain exactly one fixed point and no two-cycles. Furthermore, it is easy to see that the first row of a candidate is a cycle structure representative and that the cycle structure of each row is lexicographically larger than that of the first row. Hence, for each cycle structure there is only one universal for the first element and at any point during the tree search described in Section 2, if a row is added to a candidate such that the cycle structure of that row is lexicographically smaller than the cycle structure of the first row, the corresponding partially completed SOLS may be discarded.

Let the first row of an RSLR R be a cycle structure representative and let the cycle structure of each row be lexicographically larger than that of the first row. Suppose we wish to test whether an RSLR R is a candidate. We know at least that if there exists a lexicographically smaller RSLR, it has the same first row as R, and we want to consider pseudo-isotopisms of R for which the first row remains intact. Let r_1, r_2, \ldots, r_ℓ

be the non-empty rows in R with the same cycle structure as the first row. A pseudo-isotopism of R for which the first row remains intact thus either maps the first row to itself or maps one of these rows to the first row⁴. Therefore, these are the only pseudo-isotopisms we have to consider, and if any of these map R to a lexicographically smaller RSLR, then R is not a candidate.

To find the permutations that map a row r_1 to another row r_2 with the same cycle structure, we consider only those permutations that map each cycle of r_1 to a corresponding cycle of r_2 . If there are k cycles of equal length in both r_1 and r_2 , there are k! possible mappings of these cycles in r_1 to those in r_2 . If the cycle (x_1, x_2, \ldots, x_m) is to be mapped to the cycle (y_1, y_2, \ldots, y_m) , we may choose to map x_1 to any y_i and the remainder of the mapping will be defined uniquely. If there are a_i cycles of length i for any $i \leq n$ where n is the order of the permutations, then there are $\prod_{i=1}^n a_i l^{ia_i}$ mappings from r_1 to r_2 .

The results for the enumeration of the isotopy classes via this approach are given in Table 3.3 together with the required computing times.

| n | $\Psi(n)$ | Time |
|---|-----------|--------------|
| 4 | 1 | 0.0 |
| 5 | 1 | 0.0 |
| 6 | 0 | 0.0 |
| 7 | 4 | 1.7 |
| 8 | 4 | 72.5 |
| 9 | 175 | 2:19:33:07.4 |

Table 3.3: The number, $\Psi(n)$, of isotopy classes of SOLS of order $4 \le n \le 9$ together with the required computing times.

4 Enumeration of the isomorphism classes

Two SOLS L and L' are *isomorphic* if a single permutation performed on the rows, columns and symbol set of L or L^T results in L'. An *isomorphism* is an element of $S_n \times S_2$ acting on a SOLS and may be denoted by $p = (p_r, p_t)$, where $p_r \in S_n$ is the permutation applied to the rows, columns and symbol set, and $p_t \in S_2$ incorporates matrix transposition. For the purpose of enumerating isomorphism classes we follow the approach of McKay *et al.* [15].

A permutation p of order n is of type (a_1, a_2, \ldots, a_n) if it has a_i cycles of length i for $1 \le i \le n$. As mentioned in Section 3, if two permutations p_1 and p_2 are of the same type (a_1, a_2, \ldots, a_n) , then they are conjugates and there exist $\prod_{i=1}^n a_i! i^{a_i}$ permutations q such that $q \circ p_1 \circ q^{-1} = p_2$.

An autotopism is an isotopism that maps a SOLS \boldsymbol{L} to itself. Denote by $A(\boldsymbol{L})$ the set of all autotopisms admitted by \boldsymbol{L} . For any two isotopisms $\boldsymbol{p}=(p_r,p_s,p_t)$ and $\boldsymbol{q}=(q_r,q_s,q_t)$ the notation $\boldsymbol{p}\boldsymbol{q}=(p_r\circ q_r,p_s\circ q_s,p_t\circ q_t)$ is used to denote the action of first applying \boldsymbol{q} and then \boldsymbol{p} . Furthermore, $\boldsymbol{p}^{-1}=(p_r^{-1},p_s^{-1},p_t^{-1})$. Let $\mathcal{I}(n)$ denote a set of class representatives, one from each SOLS isotopy class of order n, and let $A'(\boldsymbol{L})$ be the set of autotopisms \boldsymbol{p} of \boldsymbol{L} for which p_r and p_s are both of the same type. For an isotopism \boldsymbol{p} in which p_r and p_s are both of type (a_1,a_2,\ldots,a_n) , define the function $\psi(\boldsymbol{p})=\prod_{i=1}^n a_i!i^{a_i}$.

All the isomorphism classes in a single isotopy class are orbits of the group $S_n \times S_2$ and we may find the number of orbits by the Cauchy-Frobenius lemma [11] (sometimes (mistakenly) referred to as Burnside's lemma [17]) which states that, if $F(\mathbf{p})$ is the number of SOLS (in a single isotopy class) fixed by $\mathbf{p} \in S_n \times S_2$, then the number of isomorphism classes of SOLS in that class is

$$\sum_{\boldsymbol{p}\in S_n\times S_2}\frac{F(\boldsymbol{p})}{|S_n\times S_2|}.$$

⁴Since we map a row to the first row by a permutation on the columns and the symbol set, the permutation on the rows is defined (uniquely) in order to ensure that the resulting RSLR is again idempotent.

In other words, the number of isomorphism classes in a single isotopy class of SOLS is the total number of distinct automorphisms over all SOLS in the class divided by the total number of possible isomorphisms. Here two automorphisms are distinct if they are either different permutations or if they are automorphisms of two different SOLS.

Theorem 4.1 If F(p) is the number of SOLS in the isotopy class of a SOLS L fixed by $p \in S_n \times S_2$, then

$$\sum_{\boldsymbol{p} \in S_n \times S_2} \frac{F(\boldsymbol{p})}{|S_n \times S_2|} = \sum_{\boldsymbol{\alpha} \in A'(\boldsymbol{L})} \frac{\psi(\boldsymbol{\alpha})}{|A(\boldsymbol{L})|}.$$

Proof: Let p be an isotopism and let $\alpha \in A(L)$. Then the isotopism $p\alpha p^{-1}$ is an autotopism of some SOLS in the isotopy class of L, and any autotopism of a SOLS in the isotopy class of L may be written in this form for some isotopism p and some $\alpha \in A(L)$.

For $p\alpha p^{-1}$ to be an automorphism it must hold that $p_r \circ \alpha_r \circ p_r^{-1} = p_s \circ \alpha_s \circ p_s^{-1}$, and hence α_r and α_s must be of the same type. The total number of isotopisms p for which $p\alpha p^{-1}$ is an automorphism is $2n!\psi(\alpha)$. This number may be found by noting that p_r may be chosen in n! ways, p_s may be chosen in $\prod_{i=1}^n a_i!i^{a_i}$ ways, given that α_r and α_s are of type (a_1, a_2, \ldots, a_n) , and finally p_t may be chosen in two ways. We thus count $\sum_{\alpha \in A'(L)} 2n!\psi(\alpha)$ automorphisms over all SOLS in the isotopy class of L, although we may have counted each automorphism more than once.

It is therefore necessary to find the number of equivalence classes of pairs (p, α) , where p is an isotopism for which $p\alpha p^{-1}$ is an automorphism and $\alpha \in A'(L)$. Here two pairs (p, α) and (q, β) are equivalent, denoted by $(p, \alpha) \sim (q, \beta)$, if and only if $p\alpha p^{-1} = q\beta q^{-1}$ and q and p both map L to the same SOLS. If we let $\gamma \in A(L)$, $q = p\gamma$ and $\beta = \gamma^{-1}\alpha\gamma$, then $p\alpha p^{-1} = q\beta q^{-1}$. Furthermore, $\beta \in A'(L)$ and q and p both map L to the same SOLS. We may therefore find, for every $\gamma \in A(L)$, a pair (q, β) such that $(p, \alpha) \sim (q, \beta)$, and these equivalence classes have cardinality at least |A(L)|.

Conversely, let $p\alpha p^{-1} = q\beta q^{-1}$ be automorphisms such that q and p both map L to the same SOLS and $\alpha, \beta \in A'(L)$. Let $\gamma = p^{-1}q \in A(L)$. Thus $p\alpha p^{-1} = q\beta q^{-1} = p\gamma\beta\gamma^{-1}p^{-1}$ and $\beta = \gamma^{-1}\alpha\gamma$. We now have the equivalence found above, and therefore the equivalence classes have size exactly |A(L)|.

The total number of distinct automorphisms over all SOLS in the isotopy class of L is therefore

$$\sum_{\boldsymbol{\alpha} \in A'(\boldsymbol{L})} \frac{2n! \psi(\boldsymbol{\alpha})}{|A(\boldsymbol{L})|}.$$

Since $|S_n \times S_2| = 2n!$ the result follows. \square

To find the number of isomorphism classes of SOLS of order n we sum over all the elements of $\mathcal{I}(n)$. The number of isomorphism classes of SOLS of order n is therefore

$$\sum_{\mathbf{L}\in\mathcal{I}(n)}\frac{1}{|A(\mathbf{L})|}\sum_{\boldsymbol{\alpha}\in A'(\mathbf{L})}\psi(\boldsymbol{\alpha}).$$

We use the isotopy class representatives generated by the method of Section 3 as the set $\mathcal{I}(n)$. The computer program nauty [13] may be used to determine the autotopy groups of these SOLS. Since nauty takes only graphs as input it is necessary to represent a SOLS \boldsymbol{L} by a graph in such a way that the isomorphisms of the graph corresponds to the isotopisms of \boldsymbol{L} . Such a graph for each class of Latin squares is described by McKay et al. [15] and we use a similar graph representation approach to find the isotopy class of SOLS.

For a SOLS L of order n, let G(L) be a vertex-coloured graph such that $V(G) = \{r_i, c_i, s_i, \ell_{ij} \mid i, j \in \mathbb{Z}_n\} \cup \{R, C\}$, where one colour is assigned to $\{r_i, c_i \mid i \in \mathbb{Z}_n\}$, another to $\{s_i \mid i \in \mathbb{Z}_n\}$, a third to $\{R, C\}$ and

a fourth colour to $\{\ell_{ij} \mid i, j \in \mathbb{Z}_n\}$. Furthermore, $E(G) = \{r_i\ell_{ij}, c_j\ell_{ij}, s_k\ell_{ij} \mid \mathbf{L}(i,j) = k\} \cup \{Rr_i, Cc_i, r_ic_i \mid i \in \mathbb{Z}_n\}$ and the isomorphisms of $G(\mathbf{L})$ are colour-preserving. For illustrative purposes a part of $G(\mathbf{L}_4)$ is shown in Figure 4.1, where

$$\boldsymbol{L}_4 = \left[\begin{array}{cccc} 0 & 2 & 3 & 1 \\ 3 & 1 & 0 & 2 \\ 1 & 3 & 2 & 0 \\ 2 & 0 & 1 & 3 \end{array} \right].$$

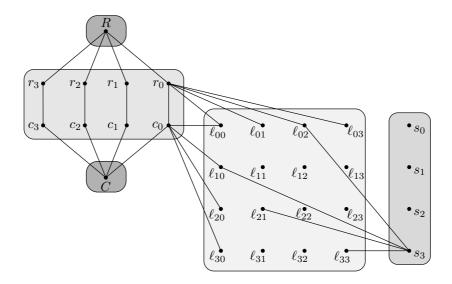


Figure 4.1: A section of the graph $G(\mathbf{L}_4)$ with some edges omitted. The isomorphisms of this graph corresponds to the isotopisms of \mathbf{L}_4 .

A SOLS L is label-isotopic to a SOLS L' if a single permutation on the symbol set of L results in L'. As validation of the correctness of the number of isomorphism classes enumerated via the method described above we employ a second (less efficient) method to enumerate the isomorphism classes for small orders $(4 \le n \le 5)$. This is achieved by means of the following proposition.

Proposition 4.1 Any SOLS L is label-isotopic to at least one SOLS from each isomorphism class in the isotopy class of L.

Proof: Let \mathcal{A} be any isomorphism class in the isotopy class of \mathbf{L} . If $\mathbf{p} = (p_1, p_2, t)$ is an isotopism from \mathbf{L} to a SOLS in \mathcal{A} , then let $\mathbf{p}' = (p_1^{-1}, p_1^{-1}, t^{-1})$ be an isomorphism from a SOLS in \mathcal{A} to another SOLS in \mathcal{A} . The isotopism $\mathbf{p}'\mathbf{p}$ is a label-isotopism from \mathbf{L} to a SOLS in \mathcal{A} . \square

It follows by Proposition 4.1 that we may perform the n! label-isotopisms on a class representative from each isotopy class and group the resulting SOLS into isomorphism classes via isomorphism testing. The test for isomorphism can easily be derived from that of isotopism.

The results obtained via the enumeration of the isomorphism classes are given in Table 4.1 together with the required computing times using the validation method of Proposition 4.1 for orders $4 \le n \le 5$. The computation of the autotopism groups via nauty was immediate for $4 \le n \le 8$ and 0.92 seconds for n = 9.

5 Enumeration of unequal and idempotent SOLS

Two SOLS L and L' are equal if L(i,j) = L'(i,j) for all i and j. We denote the number of unequal SOLS of order n by $\Lambda(n)$ and the number of idempotent SOLS of order n by $\Phi(n)$.

6 Validation of results 11

| \overline{n} | $\Upsilon(n)$ | Time |
|----------------|---------------|------|
| 4 | 5 | 0.1 |
| 5 | 11 | 1.1 |
| 6 | 0 | |
| 7 | 1986 | |
| 8 | 52060 | |
| 9 | 34564884 | |

Table 4.1: The number, $\Upsilon(n)$, of isomorphism classes of SOLS of order n together with the required computing times.

Let \mathcal{T} be a maximal set of pairwise isotopic SOLS of order n. Then \mathcal{T} forms an orbit of the group $S_n^2 \times S_2$ and it follows by a well-known property of group actions [1, 6, 11] (sometimes referred to as the orbit-stabiliser theorem) that $|\mathcal{T}| = 2(n!)^2/|A(\mathbf{L})|$. Since we have a class representative from each isotopy class in the set $\mathcal{I}(n)$, it follows that $\Lambda(n) = 2(n!)^2 \sum_{\mathbf{L} \in \mathcal{I}(n)} 1/|A(\mathbf{L})|$. It may be noted that $\Lambda(n) = n!\Phi(n)$ for any $n \in \mathbb{N}$, which is similar to the well-known result that the number of Latin squares of order n is n!(n-1)! times the number of reduced Latin squares⁵ of order n. Thus, $\Phi(n) = 2n! \sum_{\mathbf{L} \in \mathcal{I}(n)} 1/|A(\mathbf{L})|$.

As validation of the enumeration results obtained by the method described above we generated all unequal SOLS of order n and all idempotent SOLS of order n by the method described in Section 2. This was achieved by starting with an empty $n \times n$ square and a partially completed $n \times n$ square with the elements $0, 1, \ldots, n-1$ on the diagonal in order to generate all unequal and idempotent SOLS of order n, respectively.

The enumeration results for $\Lambda(n)$ and $\Phi(n)$ are shown in Table 5.1 together with the required computing times for the depth-first tree search. Where times are omitted, we were not able to complete the enumeration within an acceptable time-frame.

| \overline{n} | $\Lambda(n)$ | Time | $\Phi(n)$ | Time |
|----------------|----------------|---------|-----------|--------|
| 4 | 48 | 0.1 | 2 | 0.0 |
| 5 | 1440 | 6.5 | 12 | 0.1 |
| 6 | 0 | 33:56.1 | 0 | 0.5 |
| 7 | 19535600 | | 3840 | 4:33.4 |
| 8 | 4180377600 | | 103680 | |
| 9 | 25070769561600 | _ | 69088320 | _ |

Table 5.1: The number, $\Lambda(n)$, of unequal SOLS of order n and the number, $\Phi(n)$, of idempotent SOLS of order n together with the required computing times.

6 Validation of results

Our final result, the enumeration of different types of SOLS, is shown in Table 6.1 for orders $4 \le n \le 9$. The numbers tabulated here may also be found in [19], and the corresponding sequence reference numbers have been provided.

As a validation of our algorithmic implementations we included the case n=6 in our computations, verifying empirically the known theoretical result that $\Lambda(6)=\Phi(6)=0$. We also verified computationally that $\Lambda(n)=n!\Phi(n)$ for small orders.

A validation of the correctness of the values tabulated for $\Psi(n)$ is the fact that all idempotent SOLS of order n were enumerated by the autotopism classes of the $\Psi(n)$ non-isotopic SOLS of order n. Not all of

⁵A Latin square is *reduced* if both its first row and first column are in natural order.

7 Conclusion 12

| n | $\Lambda(n)$ | $\Phi(n)$ | $\Upsilon(n)$ | $\Psi(n)$ | |
|---|----------------|-----------|---------------|-----------|--|
| 4 | 48 | 2 | 5 | 1 | |
| 5 | 1440 | 12 | 11 | 1 | |
| 6 | 0 | 0 | 0 | 0 | |
| 7 | 19353600 | 3840 | 1986 | 4 | |
| 8 | 4180377600 | 103680 | 52060 | 4 | |
| 9 | 25070769561600 | 69088320 | 34564884 | 175 | |
| | #A160368 | #A160367 | #A160366 | #A160365. | |

Table 6.1: Enumeration of various classes of SOLS. Here $\Lambda(n)$ denotes the number of unequal SOLS of order n, $\Phi(n)$ the number of idempotent SOLS of order n, $\Upsilon(n)$ the number of isomorphism classes of SOLS of order n and $\Psi(n)$ the number of isotopy classes of SOLS of order n. The identification numbers allocated to the column sequences of the table in Sloane's Online Encyclopedia of Integer Sequences [19] are shown in the last row of the table.

the $\Phi(n)$ idempotent SOLS would have been enumerated if the value of $\Psi(n)$ were too small. Similarly, too large a value of idempotent SOLS would have been enumerated if the value of $\Psi(n)$ were too large. A final validation of the correctness of our numerical results for the isotopy classes is the fact that the two approaches of Section 3, namely completing skeletons and generating class representatives, yielded the same results.

As validation of the isomorphism class enumeration two approaches were again implemented, namely by the autotopism groups of the isotopy class representatives and by Proposition 4.1, both yielding the same results. Finally, validation of the correctness of the values tabulated for $\Lambda(n)$ and $\Phi(n)$ is the fact that both implementations of the method described in Section 2 yielded the same results for $\Lambda(n)$ and $\Phi(n)$ as enumerated by the autotopism classes of the $\Psi(n)$ non-isotopic SOLS of order n.

7 Conclusion

In this paper we enumerated the number of unequal SOLS, the number of idempotent SOLS, the number of isomorphism classes of SOLS and the number of isotopy classes of SOLS of orders $4 \le n \le 9$ by a number of different methods for each count, providing a means of validation towards the correctness of these numbers. Furthermore, we were able to build up a repository of all unequal SOLS of orders $4 \le n \le 5$, all idempotent SOLS of orders $4 \le n \le 7$ and class representatives from each of the isotopy classes of SOLS of orders $4 \le n \le 9$, all of which are available online [12].

The first level of the search-tree for SOLS of order 10 has four nodes (utilizing the orderly generation approach) while the second level has 3 825 nodes. In order to gain an understanding of the expected time complexity associated with traversing this search tree, we fathomed 13 (0.34%) of the 3 825 nodes on the second level of the tree. During this process we uncovered 494 non-isotopic SOLS of order 10 (these SOLS are available in [12]). We recorded traversal times ranging between two days and twenty days per node from which we estimate that the time required to traverse the entire tree may be between 20 years and 200 years. Our method is therefore infeasible for order 10, even if a low-level programming language (such as C^{++} or C#) were to be used instead of Mathematica, unless a massively parallel approach is adopted. Further pruning rules are required for early identification of branches of the search tree that will not result in any new SOLS, thus thinning the tree considerably. The exploration of special properties of SOLS of order 10 may also be considered in order to render the search tractable. However, once we have a class representative from each isotopy class of SOLS of a certain order $n \geq 10$, the enumeration of the number of unequal SOLS, idempotent SOLS and isomorphism classes will be neither difficult nor time-consuming.

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Appendix: Non-isotopic SOLS of orders $4 \le n \le 9$

All non-isotopic SOLS of orders $4 \le n \le 9$ are listed in this appendix. Below each SOLS the number of idempotent SOLS isotopic to it is given in bold face. This value may be multiplied by n! to obtain the cardinality of the corresponding isotopy class.

| n=4 | n = 5 | n = 7 | | | | n = 8 | | | |
|------|-------|---------|---------|---------|---------|----------|----------|------------------|----------|
| 0231 | 02143 | 0214365 | 0214365 | 0214563 | 0234561 | 02145673 | 02145673 | 02345671 | 02345671 |
| 3102 | 31402 | 3160542 | 3160524 | 3105624 | 6105243 | 31670245 | 31702456 | 31460752 | 41607352 |
| 1320 | 43210 | 4526013 | 4526031 | 4621035 | 1420635 | 43257016 | 46257301 | 65207413 | 53270146 |
| 2013 | 24031 | 5643201 | 5643102 | 6053241 | 2653014 | 20736154 | 57630124 | 74136205 | 67431025 |
| 2 | 10324 | 6351420 | 6352410 | 2536410 | 3516402 | 65314702 | 75364210 | 27654130 | 76154203 |
| | 12 | 1032654 | 2401653 | 1460352 | 4362150 | 76402531 | 13076542 | 13072546 | 14726530 |
| | | 2405136 | 1035246 | 5342106 | 5041326 | 17523460 | 20413765 | 50721364 | 20513764 |
| | | 240 | 1680 | 1680 | 240 | 54061327 | 64521037 | 46513027 | 35062417 |
| | | | | | | 80640 | 10080 | $\mathbf{11520}$ | 1440 |
| | | | | | | | | | |

m — 0

 $021436587 \ 0214$ 318507264 318064725 316078245 316578420 317502864 315874260 310257846 318764250 315784062 310274856 316278405 318027456 $472061835\ 472508361\ 452801763\ 482167305\ 482067135\ 432058716\ 452803761\ 472851306\ 472013856\ 472068135\ 452617830\ 432810765$ $207358146\ 280357416\ 260387154\ 570321864\ 576328041\ 578361024\ 576382014\ 560382741\ 587360421\ 586317240\ 580362741\ 564378012$ $180642753\ 107643852\ 105742836\ 605842731\ 658140723\ 607142835\ 763148205\ 706143825\ 760148235\ 758640321\ 768143052\ 750641823$ $746185320\ 764185203\ 738165402\ 748605213\ 764285310\ 786205143\ 148675320\ 187605432\ 238605714\ 207185463\ 204785316\ 287165340$ $853724601\ 835721640\ 874523610\ 837014652\ 835714602\ 843527601\ 805714632\ 854027613\ 854271603\ 835702614\ 837051624\ 875204631$ $635810472\ 653812074\ 683254071\ 154283076\ 140853276\ 150683472\ 284560173\ 635218074\ 146852370\ 164853072\ 645820173\ 603582174$ $564273018\ 546270138\ 547610328\ 263750148\ 203671458\ 264710358\ 637021458\ 243570168\ 603527148\ 643521708\ 173504268\ 146753208$ $90\,720\quad 362\,880\quad 181\,440\quad 362\,880\quad 725\,760\quad 725\,760\quad 725\,760\quad 725\,760\quad 725\,760$ $021436587 \ 021436587 \ 021436587 \ 021436587 \ 021436587 \ 021436587 \ 021436587 \ 021436785 \ 0214$ $316807425\ 318607254\ 318760425\ 318720465\ 316820754\ 316507842\ 314508762\ 318654207\ 310857246\ 315872046\ 314867520\ 317052846$ $582173064\ 572184036\ 562178034\ 562871034\ 582071463\ 542873016\ 562783014\ 452718036\ 472068351\ 432761850\ 402758361\ 462587103$ $170384256\ 180362745\ 180324756\ 180364752\ 178364205\ 204358761\ 206357841\ 285367140\ 548371062\ 564380127\ 560382147\ 578314062$ $765248310\ 763548120\ 705841362\ 705148326\ 705148326\ 785642130\ 783641250\ 507142863\ 687240513\ 607548231\ 678041253\ 603748251$ $208615743\ 207815463\ 273685140\ 237615840\ 237615840\ 160785324\ 140875326\ 763085412\ 136725804\ 178205364\ 243175806\ 284605317$ $834751602\ 845273601\ 834257601\ 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