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TREND-RESISTANT DESIGN OF EXPERIMENTS UNDER BUDGET CONSTRAINTS

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Abstract

When experiments are to be performed in a time sequence, the observed responses are affected by a time trend. The construction of trend-resistant run orders is extensively described in the literature. However, run orders that are optimally balanced for time trends usually involve huge costs and they are often of low practical value in view of economical considerations. This paper presents a design algorithm for the construction of trend-resistant run orders under budget constraints. The algorithm offers the experimenter a general method for solving a wide range of practical design problems.

Keywords: optimal design of experiments; time trends; trend-resistance; cost; budget constraint; run order

1 Introduction

Performing experiments in a time sequence may result in observed responses that are influenced by a temporal trend. For instance, Freeny and Lai (1997) study an experiment conducted to evaluate the performance of a polisher used in the fabrication of chips in the electronics industry. The goal was to find the maximum rate of oxide removal which could be used without degrading the uniformity of the removal over the wafer surface. However, the polisher removal rate showed a tendency to drift lower through time. Another time dependence occurs when a batch of material is created at the beginning of an experiment and treatments are to be applied to experimental units formed from the material over time. As a consequence, there will be a temporal effect due to the aging of the material. Other variables that affect observations obtained in some specific order are equipment wear-out, learning, analyst fatigue, etc.

The aim of this paper is to present a method for the construction of budget constrained designs that are highly resistant to the time trend. Section 2 gives a survey on cost-efficient and trend-resistant experimental design. Trend-resistant design of experiments under budget constraints is thoroughly dealt with in Section 3 and our proposed design algorithm is outlined in Section 4. Section 5 illustrates practical utility.

2 Trend effects and costs in experimental design

Henceforth, let y denote the response of interest and $\mathbf{f}(\mathbf{x})$ the $p \times 1$ vector representing the polynomial expansion of design point $\mathbf{x}$ for the response model. Besides, $\mathbf{g}(t)$ represents the $q \times 1$ vector of the polynomial expansion for the time trend, expressed as a function of time t. With $\boldsymbol{\alpha}$ the $p \times 1$ vector of important parameters and $\boldsymbol{\beta}$ the $q \times 1$ vector of parameters of the polynomial time trend, the model for the response is given by

$$y = \mathbf{f}'(\mathbf{x})\boldsymbol{\alpha} + \mathbf{g}'(t)\boldsymbol{\beta} + \varepsilon. \tag{1}$$

The independent error terms ε are assumed to have expectation zero and constant variance σ^2. It is convenient to rewrite (1) as

$$\mathbf{y} = \mathbf{F}\boldsymbol{\alpha} + \mathbf{G}\boldsymbol{\beta} + \boldsymbol{\varepsilon},$$

with $\mathbf{y}$ an $n \times 1$ vector of responses and $\mathbf{F}$ and $\mathbf{G}$ the $n \times p$ and the $n \times q$ extended design matrices respectively.

2.1 Trend-resistant design of experiments

There is a vast literature on the existence and the construction of trend-resistant designs. An extensive overview can be found in Tack and Vandebroek (1999). However, the approaches are mainly restricted to two or three level factorials, equally spaced time points and regular design spaces. The only exception is the approach of Atkinson and Donev

(1996) who present an algorithm to treat almost any design problem. They construct exact optimal designs that maximize the information on the important parameters $\boldsymbol{\alpha}$, whereas the q parameters modeling the time dependence are treated as nuisance parameters. We call the corresponding design the $\mathcal{D}_t$-optimal design $\delta_{\mathcal{D}_t}$ and it is found by maximizing

$$\mathcal{D}_t = |\mathbf{F}'\mathbf{F} - \mathbf{F}'\mathbf{G}(\mathbf{G}'\mathbf{G})^{-1}\mathbf{G}'\mathbf{F}|^{\frac{1}{p}}. \tag{2}$$

Note that in the absence of time trend effects, the $\mathcal{D}_t$-optimal design equals the $\mathcal{D}$-optimal design $\delta_{\mathcal{D}}$ that maximizes $\mathcal{D} = |\mathbf{F}'\mathbf{F}|^{\frac{1}{p}}$. Bradley and Yeh (1980) define a design to be trend-free if it completely eliminates the effects of the postulated time trend over the experimental units or if the least-squares estimates of the factorial effects of interest are free of bias that might be introduced from the unknown trend effects in $\boldsymbol{\beta}$. This means that a trend-resistant design is obtained if and only if each time trend component is orthogonal to the treatment effects or, equivalently, if and only if $\mathbf{F}'\mathbf{G} = \mathbf{0}$. To compare the $\mathcal{D}$- and the $\mathcal{D}_t$-optimal design with respect to information about the important parameters $\boldsymbol{\alpha}$, the generalized variance of $\boldsymbol{\alpha}$ is compared through

$$\frac{\mathcal{D}_t(\delta_{\mathcal{D}_t})}{\mathcal{D}(\delta_{\mathcal{D}})} \tag{3}$$

denoting the protection of the $\mathcal{D}_t$-optimal design $\delta_{\mathcal{D}_t}$ against time order dependence. Henceforth, we call (3) the degree of trend-resistance of the $\mathcal{D}_t$-optimal design.

Although $\mathcal{D}_t$-optimal designs have good statistical properties, there are practical circumstances where they may not be fit for use because of economical reasons. Generally speaking, the difficulty is to strike a balance between cheap but ineffective designs and costly designs with a high degree of trend-resistance. Consider as an example the response model $\mathbf{f}'(\mathbf{x}) = (1\ x_1\ x_2\ x_3\ x_1x_2\ x_1x_3\ x_2x_3)$ and design points to be taken from the 2^3-factorial. Assume also that the observed responses are influenced by a linear time trend $\mathbf{g}(t) = t$. Figure 1 shows the cost and the $\mathcal{D}_t$-value of all 8! possible run orders. The cost of a run order is calculated as the number of factor level changes over the course of the experiment. The area of the circles in Figure 1 is proportional to the number of run orders found with the associated cost and information. The plot shows that the cheapest run orders with only seven or eight level changes have rather low $\mathcal{D}_t$-values whereas the most informative run orders with a $\mathcal{D}_t$-value larger than 7.5 involve higher numbers of level changes. As a result, cost considerations often limit the usefulness of highly trend-resistant designs.

2.2 Cost-efficient design of experiments

Until recently, cost considerations have rarely been taken into account in optimal design theory. A few authors consider the costs associated with particular treatment combinations. These costs include equipment costs, the cost of material, the cost of personnel, the cost for spending time during the experiment, etc. A second cost approach results

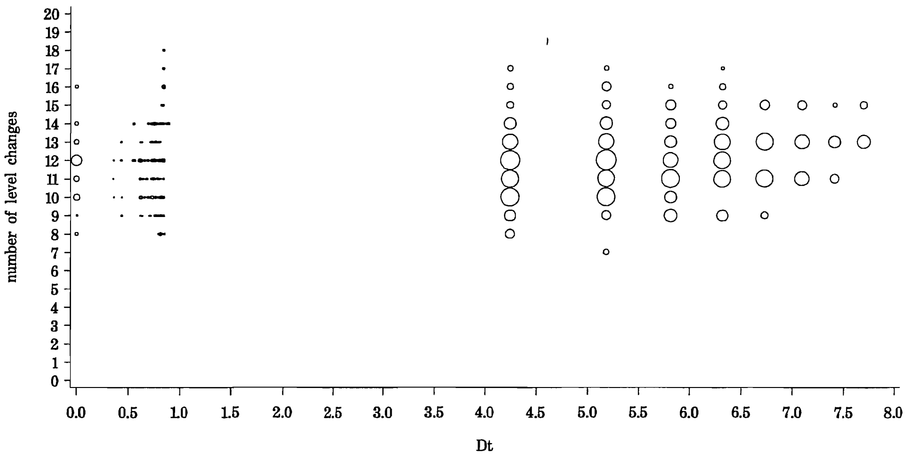


Figure 1: Cost and Information of the 2^3-Factorial Run Orders

from the fact that it is usually expensive to alter the factor levels from one observation to another. Factors such as oven temperature or line set-up are often referred to as hard-to-change factors. In order to minimize the total cost, the number of factor level changes has to be kept low. With the exception of Tack and Vandebroek (1999), we found no reference that deals with both cost approaches. They call the cost associated with the factor level combination $\mathbf{x}_i$ the measurement cost at design point $\mathbf{x}_i$, i.e. $c^m(\mathbf{x}_i)$. The mathematical representation is

$$c^m(\mathbf{x}_i) = \mathbf{m}'(\mathbf{x}_i)\boldsymbol{\varsigma},$$

where $\mathbf{m}(\mathbf{x}_i)$ is a column vector with p_m elements representing the polynomial expansion of design point $\mathbf{x}_i$ for the measurement cost and $\boldsymbol{\varsigma}$ is a $p_m \times 1$ vector of coefficients. The total measurement cost C^m of an experiment equals the weighted sum of the measurement costs at the d different design points, or, mathematically,

$$C^m = \sum_{i=1}^{d} n_i c^m(\mathbf{x}_i),$$

where n_i denotes the number of replicates at design point $\mathbf{x}_i$. The cost for changing the factor levels of design point $\mathbf{x}_i$ in the previous run to the factor levels of design point $\mathbf{x}_j$ in the next run is referred to as the transition cost $c^t(\mathbf{x}_i, \mathbf{x}_j)$ from design point $\mathbf{x}_i$ to design point $\mathbf{x}_j$. The transition cost is defined as

$$c^t(\mathbf{x}_i, \mathbf{x}_j) = \mathbf{t}'(\mathbf{x}_i, \mathbf{x}_j)\boldsymbol{\tau},$$

where $\mathbf{t}(\mathbf{x}_i, \mathbf{x}_j)$ is a $p_t \times 1$ vector representing the polynomial expansion of design points $\mathbf{x}_i$ and $\mathbf{x}_j$ for the transition cost and $\boldsymbol{\tau}$ is a column vector with p_t coefficients. The total transition cost C^t of a run order equals

$$C^t = \sum_{i=1,j=1}^{d} n_{i,j} c^t(\mathbf{x}_i, \mathbf{x}_j),$$

where $n_{i,j}$ denotes the number of transitions from design point $\mathbf{x}_i$ to design point $\mathbf{x}_j$ in the considered run order. In contrast with the total measurement cost C^m, the total transition cost C^t of a run order depends on the sequence in which the observations are taken. The total cost C of a run order simply equals the sum of the total measurement cost and the total transition cost.

2.3 Trend-resistant and cost-efficient design of experiments

Tack and Vandebroek (1999) introduce a new optimality criterion that strikes a balance between cost-efficiency and trend-resistance. This optimality criterion prefers designs that maximize the amount of information on the important parameters $\boldsymbol{\alpha}$ per unit cost. The $(\mathcal{D}_t, C)$-optimality criterion is defined as

$$(\mathcal{D}_t, C) = |\mathbf{F}'\mathbf{F} - \mathbf{F}'\mathbf{G}(\mathbf{G}'\mathbf{G})^{-1}\mathbf{G}'\mathbf{F}|^{\frac{1}{p}}/C. \tag{4}$$

Based on (4), Tack and Vandebroek (1999) present a generic design algorithm for the construction of $(\mathcal{D}_t, C)$-optimal run orders and Tack and Vandebroek (2000) extend the algorithm to incorporate designs with either fixed or random block effects.

Consider as an example an experiment with $n = 36$ observations. The design points constitute the full 3^2-factorial and the assumed response model is given by

$$\mathbf{f}'(\mathbf{x}) = (1 \ x_1 \ x_2 \ x_1x_2 \ x_1^2 \ x_2^2).$$

Besides, a linear time trend $\mathbf{g}(t) = t$ is postulated. The measurement costs are supposed to be proportional to the levels of x_1 and x_2 and they are shown in Figure 2. The horizontal axis relates to factor x_1 and the vertical axis is the x_2-axis.

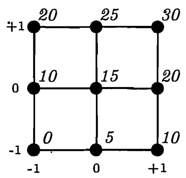


Figure 2: Measurement Costs at the Different Design Points

The transition costs for both factors are shown in Figure 3. For instance, the cost for changing factor x_1 or x_2 from level 0 in the previous run to the low or the high level in the next run equals 2.5 and changing a factor from the high level to the low level or vice versa costs 10.

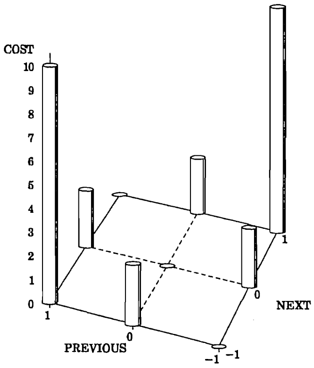
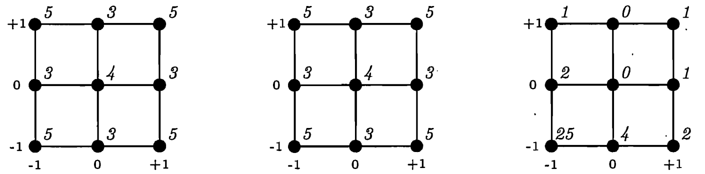


Figure 3: Transition Costs for Factors x_1 and x_2

The computed $\mathcal{D}$-, $\mathcal{D}_t$- and $(\mathcal{D}_t, C)$-optimal designs are shown in Figure 4. There is no difference between the $\mathcal{D}$- and the $\mathcal{D}_t$-optimal design, whereas the numbers of replicates n_i for the $(\mathcal{D}_t, C)$-optimal design are quite different. When costs are calculated for, the cheapest design point (-1,-1) is replicated many times more and the cheap design point (0,-1) is replicated once more. All other design points are more expensive and are replicated less.



(a) $\mathcal{D}$-optimality (b) $\mathcal{D}_t$-optimality (c) $(\mathcal{D}_t, C)$-optimality

Figure 4: Optimal Designs

As an illustration, the $\mathcal{D}_t$- and the $(\mathcal{D}_t, C)$-optimal run orders are shown in Table 1 and Table 2 respectively. It can easily be seen that the $\mathcal{D}_t$-optimal run order has more factor level changes than the $(\mathcal{D}_t, C)$-optimal one. Table 3 presents a comparison of the optimal run orders in terms of the procentual degree of trend-resistance and the total cost. The $\mathcal{D}_t$-optimal run order is nearly optimally balanced for time trends but involves a huge cost. As a matter of fact, the $(\mathcal{D}_t, C)$-optimal design is much cheaper. However, the large cost saving goes at the expense of the degree of trend-resistance. This example clearly illustrates the difficulty in striking a balance between cost-efficiency and trend-robustness. In terms of the cost per unit information, it is easy to calculate that the $(\mathcal{D}_t, C)$-optimal run order considerably outperforms the $\mathcal{D}_t$-optimal run order. For the $(\mathcal{D}_t, C)$-optimal run order, information is 59% cheaper.

time point	x_1	x_2	time point	x_1	x_2	time point	x_1	x_2
1	-1	-1	13	-1	1	25	1	-1
2	-1	1	14	-1	-1	26	1	-1
3	0	-1	15	1	1	27	1	1
4	0	0	16	1	-1	28	0	0
5	1	1	17	1	0	29	-1	-1
6	-1	1	18	0	0	30	-1	1
7	0	-1	19	-1	0	31	1	-1
8	1	0	20	1	1	32	1	0
9	1	-1	21	-1	1	33	0	1
10	1	1	22	0	-1	34	-1	-1
11	-1	0	23	0	1	35	0	1
12	0	0	24	-1	-1	36	-1	0

Table 1: The $\mathcal{D}_t$-Optimal Run Order

time point	x_1	x_2	time point	x_1	x_2	time point	x_1	x_2
1	-1	-1	13	-1	0	25	-1	-1
2	-1	-1	14	-1	0	26	-1	-1
3	-1	-1	15	-1	1	27	-1	-1
4	-1	-1	16	1	1	28	-1	-1
5	-1	-1	17	1	0	29	-1	-1
6	-1	-1	18	1	-1	30	-1	-1
7	-1	-1	19	1	-1	31	-1	-1
8	-1	-1	20	0	-1	32	-1	-1
9	-1	-1	21	0	-1	33	-1	-1
10	-1	-1	22	0	-1	34	-1	-1
11	-1	-1	23	0	-1	35	-1	-1
12	-1	-1	24	-1	-1	36	-1	-1

Table 2: The $(\mathcal{D}_t, C)$-Optimal Run Order

optimality	trend-resistance	cost
$\mathcal{D}_t$	99.99	832
$(\mathcal{D}_t, C)$	45.29	155

Table 3: Comparison of the $\mathcal{D}_t$- and the $(\mathcal{D}_t, C)$-Optimal Run Order

Figure 5 shows for both optimal run orders the cumulative costs during experimentation.

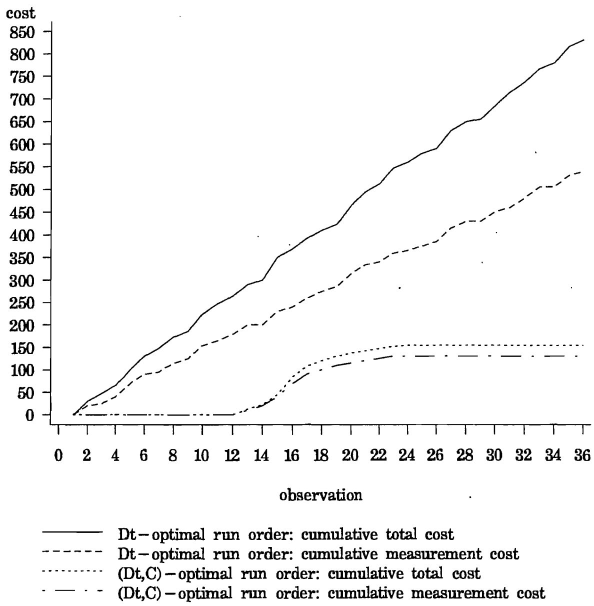


Figure 5: Cumulative Costs of Optimal Run Orders

It is clearly visible from Figure 5 that the cumulated cost of the $\mathcal{D}_t$-optimal run order is much higher than that of the $(\mathcal{D}_t, C)$-optimal run order.

It is however important to stress some major drawbacks of the $(\mathcal{D}_t, C)$-optimality criterion. Suppose for instance that the experimenter's budget is much lower than 155, then the $(\mathcal{D}_t, C)$-optimal run order has no practical utility. On the contrary, if the experimenter's budget at hand is much larger than 155, then one may wonder if it wouldn't be possible to construct a run order with a higher degree of trend-resistance. Generally speaking, the major deficiency of the $(\mathcal{D}_t, C)$-optimality criterion is that budget constraints are not allowed for.

3 Trend-resistance under budget constraints

This section goes into the subject of trend-resistant run orders under budget constraints. In the first subsection the design problem will be defined as a constrained optimization problem. Next, we will define a new optimality criterion that serves as a suitable tool for constructing optimal designs under budget constraints.

3.1 A constrained optimization problem

Let us describe the design problem at hand as follows. For a given number of observations n, determine the number of replicates n_i to be taken at the d different design points $\mathbf{x}_i$, with $i \in \{1, \ldots, d\}$ and $n = \sum_{i=1}^{d} n_i$, in order to maximize the amount of information

$$\mathcal{D}_t = |\mathbf{F}'\mathbf{F} - \mathbf{F}'\mathbf{G}(\mathbf{G}'\mathbf{G})^{-1}\mathbf{G}'\mathbf{F}|^{\frac{1}{p}}$$

subject to the constraint that the total cost C of the run order must not exceed the experimenter's budget B.

3.2 Pareto optimal run orders

In order to circumvent the previous hardly solvable problem, the search for optimal run orders is approximated by preferring run orders that maximize

$$k|\mathbf{F}'\mathbf{F} - \mathbf{F}'\mathbf{G}(\mathbf{G}'\mathbf{G})^{-1}\mathbf{G}'\mathbf{F}|^{\frac{1}{p}} - C, \tag{5}$$

with k a strictly positive weighting coefficient that strikes a balance between trend-resistance and cost-efficiency. Large values of k stress more on trend-resistance whereas low k-values put more weight on cost-efficiency. For instance, it can easily be shown that if $k \to \infty$, criterion (5) is nothing else than the $\mathcal{D}_t$-optimality criterion (2). If $k \to 0$, the resulting run order is the cost-optimal run order, i.e. the run order with the lowest total cost among all possible run orders. The determination of the weighting coefficient k and the connection with budget constraints will be extensively described in Section 4. This section goes further into some nice properties of the newly defined optimality criterion (5) that are of great interest in the sequel. It is also worthy of mention that optimality criterion (5) is a more natural criterion than the $(\mathcal{D}_t, C)$-criterion (4) in that it better relates the scales on which information and cost are measured: information is expressed as a negative cost or income and the weighting coefficient k acts as the expected income per unit information.

A relation with the familiar concept of Pareto optimality can be made as follows. A Pareto optimum in welfare economics is a situation in which no feasible reallocation of outputs and/or inputs in the economy could increase the level of utility of one or more households without lowering the level of utility of any other household. Applied to optimality criterion (5), the following theorem is proven in the appendix.

Theorem 1. An optimal run order under criterion $k\mathcal{D}_t - C$ is a Pareto optimal run order.

Theorem 1 says that no other run order than the optimal one can be found with a higher amount of information at the same or a lower cost or with a lower cost for as much information.

The following theorem elucidates the relation between the $(\mathcal{D}_t, C)$-optimal run order and the optimal run order under criterion (5). The proof is given in the appendix.

Theorem 2. The $(\mathcal{D}_t, C)$-optimal run order $\delta_{(\mathcal{D}_t,C)}$ is the Pareto optimal run order for

$$k = \frac{C(\delta_{(\mathcal{D}_t,C)})}{\mathcal{D}_t(\delta_{(\mathcal{D}_t,C)})}.$$

The corresponding criterion value (5) then equals zero. Theorem 3 relates the total cost C and the $\mathcal{D}_t$-value of the optimal run orders under criterion (5) with the constant k. Again, the proof can be found in the appendix.

Theorem 3. The total cost C and the $\mathcal{D}_t$-value of the Pareto optimal run orders are non-decreasing functions of k.

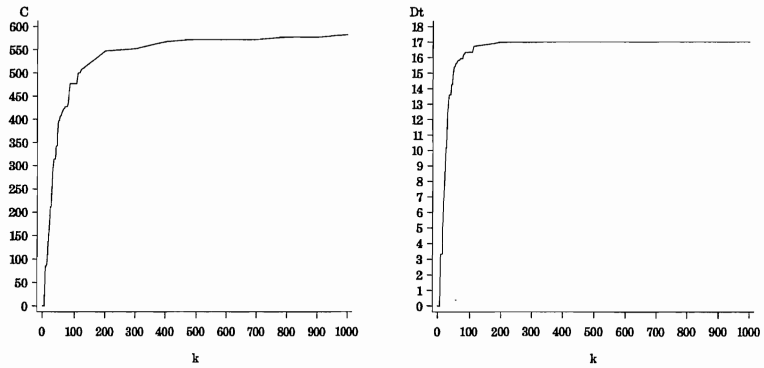
Note that these functions are in fact of a discrete form because we confine ourselves to exact designs. It follows from Theorem 3 that k can be used as a tuning constant in that an increased k-value involves at least even expensive and at least even informative run orders. As a matter of fact, the opposite holds when the k-value is lowered.

Returning to the design problem mentioned in the previous section, Pareto optimal run orders will be computed by maximizing criterion (5) for several tuning constants k. Figure 6 shows the performance of the computed Pareto optimal run orders in terms of the total cost and the $\mathcal{D}_t$-value. Note that the curves in Figure 6 are in fact discrete functions. This figure is an obvious illustration of Theorem 3. Based on Theorem 2, the cost and the $\mathcal{D}_t$-value of the $(\mathcal{D}_t, C)$-optimal run order of Table 2 is found by setting k equal to the inverse $(\mathcal{D}_t, C)$-value 20.06.

Figure 7 displays the relation between the total cost C and the degree of trend-resistance of the Pareto optimal run orders computed for varying constants k. A more general relation between both costs and information is given in Theorem 4 and is proven in the appendix.

Theorem 4. The relation between the total cost C and the $\mathcal{D}_t$-value of the Pareto optimal run orders is a strictly increasing function.

Based on Theorem 1, each point in Figure 7 represents a Pareto optimal run order and the curve in Figure 7 forms the Pareto set. This means that no other run orders can be found that are both cheaper and at least as much informative or run orders that are both more informative and equally or less expensive. The Pareto optimal run orders are to be preferred in practice. Based on this property, the next section will show how the design problems of Section 3.1 and Section 3.2 are related.



(a) total cost C (b) $\mathcal{D}_t$-value

Figure 6: Performance of Optimal Run Orders for Several Values of k

4 The design algorithm

The aim of the design algorithm is the construction of Pareto optimal run orders. At the end of this section, Theorem 5 will show that the computed Pareto optimal run orders serve as a good approximation to the constrained optimization problem of Section ??.

The input to the algorithm consists of the fixed number of observations n, the number of factors, the order and the number of parameters p of the response model, the polynomial expansion for the response model $\mathbf{f}(\mathbf{x})$, the order and the number of parameters q of the time trend, the polynomial expansion for the time trend $\mathbf{g}(t)$, cost information $\mathbf{m}$, $\mathbf{t}$, $\boldsymbol{\varsigma}$ and $\boldsymbol{\tau}$, and the list of available time points. The list of d candidate design points can be either provided or computed as shown in Atkinson and Donev (1992). Besides, the experimenter specifies the available budget B. Given the budget constraint, the aim is now the selection of n design points and the sequence in which the observations have to be taken in order to obtain maximal protection against time order dependence.

After reading the input, a direct search method iteratively computes Pareto optimal run orders δ_i for varying values $k = k_i$ in criterion (5). Let C_i denote the total cost of the

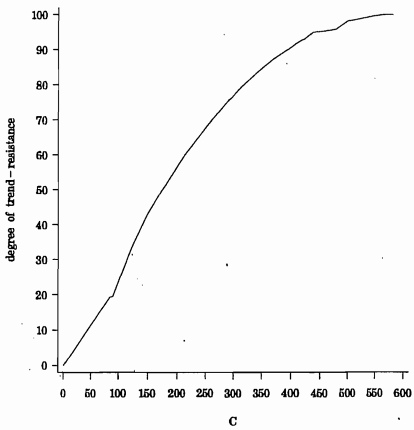


Figure 7: Total Cost and Degree of Trend-Resistance of Optimal Run Orders

Pareto optimal run order δ_i found during iteration i. Roughly speaking, the algorithm proceeds as follows. In the first iteration, k_1 is chosen as the midpoint of $K_1 = [k^-_{(1)}, k^+_{(1)}] = [0, k_{\max}]$, with $k_{\max}$ a sufficiently large number. Depending on whether the total cost C_1 of run order δ_1 exceeds the budget B or not, the search during the next iteration is restricted to $K_2 = [k^-_{(1)}, k_1] = [0, k_1]$ or $K_2 = [k_1, k^+_{(1)}] = [k_1, k_{\max}]$ respectively. Now, run order δ_2 is computed for k_2 in the middle of K_2. Again, depending on the total cost C_2, the interval K_3 for the next iteration is chosen as $[k^-_{(2)}, k_2]$ or $[k_2, k^+_{(2)}]$. In general, the tuning constant k_i during iteration i is the midpoint of $K_i = [k^-_{(i-1)}, k_{i-1}]$ or $K_i = [k_{i-1}, k^+_{(i-1)}]$ depending on whether C_{i-1} is respectively higher or lower than B. It can easily be understood that this iteration process converges to a Pareto optimal run order δ_c with a total cost C_c very close or equal to the budget B. Because of the discrete nature of the exact design problem, it is not always possible to find a run order δ_c with a total cost C_c exactly equal to the available budget B. The output of the algorithm consists of the Pareto optimal run order δ_c.

The construction of the trend-resistant run order δ_i during each iteration i is mainly based on the generic point exchange algorithm for the construction of $\mathcal{D}$-optimal designs of Atkinson and Donev (1992). The optimal run orders δ_i are obtained by selecting a random starting run order and sequentially adding and deleting design points and time points in order to maximize optimality criterion (5) for $k = k_i$. However, to avoid being stuck at a local optimum, the probability of finding the global optimum during one iteration can be increased by repeating the search several times from different starting designs or 'tries'. For a detailed description of the exchange procedures, we refer the interested reader to Tack and Vandebroek (1999, 2000).

The constructed Pareto optimal run orders usually are the solution to the constrained optimization problem. However, if $C_c \neq B$, it may be possible that the Pareto optimal run order δ_c obtained with criterion (5) does not coincide with the optimal solution for the original constrained optimization problem. In this case, the design algorithm results into a Pareto optimal run order that is close to the optimal solution for the original constrained maximization problem. Theorem 5 derives an upper bound on the difference in trend-resistance of the Pareto optimal run order and the optimal design for the constrained optimization problem.

Theorem 5. The Pareto optimal run order is at most

$$100 \times \frac{B - C}{k\,|\mathbf{F}'\mathbf{F}|^{\frac{1}{p}}}\%$$

less trend-resistant than the optimal run order for the constrained optimization problem.

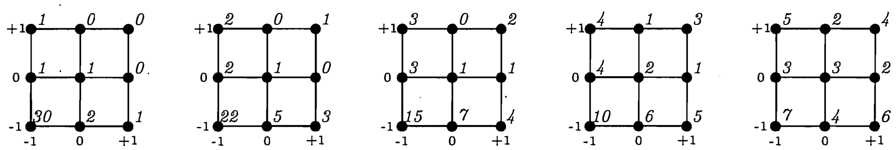
The examples in Section 5 will show that the difference in the degree of trend-resistance is small and often negligible.

5 Examples

This section presents two examples to illustrate the usefulness of the proposed design algorithm for solving practical design problems. The first example turns back to the 3^2-factorial studied in the previous sections, whereas the second example is a real-life industrial application.

5.1 A trend-resistant 3^2-factorial under budget constraints

Consider as an example the design problem described in Section 2.3 where the aim was the construction of $\mathcal{D}_t$- and $(\mathcal{D}_t, C)$-optimal run orders for an experiment with 36 observations and design points taken from the 3^2-factorial. The degree of trend-resistance and the total cost of both optimal run orders are given in Table 3. However, if we assume that the experimenter's budget is lower than 155, then neither the $\mathcal{D}_t$- nor the $(\mathcal{D}_t, C)$-optimal design have any practical value. On the other hand, if the available budget is somewhere between 155 and 832, then it may be possible to construct a run order with a higher degree of trend-resistance than that of the $(\mathcal{D}_t, C)$-optimal run order. Here, Pareto optimal run orders will be computed for five different budget constraints (Figure 8). As a matter of fact, when the budget at hand is rather low (e.g. $B = 100$ or $B = 200$), then the cheap design point (-1,-1) is replicated many times. On the other hand, when the experimenter has the disposal of a high budget (e.g. $B = 500$), then the optimal design becomes more balanced.



(a) $B = 100$ (b) $B = 200$ (c) $B = 300$ (d) $B = 400$ (e) $B = 500$

Figure 8: Optimal Designs for the 3^2-Factorial

Table 4 compares the Pareto optimal run orders in terms of trend-robustness and cost-efficiency. For example, assuming a budget $B = 100$ involves a reduction in the degree of trend-resistance from 45.29% to 17.78%. On the other hand, if the budget at hand exceeds 155, the obtained run orders are better balanced for time trends. Based on Theorem 5, Table 4 also shows how far away the Pareto optimal run orders are from the optimal run orders for the original constrained maximization problem. For instance, it is possible that for $B = 300$ there exists a budget constrained run order that is 1.74 % more trend-resistant than the Pareto optimal run order. Remark that the deviation from the optimal run orders decreases with increased budget B.

criterion	trend-resistance	cost	$100 \times (B - C)/(k\ \lvert\mathbf{F}'\mathbf{F}\rvert^{\frac{1}{p}})$
$\mathcal{D}_t$	99.99	832	-
$(\mathcal{D}_t, C)$	45.29	155	-
B = 100	17.78	85	5.97
B = 200	53.48	190	2.46
B = 300	75.38	290	1.74
B = 400	90.50	397	0.28
B = 500	98.18	500	0

Table 4: Comparison of Optimal Run Orders

5.2 The cryogenic flow meter experiment

Based on Joiner and Campbell (1976), an experimental plan will be set up to evaluate the accuracy of flow meters for use with cryogenic fluids such as liquid oxygen or liquid nitrogen. The accuracy of the flow meters is supposed to be sensitive to the temperature x_1, the pressure x_2, the flow rate of the liquid x_3 and the total weight of the liquid pumped during a test x_4. Management decides to restrain the factor levels shown in Table 5. Besides, the flow meters are known to deteriorate linearly with time and a time trend $\mathbf{g}(t) = t$ is postulated. The number of observations equals $n = 20$ and the measurement costs are given by

$$c^m(\mathbf{x}) = 20 + 5x_1 + 5x_2 - 5x_3 + 5x_4.$$

For instance, rised temperatures x_1 and/or higher pressures x_2 more heavily load the flow meter and are calculated for by means of an increased measurement cost. Rising the total weight x_4 of the liquid pumped prolongs the total execution time of the experiment and increases the measurement cost. The opposite holds for the flow rate x_3. Changing the temperature from the high level to the low level or vice versa is very time consuming and costs 100, whereas changing the pressure level is cheaper and amounts to a cost of 50. Changes in flow rate and weight could be made almost instantaneously. The transition costs for the latter two factors x_3 and x_4 are set equal to zero.

factor	coded factor levels
x_1	-1, 1
x_2	-1, 1
x_3	-1, 0, 1
x_4	-1, 0, 1

Table 5: Coded Factor Levels in Cryogenic Flow Experiment

Run orders will be computed for the following response models:

$$\begin{aligned}
(F_1)\quad \mathbf{f}'(\mathbf{x}) &= (1\ x_1\ x_2\ x_3\ x_4),\\
(F_2)\quad \mathbf{f}'(\mathbf{x}) &= (1\ x_1\ x_2\ x_3\ x_4\ x_1x_2\ x_1x_3\ x_1x_4\ x_2x_3\ x_2x_4\ x_3x_4),\\
(F_3)\quad \mathbf{f}'(\mathbf{x}) &= (1\ x_1\ x_2\ x_3\ x_4\ x_3^2\ x_4^2),\\
(F_4)\quad \mathbf{f}'(\mathbf{x}) &= (1\ x_1\ x_2\ x_3\ x_4\ x_1x_2\ x_1x_3\ x_1x_4\ x_2x_3\ x_2x_4\ x_3x_4\ x_3^2\ x_4^2).
\end{aligned}$$

The performance of the $\mathcal{D}_t$- and the $(\mathcal{D}_t, C)$-optimal run orders is shown in Table 6.

		F_1	F_2	F_3	F_4
$\mathcal{D}_t$-optimality	cost	1,900	1,480	2,360	2,150
	degree of trend-resistance	100	99.99	99.99	99.99
$(\mathcal{D}_t, C)$-optimality	cost	280	600	310	480
	degree of trend-resistance	49.17	89.97	59.25	73.11
$B = 800$	cost	800	780	745	800
	degree of trend-resistance	100	99.91	99.99	99.70
	$100 \times (B - C)/(k\ \lvert\mathbf{F}'\mathbf{F}\rvert^{\frac{1}{p}})$	0	0.018	0.006	0

Table 6: Performance of the Optimal Run Orders

Whereas the $(\mathcal{D}_t, C)$-optimal run orders considerably outperform the $\mathcal{D}_t$-optimal run orders in terms of the total cost, the $\mathcal{D}_t$-optimal run orders are better balanced for time trends. Especially for response models F_1 and F_3, the degree of trend-resistance of the $(\mathcal{D}_t, C)$-optimal run orders is quite low.

If we assume the experimenter has at his disposal a budget $B = 800$, it may be possible to construct run orders with a better balance for time trends than the $(\mathcal{D}_t, C)$-optimal run orders. The Pareto optimal run orders are given in Table 7 to Table 10 and their performance is shown in Table 6. The budget constrained run orders obviously outperform the $(\mathcal{D}_t, C)$-optimal run orders in terms of the protection against time trend effects. Based on Theorem 5, Table 6 shows that the difference in trend-resistance of the Pareto optimal run orders and the optimal constrained ones is rather negligible. Similar results were obtained for other costs.

time point	x_1	x_2	x_3	x_4	time point	x_1	x_2	x_3	x_4
1	1	1	-1	1	11	-1	1	1	-1
2	1	1	-1	-1	12	-1	-1	1	1
3	1	-1	1	-1	13	-1	-1	1	1
4	1	-1	1	1	14	-1	-1	-1	-1
5	1	-1	1	-1	15	-1	-1	-1	-1
6	-1	-1	-1	-1	16	1	-1	-1	1
7	-1	1	-1	1	17	1	-1	-1	1
8	-1	1	-1	1	18	1	1	1	1
9	-1	1	1	1	19	1	1	-1	-1
10	-1	1	1	-1	20	1	1	1	-1

Table 7: The Budget Constrained Run Order for Response Model F_1

time point	x_1	x_2	x_3	x_4	time point	x_1	x_2	x_3	x_4
1	1	1	-1	1	11	-1	1	1	-1
2	1	1	1	-1	12	-1	1	-1	-1
3	1	-1	-1	-1	13	-1	1	1	1
4	1	-1	1	1	14	-1	-1	-1	-1
5	-1	-1	-1	-1	15	-1	-1	-1	1
6	-1	-1	1	1	16	-1	-1	1	-1
7	-1	-1	1	1	17	1	-1	1	-1
8	-1	1	1	-1	18	1	-1	-1	1
9	-1	1	-1	1	19	1	1	1	1
10	-1	1	-1	1	20	1	1	-1	-1

Table 8: The Budget Constrained Run Order for Response Model F_2

time point	x_1	x_2	x_3	x_4	time point	x_1	x_2	x_3	x_4
1	1	1	-1	-1	11	-1	1	1	-1
2	1	1	0	1	12	-1	1	1	0
3	1	1	0	0	13	-1	1	-1	1
4	1	-1	1	0	14	-1	1	1	0
5	1	-1	1	1	15	-1	1	0	1
6	-1	-1	-1	-1	16	1	1	-1	0
7	-1	-1	0	0	17	1	1	0	-1
8	-1	-1	-1	0	18	1	-1	1	-1
9	-1	-1	1	1	19	1	-1	-1	1
10	-1	-1	0	-1	20	1	-1	0	0

Table 9: The Budget Constrained Run Order for Response Model F_3

time point	x_1	x_2	x_3	x_4	time point	x_1	x_2	x_3	x_4
1	1	1	-1	1	11	-1	1	-1	0
2	1	1	1	-1	12	-1	1	0	-1
3	1	-1	0	-1	13	-1	1	1	1
4	1	-1	-1	0	14	-1	-1	-1	1
5	1	-1	1	1	15	-1	-1	1	-1
6	-1	-1	1	1	16	1	-1	1	-1
7	-1	-1	-1	-1	17	1	-1	-1	1
8	-1	-1	0	0	18	1	1	1	0
9	-1	1	1	-1	19	1	1	0	1
10	-1	1	-1	1	20	1	1	-1	-1

Table 10: The Budget Constrained Run Order for Response Model F_4

As an illustration the cumulative total costs for the optimal run orders are shown in Figure 9. The $\mathcal{D}_t$-optimal run orders have the largest total cost during experimentation and the $(\mathcal{D}_t, C)$-optimal run orders are the cheapest run orders. The cumulative total cost of the budget constrained run orders is somewhere in the middle.

6 Conclusion

In practice, time trend effects often affect the observed responses. The solution to this annoying problem is the construction of run orders that are optimally balanced for time trends. In practical circumstances these run orders are of limited use because they usually involve huge transition costs. An optimal run order is not obvious and the main difficulty is how to strike the balance between cost-efficiency and trend-resistance. This paper has presented a generic design algorithm for the construction of cost-efficient run orders with an optimal protection against time trend effects. The construction algorithm enables the practitioner to tackle a wide range of practical design problems. As an example, the cryogenic flow meter experiment has shown that the algorithm serves as a proper tool for the construction of trend-resistant run orders under budget constraints.

Appendix

Theorem 1.
An optimal run order under criterion $k\mathcal{D}_t - C$ is a Pareto optimal run order.

Proof

Let δ denote the optimal run order under criterion $k\mathcal{D}_t - C$. It follows that δ maximizes $k\mathcal{D}_t - C$ or that for any run order δ_i,

$$k\mathcal{D}_t(\delta_i) - C(\delta_i) \leq k\mathcal{D}_t(\delta) - C(\delta). \tag{1}$$

Suppose now that δ is not a Pareto optimal run order. Consequently, there must be at least one run order δ_i among all possible run orders such that

$$\begin{cases} \mathcal{D}_t(\delta_i) & > & \mathcal{D}_t(\delta), \\ C(\delta_i) & = & C(\delta), \end{cases}$$

or

$$\begin{cases} \mathcal{D}_t(\delta_i) & > & \mathcal{D}_t(\delta), \\ C(\delta_i) & < & C(\delta), \end{cases}$$

or

$$\begin{cases} \mathcal{D}_t(\delta_i) & = & \mathcal{D}_t(\delta), \\ C(\delta_i) & < & C(\delta). \end{cases}$$

For each of the three cases above it then follows that

$$k\mathcal{D}_t(\delta_i) - C(\delta_i) > k\mathcal{D}_t(\delta) - C(\delta),$$

which is contrary to (1). As a result, the run order δ that maximizes $k\mathcal{D}_t - C$ is a Pareto optimal run order.

□

Theorem 2.
The $(\mathcal{D}_t, C)$-optimal run order $\delta_{(\mathcal{D}_t,C)}$ is the Pareto optimal run order for $k = C(\delta_{(\mathcal{D}_t,C)})/\mathcal{D}_t(\delta_{(\mathcal{D}_t,C)})$.

Proof

Since $\delta_{(\mathcal{D}_t,C)}$ is the $(\mathcal{D}_t, C)$-optimal run order, it follows that

$$\frac{\mathcal{D}_t(\delta_{(\mathcal{D}_t,C)})}{C(\delta_{(\mathcal{D}_t,C)})} \geq \frac{\mathcal{D}_t(\delta_i)}{C(\delta_i)}$$

for all possible run orders δ_i. Consequently,

$$\begin{aligned} C(\delta_i)\mathcal{D}_t(\delta_{(\mathcal{D}_t,C)}) &\geq C(\delta_{(\mathcal{D}_t,C)})\mathcal{D}_t(\delta_i), \\ 0 &\geq C(\delta_{(\mathcal{D}_t,C)})\mathcal{D}_t(\delta_i) - C(\delta_i)\mathcal{D}_t(\delta_{(\mathcal{D}_t,C)}), \\ C(\delta_{(\mathcal{D}_t,C)})\mathcal{D}_t(\delta_{(\mathcal{D}_t,C)}) - C(\delta_{(\mathcal{D}_t,C)})\mathcal{D}_t(\delta_{(\mathcal{D}_t,C)}) &\geq C(\delta_{(\mathcal{D}_t,C)})\mathcal{D}_t(\delta_i) - C(\delta_i)\mathcal{D}_t(\delta_{(\mathcal{D}_t,C)}), \\ \frac{C(\delta_{(\mathcal{D}_t,C)})}{\mathcal{D}_t(\delta_{(\mathcal{D}_t,C)})}\mathcal{D}_t(\delta_{(\mathcal{D}_t,C)}) - C(\delta_{(\mathcal{D}_t,C)}) &\geq \frac{C(\delta_{(\mathcal{D}_t,C)})}{\mathcal{D}_t(\delta_{(\mathcal{D}_t,C)})}\mathcal{D}_t(\delta_i) - C(\delta_i). \end{aligned} \tag{1}$$

Let $C(\delta_{(\mathcal{D}_t,C)})/\mathcal{D}_t(\delta_{(\mathcal{D}_t,C)}) = k$, then (1) can be rewritten as

$$k\mathcal{D}_t(\delta_{(\mathcal{D}_t,C)}) - C(\delta_{(\mathcal{D}_t,C)}) \;\geq\; k\mathcal{D}_t(\delta_i) - C(\delta_i).$$

Hence, the $(\mathcal{D}_t, C)$-optimal run order $\delta_{(\mathcal{D}_t,C)}$ maximizes $k\mathcal{D}_t - C$ for $k = C(\delta_{(\mathcal{D}_t,C)})/\mathcal{D}_t(\delta_{(\mathcal{D}_t,C)})$.

□

Theorem 3.
The total cost C and the $\mathcal{D}_t$-value of the Pareto optimal run orders are non-decreasing functions of k.

Proof

Let δ_1 and δ_2 denote the optimal run orders under criterion $k\mathcal{D}_t - C$ with $k = k_1$ and $k = k_2$ respectively. Besides, assume that $k_1 < k_2$. Then, because δ_1 maximizes $k_1\mathcal{D}_t - C$, it follows that

$$k_1\mathcal{D}_t(\delta_1) - C(\delta_1) \;\geq\; k_1\mathcal{D}_t(\delta_2) - C(\delta_2). \tag{1}$$

Similarly, because δ_2 maximizes $k_2\mathcal{D}_t - C$, it follows that

$$k_2\mathcal{D}_t(\delta_2) - C(\delta_2) \;\geq\; k_2\mathcal{D}_t(\delta_1) - C(\delta_1). \tag{2}$$

From (1) and (2),

$$\begin{aligned} k_1\mathcal{D}_t(\delta_1) - k_1\mathcal{D}_t(\delta_2) &\;\geq\; C(\delta_1) - C(\delta_2), \\ k_2\mathcal{D}_t(\delta_1) - k_2\mathcal{D}_t(\delta_2) &\;\leq\; C(\delta_1) - C(\delta_2), \end{aligned}$$

or,

$$k_1\mathcal{D}_t(\delta_1) - k_1\mathcal{D}_t(\delta_2) \;\geq\; k_2\mathcal{D}_t(\delta_1) - k_2\mathcal{D}_t(\delta_2).$$

Because $k_1 < k_2$, it follows that

$$\mathcal{D}_t(\delta_1) \leq \mathcal{D}_t(\delta_2). \tag{3}$$

This means that the $\mathcal{D}_t$-value is a non-decreasing function of k. Combining (1) and (3) gives

$$C(\delta_1) \leq C(\delta_2).$$

Similarly, the total cost C of the optimal run orders is a non-decreasing function of k.

□

Theorem 4.
The relation between the total cost C and the $\mathcal{D}_t$-value of the Pareto optimal run orders is a strictly increasing function.

Proof

Let δ_1 and δ_2 denote the optimal run orders under criterion $k\mathcal{D}_t - C$ for $k = k_1$ and $k = k_2$ respectively. Besides, assume that $k_1 < k_2$. Then, because δ_1 maximizes $k_1\mathcal{D}_t - C$, it follows that

$$k_1\mathcal{D}_t(\delta_1) - C(\delta_1) \;\geq\; k_1\mathcal{D}_t(\delta_2) - C(\delta_2). \tag{1}$$

Similarly, because δ_2 maximizes $k_2\mathcal{D}_t - C$, it follows that

$$k_2\mathcal{D}_t(\delta_2) - C(\delta_2) \;\geq\; k_2\mathcal{D}_t(\delta_1) - C(\delta_1). \tag{2}$$

For instance, suppose that $\mathcal{D}_t(\delta_1) = \mathcal{D}_t(\delta_2)$, then (1) and (2) respectively lead to

$$C(\delta_1) \leq C(\delta_2)$$

and

$$C(\delta_1) \geq C(\delta_2)$$

or $C(\delta_1) = C(\delta_2)$. Alternatively, if $C(\delta_1) = C(\delta_2)$, then (1) and (2) give

$$\mathcal{D}_t(\delta_1) \geq \mathcal{D}_t(\delta_2)$$

and

$$\mathcal{D}_t(\delta_1) \leq \mathcal{D}_t(\delta_2)$$

or $\mathcal{D}_t(\delta_1) = \mathcal{D}_t(\delta_2)$. Based on the these results and Theorem 3 it follows that

$$\begin{cases} \mathcal{D}_t(\delta_1) < \mathcal{D}_t(\delta_2), \\ C(\delta_1) < C(\delta_2), \end{cases}$$

or

$$\begin{cases} \mathcal{D}_t(\delta_1) = \mathcal{D}_t(\delta_2), \\ C(\delta_1) = C(\delta_2), \end{cases}$$

This means that the relation between the total cost C and the $\mathcal{D}_t$-value of the optimal run orders under criterion $k\mathcal{D}_t - C$ is a strictly increasing function.

□

Theorem 5.
The Pareto optimal run order is at most

$$100 \times \frac{B - C}{k\,|\mathbf{F}'\mathbf{F}|^{\frac{1}{p}}}\%$$

less trend-resistant than the optimal run order for the constrained optimization problem.

Proof

Let δ denote the Pareto optimal run order under criterion $k\mathcal{D}_t - C$ in the design algorithm. Then for any run order δ_i it follows that

$$k\mathcal{D}_t(\delta_i) - C(\delta_i) \leq k\mathcal{D}_t(\delta) - C(\delta)$$

or

$$\frac{\mathcal{D}_t(\delta_i)}{|\mathbf{F}'\mathbf{F}|^{\frac{1}{p}}} \leq \frac{\mathcal{D}_t(\delta)}{|\mathbf{F}'\mathbf{F}|^{\frac{1}{p}}} + \frac{C(\delta_i) - C(\delta)}{k\,|\mathbf{F}'\mathbf{F}|^{\frac{1}{p}}}. \quad (1)$$

From (1) it follows that all run orders with $C(\delta_i) \leq C(\delta)$ are equally or less trend-resistant than the Pareto optimal run order δ. However, if $C(\delta) < C(\delta_i) \leq B$ there may exist a budget constrained run order δ_i that outperforms the Pareto optimal run order δ in terms of the degree of trend-resistance. It follows from (1) that the highest outperformance occurs when $C(\delta_i) = B$ and equals

$$100 \times \frac{B - C}{k\,|\mathbf{F}'\mathbf{F}|^{\frac{1}{p}}}\%.$$

□

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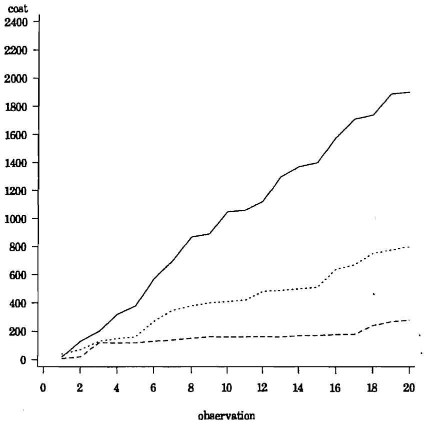
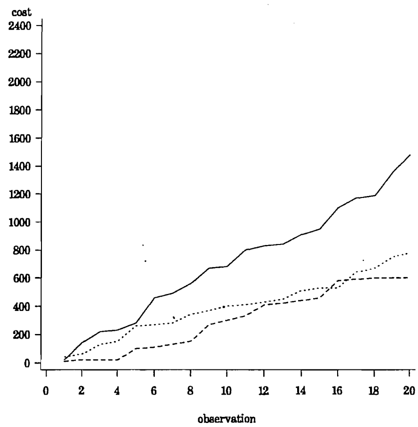
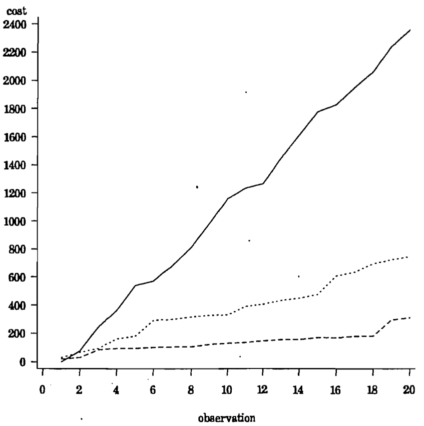


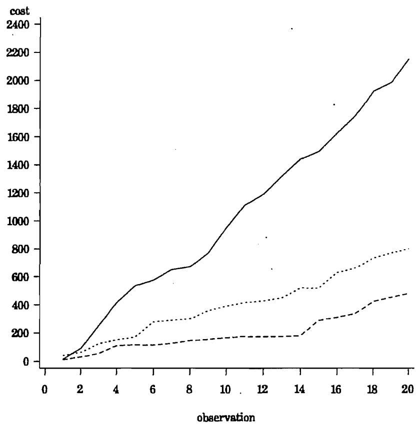
(a) Response Model F_1



(b) Response Model F_2



(c) Response Model F_3



(d) Response Model F_4

Figure 9: Cumulative Costs for Different Response Models

——— $\mathcal{D}_t$-optimal run order
- - - - - - - $(\mathcal{D}_t, C)$-optimal run order
· · · · · · · · · budget constrained run order