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Projections of Definitive Screening Designs by Dropping Columns: Selection and Evaluation

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Abstract

Definitive screening designs are increasingly used for studying the impact of many quantitative factors on one or more responses in relatively few experimental runs. In practical applications, researchers often require a design for m quantitative factors, construct a definitive screening design for more than m factors and drop the superfluous columns. This is done when the number of runs in the standard *m*-factor definitive screening design is considered too limited or when no standard definitive screening design exists for m factors. In these cases, it is common practice to arbitrarily drop the last column of the larger definitive screening design. In this paper, we show that certain statistical properties of the resulting experimental design depend on which columns are dropped and that other properties are insensitive to the exact columns dropped. We perform a complete search for the best sets of 1–8 columns to drop from standard definitive screening designs with up to 24 factors. We observed the largest differences in statistical properties when dropping four columns from 8- and 10-factor definitive screening designs. In other cases, the differences are moderate or small, or even nonexistent. Our search for optimal columns to drop necessitated a detailed study of the properties of definitive screening designs. This allows us to present some new analytical and numerical results concerning definitive screening designs.

Key words and phrases: Conference Matrix; D-efficiency; Isomorphism; Projection; Second-Order Model; Two-Factor Interaction.

1 Introduction

Screening designs permit the experimental study of many factors in a small number of runs. For a long time, the literature on screening designs concentrated on orthogonal two-level designs (Mee, 2009). In each run of a two-level screening design, each of the factors is either set at a low or at a high level. After completing all experimental runs, the responses of interest are modeled as functions of the experimental factors by statistical methods such as stepwise regression or the Dantzig selector; see Mee et al. (2017) for a recent review on two-level screening designs.

Practitioners studying quantitative factors may not feel comfortable with screening designs that restrict attention to two levels per factor. They could argue that screening also requires checking whether a factor's main effect is linear or not, and identifying active two-factor interactions. To meet these concerns, Jones and Nachtsheim (2011) developed three-level designs using a number of runs that is only one more than twice the number of factors studied. The designs are now called definitive screening designs (DSDs).

The original DSDs presented by Jones and Nachtsheim (2011) were based on a heuristic optimal design algorithm. For an odd number of factors and also for some even numbers of factors, the original DSDs were not orthogonal. Xiao et al. (2012) proposed constructing DSDs using conference matrices. A major advantage of their construction is that it guarantees that the resulting DSDs are orthogonal. A drawback is that, for certain numbers of factors, the number of runs of the resulting DSDs is larger than two times the number of factors plus one. In this paper, we refer to an *n*-factor DSD constructed from an *n*-dimensional conference matrix as a standard DSD or sDSD.

As an illustration, Table 1 shows how a 10-factor sDSD is constructed from a 10×10 conference matrix **C**. The first ten runs in the table show the original conference matrix. In general, a conference matrix **C** is an *n*-dimensional square matrix of -1s, 0s and 1s for which $\mathbf{C}^T \mathbf{C} = (n-1)\mathbf{I}_n$, where \mathbf{I}_n is the $n \times n$ identity matrix. Consequently, the columns of a conference matrix are orthogonal. This implies that a conference matrix is an ideal building block for an orthogonal experimental design. For the design in Table 1, it is easy to verify that $\mathbf{C}^T \mathbf{C} = 9\mathbf{I}_{10}$.

The second set of ten runs of the 10-factor sDSD in Table 1 contains the mirror images or the negatives of the first 10 runs. The sDSD's final run is a center run in which all factors are set at their middle level. Xiao et al. (2012) point out that their construction guarantees that the linear main effects (LEs) are orthogonal to all second-order effects (i.e., the quadratic main effects (QEs) and the two-factor interaction effects (2FIs)), and that the second-order effects are never completely aliased.

Conference matrices do not exist when n is odd, and when n is 22, 34, or 58 (Colbourn and Dinitz, 2006). For this reason, it is impossible to construct sDSDs for which the run size is as small as two times the number of factors plus one when the number of factors is odd, or when it is 22, 34, or 58. To deal with this problem, Xiao et al. (2012) recommend dropping columns from a sDSD with one, two or three columns more than the required number. Dougherty et al. (2015) followed this recommendation and generated a 9-factor design with 21 runs by dropping one column from the 10-factor sDSD in Table 1. Fidaleo et al. (2016) used the 9-factor DSD to investigate the electrochemical decolorization of the azo dye RV5, a compound used for textile dyeing.

Dropping k columns from a sDSD with n = m + k columns can result in an m-factor design

Part	Run	X_1	X_2	X_3	X_4	X_5	X_6	X_7	X_8	X_9	X_{10}
\mathbf{C}	1	0	1	1	1	1	1	1	1	1	1
	2	1	0	-1	-1	-1	-1	1	1	1	1
	3	1	-1	0	-1	1	1	-1	-1	1	1
	4	1	-1	-1	0	1	1	1	1	-1	-1
	5	1	-1	1	1	0	-1	-1	1	-1	1
	6	1	-1	1	1	-1	0	1	-1	1	-1
	7	1	1	-1	1	-1	1	0	-1	-1	1
	8	1	1	-1	1	1	-1	-1	0	1	-1
	9	1	1	1	-1	-1	1	-1	1	0	-1
	10	1	1	1	-1	1	-1	1	-1	-1	0
$-\mathbf{C}$	-10	-1	-1	-1	1	-1	1	-1	1	1	0
	-9	-1	-1	-1	1	1	-1	1	-1	0	1
	-8	-1	-1	1	-1	-1	1	1	0	-1	1
	-7	-1	-1	1	-1	1	-1	0	1	1	-1
	-6	-1	1	-1	-1	1	0	-1	1	-1	1
	-5	-1	1	-1	-1	0	1	1	-1	1	-1
	-4	-1	1	1	0	-1	-1	-1	-1	1	1
	-3	-1	1	0	1	-1	-1	1	1	-1	-1
	-2	-1	0	1	1	1	1	-1	-1	-1	-1
	-1	0	-1	-1	-1	-1	-1	-1	-1	-1	-1
0	11	0	0	0	0	0	0	0	0	0	0

Table 1: Standard definitive screening design (sDSD) with 10 factors, constructed by folding over a 10×10 conference matrix **C**.

with better aliasing properties than a sDSD with m columns. For instance, when comparing different cost-efficient screening designs, Stone et al. (2014) preferred a 6-factor design with 17 runs constructed by dropping two columns from the 8-factor sDSD to a 6-factor 13-run sDSD, due to the relatively high aliasing between pairs of 2FIs and between a QE and a 2FI in the 13-run design. Patil (2017) studied the impact of seven factors on a welding process where some 2FIs were expected to be active, and observed that the 7-factor design formed by dropping one column from the 8-factor sDSD exhibited a substantial amount of aliasing among the interactions. To reduce the aliasing, he dropped three columns from the 10-factor sDSD in Table 1, and thus used a 21-run design instead of a 17-run design. In this paper, we refer to a DSD obtained by dropping one or more columns from a sDSD as a projected DSD or pDSD.

At present, no guidelines exist concerning which subsets of k columns to drop from a sDSD with n = m + k columns. In each of the applications mentioned above, the authors arbitrarily dropped the last k columns. This is also what commercial software packages do. However, the following example shows that this procedure may be suboptimal. Suppose there is a budget of 21 runs for a study of six factors. A sensible design strategy would then be to use six of the ten columns of the 10-factor sDSD in Table 1. Dropping the last four columns of the 10-factor sDSD results in a design where nine pairs of 2FI contrast vectors possess a correlation of ± 0.75 .

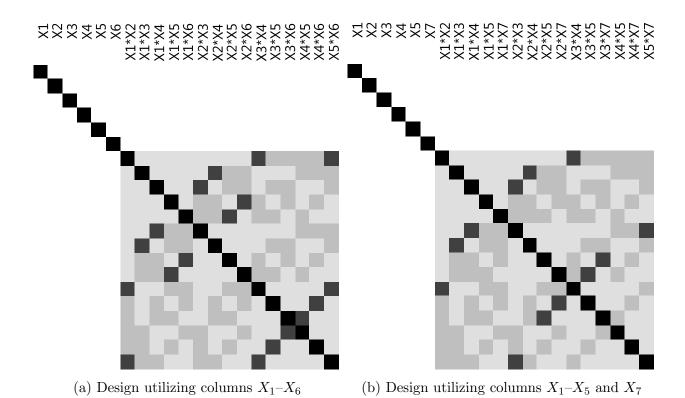


Figure 1: Color maps showing absolute correlations between LEs' and 2FIs' contrast vectors for two 6-factor pDSDs obtained from the 10-factor sDSD in Table 1.

Moreover, the sum of all squared correlations between pairs of 2FI contrast vectors equals 8.25. Dropping the columns X_6 , X_8 , X_9 and X_{10} instead of the last four columns results in a design in which only six pairs of 2FI contrast vectors have a correlation of ± 0.75 and the sum of squared correlations between pairs of 2FI contrast vectors is only 6.75. So, the aliasing between the two-factor interactions is more severe when dropping the last four columns of the design in Table 1 than when dropping columns X_6 , X_8 , X_9 and X_{10} .

The superiority of the second design option can be seen from the color maps in Figure 1, which visualize the absolute correlations between all pairs of contrast vectors corresponding to LEs and 2FIs. In the color maps, the largest absolute correlations for interactions are visualized by the darkest off-diagonal cells. In Figure 1a, there are 18 of these dark off-diagonal cells (corresponding to nine pairs of interactions), while there are only 12 in Figure 1b (corresponding to six pairs).

The difference in the number of occurrences of the maximum absolute correlations between the two design options may have major consequences for any data analysis using the two designs. To illustrate this, Table 2 compares the standard errors and the powers for the 2FIs corresponding to the last four factors (which we label C_3 , C_4 , C_5 and C_6) in the two pDSDs, assuming a model with all six LEs and the six 2FIs among the designs' last four factors. The standard errors for the pDSD using columns 1–5 and 7 of the sDSD are substantially smaller than those for the pDSD using columns 1–6. Consequently, the powers for detecting multiple significant interactions are substantially higher for that pDSD.

The purpose of this paper is to identify the best sets of k columns to drop from sDSDs.

Interaction	Columns	$X_1 - X_6$	Columns λ	$X_1 - X_5 \& X_7$
	st. error	power	st. error	power
C_3C_4	0.379	0.639	0.282	0.872
C_3C_5	0.379	0.639	0.282	0.872
C_3C_6	0.379	0.639	0.270	0.899
C_4C_5	0.379	0.639	0.270	0.899
C_4C_6	0.379	0.639	0.282	0.872
C_5C_6	0.379	0.639	0.282	0.872

Table 2: Standard errors relative to the standard deviation σ of the observations, and powers for 2FIs of size σ among the last four factors in two 6-factor pDSDs obtained from the 10-factor sDSD in Table 1.

This required us to define criteria that distinguish the designs obtained by dropping columns. It turned out that several traditional statistical criteria are insensitive to the sets of columns dropped. Therefore, in Section 2, we start by discussing statistical properties that are invariant to the sets of columns dropped. For these properties, we also present analytical expressions, which are new to the literature. In Section 3, we define three different criteria that do depend on the sets of columns dropped. These criteria are all based on correlations between 2FIs contrast vectors. In Section 4, we report the results of a complete search for the best sets of 1, 2, 3 or 4 columns to drop from sDSDs for up to 24 factors. In Section 5, we compare m-factor sDSDs to m-factor pDSDs with larger run sizes, obtained by dropping different numbers of columns from sDSDs with more than m factors. Finally, in Section 6, we conclude with a discussion and some suggestions for future research.

2 Properties that do not depend on the columns dropped

It turns out that several practically relevant properties of pDSDs do not depend on the exact set of columns dropped from a sDSD. In this section, we give an overview of all these criteria, because it provides us with a clearer picture of the properties of DSDs. We start by discussing DSDs' properties when estimating linear and quadratic main effects. Next, we discuss the projection properties of DSDs, and, finally, we study correlations between pairs of contrast vectors corresponding to 2FIs and QEs and involving at most three factors. For each of the criteria, we present analytical expressions. For the derivation of the analytical expressions, we refer to Appendix A.

2.1 Models with linear main effects only

The D-efficiencies for models with m LEs and the standard errors for the LE estimates in the models do not depend on the set of k columns dropped from a sDSD with n = m + k factors, because (i) the LEs' contrast vectors in a sDSD are orthogonal to each other and to the column of ones in the model matrix (corresponding to the intercept) and (ii) the precision is the same for each LE estimate. The D-efficiency of an m-factor pDSD with 2(m + k) + 1 runs for the

model including the intercept and all m LEs, relative to an m-factor sDSD with 2m + 1 runs, can be expressed as

$$D_{\rm le} = \left(1 + \frac{2k}{2m+1}\right)^{\frac{1}{m+1}} \left(1 + \frac{k}{m-1}\right)^{\frac{m}{m+1}}.$$
 (1)

The standard error for any LE estimate obtained from a (2(m + k) + 1)-run pDSD relative to the standard error produced by a (2m + 1)-run sDSD equals

$$SE_{le} = \sqrt{\frac{m-1}{m+k-1}}.$$
(2)

It is easy to see from Equations (1) and (2) that the relative D-efficiency increases and the relative standard error for a LE estimate decreases with the number k. In other words, the relative D-efficiency increases and the relative standard error for a LE estimate decreases with the run size of the sDSD used to construct the pDSD.

2.2 Models with linear and quadratic main effects

Just as the D-efficiency for a model with LEs only, the D-efficiency of a pDSD for a model with LEs and QEs is insensitive to the set of k columns dropped from an (m + k)-factor sDSD. The D-efficiency of a (2(m + k) + 1)-run pDSD relative to that of a (2m + 1)-run sDSD is

$$D_{\rm le+qe} = \left(1 + \frac{k}{m-1}\right)^{\frac{m}{2m+1}} \left(1 + \frac{k(m+2)}{(m-1)^2}\right)^{\frac{1}{2m+1}} \tag{3}$$

for a model including all m LEs and all m QEs. Clearly, this relative efficiency also increases with k and thus with the run size of the pDSD constructed. When estimating the model including all m LEs and all m QEs, the standard error of any QE estimate obtained from a (2(m + k) + 1)-run pDSD relative to the one produced by a (2m + 1)-run sDSD is

$$SE_{qe} = \frac{m-1}{\sqrt{(m-1)^2 + k(m+2)}} \sqrt{1 + \frac{k(m+1)}{m^2 - 3m + 5}}.$$
(4)

For any given number of factors m, this relative standard error decreases with k and thus with the run size of the pDSD. The relative standard error approaches

$$(m-1)\sqrt{(m+1)/[(m^2-3m+5)(m+2)]}$$

for large values of k. The relative standard errors for the LE estimates are not affected by the inclusion of QEs in the model. Therefore, they can still be calculated using Equation (2). This is because the LEs' contrast vectors are orthogonal to those of the QEs whenever a sDSD or a pDSD is used.

2.3 Powers for significance tests

Departing from a model including only the intercept or from a model containing the intercept and all LEs, we can conduct t tests for individual LEs, QEs and 2FIs. Four pertinent tests are

Table 3: Degrees of freedom ν and non-centrality parameters λ for various significance tests using a pDSD, assuming a signal-to-noise ratio of 1 for the effect tested. Setting k = 0 produces the results for a sDSD.

Label	Hypothesis	Model terms	ν	λ
L_1	$\beta_i = 0$	Intercept only	2(m+k) - 1	$\sqrt{2(m+k)-2}$
L_m	$\beta_i = 0$	Intercept + all LEs	2k+m	$\sqrt{2(m+k)-2}$
Q_m	$\beta_{ii} = 0$	Intercept + all LEs	2k + m - 1	$\sqrt{\frac{6(m+k-1)}{2(m+k)+1}}$
I_m	$\beta_{ij} = 0$	Intercept + all LEs	2k + m - 1	$\sqrt{2(m+k)-4}$

shown in Table 3. The first two columns in the table identify the hypothesis to be tested, while the third column shows the terms that appear in the model besides the effect to be tested. The fourth column shows the degrees of freedom ν for the t statistic. Finally, the last column is the non-centrality parameter λ of the non-central t-distribution needed to calculate the power of the test. In the table's second column, β_i , β_{ii} and β_{ij} represent the linear main effect of factor i, the quadratic main effect of factor i and the interaction between the factors i and j (where $i \neq j$), respectively.

The first test, labeled L_1 , is useful for testing whether adding a LE to a model containing only the intercept has added value. Since, in general, a pDSD involves N = 2(m + k) + 1runs and the model under study includes two parameters, the degrees of freedom for the t test equal N - 2 = 2(m + k) - 1. The second test in Table 3, labeled L_m , is useful in a scenario where the experimenter first fits a model including all m LEs and then tests whether one LE can be removed. Because models including the intercept and all m LEs require the estimation of m + 1 parameters, the degrees of freedom for the t test equal N - (m + 1) = 2k + m. The third and fourth test, labeled Q_m and I_m , are relevant in situations where the experimenter first fits a model including the intercept and all m LEs, and then tests whether adding a single QE or a single 2FI improves the model significantly. In both cases, the model under investigation involves m + 2 parameters, so that the residual degrees of freedom for the t tests equal N - (m + 2) = 2k + m - 1 in each case.

All non-centrality parameters λ listed in Table 3 are increasing functions of k. Therefore, they increase with the number of runs of the pDSD. As a result, the powers for the four significance tests will also increase with k and with the number of runs. The powers for the four significance tests can all be calculated as

$$1 - \operatorname{Prob}(-\mathbf{t}_{\nu,\alpha/2} < T_{\nu,\lambda} < \mathbf{t}_{\nu,\alpha/2}),$$

where $T_{\nu,\lambda}$ is a random variable following a non-central *t*-distribution with ν degrees of freedom and non-centrality parameter λ , and $-t_{\nu,\alpha/2}$ and $t_{\nu,\alpha/2}$ are the critical values based on a central *t*-distribution with ν degrees of freedom for a significance level equal to α . The non-centrality parameters and the resulting powers are independent of the sets of *k* columns dropped from an (m + k)-factor sDSD, and from the values of *i* and *j* in the effects tested (i.e., β_i , β_{ii} and β_{ij}). The λ values in Table 3 assume that the absolute values of β_i , β_{ii} and β_{ij} equal the standard deviation of the responses, σ . In other words, the non-centrality parameters we report correspond to signal-to-noise ratios of 1. To calculate the power for β_i , β_{ii} and β_{ij} values equal to $\delta\sigma$, the non-centrality parameter λ has to be multiplied by δ .

2.4 Correlations between specific second-order effects' contrast vectors

Regardless of which k columns are dropped from an (m + k)-factor sDSD, the correlation between the contrast vectors of any two quadratic effects β_{ii} and β_{jj} equals

$$r_{ii,jj} = \frac{1}{3} - \frac{2}{N-3},$$

where N = 2(m + k) + 1 is the run size of the design. This correlation increases with the run size and approaches 1/3 for large values of N or k. So, the QEs' contrast vectors of m-factor pDSDs exhibit larger correlations when they are based on larger sDSDs and involve more runs.

The correlation between the contrast vector of any quadratic effect β_{ii} and the contrast vector of an interaction effect β_{ij} is always zero. The correlation between the contrast vector of a quadratic effect β_{ii} and the contrast vector of an interaction effect β_{jk} is non-zero, and equals

$$r_{ii,jk} = \pm \sqrt{\frac{4N}{3(N-3)(N-5)}}.$$
(5)

If m + k is a multiple of 4, the three correlations $r_{ii,jk}$, $r_{jj,ik}$ and $r_{kk,ij}$ corresponding to any triplet of factors i, j and k are all positive, or one correlation is positive, while the other two are negative. If m + k is not a multiple of 4, two of the three correlations are positive and one is negative, or all three correlations $r_{ii,jk}$, $r_{jj,ik}$ and $r_{kk,ij}$ are negative (Schoen et al., 2017). The correlations tend to zero as the run size N or k increases. So, when using an m-factor pDSD, the correlations between the contrast vectors for the quadratic effect of one factor and the interaction between two other factors are closer to zero than when using an m-factor sDSD. In other words, the aliasing is smaller.

Finally, the correlation between the contrast vector of an interaction effect β_{ij} and the contrast vector of another interaction effect β_{ik} , involving the same factor *i*, is non-zero too, and equals

$$r_{ij,ik} = \pm \frac{2}{N-5}.$$
(6)

The correlations $r_{ij,ik}$, $r_{ji,jk}$ and $r_{ki,kj}$ exhibit the same patterns as the correlations $r_{ii,jk}$, $r_{jj,ik}$ and $r_{kk,ij}$. They also decrease with the run size. So, they are closer to zero for an *m*-factor pDSD than for an *m*-factor sDSD, which means that a pDSD reduces the aliasing between two interaction effects β_{ij} and β_{ik} .

2.5 **Projections into two or three factors**

An assumption usually adopted in a factor screening context is factor sparsity. According to this assumption, only a small subset of the factors under investigation are active. An important

Table 4: Degrees of freedom ν and non-centrality parameters λ for various significance tests when using a pDSD for fitting a full second-order response surface model in two or three factors, assuming a signal-to-noise ratio of 1. Setting k = 0 or n = m shows the results for a sDSD.

Label	Hypothesis	ν	λ	Comment
Q_2	$\beta_{ii} = 0$	2(m+k) - 5	$\sqrt{\frac{2(4m-7)}{3(m+k-1)}}$	Any $n = m + k$
I_2	$\beta_{ij} = 0$	2(m+k) - 5	$\sqrt{2(m+k)-4}$	Any $n = m + k$
Q_3	$\beta_{ii} = 0$	2(m+k) - 9	$\sqrt{\frac{2(5n^3-33n^2+51n+4)}{4n^3-21n^2+24n+2}}$	n = m + k is a multiple of 4
			$\sqrt{\frac{2(5n^3-43n^2+109n-86)}{4n^3-29n^2+54n-26}}$	Otherwise
I_3	$\beta_{ij} = 0$	2(m+k) - 9	$\sqrt{\frac{2(5n^3-33n^2+51n+4)}{5n^2-19n+14}}$	n = m + k is a multiple of 4
			$\sqrt{\frac{2(5n^3-43n^2+109n-86)}{5n^2-29n+36}}$	Otherwise

feature of a DSD is therefore its potential to form statistically efficient projections into a few factors. It is easy to see that, for any two factors, an (m + k)-factor sDSD projects into a face-centered central composite design, in which the four factorial points each appear (m+k)/2times, and the center point as well as the four axial points occur only once. This is also true for any *m*-factor pDSD obtained from an (m + k)-factor sDSD, independent of which *k* columns are dropped from the sDSD. As a result, all two-factor projections from a sDSD and any pDSD obtained from it are identical. All statistical properties of two-dimensional projections of sDSDs and pDSDs are therefore also identical.

It can be shown that the statistical properties of all three-factor projections of a given sDSD or pDSD are identical too. More specifically, it can be shown that all three-factor projections from a sDSD and from any pDSD derived from it are isomorphic (Schoen et al., 2017). The isomorphism implies that the D-efficiency for a second-order model in three factors is the same for each three-factor projection of a sDSD and for any pDSD derived from it. Similarly, the I-efficiency is the same for each three-factor projection of a sDSD of a sDSD or a pDSD obtained from it.

When fitting full second-order models in two or three quantitative factors, it is common to perform significance tests for the QEs and the 2FIs. Table 4 lists the four tests, the degrees of freedom ν for the tests as well as the values for the non-centrality parameter λ needed for calculating the powers of the tests. The tests labeled Q_2 and I_2 are concerned with a QE and a 2FI in a two-factor response surface model, while the tests labeled Q_3 and I_3 are concerned with a QE and a 2FI in a three-factor response surface model. In the expressions for the non-centrality parameters for the latter two tests, we replaced m + k by n to save space.

In Section 2.4, we pointed out that the correlations between pairs of QE contrast vectors are all equal, while the correlation between the contrast vector of a quadratic effect β_{ii} and that of an interaction β_{ij} is zero. For this reason, the non-centrality parameters λ and the powers for the two QEs in the two-factor response surface model are the same.

The power calculations for the hypotheses Q_3 and I_3 are more complex because the correlations between contrast vectors involving three factors can take different signs, depending on whether n = m + k is a multiple of 4 or not (recall that, due to the construction of sDSDs using conference matrices, n = m + k is always even). Due to these differences in signs, the expressions for the non-centrality parameters for the hypotheses Q_3 and I_3 also differ depending on whether n = m + k is a multiple of 4 or not.

3 Properties that do depend on the columns dropped

In the previous section, we showed that correlations between contrast vectors corresponding to (i) two LEs, (ii) two QEs, (iii) a LE and a QE, (iv) a LE and a 2FI, (v) a QE and a 2FI, and (vi) two 2FIs sharing a common factor do not depend on the set of k columns dropped from a sDSD. The only type of correlations that does depend on the set dropped involves contrast vectors of two 2FI effects β_{ij} and β_{kl} , corresponding to four different factors.

For an (m+k)-factor sDSD and any *m*-factor pDSD obtained from it by dropping *k* columns, the correlations between contrast vectors of pairs of interactions β_{ij} and β_{kl} , not involving a common factor, can take different values. More specifically, these correlations can take the values

$$r_{ij,kl} = \pm \frac{t}{m+k-2},$$

where $t \in \{0, 2, ..., m + k - 4\}$, provided m > 4. This follows from the results of Xiao et al. (2012). The maximum possible absolute correlation therefore is

$$1 - \frac{2}{m+k-2}.$$

This expression tends to 1 as k increases, but, even when k = 0, it can take a fairly large value. For instance, for the 10-factor sDSD in Table 1, the maximum correlation is 1-2/(10+0-2) = 3/4. While, according to the results of Xiao et al. (2012), absolute correlations of 0, 1/8, 1/4, 3/8, 1/2 and 5/8 are in theory also possible when m = 10, it turns out that the 10-factor sDSD only involves the correlations 1/4 and 3/4. None of the correlations are zero. So, certainly not all theoretically possible correlations will occur in any given sDSD or any pDSD derived from it. The 8-factor sDSD also only involves two different values for the absolute correlation, namely 0 and 2/3. For that sDSD, certain pairs of interactions β_{ij} and β_{kl} have uncorrelated contrast vectors, while other pairs of interactions have contrast vectors that have the maximum absolute correlation of 2/3. The 16-factor sDSD involves the correlations 0, 2/7, 4/7 and 6/7, but not the correlations 1/7, 3/7 and 5/7, for pairs of interactions β_{ij} and β_{kl} . Note that the correlation of 6/7 is the maximum one possible.

In any case, the maximum absolute correlations of 2/3, 3/4 and 6/7 for the 8-, 10- and 16factor sDSDs show that two interactions of the types β_{ij} and β_{kl} can be strongly aliased when sDSDs or pDSDs are used, especially when k is large. A consequence of this result is that a broad range of $r_{ij,kl}$ values is possible when an m-factor pDSD is obtained from a large (m+k)factor sDSD. The challenge then is to drop the k columns that result in a pDSD that avoids as many large correlations of the type $r_{ij,kl}$ as possible. It turns out that the average absolute

# factors in sDSD		# cc	lumns dropp	(k)
(m+k)	1	2	3	4
6	Any	Any	Any	Any
8	Any	Any	Any	Last four
10	Any	Any	Any	6, 8, 9, 10
12	Any	Any	Any	7, 8, 10, 12
14	Any	Any	Any	Last four
16	Any	8, 16	Last three	Last four
18	Any	Any	Any	Last four
20	Any	Any	Any	14, 17, 18, 20
24	Any	Any	Any	20, 22, 23, 24

Table 5: Recommended sets of k columns to drop from an (m + k)-factor sDSD.

correlations, the maximum absolute correlation and the sum of the squared correlations can be reduced by making a wise choice of the columns to drop.

A large number of large correlations $r_{ij,kl}$ in the pDSD ultimately selected results in poor precisions of the interactions in models with multiple interactions and in a low power for the corresponding significance tests. Also, the D- and I-efficiencies for models with multiple interactions will be quite low in the event there are many large correlations $r_{ij,kl}$.

4 Best sets of k columns to drop

We performed a complete search for the best sets of k columns to drop from an (m + k)-factor sDSD for $m + k \in \{6, 8, ..., 20, 24\}$ and $k \leq 8$. Detailed results on the best and worst sets of columns to drop are given in Table A1 in Appendix B and include (i) the average absolute correlations, (ii) the maximum absolute correlations, and (iii) the sum of all squared correlations between the contrast vectors for pairs of 2FI columns. In this section, we present an overview of our most important results, restricting attention to $k \leq 4$.

Table 5 shows the recommended sets of 1–4 columns to drop from each (m+k)-factor sDSD. Sometimes, there are multiple sets of columns that give rise to equally good pDSDs. In that case, we report the lexicographically maximal set of columns to drop, i.e., the set of columns that involves the largest indices. For all cases where the set of columns dropped does not affect the quality of the resulting design, we inserted the entry 'Any' in the table.

Table 5 shows that we can drop any single column, any pair of columns and any triplet of columns from a (m + k)-factor sDSD without affecting the 2FIs' contrast vectors' correlations (in other words, without affecting the aliasing among the 2FIs), except when starting from the 16-factor sDSD. As a result, Dougherty et al. (2015), Fidaleo et al. (2016), Patil (2017), and Stone et al. (2014) coincidentally used the best possible pDSD for their experiment. Any other choice of columns to drop would have resulted in an equivalent pDSD for their experiments.

Dropping different sets of four columns from a sDSD generally results in pDSDs with different values of the correlation criteria for 2FIs. To construct pDSDs for 4, 10, 12 and 14 factors from

8-, 14-, 16- and 18-factor sDSDs, respectively, the best option is to drop the last four columns. However, the introductory example showed that a 21-run 6-factor pDSD obtained by dropping columns 6, 8, 9 and 10 from a 10-factor sDSD is better than the one obtained by dropping the last four columns. Dropping columns 6, 8, 9 and 10 is in fact optimal. Similar results hold for dropping four columns from 12-, 20- and 24-factor sDSDs.

Table 6 shows to what extent the choice of the set of columns dropped from a sDSD affects the correlations among 2FI contrast vectors in a pDSD. More specifically, it shows the average and maximum absolute correlations for 2FI contrast vectors, as well as the sum of the squared correlations, for the best and the worst set of columns dropped from a sDSD. For each combination of number of factors and number of columns dropped, the results for the best set are shown first followed by the results for the worst sets. The table only covers the 10 cases in which the set of columns dropped matters (i.e., the cases for which Table 5 does not have the entry 'Any').

The difference between the best and the worst sets of k columns is most pronounced for the case in which four columns are dropped from the 8-factor sDSD. For that case, the best set provides a maximum absolute correlation as small as 0.167, an average absolute correlation of 0.133, and a sum of squared correlations of 0.333. In contrast, the worst set has a maximum absolute correlation of 0.667, an average absolute correlation of 0.267, and a sum of squared correlations of 1.667. As explained in the previous section, the value of 0.667 is the maximum possible value for the correlations between pairs of 2FI columns when m + k = 8.

In all other cases, the maximum correlation is not affected by the columns dropped. However, the average correlations and the sum of squared correlations are smaller when the optimal sets of columns are dropped. For m+k = 10, there is an appreciable difference in average correlation and in the sum of squared correlations. However, for $m + k \ge 12$, the best and worst sets of columns to drop show only minor differences in terms of the average absolute correlation and the sum of squared correlations. Also the standard errors and powers for models with many 2FIs are affected very little by the sets of columns dropped. In conclusion, dropping the last few columns from a sDSD is generally a good strategy, except when leaving out four columns from an eight factor or a ten-factor sDSD.

5 Comparing DSDs with different run sizes

Creating pDSDs by dropping columns from sDSDs is useful because it increases the number of runs for a given number of factors under investigation. This results in smaller standard errors and larger numbers of estimable 2FIs, for instance. We demonstrate the benefits of pDSDs by looking at power curves for 6-factor designs, namely the 6-factor sDSD and five 6-factor pDSDs obtained by dropping 2, 4, 6, 8 and 10 columns from 8-, 10-, 12-, 14- and 16-factor sDSDs, respectively. We used the analytical expressions in Tables 3 and 4 to determine the power curves.

5.1 Power for significance tests

Figure 2 shows the power curves for the four types of tests in Table 3, assuming a significance level of 0.05 and signal-to-noise ratios of 1 and 2. The horizontal axis in the power curves shows

# Factors $(m+k)$	$\begin{array}{c} \text{Set size} \\ k \end{array}$	$\begin{array}{c} \text{Run size} \\ 2(m+k) + 1 \end{array}$	Average correlation	Maximum correlation	Sum of squared correlations
8	4	17	$0.13333 \\ 0.26667$	$0.167 \\ 0.667$	$0.3333 \\ 1.6667$
10	4	21	$\begin{array}{c} 0.20714 \\ 0.22143 \end{array}$	$0.75 \\ 0.75$	6.75 8.25
12	4	25	$0.19048 \\ 0.19365$	$\begin{array}{c} 0.4 \\ 0.4 \end{array}$	23.76 24.24
14	4	29	$0.19394 \\ 0.19495$	$\begin{array}{c} 0.5 \\ 0.5 \end{array}$	58 58.6667
16	4	33	$0.12747 \\ 0.13467 \\ 0.12867$	$0.857 \\ 0.857 \\ 0.857$	115.0408 116.0204 117.2449
16	3	33	$0.13173 \\ 0.13458$	$0.857 \\ 0.857$	$\frac{166.0102}{166.0102}$
16	2	33	$0.13333 \\ 0.13585$	$0.857 \\ 0.857$	231.8571 231.8571
18	4	37	$0.18159 \\ 0.18178$	$0.375 \\ 0.375$	$201.1875 \\ 201.5625$
20	4	41	$0.17292 \\ 0.17311$	$\begin{array}{c} 0.444 \\ 0.444 \end{array}$	322.2222 322.8148
24	4	49	$0.13479 \\ 0.13485$	$0.364 \\ 0.364$	693.3471 693.7438

Table 6: Differences in average and maximum correlations among 2FI contrast vectors and in the sum of the squared correlations between the best and worst sets of k columns dropped from an (m + k)-factor sDSD.

the numbers of columns dropped from the larger sDSDs. These numbers correspond to run sizes 13, 17, 21, 25, 29 and 33. The figure shows that the powers for the four tests increase with k and thus with the run size. The powers for the QEs' significance tests are much lower than the powers for the other tests. Figure 2a shows that QEs with the same size as σ are unlikely to be detected, as the power is only about 25%. Figure 2b shows that QEs twice as large are quite likely to be detected. However, the power for the QEs twice the size of σ is still markedly lower than the powers for LEs and 2FIs of that size. The powers for active LEs and 2FIs that are twice as large as σ equal one for the 6-factor sDSD and any pDSD constructed from a larger sDSD.

Figure 2a shows that, when effects as large as the noise are of interest, the 6-factor sDSD involving 13 runs (and having k = 0) cannot be recommended. Instead, we recommend the

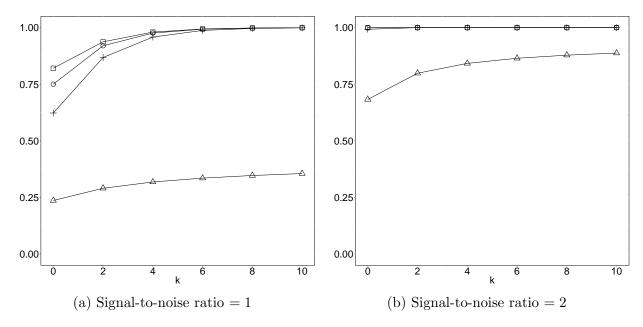


Figure 2: Statistical power for testing the hypotheses in Table 3 for the 6-factor sDSD (k = 0)and several pDSDs (k > 0). $\Box : L_1; \bigcirc : L_m; \triangle : Q_m; + : I_m$.

pDSD used by Stone et al. (2014) and constructed by dropping two columns from an 8-factor sDSD. For this option, the powers of the tests for the LEs and the 2FIs are larger than 0.86. Larger designs only marginally improve the powers. When the signal-to-noise ratio is greater than or equal to 3, the powers for all tests in Table 3 are larger than 0.90, even for the 6-factor sDSD. We conclude that it is worth considering a pDSD with four extra runs (and thus k = 2) when the interest is in detecting small effects.

Figure 3 shows the power curves for the tests in Table 4 for the 6-factor sDSD and 6-factor pDSDs constructed by dropping 2–10 columns from sDSDs with 8–16 factors, respectively. The signal-to-noise ratios assumed to construct the curves were again 1 and 2. Comparing this figure with Figure 2, we observe that the powers for hypothesis Q_2 hardly differ from the powers for hypothesis Q_m , while the powers for hypothesis I_2 lie between those for hypotheses I_m and L_m . The powers for hypotheses Q_3 and I_3 in the context of a three-factor model are lower than those for the hypotheses Q_2 and I_2 in the context of a two-factor model.

Figure 3a shows that QEs with the same size as σ are unlikely to be detected when a secondorder model in three factors is estimated. The powers for the QEs are only about 25%. The figure also shows that, for 2FIs, powers of 75% or more are achieved only when a 6-factor pDSD is formed with at least four more runs than the sDSD (by dropping two or four columns from an 8- or 10-factor sDSD). Figure 3b shows that the powers for effects that are twice as large as the standard deviation of the noise are much larger than those for effects that are as large as the standard deviation of the noise. The power for hypothesis test Q_3 , however, remains substantially smaller than 1 for any of the run sizes considered here. Signal-to-noise ratios greater than or equal to three times the noise's standard deviation result in powers larger than 0.90 for all tests listed in Table 4, except for hypothesis Q_3 , in the event the sDSD is used. In conclusion, when testing QEs end 2FIs in 2- or 3-factor second-order models, it pays off to use a pDSD involving more runs than the sDSD to detect effects with sizes equal to or twice the

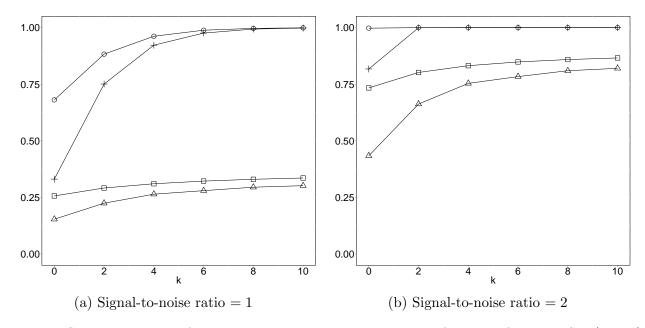


Figure 3: Statistical power for testing the hypotheses in Table 4 for the 6-factor sDSD (k = 0) and several pDSDs (k > 0). $\Box : Q_2; \bigcirc : I_2; \bigtriangleup : Q_3; + : I_3$.

standard deviation of the noise.

5.2 Aliasing of 2FIs

Based on the results reported in Section 4, we investigated whether pDSDs have the potential to improve the aliasing pattern of 2FIs in sDSDs. We studied pDSDs involving 4–18 and 20 factors constructed by dropping the optimal sets of 1–4 columns from sDSDs with up to 24 factors. For even numbers of factors up to 16, we consider the three designs obtained by dropping 0, 2 and 4 columns. For 18 and 20 factors, we consider only two different designs because there exists no 22-factor sDSD. So, 18- and 20-factor pDSDs can only be constructed starting from the 20and 24-factor sDSDs. For odd numbers of factors up to 17, we consider the pDSDs constructed from sDSDs with one and three extra factors. For 19 factors, this is impossible, again because because there is no 22-factor sDSD. For this reason, we do not discuss the 19-factor case here.

Figure 4 shows the average and maximum absolute correlations between pairs of 2FI contrast vectors for the designs under study. Figures 4a and 4b show the results for even numbers of factors m, while Figures 4c and 4d show the results for odd numbers of factors m. Figures 4a and 4c show average absolute correlations, while Figures 4b and 4d show the maximum absolute correlations.

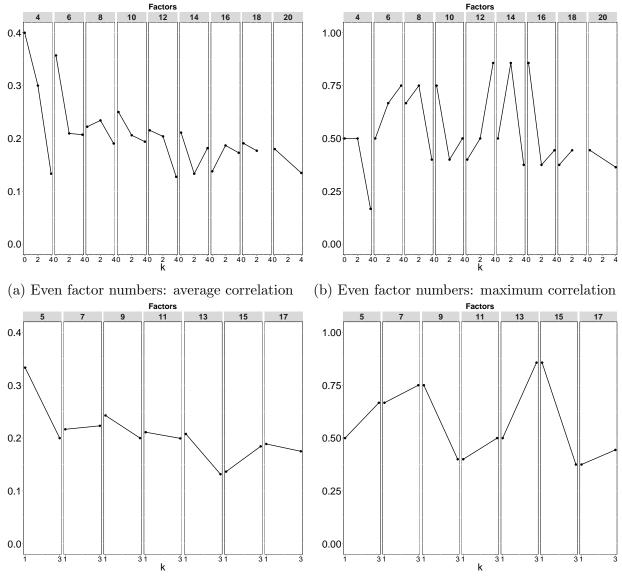
Figures 4a and 4c show that pDSDs with 4, 6, 8, 10, 12, 18 and 20 factors involve less aliasing among the 2FIs than the corresponding sDSDs and that 5-, 9-, 11-, 13- and 17-factor pDSDs with six extra runs and thus k = 3 involve less aliasing among the 2FIs than the corresponding pDSDs with only two extra runs, since the average absolute correlations decrease with k for these numbers of factors. The largest decrease in average correlation is for the 4-factor designs where the 9-run sDSD provides an average absolute correlation of 0.4, while the 17-run pDSD obtained from the 8-factor sDSD has an average as low as 0.13. For seven and 15 factors, increasing the run size by four (i.e., using k = 3 instead of k = 1) causes the average absolute correlation between pairs of 2FI contrast vectors to go up. In other words, for these cases, the larger pDSDs involve more aliasing than the smaller ones. For eight factors, the pDSD with four extra runs (corresponding to k = 2) has a larger average absolute correlation than the sDSD (k = 0), and it is the pDSD with eight extra runs (k = 4) which has the smallest average absolute correlation. For 14 and 16 factors, the best design options in terms of the average absolute correlation are the pDSD obtained by dropping two columns from the 16-factor sDSD and the 16-factor sDSD itself. The 16-factor sDSD turns out to perform well in terms of the average correlation, as the best 12-, 14- and 16-factor designs in terms of that criterion are all based on it, as well as the best 13- and 15-factor design.

Figures 4b and 4d show that, for designs with 5–7, 11–13, 17 and 18 factors, the maximum absolute correlation increases with the run size. The patterns in the maximum absolute correlations are thus quite different from those in the average absolute correlations. This means that, often, the most severe aliasing between 2FI contrast vectors is exacerbated when using pDSDs instead of sDSDs, while the total amount of aliasing goes down. The largest increase in maximum absolute correlation is for designs with 12 factors. The 12-factor sDSD provides a maximum correlation of 0.4 while the pDSD with eight extra runs (corresponding to k = 4) features a maximum of 0.857. For 8–10, 15, 16 and 20 factors however, there are pDSDs which have smaller maximum absolute correlations than the corresponding sDSDs.

Figure 4 shows that the design options used by Patil (2017) and Stone et al. (2014) were not optimal in terms of the maximum absolute correlation between pairs of 2FI contrast vectors. While the 6-factor design with 17 runs of Stone et al. (2014) provides a smaller average absolute correlation than the 6-factor sDSD, it has a larger maximum absolute correlation (0.66 versus 0.5). The 7-factor design with 21 runs and k = 3 of Patil (2017) has larger maximum and average absolute correlations between its pairs of 2FI contrast vectors than the 7-factor design with 17 runs and k = 1.

If there is one thing that Figure 4 makes clear, it is that certain sDSDs and pDSDs involve very large absolute correlations between pairs of interactions, indicating close to complete aliasing. We would feel uncomfortable using a pDSD with correlations in pairs of 2FI contrast vectors exceeding 0.5, unless one of the 2FIs involved in each pair can be assumed negligible. Particularly unfavorable in this respect are the designs constructed by dropping columns from the 16-factor sDSD, because all of these designs have quite a number of absolute correlations of 0.857 (despite the fact that the average correlations for this design are small). The figure shows that good design options (i.e., options with a maximum absolute correlation of at most 0.5) are available for all numbers of factors, except 7. For applications involving seven factors in which 2FIs are expected to be important (such as in Patil (2017)), we recommend dropping five columns from the 12-factor sDSD because the absolute correlations between the contrast vectors for the resulting design are smaller than or equal to 0.4.

Figure 4 does not show the sums of the squared correlations between pairs of 2FI contrast vectors. We found that increasing the run size of pDSDs improves the value of this criterion. The largest decrease we found was for 20-factor designs. Detailed results concerning the sums of squared correlations are given in Appendix C.



(c) Odd factor numbers: average correlation(d) Odd factor numbers: maximum correlationFigure 4: Absolute correlations between pairs of 2FI contrast vectors.

6 Discussion

In this paper, we studied pDSDs for m factors constructed by dropping sets of k columns from sDSDs with m + k factors. We considered sDSDs with 6–24 factors, and studied the pDSDs resulting from dropping sets of 1–4 columns. Table A1 in Appendix B includes additional results on dropping up to eight columns.

The sDSDs used in this study were constructed from conference matrices. This allowed us to derive analytical expressions for the relative D-efficiency to estimate models including all LEs and models including all MEs and QEs for designs with different run sizes, as well as analytical expression for the relative standard errors for LE and QE estimates. We also derived expressions for the non-centrality parameter required for calculating the power of various significance tests. We showed that the correlations between two QE contrast vectors, a QE and a 2FI contrast vector, and between two 2FI contrast vectors involving a common factor are independent of the set of k columns dropped from the (m + k)-factor sDSD. We also present analytical expressions for these correlations. Georgiou et al. (2014) provide similar expressions for the correlations between second-order effects columns but their focus is different from ours. They study the added value of extra center runs whereas we focus on the number of dropped columns. Increasing the number of dropped columns from the sDSD with m+k factors improves the statistical properties mentioned, except for the correlation between pairs of QE contrast vectors. However, this correlation cannot become larger than 1/3.

How well multiple 2FIs can be estimated at the same time depends on the selection of the sets of k columns to drop from the sDSDs. Using a complete search, we identified the best sets of columns to drop in terms of the average absolute correlation, the maximum absolute correlation, and the sum of squared correlations between pairs of 2FI contrast vectors. The differences between the best and worst sets were largest when dropping four columns from the 8- and 10-factor sDSDs. Table A1 in Appendix B shows moderate or small differences when dropping more than four columns from a sDSD except when dropping columns from the 10-factor sDSD or eight columns from the 12-factor sDSD. For these cases, the maximum absolute correlation of the worst option is at least three times larger than that of the best option. The table also shows that, in all but three cases, dropping the last columns from a sDSD is not optimal.

We compared the designs constructed by dropping columns from sDSDs in terms of the average absolute correlation, the maximum absolute correlation, and the sum of squared correlations between pairs of 2FI contrast vectors. We found that increasing the run size for a given number of factors, which is equivalent to dropping more columns from larger sDSDs, improves the sum of squared correlations between pairs of 2FI contrast vectors. However, the average and maximum absolute correlations do not necessarily improve. In fact, these values may even increase with the run size of the pDSD. Thus, in order to limit the amount of aliasing between 2FIs, a careful design selection is needed. For certain sDSDs and pDSDs, quite large numbers of 2FIs are nearly completely aliased.

A major result of the research leading to this paper is that, for a given sDSD, all three-factor projections are isomorphic. This implies that any 3-factor pDSD obtained from any given sDSD provides the same D-efficiency and the same I-efficiency for the full second-order model in these factors. Due to the isomorphism, the properties of three-factor projections from any pDSD do not depend on the set of k columns dropped from a sDSD. There is no such result for 4-factor

projections, because the 4-factor projections from a sDSD can differ in statistical properties. Evaluating all pDSDs that can be obtained by dropping k columns from an (m+k)-factor sDSD in terms of their four-, five- or six-factor projections is a major computational task, which would be an interesting topic for future research.

In this article, we focused on completely randomized DSDs involving quantitative factors only. The sDSDs have, however, also been adapted to deal with two-level categorical factors and with blocking factors. The methods developed by Jones and Nachtsheim (2013) and Nguyen and Pham (2016) to include k two-level categorical factors in a DSD transform the last kcolumns into two-level columns. Picking other columns than the last k may yield better designs. Similarly, the blocking schemes of Jones and Nachtsheim (2016) convert the last k columns of DSDs into blocking factors. Possibly, better designs can be obtained by using other columns to create the blocking factor. Investigating these issues would be an interesting avenue for future research too.

Appendices

A Derivations of design properties

In this section, we derive the properties of pDSDs constructed by dropping columns from sDSDs. For notational simplicity, we assume that the pDSD with m factors and N = 2(m+k) + 1 runs is constructed by dropping k columns from an (m+k)-factor sDSD. Note that, if k = 0, then the design is the original sDSD; otherwise, it is a pDSD.

A.1 Estimation efficiency

A.1.1 Efficiency to estimate the model with linear effects.

Consider the $N \times (m+1)$ matrix \mathbf{X}_l including the intercept and all linear effect (LE) columns of the pDSD. It is easy to show that $\mathbf{X}_l^T \mathbf{X}_l$ is a diagonal matrix with determinant $|\mathbf{X}_l^T \mathbf{X}_l| = [2(m+k)+1][2(m+k)-2]^m$. For an *m*-factor sDSD, this determinant equals $(2m+1)(2m-2)^m$. Therefore the relative D-efficiency of the pDSD and the *m*-factor sDSD for a model with all the LEs is

$$D_{le} = \left[\frac{2(m+k)+1}{2m+1} \left(\frac{2(m+k)-2}{2m-2}\right)^m\right]^{\frac{1}{m+1}}$$

After simplification, we obtain the expression for D_{me} in Section 2.1.

A.1.2 Relative standard error for a linear main effect.

The variances for the ordinary least squares (OLS) estimators of the intercept and all LEs in the pDSD are calculated from the matrix $\sigma^2(\mathbf{X}_l^T\mathbf{X}_l)^{-1}$, where σ^2 denotes the variance of the residual errors. It is easy to see that the variance for any LE equals $\sigma^2(2(m+k)-2)^{-1}$. For the *m*-factor sDSD, this variance equals $\sigma^2(2m-2)^{-1}$. Thus the relative standard error of the pDSD and the m-factor sDSD is

$$SE_{le} = \left(\frac{2m-2}{2(m+k)-2}\right)^{1/2}$$

After simplification, we obtain the expression for SE_{me} in Section 2.1.

A.1.3 Efficiency to estimate the model with linear and quadratic main effects.

Consider the $N \times (2m+1)$ model matrix $\mathbf{X}_{lq} = [\mathbf{1}_n, \mathbf{Q}, \mathbf{L}]$, where $\mathbf{1}_n$ is an $N \times 1$ column vector of ones (the intercept column), \mathbf{Q} the $N \times m$ matrix including the quadratic main effect (QE) columns, and \mathbf{L} the $N \times m$ matrix including the LE columns of the pDSD. The information matrix is

$$\mathbf{X}_{lq}^{T}\mathbf{X}_{lq} = \begin{pmatrix} N & 2(n-1)\mathbf{1}_{1\times m} & \mathbf{0}_{1\times m} \\ 2(n-1)\mathbf{1}_{m\times 1} & 2(n-2)\mathbf{J}_{m\times m} + 2\mathbf{I}_{m\times m} & \mathbf{0}_{m\times m} \\ \mathbf{0}_{m\times 1} & \mathbf{0}_{m\times m} & 2(n-1)\mathbf{I}_{m\times m} \end{pmatrix},$$
(7)

where $\mathbf{I}_{m \times m}$ is the identity matrix of order m, $\mathbf{J}_{m \times m}$ is the matrix with all its entries equal to 1, $\mathbf{0}_{p \times q}$ denotes a $p \times q$ matrix of zeroes, and n = m + k. Note that matrix (7) is a block diagonal matrix and can be expressed as

$$\mathbf{X}_{lq}^{T}\mathbf{X}_{lq} = \begin{pmatrix} \mathbf{A} & \mathbf{0}_{(m+1)\times m} \\ \mathbf{0}_{m\times(m+1)} & \mathbf{B} \end{pmatrix},$$

where

$$\mathbf{A} = \begin{pmatrix} N & 2(n-1)\mathbf{1}_{1\times m} \\ 2(n-1)\mathbf{1}_{m\times 1} & 2(n-2)\mathbf{J}_{m\times m} + 2\mathbf{I}_{m\times m} \end{pmatrix}, \text{ and } \mathbf{B} = 2(n-1)\mathbf{I}_{m\times m}.$$

Using Harville (2011, p.p. 187), we have that $|\mathbf{X}_{lq}^T \mathbf{X}_{lq}| = |\mathbf{A}||\mathbf{B}|$. We can calculate the determinant of \mathbf{A} by taking $c_0 = N$, c = 2(n-1), a = 2(n-2), and b = 2, and applying lemma 2*iii* of Zhou and Xu (2016). The determinant of the information matrix $|\mathbf{X}_{lq}^T \mathbf{X}_{lq}|$ is then $2^{2m}(m+k-1)^m [(m-1)^2 + k(m+2)]$. For the *m*-factor sDSD, this determinant equals $2^{2m}(m-1)^{m+2}$ for the information matrix of a model including the intercept, all QEs, and all LEs. As a result, the relative D-efficiency of the pDSD and the *m*-factor sDSD is

$$D_{le+qe} = \left\{ \left(\frac{m+k-1}{m-1}\right)^m \left[\frac{(m-1)^2 + k(m+2)}{(m-1)^2}\right] \right\}^{\frac{1}{2m+1}}.$$

Simplification yields the expression for D_{le+qe} in Section 2.1.

A.1.4 Relative standard errors for quadratic effect estimates.

Consider the information matrix (7) for the pDSD. Using Harville (2011, p.p. 89), we have that the variances for the OLS estimators of the model including the intercept, all LEs, and all QEs in the pDSD are calculated from the matrix

$$\sigma^{2} \left(\mathbf{X}_{lq}^{T} \mathbf{X}_{lq} \right)^{-1} = \sigma^{2} \left(\begin{array}{cc} \mathbf{A}^{-1} & \mathbf{0}_{(m+1) \times m} \\ \mathbf{0}_{m \times (m+1)} & \mathbf{B}^{-1} \end{array} \right).$$

Note that sub-matrix $\sigma^2 \mathbf{A}^{-1}$ contains the variances for the OLS estimators of the QEs. Consider the following sub-matrices

$$\mathbf{W} = N, \mathbf{T} = 2(n-2)\mathbf{J}_{m \times m} + 2\mathbf{I}_{m \times m}, \text{ and } \mathbf{V} = \mathbf{U}^T = 2(n-1)\mathbf{1}_{1 \times m},$$

that partition matrix A into four parts. Using Harville (2011, p.p. 99) and Lemma 2*i* of Zhou and Xu (2016), it is straightforward to show that the variance of the OLS estimator for any QE, denoted as $\hat{\beta}_{ii}$, in a model including the intercept, all LEs and all QEs based on the pDSD is

$$\operatorname{Var}(\hat{\beta}_{ii}) = \sigma^2 \frac{(m-1)^2 + m(k-1) + k + 4}{2\left[(m-1)^2 + k(m+2)\right]},$$

For the *m*-factor sDSD, $\operatorname{Var}(\hat{\beta}_{ii}) = \sigma^2 (m^2 - 3m + 5)/(2(m - 1)^2)$. Then the relative standard error of the OLS estimate of any QE in the pDSD and the *m*-factor sDSD is

$$SE_{qe} = \left\{ \left[\frac{(m-1)^2}{(m-1)^2 + k(m+2)} \right] \left[\frac{m^2 - 3m + 5 + k(m+1)}{m^2 - 3m + 5} \right] \right\}^{1/2}$$

After simplification, we obtain the expression for SE_{qe} in Section 2.2.

A.2 Pairwise correlations among contrast vectors

A.2.1 Correlation between a quadratic effect column and a two-factor interaction column.

The expression for $r_{ss,tt}^c r_{ss,tu}^c$ and $r_{st,su}^c$ in Section 2.4 are obtained by substituting m + k for m in the corresponding expressions given in Jones and Nachtsheim (2011).

A.2.2 Correlation between pairs of two-factor interaction columns with a common factor.

Consider two two-factor interaction (2FI) columns \mathbf{x}_{st} and \mathbf{x}_{su} formed by the element-wise multiplications of the LE columns s and t and the element-wise multiplication of the LE columns s, and u, respectively, in the pDSD. Denote the elements in \mathbf{x}_{st} and \mathbf{x}_{su} as $x_{i,st}$ and $x_{i,su}$, respectively; $i = 1, \ldots, N$. Note that the average of these elements, denoted as $\bar{x}_{i,st}$, equals zero and that their sum of squares equals 2(m + k) - 4. The correlation between two 2FI columns with a common factor is then

$$r_{st,su}^{c} = \frac{\sum [x_{i,st} - \bar{x}_{st}] [x_{i,su} - \bar{x}_{su}]}{\sqrt{\sum [x_{i,st} - \bar{x}_{st}]^{2} \sum [x_{i,su} - \bar{x}_{su}]^{2}}} = \frac{\sum x_{i,st} x_{i,su}}{\sqrt{\sum (x_{i,st})^{2} \sum (x_{i,su})^{2}}} = \frac{\sum x_{i,st} x_{i,su}}{2(m+k) - 4}, \quad (8)$$

where all sums run from $i = 1, \ldots, N$.

The numerator in (8) is calculated as follows. We first note that $\sum x_{i,st}x_{i,su} = \sum x_{i,ss}x_{i,tu}$, where $x_{i,ss}$ is the *i*-th element of the QE column \mathbf{x}_{ss} . It is easy to show that $\sum x_{i,ss}x_{i,tu} = \pm 2$. If we substitute $\sum x_{i,st}x_{i,su} = \pm 2$ and 2(m+k) + 1 by N in expression (8) and simplify, we obtain the expression for $r_{st,su}^c$ in Section 2.4.

A.2.3 Correlation between pairs of two-factor interaction columns not sharing a common factor.

The derivations for possible values and the maximum absolute value for the correlations between pairs of 2FI columns in the pDSD are straightforward and therefore omitted.

A.3 Power calculations

In Sections 2.1 and 2.2 of the main paper, powers for t tests of the hypotheses L_1 , L_m , Q_m , I_m , Q_3 and I_3 are discussed. The statistical power provided by the pDSD to test these hypotheses is computed as Power = $1 - \text{Prob}(-t_c < \underline{t}_{[df,\lambda]} < t_c)$, where $\underline{t}_{[df,\lambda]}$ is a random variable following a non-central t distribution with df degrees of freedom, and non-centrality parameter λ , t_c is the critical value of the null distribution at level α , and $\alpha = \text{Prob}(|t_{[df,0]}| > t_c)$. For all the hypothesis tests df = N - p, where p is the number of parameters included in the model. The non-centrality parameter of the t distribution is given by

$$\lambda = \frac{\beta_i / \sigma}{\sqrt{\operatorname{Var}(\hat{\beta}_i)}},$$

where the OLS estimate $\hat{\beta}_i$ is computed for a given model. Showing that the power calculations are independent of the set of k columns to drop from the (m + k)-factor sDSD is equivalent to showing that the value of $\operatorname{Var}(\hat{\beta}_i)$, and thus of λ , is the same for any subset. We show below that λ for a given δ , only depends on the values of m and k.

A.3.1 Power for L_1 .

Since the all LE columns are orthogonal to the intercept, it is easy to see that the variance for the OLS estimator of any main effect is $\sigma^2(2(m+k)-2)^{-1}$. Since only the intercept and a main effect are included in the model, df = N - 2 = 2(m+k) - 1, and the expression for the power calculations follows.

A.3.2 Power for L_m .

Using the model matrix \mathbf{X}_l and the calculations in Section A.1.2, it is easy to show that the variance for the OLS estimator is the same as for L_1 . Since the number of parameters already in the model is one plus the number of factors, the expression for the power calculations follows.

A.3.3 Power for Q_m .

Consider the $N \times (m+2)$ matrix, \mathbf{X}_{qm} , including the intercept column, one QE column, and all LE columns of the pDSD. For whatever QE column is chosen, the information matrix is

$$\mathbf{X}_{qm}^{T}\mathbf{X}_{qm} = \begin{pmatrix} N & 2(n-1) & \mathbf{0}_{1 \times m} \\ 2(n-1) & 2(n-1) & \mathbf{0}_{1 \times m} \\ \mathbf{0}_{m \times 1} & \mathbf{0}_{m \times 1} & 2(n-1)\mathbf{I}_{m \times m} \end{pmatrix},$$

where n = m + k. Note that this matrix is a block diagonal matrix with blocks

$$\mathbf{A} = \begin{pmatrix} N & 2(n-1) \\ 2(n-1) & 2(n-1) \end{pmatrix}, \text{ and } \mathbf{B} = 2(n-1)\mathbf{I}_{m \times m},$$

Using Harville (2011, p.p. 89), we can easily calculate the inverse of the information matrix:

$$\begin{pmatrix} \mathbf{X}_{qm}^T \mathbf{X}_{qm} \end{pmatrix}^{-1} = \begin{pmatrix} \mathbf{A}^{-1} & \mathbf{0}_{2 \times m} \\ \mathbf{0}_{m \times 2} & \mathbf{B}^{-1} \end{pmatrix} = \begin{pmatrix} 1/3 & -1/3 & \mathbf{0}_{1 \times m} \\ -1/3 & (2n+1)/(6n-6) & \mathbf{0}_{1 \times m} \\ \mathbf{0}_{m \times 1} & \mathbf{0}_{m \times 1} & (2n-2)^{-1} \mathbf{I}_{m \times m} \end{pmatrix}.$$

Therefore the variance for the OLS estimator of any QE is $\sigma^2(2n+1)/(6n-6)$. Given that the number of parameters already included in the model is m+1, the expression for the power follows.

A.3.4 Power for I_m .

Consider the $N \times (m+2)$ matrix, \mathbf{X}_{im} , including the intercept column, a single 2FI column, and all LE columns for the pDSD. Regardless of the 2FI chosen, the information matrix is

$$\mathbf{X}_{im}^T \mathbf{X}_{im} = \begin{pmatrix} 2n+1 & 0 & \mathbf{0}_{1 \times m} \\ 0 & 2n-4 & \mathbf{0}_{1 \times m} \\ \mathbf{0}_{m \times 1} & \mathbf{0}_{m \times 1} & 2(n-1)\mathbf{I}_{m \times m} \end{pmatrix},$$

which is a diagonal matrix. Then the variance for the OLS estimate of the 2FI is $\sigma^2(2n-4)^{-1}$. Given that the number of parameters already included in the model is m+1, the expression for the power follows.

A.3.5 Power for Q_2 and I_2 .

Consider the $N \times 6$ matrix, \mathbf{X}_{q2} , including the intercept column, the two QE columns, the two LE columns, and the 2FI column of any two-factor projection of the pDSD. It is easy to see that the information matrix for any two-factor projection is

$$\mathbf{X}_{q2}^{T}\mathbf{X}_{q2} = \begin{pmatrix} N & 2n-2 & 2n-2 & 0 & 0 & 0 \\ 2n-2 & 2n-2 & 2n-4 & 0 & 0 & 0 \\ 2n-2 & 2n-4 & 2n-2 & 0 & 0 & 0 \\ 0 & 0 & 0 & 2n-2 & 0 & 0 \\ 0 & 0 & 0 & 0 & 2n-2 & 0 \\ 0 & 0 & 0 & 0 & 0 & 2n-4 \end{pmatrix}$$

Using Harville (2011, p.p. 89, 99), it is easy to show that the inverse of this information matrix equals

$$\left(\mathbf{X}_{q2}^{T} \mathbf{X}_{q2} \right)^{-1} = \begin{pmatrix} \frac{2n-3}{4n-7} & \frac{1-n}{4n-7} & \frac{1-n}{4n-7} & 0 & 0 & 0 \\ \frac{1-n}{4n-7} & \frac{3(n-1)}{2(4n-7)} & \frac{-(n-4)}{2(4n-7)} & 0 & 0 & 0 \\ \frac{1-n}{4n-7} & \frac{-(n-4)}{2(4n-7)} & \frac{3(n-1)}{2(4n-7)} & 0 & 0 & 0 \\ 0 & 0 & 0 & (2n-2)^{-1} & 0 & 0 \\ 0 & 0 & 0 & 0 & (2n-2)^{-1} & 0 \\ 0 & 0 & 0 & 0 & 0 & (2n-4)^{-1} \end{pmatrix}.$$

So the variances for the OLS estimates of the 2FI, and of any QE equal $\sigma^2(2n-4)^{-1}$ and $\sigma^2(3n-3)/(8n-14)$, respectively. Since the number of parameters already included in the model is N-6, the power expressions for I_2 and Q_2 follow.

A.3.6 Power for Q_3 and I_3 .

Schoen et al. (2017) considered pDSDs in three factors. They made a distinction between DSDs with $n \equiv 0 \pmod{4}$ and those with $n \equiv 2 \pmod{4}$, where n = (N - 1)/2 and they showed that for a given N all three-factor pDSDs are isomorphic or statistically equivalent.

Consider now the second order model matrix of a three-factor projection of a DSD, \mathbf{X}_{q3} . This is an $N \times 10$ model matrix including the intercept column, three QE columns, three LE columns and three 2FI columns. When $(N-1) \equiv 0 \pmod{8}$, the information matrix for one of the isomorphic DSDs is

Alternatively, when $(N-1) \equiv 4 \pmod{8}$, the information matrix for one of the isomorphic DSDs is

We calculated the inverses of the information matrices using Mathematica. For both information matrices, the output of Mathematica (not included here) showed that the variance of the OLS estimates for any QE is the same. The output also showed that the variances of the OLS estimates of the three 2FIs are equal. The variances in case $(N-1) \equiv 0 \pmod{8}$ differ from the corresponding variances when $(N-1) \equiv 4 \pmod{8}$. For $n \equiv 0 \pmod{4}$, the variances for a QE estimate, $\hat{\beta}_{ii}$, and a 2FI estimate, $\hat{\beta}_{ij}$, are:

$$\operatorname{Var}(\hat{\beta}_{ii}) = \frac{4(m+k)^3 - 21(m+k)^2 + 24(m+k) + 2}{10(m+k)^3 - 66(m+k)^2 + 102(m+k) + 8}$$
$$\operatorname{Var}(\hat{\beta}_{ij}) = \frac{5(m+k)^2 - 19(m+k) + 14}{10(m+k)^3 - 66(m+k)^2 + 102(m+k) + 8}.$$

For $n \equiv 2 \pmod{4}$, the variances for a QE estimate, $\hat{\beta}_{ii}$, and a 2FI estimate, $\hat{\beta}_{ij}$, are:

$$\operatorname{Var}(\hat{\beta}_{ii}) = \frac{4(m+k)^3 - 29(m+k)^2 + 54(m+k) - 26}{10(m+k)^3 - 86(m+k)^2 + 218(m+k) - 172}$$
$$\operatorname{Var}(\hat{\beta}_{ij}) = \frac{5(m+k)^2 - 29(m+k) + 36}{10(m+k)^3 - 86(m+k)^2 + 218(m+k) - 172}.$$

Since the number of parameters already included in the model is N - 10, the power expressions for I_3 and Q_3 follow for the two cases.

B Table with detailed results

Table A1 shows the best and worst sets of columns to drop from sDSDs for $m+k \in \{6, 8, \ldots, 22, 24\}$ and $k \leq 8$. The table includes (i) the average absolute correlations, (ii) the maximum absolute correlations, and (iii) the sum of all squared correlations between contrast vectors for pairs of 2FI columns. Each set of columns is labeled as *i.criteria*, where *i* can be "b" for best option or "w" for worst option. The *criteria* can include the letters "a", "m", or "s" corresponding to the average absolute correlation, maximum absolute correlation, and sum of squared correlations criteria, respectively. For instance, a set of columns labeled "b.ams" thus is best in terms of all three criteria, while a design labeled "w.a" is worst in terms of the average absolute correlation criterion.

C Sum of squared correlations between pairs of twofactor interactions

Figures A1 shows the logarithm of the sum of squared correlations between pairs of 2FI contrast vectors for the designs discussed in Section 5.2.

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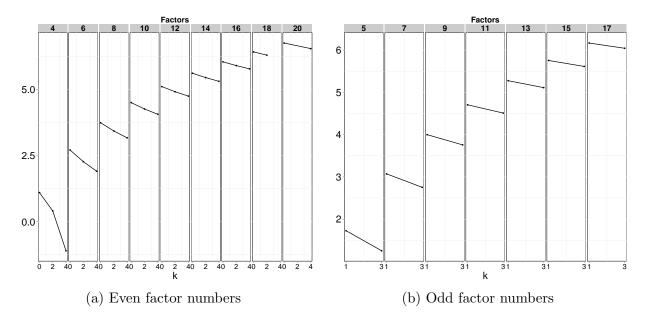


Figure A1: Sum of squared correlations between pairs of 2FI contrast vectors on a logarithmic scale.

Table A1: Columns to drop from sDSDs. b: best option. w: worst option. a: average correlation. m: maximum correlation. s: sum of squared correlations.

Columns in sDSD	Number of columns to drop	Option	Subset of columns to drop	Average correlation	Maximum correlation	Sum of Squared Correlations	Columns in standard DSD	Number of columns to drop	Option	Subset of columns to drop	Average correlation	Maximum correlation	Sum of Squared Correlations
8	4	b.ams		0.133333	0.167	0.3333	18	4	b.as	$15 \ 16 \ 17 \ 18$	0.181593	0.375	201.1875
		w.ams	4578	0.266667	0.667	1.6667			w.as	$14 \ 16 \ 17 \ 18$	0.181777	0.375	201.5625
10	4	b.as	68910	0.207143	0.75	6.75		ъ	b.as	12 15 16 17 18	0.178072	0.375	143.3672
		w.as	78910	0.221429	0.75	8.25			W.as	$13 \ 15 \ 16 \ 17 \ 18$	0.178821	0.375	144.4922
	5	b.ams	$4\ 6\ 7\ 9\ 10$	0.166667	0.25	1.4063		9	b.as	$9\ 12\ 13\ 14\ 15\ 18$	0.172902	0.375	97.7813
		w.ams		0.2	0.75	2.9063			W.as	$9 \ 13 \ 15 \ 16 \ 17 \ 18$	0.176049	0.375	101.1563
	9	b.ams	$4\ 6\ 7\ 8\ 9\ 10$	0.15	0.25	0.375		7	b.as	$9\ 12\ 13\ 14\ 15\ 17\ 18$	0.168813	0.375	65.4023
		w.ams	$5\ 6\ 7\ 8\ 9\ 10$	0.25	0.75	1.875			W.as	$9 \ 10 \ 13 \ 15 \ 16 \ 17 \ 18$	0.172348	0.375	68.0273
12	4	b.as	7 8 10 12	0.190476	0.4	23.76		×	b.as	$9 \ 10 \ 12 \ 13 \ 14 \ 15 \ 17 \ 18$	0.162121	0.375	40.875
		w.as	$9 \ 10 \ 11 \ 12$	0.193651	0.4	24.24			w.as	$8 \ 10 \ 11 \ 12 \ 14 \ 15 \ 16 \ 18$	0.168939	0.375	44.25
	ю	b.as	7 8 10 11 12	0.181429	0.4	12.09	20	4	b.as	$14\ 17\ 18\ 20$	0.172923	0.444	322.2222
		W.as	8 9 10 11 12	0.192857	0.4	13.05			W.as	$14\ 18\ 19\ 20$	0.173109	0.444	322.8148
	9	b.as	$5\ 7\ 8\ 10\ 11\ 12$	0.16	0.4	4.92		ъ	b.as	$14 \ 16 \ 17 \ 19 \ 20$	0.170543	0.444	241.6944
		W.aS	789101112	0.182857	0.4	5.88			W.as	$12 \ 16 \ 17 \ 19 \ 20$	0.171032	0.444	242.8796
	7	b.as	$5\ 7\ 8\ 9\ 10\ 11\ 12$	0.146667	0.4	1.74		9	b.as	$11 \ 13 \ 15 \ 18 \ 19 \ 20$	0.167359	0.444	176.5556
		W.aS	$6\ 7\ 8\ 9\ 10\ 11\ 12$	0.2	0.4	2.7			W.as	$12 \ 13 \ 16 \ 17 \ 19 \ 20$	0.168661	0.444	178.9259
	x	h as	45678101112	0.08	0.1	0.12		1-	h as	11 13 15 16 18 19 20	0.164391	0.444	126.3519
)	W. AS	56789101112	0.16	0.4	0.6			W. AS	$12\ 13\ 15\ 16\ 17\ 19\ 20$	0.166167	0.444	128.4259
14	4	h.as	11 12 13 14	0.193939	0.5	58		x	h.as	10 12 13 14 17 18 19 20	0.159751	0.444	86.9259
		W.as	$9\ 12\ 13\ 14$	0.194949	0.5	58.6667)	W.as	$9\ 12\ 13\ 14\ 15\ 16\ 17\ 20$	0.164413	0.444	90.037
	ьc	h.as	$10\ 11\ 12\ 13\ 14$	0.185714	0.5	34.25	24	4	h.as	20 22 23 24	0.134792	0.364	693.3471
	,	W. AS	$9\ 11\ 12\ 13\ 14$	0.188889	0.5	35.5833	l	,	W. AS	21 22 23 24	0.134852	0.364	693.7438
	9	b.as	$9 \ 10 \ 11 \ 12 \ 13 \ 14$	0.177249	0.5	19		ю	b.as	$17\ 20\ 22\ 23\ 24$	0.13368	0.364	554.6343
	5	W. as	7 9 10 11 12 14	0.185185	0.5	21		ŀ	W. as	$20\ 21\ 22\ 23\ 24$	0.133831	0.364	555.626
	7	h.as	67810121314	0.158333	0.5	8.3125		9	h.as	$16\ 17\ 20\ 22\ 23\ 24$	0.132283	0.364	437.0579
		W.aS	$6 \ 8 \ 9 \ 11 \ 12 \ 13 \ 14$	0.182143	0.5	11.6458			W.as	$19\ 20\ 21\ 22\ 23\ 24$	0.132845	0.364	440.0331
	×	h.as	6781011121314	0.147619	0.5	3.6667		7	h.as	$15\ 17\ 19\ 20\ 22\ 23\ 24$	0.130838	0.364	340.0165
)	W. AS	-1-	0.176190	0.5	5.6667			W AS	18 19 20 21 22 23 24	0.131788	0.364	343 3884
16	6	h.a.	8 16 8 16	0.133333	0.857	231.8571		x	h as	20 22	0.128953	0.364	258.9421
2	ı	0.10	51 X	0.135845	0.857	931 8571)	MI C		0.13004	0.364	264 4959
	ç	ۍ د ۲	0 TU 1 / 1 K 1 K	0.121795	0.857	166 0109			6.W	90 91 93	0.131009	0.364	963 7095
	5	e M	8 14 15	0.134580	0.857	166.0102			3		100101-0	100.0	01001
	4	h.as	13 14 15 16	0.127473	0.857	115.0408							
	4	e M	7 8 12 14	0 134665	0.857	116 0204							
		5 M	19 14 15 16	0.128671	0.857	117.9440							
	ьc	s S S	8 13 14 15 16	0 124242	0.857	75 9949							
	,	S M	12 13 14 15 16	0.123088	0.857	78 4439							
		h.a.	$12\ 13\ 14\ 15\ 16$	0.123088	0.857	78 4439							
		a M	7 8 19 13 14	0.133478	0.857	77 464							
	9	9. v S	7811191315	0.194675	0.857	47 3878							
	>	S M	11 19 13 14 15 16	0.119481	0.857	53 2653							
		, 4 , 4	8 11 13 14 15 16	0.118615	0.857	48.6122							
		5 M	678101913	0.135065	0.857	53 8163							
	4	b ac	7 8 11 19 13 15 16	0.110204	0.857	97 7347							
	-	S M	10 11 12 13 14 15 16	0.123810	0.857	39							
		e W	6789101113	0.140136	0.857	34 5918							
	x	n s q	467811191315	0.117914	0.857	01:0010 14.5714							
	D	6.0 8	7 8 11 12 13 14 15 16	0.104308	0.857	15.551							
						100.0							

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