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Making Experimental Designs Robust Against Time Trend

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Abstract

In numerous experimental settings, engineers and scientists might be obliged to run their experiments in sequence and so the run order of the experimental units must be taken into account. This paper describes an approach to construct experimental designs such that the main effects, 2-factor interactions and quadratic effects are orthogonal or near-orthogonal to the linear and quadratic trends. Some constructed designs will then be compared with those of John (1990). Some trend-free Box-Behnken designs will also be given.

Keywords: Box-Behnken designs; computer-aided designs; A-optimality; D-optimality; optimality; fractional factorial designs; interchange algorithm; response surface designs; trend-free designs.

1 Introduction

Certain experimenal materials such as food may deteriorate over time and therefore, there is a need for designs which are robust against time trend (or trend-free designs). Consider an experiment to study the effects of processing time, temperature and shear stress caused by pumping on the quality of skim milk powder. The milk for this entire experiment is blended and stored at 4^0C in milk cans. It is used over a week for a series of experimental runs. Because the milk quality will deteriorate over the week, the scientist is keen to have a design whose runs are in a particular order such that its main effects, interactions and quadratic effects are orthogonal or near-orthogonal to the time trend.

Daniel & Wilcoxon (1966) constructed plans for 2^n factorial designs whose main effects are orthogonal to the time trend. Noting the connection between these designs and fold-over designs, John (1990) developed trend-free sequences for both 2^n and 3^n factorials. Atkinson & Donev (1996) developed the first determinant-based algorithm, called BT, to construct trend-free designs. These designs include factorial designs and response surface designs. The BT algorithm generates designs from scratch. The paper of Atkinson & Donev (1996) also includes extensive references on trend-free designs.

The approach used in this paper is to arrange the runs of an experimental design such that the main effects, 2-factor interactions and quadratic effects (derived variables), are orthogonal or near-orthogonal to the linear (and quadratic) time trend. This approach is similar to the design blocking approach used in Nguyen (2001) where the runs are arranged such that the mentioned variables are orthogonal or near-orthogonal to the blocking variables. Section 2 describes a design criterion which is closely related to the D-optimality criterion used by Atkinson & Donev (1996) and an algorithm called RAT (robust against trend) which implements the mentioned approach and design criterion. Section 3 compares designs constructed by RAT and those of John (1990). Section 4 presents some Box-Behnken designs which are $L+$ (orthogonal to the linear trends).

2 A new approach to constructing trend-free designs

The uth row of the extended design matrix X for n runs with t trend columns, m factors and $p-1-m-t$ derived variables is $(w_{u1}, \ldots, w_{ut}, 1, x_{u1}, \ldots, x_{um}, \ldots, x_{u(p-1-t)})$. Partition X as $(\mathbf{W}|\mathbf{X})$ and $X'X$ as:

$$\left(\begin{array}{c|c} \mathbf{W}'\mathbf{W} & \mathbf{W}'\mathbf{X} \\ \hline \mathbf{X}'\mathbf{W} & \mathbf{X}'\mathbf{X} \end{array}\right). \tag{1}$$

The condition for columns of $\mathbf{X}$ to be trend-free is that these columns be orthogonal to the columns of $\mathbf{W}$, i.e. $\mathbf{W}'\mathbf{X}=\mathbf{0}$. Our suggested approach is to first find a suitable design and then allocate the n runs of this design to the n time points such that the resulting design is A- or D-optimal. In the next paragraph, we will show that a quick way to do this is to minimize f where f is the sum of squares of the elements of $\mathbf{W}'\mathbf{X}$.

Let $M = X'X$. Without loss of generality, let's assume that M to be of full rank. Let $\lambda_1, \ldots, \lambda_p$ be the eigenvalues of M. Since trace$(M) = \sum \lambda_i$ =constant and trace$(MM) = \sum \lambda_i^2$, minimizing f (*i.e.* minimizing the sum of squares of the elements of $\mathbf{W}'\mathbf{X}$) which is equivalent to minimizing trace(MM) is the same as making the λ_i's as equal as possible with $\sum \lambda_i$=constant. This is an approximation of A-optimality criterion which requires the minimization of $\sum \lambda_i^{-1}$ (=trace(M^{-1})), or the D-optimality criterion which requires the maximization of $\Pi\lambda_i$ (=$|M|$)(see Kiefer 1959). In a sense, it is closely allied to the (M, S)-optimality criterion introduced by Eccleston & Hedayat (1974) in the incomplete block designs context.

Before discussing the RAT algorithm which implements the aforementioned approach, we will present some matrix results. Let the ith and uth row vectors of $\mathbf{X}$ be $\mathbf{x}_i$ and $\mathbf{x}_u$. The corresponding vectors $\mathbf{W}$ are $\mathbf{w}_i$ and $\mathbf{w}_u$. It can then easily be shown that the effect on M by swapping the ith and uth row of $\mathbf{X}$ is the same as adding the following matrix to $\mathbf{W}'\mathbf{X}$:

$$-(\mathbf{w}_i - \mathbf{w}_u)'(\mathbf{x}_i - \mathbf{x}_u). \tag{2}$$

The RAT algorithm based on the above matrix result is as follows:

1. Construct a starting trend-free design $\mathbf{X}$ by randomly allocating the design runs to the time points. Calculate f, the sum of squares of the elements of $\mathbf{W}'\mathbf{X}$.

2. Repeat searching a pair of ith and uth runs of $\mathbf{X}$ such that the swap of these two rows results in the biggest reduction in f. If the search is successful, swap these two rows, update $\mathbf{W}'\mathbf{X}$ using (2). This process is repeated until $f = 0$ or f cannot be reduced further.

3. Calculate $|M|$ and $TF = \{(|X'X|/|\mathbf{W}'\mathbf{W}|)/|\mathbf{X}'\mathbf{X}|\}^{1/(p-t)}$, the trend factor (See Atkinson & Donev, 1996, p. 334).

Each *try* consists of Steps 1-3. Several tries are made for each design and the one with the smallest f will be chosen. The algorithm stops when the number of tries is exhausted or when $f = 0$ (i.e. $TF = 1$).

The following example will illustrate the steps of the RAT algorithm in constructing a 2^3 fractional factorial in 15 runs when three runs are allowed at each time point:

(A)				(B)				(C)			
-1	1	1	1	-1	1	1	1	-1	1	1	1
-1	-1	-1	1	-1	1	-1	-1	-1	1	-1	-1
-1	1	-1	-1	-1	1	-1	1	-1	-1	-1	-1
-0.5	-1	1	-1	-0.5	-1	1	1	-0.5	-1	1	1
-0.5	1	1	-1	-0.5	-1	-1	1	-0.5	-1	-1	1
-0.5	-1	1	1	-0.5	-1	1	-1	-0.5	-1	1	-1
0	-1	1	1	0	1	1	-1	0	1	1	-1
0	1	-1	-1	0	1	1	-1	0	1	1	-1
0	-1	-1	-1	0	-1	-1	-1	0	1	-1	1
0.5	-1	-1	1	0.5	-1	-1	1	0.5	-1	-1	1
0.5	-1	-1	-1	0.5	-1	1	-1	0.5	-1	1	-1
0.5	1	1	-1	0.5	-1	1	1	0.5	-1	1	1
1	1	1	1	1	1	-1	-1	1	1	-1	-1
1	1	-1	1	1	-1	-1	-1	1	-1	-1	-1
1	-1	1	-1	1	1	1	1	1	1	1	1

(A) is the design D4 in Table 5 of Atkinson & Donev (1996), p. 337. For this design $f = 20$, $|M| = 9.060E + 8$ and $TF = 0.9686$. (B) illustrates Step 1 where the runs of D4 (columns 2-4) are randomly allocated to the time point (column 1). The resulting design has $f = 16$. (C) illustrates Step 2 where the 3rd and 9th runs are swapped. The resulting design is trend free with $f = 0$, $|M| = 1.133E + 9$ and $TF = 1$.

3 Comparing RAT designs with those of John (1990)

Most trend-free designs constructed by John (1990) and those of RAT are similar. There are exceptions which will be dealt with later. The following is an example of an orthogonal array (OA) $L_{16}(2^{11})$ which is $L+$ constructed by allocating the rows of an $L_{16}(2^{11})$ to the time points (the first column).

-1.0000	1	1	-1	-1	-1	1	-1	-1	1	1	-1
-0.8667	-1	-1	-1	1	-1	-1	1	1	-1	1	-1
-0.7333	-1	1	-1	1	1	1	1	-1	-1	-1	1
-0.6000	1	-1	-1	-1	1	-1	-1	1	1	-1	1
-0.4667	1	1	1	1	-1	-1	-1	1	-1	-1	1
-0.3333	-1	-1	1	-1	-1	1	1	-1	1	-1	1
-0.2000	-1	1	1	-1	1	-1	1	1	1	1	-1
-0.0667	1	-1	1	1	1	1	-1	-1	-1	1	-1
0.0667	1	-1	1	-1	1	1	1	1	-1	-1	-1
0.2000	-1	1	1	1	1	-1	-1	-1	1	-1	-1
0.3333	-1	-1	1	1	-1	1	-1	1	1	1	1
0.4667	1	1	1	-1	-1	-1	1	-1	-1	1	1
0.6000	1	-1	-1	1	1	-1	1	-1	1	1	1
0.7333	-1	1	-1	-1	1	1	-1	1	-1	1	1
0.8667	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1
1.0000	1	1	-1	1	-1	1	1	1	1	-1	-1

The trend column (first column) was constructed by scaling a column of numbers $(1, \ldots, 16)'$, i.e. by subtracting each number from their mean and then dividing the resulting number by the biggest one. The 1st, 4th, 6th and 11th columns of the above designs are *kept* columns (a column whose elements in the second half are the same as those in the first half). The remaining columns are *folded* columns (columns whose elements in the second half are obtained by reversing the signs of those in the first half). The concept of *kept* and *folded* columns are due to John (1990). This design corresponds to Plan 7 of John (1990), p. 278. John used the 11 interactions of the 2^4 factorial to construct this design.

Another method to construct the above design is to start with an orthogonal array $L_8(2^7)$ and fold it over. We then use the NOA program of Nguyen (1996a,b) to add four 2-level columns to this design such that the new columns are orthogonal to one another, to the column representing the linear trend and to the folded columns.

The following is a trend-free 2^4 factorial constructed by allocating the runs of a 2^4 factorial to the time points (the first two columns):

-1.0000	1.0000	1	1	-1	1
-0.8667	0.6000	-1	-1	-1	-1
-0.7333	0.2571	-1	1	1	-1
-0.6000	-0.0286	1	-1	1	1
-0.4667	-0.2571	1	-1	1	-1
-0.3333	-0.4286	-1	1	1	1
-0.2000	-0.5429	-1	-1	-1	1
-0.0667	-0.6000	1	1	-1	-1
0.0667	-0.6000	-1	-1	1	-1
0.2000	-0.5429	1	1	1	1
0.3333	-0.4286	1	-1	-1	1
0.4667	-0.2571	-1	1	-1	-1
0.6000	-0.0286	-1	1	-1	1
0.7333	0.2571	1	-1	-1	-1
0.8667	0.6000	1	1	1	-1
1.0000	1.0000	-1	-1	1	1

The second trend column was constructed by scaling a column obtained by squaring each element of the first trend column. All columns in this design are folded columns. Like plan DW of John (1990), p. 275, all main effects are $L+$ and $Q+$ (orthogonal to the linear and quadratic trends). The correlations of the interactions AD, BD and CD with the linear trend are 0.217, -0.108 and 0.434 (see additional discussion in John, 1990).

To construct the above design, RAT uses two objective functions g and f. Partition $\mathbf{X}$ as $(\mathbf{X}_1|\mathbf{X}_2)$ where $\mathbf{X}_1$ is an $n \times (1+m)$ matrix, then g is the sum of squares of the elements $\mathbf{W}'\mathbf{X}_1$. A design is selected if it has a smaller g than the previous design or the same g but smaller f (the sum of squares of the elements of $\mathbf{W}'\mathbf{X}$).

The following is a coded plan of an $L_{18}(3^6)$ which is $L+$. This plan was constructed by coding levels 1, 2 and 3 in columns 2-7 of the $L_{18}(2 \cdot 3^7)$ in Taguchi (1987) p. 36 with the corresponding coefficients in the orthogonal polynomials, i.e. $(-1\ 1), (0\ \ -2)$ and $(1\ 1)$ and allocating the rows of the coded plan to the time points (the first column).

-1.0000	0	-2	-1	1	-1	1	0	-2	0	-2	1	1
-0.8824	0	-2	0	-2	0	-2	1	1	1	1	-1	1
-0.7647	0	-2	1	1	1	1	-1	1	-1	1	0	-2
-0.6471	-1	1	1	1	1	1	1	1	1	1	1	1
-0.5294	-1	1	-1	1	-1	1	-1	1	-1	1	-1	1
-0.4118	-1	1	0	-2	0	-2	0	-2	0	-2	0	-2
-0.2941	1	1	-1	1	0	-2	-1	1	1	1	0	-2
-0.1765	1	1	0	-2	1	1	0	-2	-1	1	1	1
-0.0588	1	1	1	1	-1	1	1	1	0	-2	-1	1
0.0588	1	1	0	-2	-1	1	1	1	-1	1	0	-2
0.1765	1	1	1	1	0	-2	-1	1	0	-2	1	1
0.2941	1	1	-1	1	1	1	0	-2	1	1	-1	1
0.4118	-1	1	1	1	0	-2	0	-2	-1	1	-1	1
0.5294	-1	1	-1	1	1	1	1	1	0	-2	0	-2
0.6471	-1	1	0	-2	-1	1	-1	1	1	1	1	1
0.7647	0	-2	0	-2	1	1	-1	1	0	-2	-1	1
0.8824	0	-2	1	1	-1	1	0	-2	1	1	0	-2
1.0000	0	-2	-1	1	0	-2	1	1	-1	1	1	1

The transpose of the decoded plan is given below. Unlike Plan 16 of John (1990), no pattern is observed in this plan.

2	2	2	1	1	1	3	3	3	3	3	3	1	1	1	2	2	2
1	2	3	3	1	2	1	2	3	2	3	1	3	1	2	2	3	1
1	2	3	3	1	2	2	3	1	1	2	3	2	3	1	3	1	2
2	3	1	3	1	2	1	2	3	3	1	2	2	3	1	1	2	3
2	3	1	3	1	2	3	1	2	1	2	3	1	2	3	2	3	1
3	1	2	3	1	2	2	3	1	2	3	1	1	2	3	1	2	3

Most trend free designs in John (1990) relate to an orthogonal structure. When there is no related orthogonal structure, then RAT designs are better than those of John (1990). (A) is a near-OA $L'_{12}(2^5)$ of John (1990) which is $L+$ and near-$Q+$ (Plan 8). This plan is constructed by folding a resolution III plan for five factors in six runs. (B) is an OA $L_{12}(2^5)$ which is near-$L+$ and near-$Q+$. This design is constructed by allocating the runs of an $L_{12}(2^5)$ to the time points (the first two columns). Although the columns of this design are not $L+$ like Plan 8 of John (1990), it has two main advantages over John's: (i) its columns are mutually orthogonal and (ii) the correlations of its columns with the trend columns in term of absolute value are very small (< 0.01).

(A)

-1.0000	1.0000	-1	-1	-1	-1	-1
-0.8182	0.4546	1	1	1	1	-1
-0.6364	0.0182	1	1	1	-1	1
-0.4546	-0.3091	1	-1	-1	1	1
-0.2727	-0.5273	-1	1	-1	1	1
-0.0909	-0.6364	-1	-1	1	-1	-1
0.0909	-0.6364	1	1	1	1	1
0.2727	-0.5273	-1	-1	-1	-1	1
0.4546	-0.3091	-1	-1	-1	1	-1
0.6364	0.0182	-1	1	1	-1	-1
0.8182	0.4546	1	-1	1	-1	-1
1.0000	1.0000	1	1	-1	1	1

(B)

-1.0000	1.0000	-1	-1	-1	-1	-1
-0.8182	0.4545	1	1	1	-1	1
-0.6364	0.0182	1	1	-1	1	1
-0.4545	-0.3091	1	-1	1	1	-1
-0.2727	-0.5273	-1	1	1	1	-1
-0.0909	-0.6364	-1	-1	-1	1	1
0.0909	-0.6364	-1	1	1	-1	1
0.2727	-0.5273	1	-1	-1	-1	1
0.4545	-0.3091	1	-1	1	-1	-1
0.6364	0.0182	-1	1	-1	-1	-1
0.8182	0.4545	1	1	-1	1	-1
1.0000	1.0000	-1	-1	1	1	1

4 $L+$ *Box-Behnken* designs

Box & Behnken (1960) proposed some response surface designs with factors at three levels (-1, 0, 1) known as Box-Behnken designs (BBDs). BBDs are formed by combining 2^k factorials with incomplete block designs. BBDs are very popular as there are many situations where researchers are restricted to three equally-spaced levels. Hinkelmann & Jo (1998) described a mathematical approach to construct $L+$ BBDs. The webpage `http://designcompting.net/LplusBBD/` lists $L+$ BBDs constructed by the RAT approach for three factor in 15 runs, four factors in 27 runs, five factors in 46 runs, six factors in 54 runs and seven factors in 62 runs. The main effects, interactions and quadratic effects of the listed BBDs are all orthogonal to the linear trend. In the presence of time trend, these designs are better alternative to randomized BBDs or blocked BBDs.

The byte code of the Java program implementing the RAT algorithm discussed in this paper is available free of cost from the author. Additional examples of designs obtained by RAT can be found at `http://designcomputing.net/gendex/rat/`.

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