# Small, Efficient, Equireplicated Resolution V Fractions of $2^k$ designs and their Application to Central Composite Designs

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#### **Summary**

We present class of equireplicated, irregular fractions of two-series designs constructed algorithmically using the D-optimality criterion. These designs can be constructed for even numbers of runs and can take a wider variety of sizes than usual regular and irregular fractions. We present examples of minimal designs of resolution V and compare them to some alternatives. We use these designs to form central composite designs and show that the present designs are more efficient than most competitors.

Key words: optimal design, columnwise-pairwise algorithm, D-optimality, response surfaces

### 1 Introduction

Resolution V fractions of  $2^k$  designs are frequently used in experimentation when we want all estimates of main effects and two-factor interactions unaliased with other main effects and two factor interactions. Regular fractions may be constructed using well-known group theoretic methods; estimated effects using such fractions are all independent, and the designs are highly efficient. In many situations, however, regular fractions contain considerably more runs than are necessary to estimate the p = 1 + k + k(k-1)/2 effects in the model containing effects up to two-way interactions. For example, the smallest regular resolution V fraction when k = 7 uses 64 runs to estimate the 29 parameters in the model. Because of this, numerous irregular fractions have been developed to provide resolution V designs using fewer runs.

Most irregular fractions are constructed by combining regular fractions. John (1969) constructs irregular resolution V fractions that contain only three fourths the runs of a regular resolution V fraction. Addelman (1969) considers designs formed by first producing a very small regular fraction, and then adding additional fractions from the same family until the combined design has

resolution V. This is a multistep version of John's method. Pajak and Addelman (1975) investigate using fractions from different low-resolution fractional families to form resolution V designs.

A second approach is the use of balanced, saturated designs (Rechtschaffner 1967; Srivastava and Chopra 1971). These designs are constructed in n = 1 + k + k(k-1)/2 runs as the treatment combination with all factors low, the k combinations with one factor low and all others high, and the k(k-1)/2 combinations that have only two factors high. (Other high/low patterns may work, but this pattern is optimal. See Kim 1993.) This design is balanced in the sense that all the main effect variances are equal, all the main effect covariances are equal, all the two-factor interaction covariances are equal, and all covariances between main effects and two-factor interactions are equal. Saturated designs are the smallest possible designs for a given model, but they have no degrees of freedom for estimating pure error or lack-of-fit.

Mee (1999) describes a third approach that uses a point exchange search algorithm on a candidate set of treatment combinations to find good designs in the D-optimal sense. In particular, Mee finds good 64-point designs for k equal to 9 and 10. Mee also gives a catalog of recommended designs of various pedigrees for k from 5 to 11.

Central composite designs are used for collecting data to fit second order models in response surfaces (Box and Wilson 1951). The central composite design for k factors comprises  $n_0 + n_f + 2k$  points:  $n_0$  center points at the origin,  $n_f$  factorial points taken from a full  $2^k$  factorial at levels  $\pm 1$ , and 2k axial points at locations  $\pm \alpha$  along each coordinate axis. If the factorial points form a resolution V design, then the resulting central composite design will be capable of estimating the full quadratic model, which has q = 1 + 2k + k(k-1)/2 parameters. The overall efficiency of the resulting design depends on the quality of the factorial points and number of center points.

In fact, the factorial portion of the design need not be resolution V (Hartley 1959); fractions down to resolution III may be used provided only that two-factor interactions not be aliased to other two-factor interactions. This allows smaller factorial fractions to be used, and Hartley published several examples where the recommended fractional design for the central composite differs dramatically from the recommend fractional design standing alone. Several authors have continued the quest for smaller designs. Westlake (1965) published smaller fractions for k of 5, 7, and 9. Draper (1985) uses Plackett-Burmann designs to form even smaller designs than Westlake's, again for k of 5, 7, and 9. Draper and Lin (1990) follows up on this work. Lucas (1974) computes the D-criterion for saturated composite designs constructed using a subset of points from the saturated resolution V designs of Rechtschaffner (1967).

Some alternatives to central composite designs include Box-Behnken designs (Box and Behnken 1960), noncentral composite designs (Mee 2001), and augmented pairs designs Morris (2000).

In this article we construct two-level equireplicated irregular fractions with resolution V. A design is equireplicated if each factor occurs an equal number of times at the high and low levels. Obviously, equireplicated designs must have an even number of runs. Equireplication is not the same thing as balance (described above); either can occur without the other. These new designs are constructed algorithmically to optimize the D-criterion using the columnwise-pairwise algorithm. The designs may be used on their own as resolution V irregular fractions, and they may also be used as the factorial component of central composite designs. Section 2 of this paper describes the algorithm for constructing these designs. Section 3 compares these new designs to existing resolution V fractions, and Section 4 compares central composite designs constructed using these fractions to other small central composite designs.

## 2 Constructing the designs

Suppose that we wish to construct a resolution V fraction of a k-factor design in n runs. Let X be the n by k design matrix, with high levels of a factor denoted by 1, and low levels denoted by -1. We only consider equireplicated designs, so each column contains an equal number of 1's and -1's. Because there are p = 1 + k + k(k - 1)/2 model degrees of freedom, n can be any even number at least that large. The second-order model includes a constant, all main effects, and all two-factor interactions. Let  $\tilde{X}$  be the n by p model matrix for the second-order model. The D-criterion is  $|\tilde{X}'\tilde{X}|$ , and we seek designs that give us large values of D. (Alternatively, the D-criterion can be written as  $|(\tilde{X}'\tilde{X})^{-1}|$ , and we seek small values of D.)

In principle, we can find the D-optimal design by enumerating and evaluating all eligible designs. In practice, this is usually not feasible. For example, the smallest possible resolution V design for k=6 has n=22, so there are more than  $10^{35}$  potential designs (though many are equivalent and many others are resolution less than five). Thus we are forced to use some algorithm to search through a restricted class of test designs.

The most common optimal design algorithms are single-point exchange algorithms. That is, they use a search that involves replacing a single design point (row of X) with an alternative design point; the replacement is accepted if it increases D. We cannot use those algorithms in our situation, because we seek equireplicated designs, and the current design point is the only one that maintains equireplication. Thus any point exchanges must involve an even number of design points.

We use the columnwise-pairwise (CP) algorithm of Li and Wu (1997) to find our designs. As might be expected from the "pairwise" in the name, CP is a two-point exchange algorithm. The idea is as follows. Begin with a equireplicated resolution V design. Consider all designs that are in a neighborhood of that design, and move to the neighbor that has best D. Now consider all neighbors of the new design, and continue until we reach a design which has no neighbors with a better D. The CP algorithm is a typical "greedy" optimization algorithm, always taking the biggest possible step up, and often finding a local rather than a global optimum.

In the CP algorithm, we consider two design matrices X and  $X_t$  to be neighbors if they differ in only two elements, with both elements in the same column. That is, two designs are neighbors if one can reach the other design by swapping a +1 and a -1 in the same column, hence columnwise-pairwise.

As described above, all neighbors are checked at every step, which is  $k(n/2)^2$  neighbors. This is feasible for small values of n and k, but again becomes burdensome as n and k increase. For large n and k, we revise the search to limit the computations. For each column, we first find the +1 value that most improves D if switched to a -1, and having made that change, we find the -1 value in that same column that most improves D if switched to a +1. This restricted neighborhood search will not, in general, find as good a candidate switch, but it reduces the computations by a factor of n, which can make the exercise possible.

In the discussion below, we will refer to designs obtained using the full CP algorithm as CP designs, and those obtained using the faster restricted algorithm as CP\* designs.

We must have an initial resolution V design to begin the search. These can generally be constructed by hand by using the following types of points:

- base points: all levels at -1;
- linear points: all levels –1 except for a single +1;

• lag j points: all levels -1 except for two +1's that are j elements apart (wrapping around to the start of the list if necessary).

The combination of a base point, all linear points, and all lag j points up to  $j \leq \lfloor k/2 \rfloor$  provides a resolution V design. Add an additional base point if necessary to make n even. The design can be made equireplicated by changing the signs of the points. For example, for k=7, use linear points and lag 1 points as given above, and use lag 2 and lag 3 points and two base points with reversed signs. With this design, every factor has 15 each of the high and low levels.

The CP algorithm often finds a local optimum rather than a global optimum. It thus makes sense to try several different starting designs and choose the best of the resulting local optima. We find alternate starting designs by taking the standard starting design and making random columnwise-pairwise swaps, accepting any swap that results in a resolution V design. Specifically, we make 100 passes through the columns for  $k \le 11$ , 200 passes for  $12 \le k \le 17$ , 300 passes for  $18 \le k \le 23$ , and 400 passes for  $24 \le k \le 26$ . For the designs described below we have used 200 random starting designs.

The major portion of the computational burden is computing the D-criterion after exchanging points. This computation can be done efficiently by using a Choleski decomposition and rank one up- and down-dates. Write  $\tilde{X}'\tilde{X}$  as LL', where L is lower triangular; D is simply the square of the product of the diagonal elements of L. Rank one up- and down-date algorithms (for example, DCHUD and DCHDD in LINPACK) can be used to update L when a row is added or removed from  $\tilde{X}$ . These algorithms are much more efficient than recomputing L or D from scratch.

## 3 Efficiency as Fractions

Several criteria can be used to evaluate the quality of experimental designs. These criteria are based on  $C = \tilde{X}'\tilde{X}$  and  $V = (\tilde{X}'\tilde{X})^{-1}$ . As we are designing for D-optimality, it makes sense to compare designs based on their D-criterion: D = |C|. A related criterion is the average information per parameter per observation:  $D_e = |C|^{1/p}/n$ . In the case of two-series designs with all factors at levels  $\pm 1$ , the maximum value of  $D_e$  is 1 (obtained for orthogonal designs), so that  $D_e$  can be taken as an absolute measure of efficiency.

Many other optimality criteria related to C or V are available. One important criterion is A-efficiency  $A=p/(n{\rm tr}(V))$ , which gives us the average variance of the estimated parameters relative to the average variance for an orthogonal design. Further exploration of V can consider the average variances of the main effects relative to orthogonal designs  $A_1=k/(n{\rm tr}_m(A))$  (where  ${\rm tr}_m$  indicates the sum of the diagonal elements corresponding to main effects) and interactions  $A_2=k(k-1)/(2n{\rm tr}_i(A))$ , or the maximal absolute correlations between main effects  $r_m$ , interactions  $r_i$ , and main effects and interactions  $r_{mi}$ .

Table 1 compares CP and CP\* designs to several designs given in the literature, including all of those recommended in Mee (1999). The CP and CP\* designs are the best found using 200 random perturbations of a standard starting design. We have used the CP search for  $n \le 50$ , and the CP\* search for n > 50. These new designs are compared to the saturated designs of Rechtschaffner (1967) for k = 6, 7, 8, 9; the mixed family fraction sequences of Pajak and Addelman (1975) for k = 6, 9, the 3/4 replicates of resolution V fractions of John (1969) for k = 7, 8, 9, 10, 11; the irregular fraction sequences of Addelman (1969) for k = 7, 9, 10, 11; and the point exchange D-

Table 1: Factorial Efficiencies

k	n	Design	$\log(D)$	$D_e$	A	$A_1$	$r_m$	$r_i$	$r_{mi}$
6	22	saturated	66.31	.936	.868	.870	.069	.069	.069
	22	CP	64.48	.852	.615	.545	.365	.300	.365
	24	Pajak and Addelman $3 \times 2^{6-3}$	60.71	.658	.284	.421	.722	.817	.722
	24	CP	66.76	.867	.719	.769	.447	.500	.447
7	29	saturated	90.92	.793	.673	.685	.086	.086	.086
	30	CP	93.28	.831	.636	.623	.408	.444	.408
	40	Addelman's (5/16) 2 <sup>7</sup>	103.68	.893	.757	.862	.408	.714	.408
	40	CP	105.59	.953	.918	.925	.200	.143	.200
	48	John's (3/4) 2 <sup>7-1</sup>	110.16	.930	.847	.811	.500	.500	.500
	48	CP	111.10	.961	.918	.931	.200	.200	.200
8	37	saturated	118.37	.662	.515	.536	.091	.091	.091
	38	CP	126.27	.799	.577	.511	.637	.440	.637
	48	John's (3/4) 2 <sup>8-2</sup>	139.03	.893	.767	.762	.500	.500	.500
	48	CP	139.58	.906	.808	.857	.328	.328	.328
9	46	saturated	148.70	.551	.399	.426	.089	.089	.089
	46	CP	163.12	.754	.505	.476	.418	.395	.418
	48	Pajak and Addelman $3 \times 2^{9-5}$	163.30	.725	.358	.545	.791	.894	.791
	48	CP	166.92	.785	.539	.550	.464	.631	.464
	64	Addelman's (4/32) 2 <sup>9</sup>	182.99	.835	.657	.750	.577	.577	.577
	64	Mee's D-optimal	185.63	.884	.745	1	.000	.612	.000
	64	CP*	187.55	.922	.840	.818	.281	.239	.281
	96	John's (3/4) 2 <sup>9-2</sup>	206.11	.920	.814	.935	.333	.500	.333
	96	CP*	209.04	.980	.960	.955	.103	.126	.103
10	56	CP*	208.32	.737	.453	.464	.440	.589	.440
	64	Addelman's (4/64) 2 <sup>10</sup>	218.34	.771	.538	.588	.707	.707	.707
	64	Mee's D-optimal	222.04	.824	.646	1.	.000	.500	.000
	64	CP*	222.74	.834	.657	.650	.351	.386	.351
	96	John's (3/4) 2 <sup>10-3</sup>	250.93	.920	.821	.909	.333	.500	.333
	96	CP <sup>⋆</sup>	253.16	.957	.913	.921	.143	.158	.143
11	68	CP*	263.81	.754	.438	.434	.582	.631	.582
	80	Addelman's (5/128) 2 <sup>11</sup>	267.78	.680	.385	.451	.750	.756	.750
	80	CP*	285.20	.882	.736	.750	.323	.324	.323
	96	John's (3/4) 2 <sup>11-4</sup>	299.10	.905	.791	.815	.500	.500	.500
	96	CP*	301.54	.938	.873	.873	.166	.185	.166
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optimal designs of Mee (1999). All of these designs, except for the saturated designs with k of 7 or 8, are equireplicated designs. The minimal run CP designs are listed in the Appendix.

We can draw several conclusions from Table 1. First, except for the saturated design with k=6, the CP algorithm was always able to find an equireplicated design with higher D than the alternatives from the literature. Second, although we did not show both CP and CP\* results for the same n, k pairs, the CP and CP\* algorithms generally give similar optima, with the CP usually, but not always, yielding a higher D. The difference between the two is typically not enough to encourage the use of the slower CP algorithm. Third, information per observation generally increases as n increases for fixed k.

Although we have not shown all 200 local optima found for each n and k combination, it is of interest to know how good the other 199 designs are. Consider the  $D_e$  criterion for a given n and k combination, and divide all 200  $D_e$ 's obtained from the different starts by the maximal  $D_e$ . For 16 different n,k pairs studied, the upper quartile of the relative  $D_e$  was .94 for one pair and was above .97 for the remaining 15 pairs. Thus the best of ten random starts will typically be very close to the best of 200 random starts. The worst case designs had relative  $D_e$  of about .4.

Mee (1999) stated that saturated designs should not be used for k larger than 7, and we certainly agree. Both  $D_e$  and A drop rather dramatically for k > 7, although the saturated designs do have low correlations between estimated effects.

The equivalent family fractional designs of Pajak and Addelman (1975) for k = 6, n = 24 and k = 9, n = 48 are also not very attractive. Both have low  $D_e$ , very low A, and correlations greater than .7; corresponding CP and CP\* designs are better on every measure.

The sequence of fractions designs of Addelman (1969) are reasonably competitive on  $D_e$ , but tend to have poor A criteria and large correlations. The corresponding CP and CP\* designs are better on every measure.

The 3/4 replicate designs of John (1969) have good D-criteria, but are a little lower on the A criteria. The major problem with these designs is several correlations of .5 between estimates. Once again, the CP and CP\* designs are better on every measure.

Finally, the designs of Mee (1999) are good on  $D_e$  and A, and are outstanding for the main effects: orthogonal and fully A-efficient. They do have some large correlations between main effects and interactions.

Overall, the algorithmically-produced designs, either the CP-type designs presented here or those of Mee, have better properties than the algebraically-derived designs. They can also be constructed for a much broader range of n. Algorithmic designs do, of course, suffer from the necessity of searching for the optimal design.

# 4 Efficiency in Central Composite Designs

When a resolution V fraction is combined with axial points, we obtain a central composite design that can fit a second-order polynomial model. Classical CCD's use regular resolution V fractions, but these can be larger than is necessary. As was described in Section 1, considerable work has been done to find smaller composite designs that still enable estimate of the second-order model.

In this section we investigate the use of our CP fractions in CCD's. These designs will not usually be saturated designs; that is, CCD formed using our CP fractions will not usually be the

Table 2: CCD Efficiencies

k	n	Design	$df_e$	$D_e$	$D_l$	$D_q$	$D_i$
5	22	Draper & Lin's P-B	.955	.259	.130	.140	.197
	22	Westlake's irregular	.955	.272	.141	.117	.226
	26	Saturated	.808	.440	.692	.122	.615
6	28	Draper & Lin's P-B	1	.263	.071	.111	.237
	34	CP	.824	.395	.488	.091	.527
7	38	Draper & Lin's P-B	.947	.229	.083	.082	.209
	38	Westlake's irregular	.947	.229	.088	.069	.214
	44	CP	.818	.391	.492	.071	.539
	62	John's 3/4	.581	.439	.666	.052	.702
	62	CP	.581	.450	.758	.052	.734
8	52	Draper & Lin's P-B	.865	.284	.157	.060	.323
	54	CP	.833	.384	.434	.057	.532
	64	John's 3/4	.703	.427	.609	.049	.648
	64	CP	.703	.431	.631	.049	.659
9	58	Draper & Lin's P-B	.948	.155	.050	.036	.137
	62	Westlake's irregular	.887	.245	.078	.049	.267
	64	CP	.859	.372	.407	.047	.509
	82	Mee's irregular	.671	.433	.805	.038	.667
	82	CP	.671	.449	.670	.038	.705
	114	John's 3/4	.482	.451	.817	.027	.759
	114	CP	.482	.476	.823	.027	.821
10			0.54	100	0.45	0.4.4	201
10	68	Draper & Lin's P-B	.971	.199	.046	.044	.201
	76	CP	.868	.372	.412	.039	.511
	84	Mee's irregular	.786	.411	.786	.036	.599
	84	CP	.786	.416	.533	.036	.611
	116	John's 3/4	.569	.460	.693	.025	.722
	116	CP	.569	.475	.731	.025	.754

smallest possible design. Nevertheless, these designs are smaller than the standard regular fractions and are fairly efficient per unit.

We propose the following measures of efficiency for the CCD's that we will compare. First is degree of freedom efficiency,  $df_e = q/n$ , which is essentially a measure of design size relative to minimum size. The other four measures are forms of D-efficiency:

$$D_{e} = |V|^{-1/q}/n$$

$$D_{l} = |V_{l}|^{-1/k}/n$$

$$D_{q} = |V_{q}|^{-1/k}/n$$

$$D_{i} = |V_{i}|^{-2/(k(k-1))}/n$$

where  $V=(\tilde{X}'\tilde{X})^{-1}$ , and  $V_l$ ,  $V_q$ , and  $V_i$  are the submatrices of V corresponding to linear, quadratic, and interaction terms. These D-efficiencies are information per parameter per observation. All of our designs will have  $\alpha=1$ , so the maximum value of the D-efficiencies is 1. Higher  $df_e$  designs are smaller, but lower  $df_e$  designs tend to have better D-efficiencies.

We compare the CP-based CCD's to those suggested by Westlake (1965) and Draper and Lin (1990), as well as those using the irregular resolution V fractions of John (1969) and Mee (1999). From Table 2 we can see that CP-based designs are generally higher on all all D-criteria than competitors with the same n. The notable exceptions are for estimating linear effects with k = 9, 10, for which Mee's designs are much more efficient. As with Table 1, information per observation generally increases as sample size increases; a slightly larger design can often have much larger D-efficiency.

#### 5 Discussion and Conclusions

Resolution V CP designs have attractive efficiencies when used both as irregular fractions and as a basis for central composite designs. They can be constructed for a much broader range of sample sizes than are available with standard irregular fractions, giving experimenters more flexibility in trading off size and availability of efficient designs.

Computation time is an issue for larger designs. Running on a 1.4 GHz Pentium IV, a n=22, k=6 optimization takes about .6 seconds, whereas a n=116, k=10 optimization takes about 9.3 seconds with our current code. Large designs, say n=212, k=20, cannot be done interactively.

The CP algorithm as described is optimizing the D criterion. There is nothing to prevent optimization of an alternate criterion. For example, modifying the algorithm so that it maximizes the A-efficiency is straightforward. Using A-optimality, the CP algorithm yields the same design as D-optimality for n=22, k=6, but for n=64, k=9 yields a design with a slightly lower A-efficiency criterion than the design found when optimizing D-efficiency!

The optimality criteria tend to have many local optima, suggesting that several random starts should be attempted to try to avoid poor local optima. Simulation results indicate that 20 random starts should be sufficient with high probability.

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Table 1: Resolution V CP design for k = 6 and n = 22.

# 7 Appendix: CP Designs

Table 2: Resolution V CP design for k=7 and n=30.

Table 3: Resolution V CP design for k = 8 and n = 38.

Table 4: Resolution V CP design for k = 9 and n = 46.

Table 5: Resolution V CP design for k=10 and n=56.

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Table 6: Resolution V CP design for k=11 and n=68.

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