Optimal and efficient semi-Latin squares

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Abstract

An $(n \times n)/k$ *semi-Latin square* is an $n \times n$ square array in which nk distinct symbols (representing treatments) are placed in such a way that there are exactly k symbols in each cell (row-column intersection) and each symbol occurs once in each row and once in each column. Semi-Latin squares form a class of row-column designs generalising Latin squares, and have applications in areas including the design of agricultural experiments, consumer testing, and via their duals, human-machine interaction. In the present paper, new theoretical and computational methods are developed to determine optimal or efficient $(n \times n)/k$ semi-Latin squares for values of n and k for which such semi-Latin squares were previously unknown. The concept of subsquares of uniform semi-Latin squares is studied, new applications of the DESIGN package for GAP are developed, and exact algebraic computational techniques for comparing efficiency measures of binary equireplicate block designs are described. Applications include the complete enumeration of the $(4 \times 4)/k$ semi-Latin squares for $k = 2, \ldots, 10$, and the determination of those that are A-, D- and E-optimal, the construction of efficient $(6 \times 6)/k$ semi-Latin squares for $k = 4, 5, 6$, and counterexamples to a long-standing conjecture of R.A. Bailey and to a similar conjecture of D. Bedford and R.M. Whitaker.

Keywords: Semi-Latin square, Design optimality, Mutually orthogonal Latin squares, Block design, Block design efficiency measures, Construction and enumeration of combinatorial designs, DESIGN package for GAP, Algebraic computation

1. Introduction

An $(n \times n)/k$ *semi-Latin square* is an $n \times n$ square array in which nk distinct symbols (representing treatments) are placed in such a way that there are exactly k symbols in each cell (row-column intersection) and each symbol occurs once in each row and once in each column. The order of symbols within a cell is immaterial, and to avoid trivialities, we assume throughout that $n > 1$ and $k > 0$. Since no symbol can occur more than once within a cell, it is convenient to consider the contents of a cell to be a k-element subset of the set of symbols, and we call such a subset a *block* of a semi-Latin square.

We consider two $(n \times n)/k$ semi-Latin squares to be *isomorphic* if one can be obtained from the other by applying one or more of: a row permutation, a column permutation,

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transposing, and renaming symbols. The *underlying block design* $\Delta(S)$ of a semi-Latin square S is obtained by ignoring the row and column structure of S, so $\Delta(S)$ is a block design whose treatments are the symbols of S and whose blocks are the blocks of S (including any repeats). The *dual* S^* of an $(n \times n)/k$ semi-Latin square S is the block design whose n^2 treatments are the ordered pairs (i, j), with $i, j \in \{1, \ldots, n\}$, and whose nk blocks correspond to the symbols of S, with the block corresponding to a symbol α consisting precisely of the ordered pairs (i, j) such that α is in the (i, j)-cell of S (see Bailey (2011)). Note that, up to the naming of its symbols, a semi-Latin square S can be recovered from its dual S^*.

For example, here is a $(3 \times 3)/2$ semi-Latin square with symbol-set $\{1, \ldots, 6\}$:

1 4	2 5	3 6
3 5	1 6	2 4
2 6	3 4	1 5

, (1)

and the blocks of its dual are:

$$\begin{array}{lll} \{(1,1),(2,2),(3,3)\}, & \{(1,2),(2,3),(3,1)\}, & \{(1,3),(2,1),(3,2)\}, \\ \{(1,1),(2,3),(3,2)\}, & \{(1,2),(2,1),(3,3)\}, & \{(1,3),(2,2),(3,1)\}. \end{array}$$

Note that an $(n \times n)/1$ semi-Latin square is the same thing as a Latin square of order n.

Semi-Latin squares have applications in the design of comparative experiments, including the design of agricultural experiments, consumer testing, and via their duals, human-machine interaction (see Preece and Freeman (1983); Bailey (1988, 1992, 2011); Edmondson (1998), and their references). Thus, it is important to know statistically optimal, or at least efficient, $(n \times n)/k$ semi-Latin squares for given values of n and k. Following the analysis by Bailey (1992), an $(n \times n)/k$ semi-Latin square is *optimal* (in the class of $(n \times n)/k$ semi-Latin squares) with respect to a given optimality criterion if and only if its underlying block design is optimal with respect to that criterion in the class of underlying block designs of $(n \times n)/k$ semi-Latin squares. In addition, as shown by Bailey (2011), the dual of an $(n \times n)/k$ semi-Latin square S is optimal (in the class of duals of $(n \times n)/k$ semi-Latin squares) if and only if S is optimal, for a wide range of statistical optimality criteria, including A, D and E.

A *binary equireplicate design* with *parameters* (v, b, r, k), or simply a (v, b, r, k)-*design*, is a block design having $v > 1$ treatments and b blocks, such that each block is a set consisting of $k > 0$ distinct treatments, and each treatment is in exactly $r > 0$ blocks. Note that the underlying block design of an $(n \times n)/k$ semi-Latin square is an (nk, n^2, n, k)-design.

The *concurrence matrix* Λ of a (v, b, r, k)-design Δ is the $v \times v$ matrix whose rows and columns are indexed by the treatments of Δ, and whose (α, β)-entry is the number of blocks containing both α and β. The *scaled information matrix* of Δ is

$$F(\Delta) := I_v - (rk)^{-1}\Lambda,$$

where I_v is the $v \times v$ identity matrix (see Bailey and Cameron (2009)). The eigenvalues of $F(\Delta)$ are all real and lie in the interval $[0, 1]$. At least one eigenvalue is zero: an associated eigenvector is the all-1 vector. The remaining eigenvalues $\delta_1 \le \delta_2 \le \cdots \le \delta_{v-1}$ of $F(\Delta)$ are called the *canonical efficiency factors* of Δ (see John and Williams (1982); Bailey and Cameron (2009)). These are all non-zero if and only if Δ is connected (that is, the treatment-block incidence graph of Δ is a connected graph). If Δ is not connected, then we define $\mathrm{A}_\Delta = \mathrm{D}_\Delta = \mathrm{E}_\Delta := 0$. Otherwise, these *efficiency measures* are defined by $\mathrm{A}_\Delta := (v-1)/\sum_{i=1}^{v-1} 1/\delta_i$, $\mathrm{D}_\Delta := \left(\prod_{i=1}^{v-1}\delta_i\right)^{1/(v-1)}$, and $\mathrm{E}_\Delta := \delta_1 = \min\{\delta_1,\ldots,\delta_{v-1}\}$. We say that Δ is *A-optimal* in a class $\mathcal{C}$ of (v,b,r,k)-designs containing Δ if $A_\Delta \geq A_\Gamma$ for each $\Gamma \in \mathcal{C}$. D-optimal and E-optimal are defined similarly. We refer the reader to Bailey and Cameron (2009) and Shah and Sinha (1989) for more background on block design optimality, and for the respective definitions of Schur-optimality and MV-optimality.

When we apply the terms canonical efficiency factors, connected, and efficiency measure to a semi-Latin square S, we shall always mean the same as when those terms are applied to the underlying block design of S.

In this paper, new theoretical and computational methods are developed and applied to determine optimal, or at least efficient, $(n\times n)/k$ semi-Latin squares for values of n and k for which such semi-Latin squares were previously unknown.

We start by providing background results, including a discussion of the "pseudo-Trojan" semi-Latin squares constructed and analysed by Bailey (1992), and which were conjectured to be optimal.

We then describe the enumeration of the $(4\times4)/k$ semi-Latin squares for $k = 2,\ldots,10$, including determining those that are A-, D- and E-optimal. The results for $k = 5,\ldots,10$ are completely new.

A semi-Latin square U is *uniform* if any two blocks of U not in the same row or column meet in a constant number $\mu = \mu(U)$ of symbols, and we say that an $n\times n$ semi-Latin square S is a *subsquare* of an $n\times n$ semi-Latin square T if $S = T$ or T is obtained by superimposing S and another $n\times n$ semi-Latin square (with a disjoint symbol-set). Pseudo-Trojan semi-Latin squares, as well as the semi-Latin squares constructed by Bedford and Whitaker (2001), can be viewed as certain $(n\times n)/k$ subsquares of $(n\times n)/u$ uniform semi-Latin squares, with $u-k < n-1$, and we study the canonical efficiency factors of such subsquares. One outcome of this study is to explain certain numerical observations of Bedford and Whitaker (2001). We then enumerate the uniform $(5\times5)/8$ semi-Latin squares, and examine their subsquares, obtaining $(5\times5)/6$ counterexamples to both Bailey's conjecture and one of Bedford and Whitaker.

Pseudo-Trojan semi-Latin squares provide efficient (although we now know, not necessarily optimal) $(n\times n)/k$ semi-Latin squares when n is a prime power. We then discuss the situation for 6×6 semi-Latin squares, with our particular contribution being efficient $(6\times6)/k$ semi-Latin squares for $k = 4,5,6$, the $(6\times6)/6$ example being especially noteworthy.

Throughout, we make extensive use of the author's DESIGN package (Soicher, 2011) for GAP (The GAP Group, 2012), and in Appendix A we present the group-theoretical framework to use this package in the enumeration of semi-Latin squares with given properties. Readers unfamiliar with permutation groups and group actions should consult Cameron (1999), or may want to skim over much of Appendix A.

One especially novel aspect of this paper is that exact algebraic computation is used for the comparison of efficiency measures, and these techniques are discussed in Appendix B. Thus, when determining the optimal designs amongst those enumerated, or determining a counterexample to a conjecture on optimality, there is no danger of numerical error producing an erroneous result.

2. Background

Let s be a positive integer. An *s-fold inflation* of an $(n \times n)/k$ semi-Latin square is obtained by replacing each symbol α in the semi-Latin square by s symbols $\sigma_{\alpha,1}, \ldots, \sigma_{\alpha,s}$, such that $\sigma_{\alpha,i} = \sigma_{\beta,j}$ if and only if $\alpha = \beta$ and $i = j$. The result is an $(n \times n)/(ks)$ semi-Latin square. For example, here is a 2-fold inflation of a Latin square of order 3:

1 4	2 5	3 6
3 6	1 4	2 5
2 5	3 6	1 4

.

The *superposition* of an $(n \times n)/k$ semi-Latin square with an $(n \times n)/\ell$ semi-Latin square (with disjoint symbol sets) is performed by superimposing the first square upon the second, resulting in an $(n \times n)/(k+\ell)$ semi-Latin square. An $(n \times n)/k$ semi-Latin square is *Trojan* if it is the superposition of k mutually orthogonal Latin squares (MOLS) of order n with pairwise disjoint symbol sets. For example, the semi-Latin square (1) is Trojan. The canonical efficiency factors of (the underlying block design of) an $(n \times n)/k$ Trojan semi-Latin square are $1-1/k$ ($k(n-1)$ times), and 1 ($k-1$ times); see Bailey (1992, Corollary 5.2). Cheng and Bailey (1991) proved that each $(n \times n)/k$ Trojan semi-Latin square is A-, D- and E-optimal. Indeed, they proved that the underlying block design of an $(n \times n)/k$ Trojan semi-Latin square is optimal in the class of all (nk, n^2, n, k)-designs, with respect to a wide range of optimality criteria, including the A-, D- and E-efficiency measures. Of course, there may not exist k MOLS of order n, as when $k \geq n$ or when $n = 6$ and $k > 1$.

An $(n \times n)/k$ *pseudo-Trojan* semi-Latin square $P(n, k)$ is either Trojan or $k \geq n$ and there must exist $n-1$ MOLS $L_1, \ldots, L_{n-1}$ of order n from which $P(n, k)$ is constructed as follows. (The only n currently known with the property that there exist $n-1$ MOLS of order n are the prime powers.) Let $k = a(n-1)+b$, with a and b integers with $a > 0$ and $0 \leq b < n-1$. Then $P(n, k)$ is formed by superimposing $(a+1)$-fold inflations of $L_1, \ldots, L_b$ and a-fold inflations of $L_{b+1}, \ldots, L_{n-1}$. The canonical efficiency factors of such a $P(n, k)$ are $1-(a+1)/k$ ($b(n-1)$ times), $1-a/k$ ($(n-1-b)(n-1)$ times), and 1 ($nk-(n-1)^2-1$ times); see Bailey (1992, Corollary 5.3). Thus every (Trojan or not) $(n \times n)/k$ pseudo-Trojan semi-Latin square has the same canonical efficiency factors, and from these we can compute its A-, D- and E-efficiency measures. For example, a pseudo-Trojan $(5 \times 5)/6$ semi-Latin square $P(5, 6)$ has

$$\mathrm{A}_{P(5,6)} = 145/173 \approx .838150,\ \mathrm{D}_{P(5,6)} = (390625/43046721)^{1/29} \approx .850315, \tag{2}$$

and $\mathrm{E}_{P(5,6)} = 2/3$.

Bailey (1992) introduced and analysed pseudo-Trojan squares (but did not name them), and conjectured that each $(n \times n)/k$ pseudo-Trojan semi-Latin square is "optimal". In the context of Bailey (1992), we take this to mean:

Conjecture 1 (Bailey). *Each $(n \times n)/k$ pseudo-Trojan semi-Latin square is A-, D- and E-optimal.*

In the same paper, Bailey showed that this conjecture is true when $n-1$ divides k, and also when $n < 4$. Chigbu (1996) established the conjecture in the case $n = k = 4$.

An $(n \times n)/k$ semi-Latin square in which any two distinct symbols occur together in at most one block is called a SOMA(k, n). It is believed that a SOMA(k, n) that is optimal in the class of all SOMA(k, n)s is in fact optimal in the class of all $(n \times n)/k$ semi-Latin squares (see Bailey and Royle (1997); John and Williams (1982)). Note that each $(n \times n)/k$ Trojan semi-Latin square is a SOMA(k, n), but a SOMA(k, n) may exist when there do not exist k MOLS of order n. However, a SOMA(k, n) always has $k < n$.

Bailey and Royle (1997) enumerated the underlying block designs of the SOMA$(2, 6)$s, and determined optimal SOMA$(2, 6)s$ for each of the efficiency measures A, D, E and MV (although MV is called by the less common name E$'$). All SOMA$(k, n)s$ with $n \leq 6$ were enumerated by the author and are available from his "SOMA Update" webpage (Soicher, 2012). Up to (semi-Latin square) isomorphism there are just 2799 SOMA$(2, 6)$s and four SOMA$(3, 6)$s. (See also Phillips and Wallis (1996) and Preece and Phillips (2002) regarding the enumeration of SOMA$(3, 6)$s.) We find that the two SOMA$(3, 6)$s which are superpositions of a Latin square of order 6 and a SOMA$(2, 6)$ have the same canonical efficiency factors and are A-, D-, E- and MV-optimal amongst the SOMA$(3, 6)$s; see also (Bailey, 2011). There is no SOMA$(k, 6)$ with $k > 3$, so we shall focus in this paper on efficient $(6 \times 6)/k$ semi-Latin squares with $k > 3$.

Recall that a semi-Latin square U is *uniform* if any two blocks of U not in the same row or column meet in a constant number $\mu = \mu(U)$ of symbols. Soicher (2012) introduced and studied uniform semi-Latin squares. An $(n \times n)/k$ uniform semi-Latin square U has $k = \mu(U)(n - 1)$, with $\mu(U) = 1$ if and only if U is a superposition of $n - 1$ MOLS of order n. Soicher (2012) also proved that each $(n \times n)/k$ uniform semi-Latin square is Schur-optimal. In particular, each uniform semi-Latin square is A-, D- and E-optimal (see Giovagnoli and Wynn (1981)). In addition, Soicher gave a construction to make an $(n \times n)/k$ semi-Latin square SLS(G) from a transitive permutation group G of degree n and order nk, and proved that SLS(G) is uniform if and only if G is 2-transitive. He also constructed uniform $(6 \times 6)/(5\mu)$ semi-Latin squares for all integers $\mu > 1$.

3. Enumeration of $(4 \times 4)/k$ semi-Latin squares

Each 2×2 semi-Latin square is simply an inflation of a Latin square of order 2, and is not connected. Bailey (1992) enumerated the 3×3 semi-Latin squares. Applying the methods discussed in Appendix A, we used the DESIGN package function `SemiLatinSquareDuals` to enumerate the $(4 \times 4)/k$ semi-Latin squares up to isomorphism (via their duals), for $k = 2, \ldots, 10$. This required under an hour of CPU-time on a 3.1 GHz PC running Linux. Analysing these squares (using exact algebraic computation as described in Appendix B), we found that each A-optimal square is in fact A-, D- and E-optimal, and has the same canonical efficiency factors as a pseudo-Trojan square of the same size. This verifies that Bailey's conjecture holds in the case of $(4 \times 4)/k$ semi-Latin squares with $k \leq 10$, and so for these sizes, a pseudo-Trojan square is A-, D- and E-optimal.

A summary of the results is given in Table 1. We record k, the number of $(4 \times 4)/k$ semi-Latin squares (up to isomorphism), and the number of (pairwise nonisomorphic) optimal $(4 \times 4)/k$ semi-Latin squares. By optimal we mean here A-, D- and E-optimal, and remark that for $2 \leq k \leq 10$, an A-, D- and E-optimal $(4 \times 4)/k$ semi-Latin square is MV-optimal if and only if $k \notin \{4, 7, 10\}$.

k	no. squares	no. optimal
2	10	1
3	40	1
4	164	3
5	621	3
6	2298	2
7	7905	5
8	25657	4
9	77744	2
10	221201	6

Table 1: $(4 \times 4)/k$ semi-Latin squares.

Preece and Freeman (1983) enumerated by hand the $(4 \times 4)/2$ semi-Latin squares, up to both isomorphism and "strong isomorphism" (strong isomorphism is defined in Appendix A), and our results agree with theirs. Using a mixture of hand and machine computation, Chigbu (1996) (see also Bailey and Chigbu (1997)) enumerated the $(4 \times 4)/3$ and $(4 \times 4)/4$ semi-Latin squares, up to both isomorphism and strong isomorphism. Our results disagree with his, and our consistency checks indicate that he missed some isomorphism classes. For the record, we calculate that, up to strong isomorphism, there are exactly 46 $(4 \times 4)/3$ and 201 $(4 \times 4)/4$ semi-Latin squares.

We remark that complete enumerations of the kind described here are useful for other statistical purposes than determining optimal designs with respect to a given optimality criteria. For example, we may wish to evaluate designs with respect to other properties, such as robustness. In Section 5, we enumerate all uniform (and hence known to be A-, D- and E-optimal) $(5 \times 5)/8$ semi-Latin squares in order to determine the most efficient subsquares of these.

4. On subsquares of uniform semi-Latin squares

Let S and U be $n \times n$ semi-Latin squares. Recall that S is a *subsquare* of U if $S = U$ or U is a superposition of S and another $n \times n$ semi-Latin square. A subsquare S of U is *proper* if $S \neq U$.

In this section, we prove a theorem about the canonical efficiency factors of the $(n \times n)/k$ subsquares of uniform $(n \times n)/u$ semi-Latin squares, such that $u - k < n - 1$. Such subsquares include pseudo-Trojan squares and the semi-Latin squares constructed by Bedford and Whitaker (2001). Our theorem explains certain numerical observations by Bedford and Whitaker (2001), and leads us, in the next section, to finding counterexamples to Bailey's conjecture and a similar conjecture of Bedford and Whitaker.

It is convenient to study subsquares via their duals, and the reader should keep in mind that the canonical efficiency factors not equal to 1 of a semi-Latin square S, and their multiplicities, are the same as those of the dual S^* of S (see Bailey and Cameron (2009, Section 3.1.1)).

Lemma 1. *Let S and T be $n \times n$ semi-Latin squares with disjoint symbol sets, and let U be the superposition of S and T. Then the concurrence matrix of U^* is the sum of the concurrence matrices of S^* and T^*.*

Proof. Straightforward.

Theorem 2. *Let $n > 2$ and let S be an $(n \times n)/k$ subsquare of a uniform $(n \times n)/u$ semi-Latin square U, such that $u - k < n - 1$. Then:*

1. $\mathrm{E}_S = 1 - u/(k(n-1)) = 1 - \mu(U)/k$;
2. *if P is a pseudo-Trojan $(n \times n)/k$ semi-Latin square, then $\mathrm{E}_S = \mathrm{E}_P$;*
3. *if P is a pseudo-Trojan $(n \times n)/k$ semi-Latin square and U is the superposition of S and an $n \times n$ Trojan square (in particular, if $u - k = 1$), then the canonical efficiency factors of S and their multiplicities are the same as those of P.*

Proof. First suppose that S is a proper subsquare of U, so that U is the superposition of S and some $(n \times n)/(u-k)$ semi-Latin square T. Let L be the concurrence matrix of T^* and let M be the concurrence matrix of U^*. Then L and M are real, symmetric, positive semi-definite matrices whose rows and columns are indexed by $\{1, \ldots, n\}^2$, as are the co-ordinates of the (column) vectors in what follows.

Since U is a uniform semi-Latin square, U^* is a partially balanced incomplete-block design with respect to the L_2-type association scheme, and the eigenvalues of M are nu with multiplicity 1, 0 with multiplicity $2n-2$, and $nu/(n-1)$ with multiplicity $(n-1)^2$ (see, for example, Vartak (1959)). Denote the eigenspaces corresponding to these (distinct) eigenvalues by V_0, V_1, and V_2, respectively. From the proof of Theorem 3.4 of Soicher (2012), we observe that $L\mathbf{v} = n(u-k)\mathbf{v}$ if $\mathbf{v} \in V_0$, and $L\mathbf{v} = \mathbf{0}$ if $\mathbf{v} \in V_1$. Thus, there is a basis $\mathbf{v}_1, \ldots, \mathbf{v}_{(n-1)^2}$ of $V_2 = (V_0 + V_1)^\perp$ consisting of pairwise orthogonal eigenvectors of L. Let τ_i be the eigenvalue of L corresponding to $\mathbf{v}_i$ ($i = 1, \ldots, (n-1)^2$).

By Lemma 1, the concurrence matrix of S^* is $M - L$. From the discussion above, the eigenvalues of $M - L$ are nk (once), 0 ($2n-2$ times), and $nu/(n-1) - \tau_i$, for $i = 1, \ldots, (n-1)^2$. Now S^* has scaled information matrix

$$I_{n^2} - (nk)^{-1}(M - L),$$

and so the canonical efficiency factors of S^* are 1 ($2n-2$ times), and $1 - u/(k(n-1)) + \tau_i/(nk)$, for $i = 1, \ldots, (n-1)^2$. In particular, the least canonical efficiency factor of S^* (and so of S) is $1 - u/(k(n-1)) + \tau/(nk)$, where $\tau := \min\{\tau_1, \ldots, \tau_{(n-1)^2}\}$.

Now T is an $(n \times n)/(u-k)$ semi-Latin square, and by assumption, $u - k < n - 1$. Thus $(n-1)^2 > (u-k)n - 1$, so T has fewer than $(n-1)^2$ canonical efficiency factors, so T^* has more than $2n-2$ canonical efficiency factors equal to 1, so $\tau = 0$, and we have

$$\mathrm{E}_S = \mathrm{E}_{S^*} = 1 - u/(k(n-1)).$$

We complete the proof of part 1 by noting that if $S = U$ then $\mathrm{E}_S = \mathrm{E}_U = 1 - 1/(n-1)$, as required.

Suppose now that P is a pseudo-Trojan $(n \times n)/k$ semi-Latin square, and let $\mu := \mu(U) = u/(n-1)$. Then P is an $(n \times n)/k$ subsquare of some μ-fold inflation Q of a superposition of $n-1$ MOLS of order n (since $k \le u$), and Q is a uniform $(n \times n)/u$ semi-Latin square. Thus, both S and P are $(n \times n)/k$ subsquares of certain uniform $(n \times n)/u$

semi-Latin squares, with $u - k < n - 1$, and so by part 1, we have $E_S = E_P = 1 - \mu/k$, and the proof of part 2 is complete.

Now suppose that U is the superposition of S and a Trojan square T, We know that Q above is the superposition of P and some Trojan square T' having the same size as T. By Bailey (1992), T and T' have the same canonical efficiency factors, so it follows from the proof of part 1 that both S^* and P^* have the same canonical efficiency factors, and so too must S and P.

Bedford and Whitaker (2001) used sets of $n - 1$ MOLS of order n to construct efficient $(n \times n)/k$ semi-Latin squares for certain $k \geq n$, when n is a prime power. Their construction starts by superimposing certain superpositions of $n - 1$ MOLS of order n, which makes a uniform semi-Latin square U, and then if required, removing an $n \times n$ Trojan semi-Latin square from U. Thus, by part 3 of the result above, an $(n \times n)/k$ semi-Latin square constructed by their method has the same canonical efficiency factors as a pseudo-Trojan $(n \times n)/k$ semi-Latin square $P(n, k)$. This explains the numerical observation by Bedford and Whitaker (2001) that the A-, D- and E-efficiency measures of the squares they construct appear to be the same as the pseudo-Trojan squares of the same size constructed by Bailey (1992). (However, Bedford and Whitaker's calculation of MV-efficiency measures of pseudo-Trojan squares is erroneous, and so their comparison with that measure for their squares is not valid.) Bedford and Whitaker (2001) also conjectured that the semi-Latin squares coming from their construction are A-, D- and E-optimal. However, one such square is a $(5 \times 5)/6$ semi-Latin square, so the following section provides counterexamples to their conjecture, as well as to Bailey's.

5. Counterexamples to Bailey's conjecture

The theory of the previous section shows that we cannot get a counterexample to Bailey's conjecture simply by removing a Trojan subsquare from some uniform semi-Latin square, but suggests it may be fruitful to examine other subsquares of uniform squares. Having found no counterexample to Bailey's conjecture when $n = 4$, we enumerated the uniform $(5 \times 5)/8$ semi-Latin squares and studied their subsquares. It turns out that, up to isomorphism, there are exactly 10 uniform $(5 \times 5)/8$ semi-Latin squares. This enumeration, via their duals, is easily accomplished by the DESIGN package, by applying Corollary 6.

1 2 3 4 5 6	7 8 9 10 11 12	13 14 15 16 17 18	19 20 21 22 23 24	25 26 27 28 29 30
7 13 14 19 25 26	1 15 16 20 21 27	2 8 22 23 28 29	3 4 9 10 17 30	5 6 11 12 18 24
9 11 15 20 22 28	3 5 13 23 25 29	1 6 7 10 24 30	2 12 14 18 26 27	4 8 16 17 19 21
8 12 17 23 24 27	6 14 18 19 22 30	4 9 11 21 25 26	1 5 7 16 28 29	2 3 10 13 15 20
10 16 18 21 29 30	2 4 17 24 26 28	3 5 12 19 20 27	6 8 11 13 15 25	1 7 9 14 22 23

Figure 1: $B(5, 6)$: a $(5 \times 5)/6$ counterexample to Bailey's conjecture.

We then used the `BlockDesigns` function to enumerate the $(5 \times 5)/k$ subsquares of each of these uniform squares, for $k = 5, 6$, up to the action of the automorphism group of each such uniform square and the naming of symbols. This was done by enumerating the $(25, 5k, k, 5)$-subdesigns (for $k = 5, 6$) of the duals of the $(5 \times 5)/8$ uniform squares,

31 32	33 34	35 36	37 38	39 40
33 37	31 39	32 34	35 40	36 38
36 40	35 38	37 39	31 34	32 33
35 39	32 40	31 38	33 36	34 37
34 38	36 37	33 40	32 39	31 35

Figure 2: A SOMA$(2, 5)$ whose superposition with $B(5, 6)$ is uniform.

up to the actions of their respective automorphism groups. We then analysed these $(5 \times 5)/k$ subsquares, and found that, up to isomorphism, exactly 29 of these have a higher A-measure than a pseudo-Trojan $(5 \times 5)/k$ semi-Latin square. All these 29 have $k = 6$, and of these 29, exactly 24 come from removing a (non-Trojan) SOMA$(2, 5)$ from a uniform square, and these 24 are precisely the ones with both A-measure and D-measure higher than those of a $(5 \times 5)/6$ pseudo-Trojan square $P(5, 6)$. Of course, all 29 have the same E-measure, 2/3, as $P(5, 6)$. We give in Figure 1 the unique (up to isomorphism) $(5 \times 5)/6$ semi-Latin square $B(5, 6)$ with the best A-measure of the 29. It turns out also to be uniquely D-optimal amongst the $(5 \times 5)/6$ subsquares of uniform $(5 \times 5)/8$ semi-Latin squares. In Figure 2 we display a SOMA$(2, 5)$ such that the superposition of $B(5, 6)$ with this SOMA is uniform. We have:

$$\begin{aligned} A_{B(5,6)} &= 309578045/369257731 \approx .838379, \\ D_{B(5,6)} &= (30592715909/3363025078125)^{1/29} \approx .850387 \end{aligned}$$

(compare with (2)).

6. Efficient 6×6 semi-Latin squares

Pseudo-Trojan semi-Latin squares provide easy to construct and efficient (although not necessarily optimal) $(n \times n)/k$ semi-Latin squares when n is a prime power. In the case of $n = 6$, however, efficient $(n \times n)/k$ semi-Latin squares were known only for $k = 2$ and 3. Here we provide new efficient $(6 \times 6)/k$ semi-Latin squares for $k = 4, 5, 6$, obtained as subsquares of a certain remarkable $(6 \times 6)/6$ semi-Latin square. We remark that efficient $(6 \times 6)/k$ semi-Latin squares for $k = 7, 8, 9, 10$ are calculated and presented in (Soicher, to appear), and are found as subsquares of a certain uniform $(6 \times 6)/10$ semi-Latin square.

6.1. *A remarkable* $(6 \times 6)/6$ *semi-Latin square*

Let

$A :=$

1 13 31	14 20 26	21 27 33	4 10 16	11 23 29	6 12 36
16 29 33	1 10 23	6 13 20	12 14 27	4 21 36	11 26 31
14 23 36	4 27 31	1 12 29	11 13 21	6 16 26	10 20 33
4 12 26	6 11 33	16 23 31	1 20 36	10 13 27	14 21 29
11 20 27	12 16 21	10 26 36	6 29 31	1 14 33	4 13 23
6 10 21	13 29 36	4 11 14	23 26 33	12 20 31	1 16 27

.

Then, up to isomorphism, A is the unique SOMA$(3,6)$ having an automorphism group of order 72 (A is not an optimal SOMA). Let H be this automorphism group. It turns out that, up to the naming of symbols, there is just one further H-invariant SOMA$(3,6)$, which can be taken to be:

$B :=$

7 19 25	2 8 32	3 9 15	22 28 34	5 17 35	18 24 30
2 9 24	15 30 34	7 28 35	5 19 32	8 18 25	3 17 22
3 8 28	7 17 24	18 22 32	2 30 35	9 19 34	5 15 25
15 22 35	18 19 28	5 8 30	9 17 25	3 24 32	2 7 34
5 18 34	3 25 35	2 17 19	8 15 24	7 22 30	9 28 32
17 30 32	5 9 22	24 25 34	3 7 18	2 15 28	8 19 35

Now consider the superposition X_6 of A and B. The symbols of X_6 have been chosen to highlight the fact that it is the superposition of six Latin squares, call them $L_1, \ldots, L_6$, with respective symbol sets

$$\{1,2,3,4,5,6\}, \{7,8,9,10,11,12\}, \ldots, \{31,32,33,34,35,36\}.$$

Note that a semi-Latin square S is a superposition of Latin squares if and only if its dual S^* is resolvable. (This can be checked and resolutions can be determined using the DESIGN package.) Moreover, any two blocks of X_6, not in the same row or column, meet in 1 or 2 symbols. We have also determined that the group of all (semi-Latin square) automorphisms of X_6 has order 144, and that this group acts transitively on both the union and the Cartesian product of the rows and columns of X_6.

The canonical efficiency factors of X_6 are 3/4 with multiplicity 16, 8/9 with multiplicity 9, and 1 with multiplicity 10. As shown in Table 2, even if there were five MOLS of order six, then each of the A-, D- and E-efficiency measures for X_6 would be larger than the corresponding measures for a pseudo-Trojan $(6 \times 6)/6$ semi-Latin square. Note also that X_6 cannot be a subsquare of a uniform $(6 \times 6)/10$ semi-Latin square, for otherwise, the E-efficiency measure of X_6 would be 2/3.

Now let X_k be the semi-Latin square formed by the superposition of $L_1, \ldots, L_k$. For $k = 2, \ldots, 6$, Table 2 records approximations to the A- and D-measures, as well as the E-measure, of X_k. For $k = 2, 3, 4, 5$, the table also records (approximations to) the relative efficiency measures of X_k compared to a hypothetical optimal superposition $P(6,k)$ of k MOLS of order 6 (were k MOLS of order 6 to exist), as well as the relative efficiency measures of X_6 compared to a hypothetical $(6 \times 6)/6$ pseudo-Trojan semi-Latin square $P(6,6)$ (were five MOLS of order 6 to exist). The approximations were determined in GAP by rounding exactly determined values in the case of A-efficiency measures, and rounding numerical approximations of $(6k-1)$-th roots of exactly determined values in the case of D-efficiency measures.

Now X_2 and X_3 are not quite as efficient as certain SOMAs of the same respective sizes, but X_4, X_5 and X_6 are new and efficient. Indeed, we conjecture that X_5 and X_6 are A-, D- and E-optimal.

7. Conclusion

This paper developed theoretical and computational methods to determine optimal and efficient semi-Latin squares. The main theoretical advance was the study of efficiency

k	A_{X_k}	D_{X_k}	E_{X_k}	$A_{X_k}/A_{P(6,k)}$	$D_{X_k}/D_{P(6,k)}$	$E_{X_k}/E_{P(6,k)}$
2	.511628	.526849	1/3	.976744	.989350	2/3
3	.674492	.689909	1/2	.972062	.986658	3/4
4	.761394	.771929	5/8	.982088	.991334	5/6
5	.811126	.819262	7/10	.985938	.993038	7/8
6	.844221	.850612	3/4	1.00101	1.00031	9/8

Table 2: Efficiency measures of X_k.

properties of subsquares of uniform semi-Latin squares. The main computational methods were a group-theoretic framework for the enumeration of semi-Latin squares via their duals, and the use of exact algebraic computing in the comparison of efficiency measures. Both methods are implemented in the author's DESIGN package, and the latter method in particular has applications beyond semi-Latin squares.

All $(4 \times 4)/k$ semi-Latin squares were enumerated for $k = 2, \ldots, 10$, and those that are A-, D- and E-optimal were determined. We constructed efficient $(6 \times 6)/k$ semi-Latin squares for $k = 4, 5, 6$, the example with $k = 6$ being particularly noteworthy. We also applied our methods to find counterexamples to a long-standing conjecture of R.A. Bailey and to a similar conjecture of D. Bedford and R.M. Whitaker.

At present, efficient $(n \times n)/k$ semi-Latin squares are known when there are k MOLS of order n, when n is a prime-power, when $n = 6$ and $k \leq 10$, when $n = 6$ and $k = 5\mu$ for some integer $\mu \geq 2$, and when there is a doubly transitive permutation group of degree n and order nk. As far as $n = 10$ goes, there are two MOLS of order 10 (whose superposition forms an A-, D- and E-optimal semi-Latin square), but it is a major unsolved problem as to whether there are three MOLS of this order. Soicher (1999) constructed the first SOMA(3, 10)s, and at present, the SOMA(3, 10) with the best known A-efficiency measure is that in Figure 4 of (Soicher, 1999). The first SOMA(4, 10) is displayed on the webpage (Soicher, 2012), and the construction of an efficient $(10 \times 10)/6$ semi-Latin square is given as an example in (Soicher, to appear).

Appendix A. Enumerating semi-Latin squares via their duals

The author's DESIGN package (Soicher, 2011) is a refereed and officially accepted GAP (The GAP Group, 2012) package which provides functionality for constructing, enumerating, partitioning and studying block designs. The most important DESIGN package function is `BlockDesigns`, which can construct and enumerate block designs satisfying a wide range of user-specified properties. More generally, `BlockDesigns` can enumerate subdesigns of a given block design Δ, such that the subdesigns each have the same user-specified properties, such as each being a binary equireplicate block design with the same given parameters. (Here a *subdesign* of Δ means a block design with the same treatment set as Δ and whose block multiset is a submultiset of the blocks of Δ.) The subdesigns are enumerated up to the action of a given subgroup G of the automorphism group of Δ, and it can be required that each subdesign be invariant under a given subgroup H of G.

In this appendix we show how to transform certain enumeration problems for semi-Latin squares into enumeration problems for block designs (see also Bailey and Chigbu

(1997)), in a way which allows the application of the function `BlockDesigns` in the DESIGN package to perform the required enumerations. Explicit GAP code implementing this approach can be found in (Soicher, to appear).

Let S_n denote the group of all permutations of $\{1,\dots,n\}$, let $n>1$, and let

$$W_n := \langle S_n \times S_n, \tau \mid \tau^2 = 1, \tau(a,b)\tau = (b,a) \text{ for all } a,b \in S_n\rangle.$$

Then W_n (which is isomorphic to the wreath product of S_n with the cyclic group of order 2) acts on the set of duals of $(n\times n)/k$ semi-Latin squares as follows. Let $S^* = (V,\mathcal{B})$ be such a dual, with treatment set $V := \{1,\dots,n\}^2$ and block multiset $\mathcal{B}$, and let $g \in W_n$. (We consider a multiset to be a list, where order does not matter.) Then $g = (a,b)$ or $g = (a,b)\tau$ for some $a,b \in S_n$. For $(i,j)\in V$, define $(i,j)^{(a,b)} := (i^a, j^b)$ and $(i,j)^{(a,b)\tau} := (j^b, i^a)$. In this way, W_n acts on V. We find the g-image $\mathcal{B}^g$ of the block multiset $\mathcal{B}$ of S^* by applying g to each treatment in each block in $\mathcal{B}$. It is not difficult to see that $(S^*)^g := (V,\mathcal{B}^g)$ is the dual of a semi-Latin square T isomorphic to S. Indeed, if $g=(a,b)$ then T is obtained from S by permuting its rows by a and its columns by b, and if $g=(a,b)\tau$ then T is obtained from S by permuting its rows by a, its columns by b, and then transposing. Conversely, suppose S and T are isomorphic $(n\times n)/k$ semi-Latin squares, with respective duals S^* and T^*. Then T can be obtained from S by applying some row permutation a, some column permutation b, followed possibly by transposing and/or renaming symbols. Then $(S^*)^{(a,b)} = T^*$ if transposing does not take place, and otherwise $(S^*)^{(a,b)\tau} = T^*$. To summarize, we have proved the following:

Theorem 3. *The orbits of W_n acting on the duals of $(n\times n)/k$ semi-Latin squares are in one-to-one correspondence with the isomorphism classes of $(n\times n)/k$ semi-Latin squares.*

We now define a W_n-invariant block design $U_{n,k} = (V,\mathcal{B}_{n,k})$, which contains the dual of every $(n\times n)/k$ semi-Latin square. As before, $V=\{1,\dots,n\}^2$. The block multiset $\mathcal{B}_{n,k}$ consists of all the subsets of V of the form

$$\{(1,1^\pi),(2,2^\pi),\dots,(n,n^\pi)\},$$

with $\pi\in S_n$, and with each such block having multiplicity k (giving a total of $kn!$ blocks). Now if $D=(V,\mathcal{B})$ is the dual of an $(n\times n)/k$ semi-Latin square, then D is an (n^2,nk,k,n)-design and D is a subdesign of $U_{n,k}$ (i.e. D and $U_{n,k}$ have the same treatment set and $\mathcal{B}$ is a submultiset of $\mathcal{B}_{n,k}$). The converse clearly holds: if D is an (n^2,nk,k,n)-subdesign of $U_{n,k}$ then D is the dual of some $(n\times n)/k$ semi-Latin square.

We have thus proved the following:

Theorem 4. *The isomorphism classes of the $(n\times n)/k$ semi-Latin squares are in one-to-one correspondence with the W_n-orbits of (n^2,nk,k,n)-subdesigns of $U_{n,k}$. Representatives of these orbits give the duals of isomorphism class representatives of the $(n\times n)/k$ semi-Latin squares.*

We may thus enumerate (the duals of) the $(n\times n)/k$ semi-Latin squares by using the function `BlockDesigns` to enumerate the (n^2,nk,k,n)-subdesigns of $U_{n,k}$, up to the action of W_n. However, there appear to be far too many semi-Latin squares for a complete enumeration when $n>4$ and $k>1$, so additional constraints must be specified, such as all the required duals being invariant under a given non-trivial subgroup of W_n.

Adaptations of Theorem 4 allow for enumerations (using the function `BlockDesigns`) of semi-Latin squares satisfying certain W_n-invariant properties. For example:

Corollary 5. *The isomorphism classes of the SOMA(k,n)s are in one-to-one correspondence with the W_n-orbits of the binary equireplicate subdesigns of $U_{n,1}$ having parameters (n^2, nk, k, n) and the property that each pair of distinct blocks meet in at most one treatment. Representatives of these orbits give the duals of isomorphism class representatives of the SOMA(k,n)s.*

Corollary 6. *Suppose $n-1$ divides k and let $\mu := k/(n-1)$. The isomorphism classes of the uniform $(n \times n)/k$ semi-Latin squares are in one-to-one correspondence with the W_n-orbits of the subdesigns of $U_{n,\mu}$ with the property that any two treatments having no co-ordinate in common occur together in exactly μ blocks. Representatives of these orbits give the duals of isomorphism class representatives of the uniform $(n \times n)/k$ semi-Latin squares.*

For example, we find that, up to isomorphism, there are just 277 uniform $(5 \times 5)/12$ semi-Latin squares. In (Soicher, to appear), we give explicit GAP code used to enumerate the 98 uniform $(6 \times 6)/10$ semi-Latin squares with the property that no two distinct symbols occur together in more than two blocks.

Some call the isomorphism of semi-Latin squares defined in this paper "weak isomorphism", with "strong isomorphism" not allowing the operation of transposing to be used (see Bailey and Chigbu (1997)). More precisely, two $(n \times n)/k$ semi-Latin squares are *strongly isomorphic* if one can be obtained from the other by applying one or more of: a row permutation, a column permutation, and renaming symbols. This notion of isomorphism can be accommodated simply by replacing W_n by its subgroup $S_n \times S_n$.

Some straightforward applications of the methods of this appendix are implemented in the DESIGN package function `SemiLatinSquareDuals`, which calls the function `BlockDesigns` appropriately. For example, the function call `SemiLatinSquareDuals(4,5)` returns a list of the duals of the elements of a set of isomorphism class representatives of the $(4 \times 4)/5$ semi-Latin squares, and the function call `SemiLatinSquareDuals(6,3,"default",[0,1])` returns a list of the duals of the elements of a set of isomorphism class representatives of the SOMA$(3,6)$s. Further information can be obtained from the DESIGN package documentation.

Appendix B. Exact algebraic computation for comparing efficiency measures

In this appendix we outline the exact computational techniques implemented in the DESIGN package function `BlockDesignEfficiency`, and which are used in this paper for comparing the A-, D- and E-efficiency measures of binary equireplicate designs.

Let Δ be a (v, b, r, k)-design that we wish to compare with other such designs. We first compute the scaled information matrix $F := F(\Delta)$ and its characteristic polynomial $\chi_F(x)$. (It appears that GAP is efficient at calculating characteristic polynomials with many low-degree factors, such as we often encounter in our current situation.) Let

$$e_\Delta(x) := \chi_F(x)/x = x^{v-1} + e_{v-2}x^{v-2} + \cdots + e_1 x + e_0,$$

so that the zeros of $e_\Delta(x)$ (counting repeats) are the canonical efficiency factors $\delta_1 \leq \cdots \leq \delta_{v-1}$ of Δ. We have $e_0 \neq 0$ if and only if Δ is connected, which we now assume is the case. Moreover,

$$(-1)^{v-1}e_0 = \prod_{i=1}^{v-1} \delta_i = (\mathrm{D}_\Delta)^{v-1},$$

and we can compare D-measures by comparing their $(v-1)$-th powers. Now the polynomial

$$e_0^{-1}(e_0x^{v-1} + e_1x^{v-2} + \cdots + e_{v-2}x + 1)$$

is monic and its zeros are $1/\delta_1, \ldots, 1/\delta_{v-1}$, so $-e_1/e_0 = \sum_{i=1}^{v-1} 1/\delta_i$, and so

$$\mathrm{A}_\Delta = -(v-1)e_0/e_1.$$

We now outline how we determine E_Δ exactly if it is rational, and otherwise, how we determine an interval $[a, b]$ containing E_Δ, such that a and b are rational and the length of $[a, b]$ is at most a given $\epsilon > 0$. All computations take place over the rational numbers and are performed exactly in GAP.

Let $e(x) := e_\Delta(x)$, let $e'(x)$ denote the derivative of $e(x)$, and let

$$f(x) := e(x)/\gcd(e(x), e'(x)).$$

Then $f(x)$ has the same zeros as $e_\Delta(x)$, but each with multiplicity 1. We then determine the set R of rational zeros of $f(x)$ and set

$$g(x) := f(x)/\prod_{r\in R}(x-r).$$

If R is non-empty we apply a Sturm sequence (see Childs (1995, p.280–285)) to determine the number of (real) zeros of $g(x)$ in $[0, \min(R)]$. If there are none, then we have that $\mathrm{E}_\Delta = \min(R)$, and otherwise, we apply bisection and Sturm sequences repeatedly, starting with the interval $[0, \min(R)]$, to find the required interval $[a, b]$ containing E_Δ. If R is empty then we again apply bisection and Sturm sequences repeatedly, this time starting with the interval $[0, 1]$. The bisection process works as follows, given an initial interval $[c, d]$, with c, d rational, $d - c > 0$, and $g(c) \neq 0 \neq g(d)$. If $d - c \leq \epsilon$ we stop, with $a := c$ and $b := d$. Otherwise, we calculate a Sturm sequence to find the number of zeros of $g(x)$ in $[c, (c + d)/2]$. If this number is not zero, we continue the process with the interval $[c, (c + d)/2]$; otherwise, we continue with the interval $[(c + d)/2, d]$.

Since Δ is a binary equireplicate design, the canonical efficiency factors of Δ not equal to 1, and their multiplicities, are the same as those of the dual block design Δ^* of Δ (see Bailey and Cameron (2009, Section 3.1.1)). Thus, if v exceeds the number b of blocks of the connected design Δ, and $b > 1$, we may reduce the size of the calculations above by applying them to Δ^*. We then have $\mathrm{A}_\Delta = (v-1)/((b-1)/\mathrm{A}_{\Delta^*} + v - b), (\mathrm{D}_\Delta)^{v-1} = (\mathrm{D}_{\Delta^*})^{b-1}, \mathrm{E}_\Delta = \mathrm{E}_{\Delta^*}$.

There are of course other measures of efficiency for binary equireplicate designs than the A-, D- and E-measures. One such measure, which is rational and can be computed exactly by the function `BlockDesignEfficiency` is the MV-measure (see Bailey and Royle (1997); Soicher (2011)).

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