ScienceDirect

Factorial Experiment

A factorial experiment can be defined as an experiment in which the response variable is observed at all factor-level combinations of the independent variables.

Related terms:

Sum of Squares, Analysis of Variance, Experimental Design, Factorials, Response Variable

Factorial Experiments

Rudolf J. Freund, ... Donna L. Mohr, in Statistical Methods (Third Edition), 2010

9.7 Three or More Factors

Obviously factorial experiments can have more than two factors. As we have noted, fertilizer experiments are concerned with three major fertilizer ingredients, N, P, and K, whose amounts in a fertilizer are usually printed on the bag. The fundamental principles of the analysis of factorial experiments such as the model describing the data, the partitioning of sums of squares, and the interpretation of results are relatively straightforward extensions of the two-factor case. Since such analyses are invariably performed by computers, computational details are not presented here.

The model for a multifactor factorial experiment is usually characterized by a large number of parameters. Of special concern is the larger number and greater complexity of the interactions. In the three-factor fertilizer experiment, for example, the model contains parameters describing

- three main effects: N, P, and K,
- three two-factor interactions: $\mathbf{N} \times \mathbf{P}$, $\mathbf{N} \times \mathbf{K}$, and $\mathbf{P} \times \mathbf{K}$, and
- one three-factor interaction: $\mathbf{N} \times \mathbf{P} \times \mathbf{K}$.

The interpretations of main effects and two-factor interactions remain the same regardless of the number of factors in the experiment. Interactions among more than two factors, which are called higher order interactions, are more difficult to interpret. One interpretation of a three-factor interaction, say, $\mathbf{N} \times \mathbf{P} \times \mathbf{K}$, is that it reflects the inconsistency of the $\mathbf{N} \times \mathbf{P}$ interaction across levels of K. Of course, this is equivalent to the inconsistency of the $\mathbf{P} \times \mathbf{K}$ interaction across N, etc.

Example 9.6

It is of importance to ascertain how the lengths of steel bars produced by several screw machines are affected by heat treatments and the time of day the bars are produced. A factorial experiment using four machines and two heat treatments was conducted at three different times in one day. This is a three-factor factorial with factors:

- Heat treatment, denoted by HEAT, with levels W and L,
- Time of experiment, denoted by TIME, with levels 1, 2, and 3 representing 8:00 a.m., 11:00 a.m., and 3:00 p.m., and
- Machine, denoted by MACHINE with levels A, B, C, and D.

Each factor level combination was run four times. The response is the (code) length of the bars. The data are given in Table 9.16.

Table 9.16. Steel Bar Data for Three-Factor Factorial

	HEAT TREATMENT W MACHINES				HEAT TREATMENT L MACHINES			
Time	**A**	**B**	**C**	**D**	**A**	**B**	**C**	**D**
8:00 AM	6	7	1	6	4	6	**−1**	4
	9	9	2	6	6	5	0	5
	1	5	0	7	0	3	0	5
	3	5	4	3	1	4	1	4
11:00 AM	6	8	3	7	3	6	2	9
	3	7	2	9	1	4	0	4
	1	4	1	11	1	1	**−1**	6
	−1	8	0	6	**−2**	3	1	3
3:00 PM	5	10	**−1**	10	6	8	0	4
	4	11	2	5	0	7	**−2**	3
	9	6	6	4	3	10	4	7
	6	4	1	8	7	0	**−4**	0

Solution

The analysis of variance for the factorial experiment is performed with PROC ANOVA of the SAS System with the results, which are quite straightforward, shown in Table 9.17. The HEAT and MACHINE effects are clearly significant, with no other factors approaching significance at the 0.05 level. In fact, some of the F values are suspiciously small, which may raise doubts about the data collection procedures.

Table 9.17. Analysis of Variance for Steel Bar Data

Analysis of Variance Procedure
Dependent Variable: LENGTH

Analysis of Variance Procedure				
Source	DF	Sum of Squares	Mean Square	F Valu
Dependent Variable: LENGTH				
Model	23	590.3333333	25.6666667	4.13
Error	72	447.5000000	6.2152778	
Corrected Total	95	1037.8333333		
Source	DF	Sum of Squares	Mean Square	F Valu
	R Square	C.V.	Root MSE	LEN
	0.568813	62.98221	2.493046	3.9
Source	DF	Anova SS	Mean Square	F Valu
TIME	2	12.8958333	6.4479167	1.04
HEAT	1	100.0416667	100.0416667	16.1
TIME*HEAT	2	1.6458333	0.8229167	0.13
MACHINE	3	393.4166667	131.1388889	21.1
TIME*MACHINE	6	71.0208333	11.8368056	1.90
HEAT*MACHINE	3	1.5416667	0.5138889	0.08
TIME*HEAT*MACHINE	6	9.7708333	1.6284722	0.26

No specifics are given on the structure of the factor levels; hence post hoc paired comparisons are in order. The HEAT factor has only two levels; hence the only statement to be made is that the sample means of 2.938 and 4.979 for L and W indicate that W produces longer bars. Duncan's multiple range test is applied to the MACHINE factor with results given in Table 9.18.

Table 9.18. Analysis of Variance for Steel Bar Data, Duncan's Multiple Range Test for Machine

Alpha = 0.05 cdf = 72 cMSE = 6.215278			
Number of Means	2	3	4
Critical Range	1.436	1.510	1.558
Means with the same letter are not significantly different.			
Duncan Grouping	Mean	N	MACHINE
A	5.875	24	B
A	5.667	24	D
B	3.417	24	A
C	0.875	24	C

Figure 9.5 is a profile plot illustrating the HEAT by MACHINE means. In general, for any machine, heat W gives a longer bar and the differences among machines are relatively the same for each heat. This is consistent with the lack of interaction.

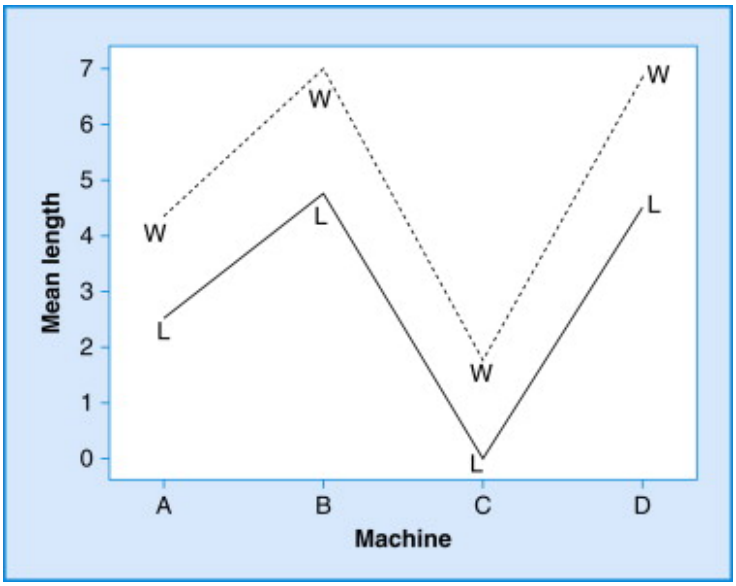

FIGURE 9.5. Profile Plot for Steel Bar Data in Example 9.6.

Factorial experiments with many factors often produce a large number of factor level combinations. The resulting requirement for a large number of observations may make it impossible to provide for replicated values in the cells. Since higher order interactions are difficult to interpret, their mean squares make good candidates for the estimate of σ^2. Of course, if these interactions do exist, the resulting tests are biased.

9.7.1 Additional Considerations

ecial experimental designs are available to overcome partially the often excessive number of experimental units required for factorial experiments. For example, the estimation of a polynomial response regression does not require data from all the factor level combinations provided by the factorial experiment; hence special response surface designs are available for use in such situations. Also, since higher order interactions are often of little interest, designs have been developed that trade the ability to estimate these interactions for a reduction in sample size. For additional information on such topics, refer to a book on experimental design (for example, Kirk (1995)).

Read full chapter

URL: https://www.sciencedirect.com/science/article/pii/B9780123749703000093

Design of Experiments

Kandethody M. Ramachandran, Chris P. Tsokos, in Mathematical Statistics with Applications in R (Second Edition), 2015

9.3.3 Fractional Factorial Design

In a fractional factorial experiment, only a fraction of the possible treatments are actually used in the experiment. A full factorial design is the ideal design, through which we could obtain information on all main effects and interactions. But because of the prohibitive size of the experiments, such designs are not practical to run. For instance, consider Example 9.2.2. Now if we were to add say, two different densities, three sizes of fish, and three types of food, the number of factors becomes five, and total number of distinct treatments will be $4 \times 4 \times 2 \times 3 \times 3 = 288$. This method becomes very time consuming and expensive. The number of relatively significant effects in a factorial design is relatively small. In these types of situations, fractional factorial experiments are used in which trials are conducted on only a well-balanced subset of the possible combinations of levels of factors. This allows the experimenter to obtain information about all main effects and interactions while keeping the size of the experiment manageable. The experiment is carried out in a single systematic effort. However, care should be taken in selection of treatments in the experiment so as to be able to answer as many relevant questions as possible. The fractional factorial design is useful when the number of factors is large. Because we are reducing the number of factors, a fractional factorial design will not be able to evaluate the influence of some of the factors independently. Of course, the question is how to choose the factors and levels we should use in a fractional factorial design. The question of how fractional factorial designs are constructed is beyond the scope of this book.

Design of Experiments

Rudolf J. Freund, ... Donna L. Mohr, in Statistical Methods (Third Edition), 2010

Example 10.1

A Factorial Experiment with Different Plot Sizes

We are interested in the yield response of corn to the following factors:

WTR: levels of irrigation with levels 1 and 2,

NRATE: rate of nitrogen fertilization with levels 1, 2, and 3, and

P: planting rates with levels 5, 10, 20, and 40 plants per experimental plot.

The response variable is total dry matter harvested (TDM).[1] The experiment is a $\mathbf{2 \times 3 \times 4}$ factorial experiment. Because of physical limitations the experiment was conducted as follows:

- The experiment used four fields with 24 plots to accommodate all factor level combinations.
- Normally each of the 24 plots would be randomly assigned one factor level combination. However, because it is physically impossible to assign different irrigation levels to the individual plots, each field was divided in half and each half randomly assigned an irrigation level.
- The 12 factor levels of the other factors (NRATE and P) were randomly assigned to each half field.

A possible additional complication arises from the fact that the specified planting rates do not always produce that exact number of plants in each plot. Therefore the actual plants per plot are also recorded. For the time being, we will assume that this complication does not affect the analysis of the data. We will return to this problem in Chapter 11, Exercise 14 where the effect of the different number of plants in each plot will be examined. The data are shown in Table 10.1. The NRATE and WTR combinations are identified as rows, and the four sets of columns correspond to the four planting rates (P). The two entries in the table are the actual number of plants per plot (NO) and the total dry matter (TDM). The solution is presented in Section 10.6.

Table 10.1. Example of an Experimental Design

		$P = 5$		$P = 10$		$P = 30$		$P = 40$	
WTR	NRATE	NO	TDM	NO	TDM	NO	TDM	NO	TDM
REP = 1									
1	1	7	3.426	13	2.084	20	2.064	37	2.851
1	2	7	7.070	12	7.323	24	7.321	38	7.865
1	3	6	4.910	10	6.620	22	8.292	43	7.528
2	1	5	2.966	12	3.304	20	4.055	37	2.075
2	2	7	3.484	12	2.894	22	5.662	26	3.485
2	3	5	1.928	10	4.347	20	3.178	33	3.900
REP = 2									
1	1	6	3.900	11	3.015	27	3.129	38	3.175
1	2	7	5.581	14	7.908	19	6.419	37	7.685
1	3	5	3.350	13	5.986	20	6.515	32	10.515
2	1	5	2.574	12	4.390	20	2.855	42	3.042
2	2	5	3.952	11	4.744	21	5.472	30	5.125
2	3	6	4.494	11	5.480	20	4.871	36	5.294
REP = 3									
1	1	5	3.829	10	3.173	18	2.741	33	2.166
1	2	5	3.800	13	7.568	19	7.797	34	6.474
1	3	8	6.156	15	7.034	23	7.754	40	8.458
2	1	6	2.872	12	5.759	21	4.512	42	4.864
2	2	5	2.826	14	3.840	21	4.494	30	4.804
2	3	5	3.107	10	3.620	20	4.620	32	5.376
REP = 4									

		$P = 5$		$P = 10$		$P = 30$		$P = 40$	
WTR	NRATE	NO	TDM	NO	TDM	NO	TDM	NO	TDM
1	1	5	3.325	11	4.193	20	3.409	40	4.877
1	2	6	4.984	12	7.627	20	6.562	39	9.093
1	3	6	4.067	12	4.394	20	7.089	28	7.088
2	1	6	2.986	11	5.327	20	5.390	43	5.632
2	2	5	2.417	11	3.592	20	4.311	33	5.975
2	3	9	4.180	12	5.282	19	4.498	35	6.519

Source: Personal communication from R. M. Jones and M. A. Sanderson, Texas Agricultural Experiment Station, Stephenville, and J. C. Read, Texas Agricultural Experiment Station, Dallas.

Read full chapter

URL: https://www.sciencedirect.com/science/article/pii/B978012374970300010X

Unbalanced Designs and Missing Data

Barry Kurt Moser, in Linear Models, 1996

In complete, balanced factorial experiments, the same number of replicate values is observed within each combination of the factors. Kronecker products may be used in such experiments to construct covariance and sum of squares matrices. However, in other types of experiments, the number of replicates per combination of the factors varies, or certain factor combinations may have no observations at all. Kronecker products are often not useful for constructing covariance and sums of squares matrices in such unbalanced and missing data experiments. To accommodate these unbalanced and missing data situations, replication and pattern matrices are introduced.

Read full chapter

URL: https://www.sciencedirect.com/science/article/pii/B9780125084659500077

Maximum Likelihood Estimation and Related Topics

Barry Kurt Moser, in Linear Models, 1996

Example 6.3.2

Consider the two-way balanced factorial experiment given in Example 6.3.1. The model can be written as $\mathbf{Y} = \mathbf{X}\beta+\mathbf{E}$ where $\mathbf{X} = \mathbf{1}_b \otimes \mathbf{I}_t$, $\beta = (\beta_1 \ldots, \beta_t)'$ and

$$\Sigma = \sigma_B^2 \left[\mathbf{I}_b \otimes \mathbf{J}_t\right] + \sigma_{BT}^2 \left[\mathbf{I}_b \otimes \left(\mathbf{I}_t - \tfrac{1}{t}\mathbf{J}_t\right)\right] \cdot$$

Let the sums of squares due to the overall mean, the random blocks, the fixed treatments, and the random interaction of blocks and treatments be represented

by $\mathbf{Y}'\mathbf{B}_1\mathbf{Y}$, $\mathbf{Y}'\mathbf{C}_1\mathbf{Y}$, $\mathbf{Y}'\mathbf{B}_2\mathbf{Y}$, and $\mathbf{Y}'\mathbf{C}_2\mathbf{Y}$, respectively, where $p_1 = 1$, $r_1 = b - 1$, $p_2 = t - 1$, $r_2 = (b - 1)(t - 1)$ and

$$\mathbf{B}_1 = \tfrac{1}{b}\mathbf{J}_b \otimes \tfrac{1}{t}\mathbf{J}_t$$
$$\mathbf{C}_1 = \left(\mathbf{I}_b - \tfrac{1}{b}\mathbf{J}_b\right) \otimes \tfrac{1}{t}\mathbf{J}_t$$
$$\mathbf{B}_2 = \tfrac{1}{b}\mathbf{J}_b \otimes \left(\mathbf{I}_t - \tfrac{1}{t}\mathbf{J}_t\right)$$
$$\mathbf{C}_2 = \left(\mathbf{I}_b - \tfrac{1}{b}\mathbf{J}_b\right) \otimes \left(\mathbf{I}_t - \tfrac{1}{t}\mathbf{J}_t\right).$$

Note that $\mathbf{I}_b \otimes \mathbf{I}_t = \mathbf{B}_1 + \mathbf{C}_1 + \mathbf{B}_2 + \mathbf{C}_2$. Furthermore, $\mathbf{B}_1\Sigma = t\sigma_B^2\mathbf{B}_1$, $\mathbf{C}_1\Sigma = t\sigma_B^2\mathbf{C}_1$, $\mathbf{B}_2\Sigma = \sigma_{BT}^2\mathbf{B}_2$, and $\mathbf{C}_2\Sigma = \sigma_{BT}^2\mathbf{C}_2$. Therefore, $\Sigma_{i=1}^2 a_i(\mathbf{B}_i + \mathbf{C}_i) = t\sigma_B^2[\mathbf{I}_b \otimes \frac{1}{t}\mathbf{J}_t] + t\sigma_{BT}^2[\mathbf{I}_b \otimes (\mathbf{I}_t - \frac{1}{t}\mathbf{J}_t)]$ where $a_1 = t\sigma^2{}_B$ and $a_2 = \sigma^2{}_{BT}$. Furthermore,

$$\sum_{i=1}^{2}\mathbf{B}_i\mathbf{X} = \left[\left(\tfrac{1}{b}\mathbf{J}_b \otimes \tfrac{1}{t}\mathbf{J}_t\right) + \left(\tfrac{1}{b}\mathbf{J}_b \otimes \left(\mathbf{I}_t - \tfrac{1}{t}\mathbf{J}_t\right)\right)\right][1_b \otimes \mathbf{I}_t]$$
$$= 1_b \otimes \mathbf{I}_t$$
$$= \mathbf{X}.$$

Therefore, by Theorem 6.3.1, the MLE of β is given by

$$\begin{aligned}\tilde{\beta} &= (\mathbf{X}'\mathbf{X})^{-1}\mathbf{X}'\mathbf{Y} \\ &= \left[(1_b \otimes \mathbf{I}_t)'(1_b \otimes \mathbf{I}_t)\right]^{-1}(1_b \otimes \mathbf{I}_t)'\mathbf{Y} \\ &= (\overline{Y}_{\cdot 1}, \ldots, \overline{Y}_{\cdot t})'\end{aligned}$$

and the MLEs of a_1 and a_2 are

$$\tilde{a}_1 = t\tilde{\sigma}_B^2 = \mathbf{Y}'\mathbf{C}_1\mathbf{Y}/b$$

and

$$\tilde{a}_2 = \tilde{\sigma}_{BT}^2 = \mathbf{Y}'\mathbf{C}_2\mathbf{Y}/[b(t-1)].$$

Therefore, the MLEs of $\sigma^2{}_B$ and $\sigma^2{}_{BT}$ are

$$\tilde{\sigma}_B^2 = \mathbf{Y}'\left[\left(\mathbf{I}_b - \tfrac{1}{b}\mathbf{J}_b\right) \otimes \tfrac{1}{t}\mathbf{J}_t\right]\mathbf{Y}/(bt)$$

and

$$\tilde{\sigma}_{BT}^2 = \mathbf{Y}'\left[\left(\mathbf{I}_b - \tfrac{1}{b}\mathbf{J}_b\right) \otimes \left(\mathbf{I}_t - \tfrac{1}{t}\mathbf{J}_t\right)\right]\mathbf{Y}/[b(t-1)].$$

These are the same MLEs derived in Example 6.3.1.

Although this chapter deals mainly with maximum likelihood estimators of multivariate normal models, Theorem 6.3.1 also motivates a further generalization of the Gauss–Markov theorem. The Gauss–Markov theorem was introduced in Section 5.2 for the model $\mathbf{Y} = \mathbf{X}\beta + \mathbf{E}$ when the $n \times 1$ error vector $\mathbf{E}$ had a distribution with $E(\mathbf{E}) = \mathbf{0}$ and $\text{cov}(\mathbf{E}) = \sigma^2\mathbf{I}_n$. In Section 5.4 the Gauss–Markov theorem was extended to include the model $\mathbf{Y} = \mathbf{X}\beta + \mathbf{E}$ with $E(\mathbf{E}) = \mathbf{0}$ and $\text{cov}(\mathbf{E}) = \sigma^2\mathbf{V}$ where $\mathbf{V}$ is an $n \times n$ positive definite matrix of known constants. In the next theorem, the Gauss–Markov theorem is again extended to include an even broader class of covariance matrices.

Read full chapter

URL: https://www.sciencedirect.com/science/article/pii/B9780125084659500065

Experimental Design for Mixture Studies

D. Voinovich, ... R. Phan-Tan-Luu, in Comprehensive Chemometrics, 2009

1.13.4.2 *D*-Optimal Designs

As occurs in experimental situations involving factorial experiments, also in mixture design the number of experiences increases rapidly along with the number of the various dimensional faces when $q \geq 5$. Moreover, the ultimate size of the design will also be a function of the number of model coefficients to be calculated. To reduce the size of the design for conducting experiments, in particular within irregularly shaped experimental regions due to physical or economic constraints on the design variables, the modern iterative methods for generating optimal designs for experiments can be applied.[20,21]

Let us consider again the four-component system presented in Example 7, where the constrained experimental domain of interest was defined through the composition of a set of remarkable points of the domain itself:

- the 10 vertices
- the 15 midpoints of the edges
- the 7 face centroids
- the overall centroid

This set of points may be used to estimate the response surface enabling the exploration of the entire region of interest. Generally, the investigator may wish to know the value of one or more responses at any point of the experimental domain. In this way, it will be possible to know the evolution of each response within the experimental domain. In this example, we initially assume that the special cubic polynomial may be adequate to model the response under study within the region of interest defined by Equations (36) and (53) and is shown in **Figure 13**:

$$\eta = \beta_1 x_1 + \beta_2 x_2 + \beta_3 x_3 + \beta_4 x_4 + \beta_{12} x_1 x_2 + \beta_{13} x_1 x_3 + \beta_{23} x_2 x_3 + \beta_{14} + \beta_{34} x_3 x_4 + \beta_{123} x_1 x_2 x_3 + \beta_{124} x_1 x_2 x_4 + \beta_{134} x_1 x_3 x_4 + \beta_{234} x_2 x_3 x_4 \quad (57)$$

This model for a four-component system has $p = 14$ parameters to be estimated by taking observations in the constrained composition space. The composition points for measuring the considered responses must be chosen in an appropriate way to ensure that the experimental data will provide the desired information. In other words, results of mixture experiments must enable the coefficient estimation of a model that, once its adequacy to represent the evolution of the measured response has been established, can be used for prediction in any point of the domain of interest with an acceptable precision (see Chapter 1.12).

The simplest strategy might be carrying out the experiments on the 33 candidate points listed in **Table 9**. However, given the large expenditures in terms of time and cost of experimentation frequently involved in research projects, reducing the number of experiments may be a requirement to be considered. If this be the case, then the objective is to select a subset of points from a list of candidate design points covering the feasible region (here, the 33 experiments), which will provide precise estimates of the parameters in the model (given in Equation (57)). To be able to compare various experimental designs for selecting an optimum design, the use of some quantitative criterion is recommended.[20]

Table 9. The candidate design points for exploring the constrained region defined in Equations (36) and (53)

Design points	X_1	X_2	X_3	X_4
1	0.150	0.050	0.100	0.700
2	0.020	0.200	0.100	0.680
3	0.150	0.050	0.700	0.100
4	0.020	0.180	0.100	0.700
5	0.020	0.180	0.700	0.100
6	0.020	0.200	0.680	0.100
7	0.150	0.150	0.100	0.600
8	0.100	0.200	0.100	0.600
9	0.150	0.150	0.600	0.100
10	0.100	0.200	0.600	0.100
11	0.150	0.050	0.400	0.400
12	0.085	0.115	0.100	0.700
13	0.150	0.100	0.100	0.650
14	0.020	0.190	0.100	0.690
15	0.020	0.200	0.390	0.390
16	0.060	0.200	0.100	0.640
17	0.085	0.115	0.700	0.100
18	0.150	0.100	0.650	0.100
19	0.020	0.180	0.400	0.400
20	0.020	0.190	0.690	0.100
21	0.060	0.200	0.640	0.100
22	0.125	0.175	0.100	0.600
23	0.150	0.150	0.350	0.350
24	0.100	0.200	0.350	0.350
25	0.125	0.175	0.600	0.100
26	0.125	0.175	0.350	0.350
27	0.085	0.115	0.400	0.400
28	0.020	0.190	0.395	0.395
29	0.150	0.100	0.375	0.375
30	0.060	0.200	0.370	0.370
31	0.088	0.156	0.100	0.656

Design points	X_1	X_2	X_3	X_4
32	0.088	0.156	0.656	0.100
33	0.088	0.156	0.378	0.378

Among the most useful criteria for assessing the quality of a particular design, there is the minimum–maximum variance, the *G*-optimality criterion, referring to the maximum variance function over the experimental region. If this is the design criterion selected, starting from a set of candidate points, all possible forms of the model matrix (**X**), along with their corresponding information matrix (**X′X**) and the dispersion matrix $(\mathbf{X'X})^{-1}$ can be calculated for some determined number of runs (representing fractions of the starting design). In this way, at any point of the experimental domain of interest the variance function, $\sigma^2 d$, where $d = \mathbf{x}(\mathbf{X'X})^{-1}\mathbf{x'}$, can be computed and thus its maximum value, $d_{\max}$, be known. The maximum variance function provides a measure of how close a given design is to optimum. However, to assess the optimum in percentage terms, the *G*-efficiency (*G* stands for global) of a design, involving also the number of model parameters and the number of observations in the design, may also be considered:

$$G - \text{efficiency} = \frac{100p}{Nd}$$

Let us apply the strategy to this example. The approach will involve a step-by-step procedure, as illustrated earlier in Chapter 1.12.

Step 1. Find if there exists a subset of experiments, $N < 33$, providing information of sufficient quality.

- Fix the minimal value of $N \geq N_I = 15$ (since the number of coefficient in the model is 14).
- Fix the maximal value of $N \leq N_F = 25$.
- Select an optimum experimental design ξ_{N^*} for fitting the assumed 14-term mixture model from a set Ξ of possible designs ξ_N based on a specific optimality criterion (a type I criterion). The set Ξ contains a number of different experimental designs given by

$$\frac{33!}{[(33-N)!N!]} \tag{58}$$

- Repeat this algorithm for different values of N ($N_I \leq N \leq N_F$) to obtain the optimal solution set ξ_{N^*}. Here, we refer to the *D*-optimality criterion, requiring the maximization of the determinant of the information matrix as the selected type I criterion. In **Table 10** some design properties of the generated optimal design solutions are given. The determinant of the moment matrix ($|\mathbf{M}|$), trace $(\mathbf{X'X})^{-1}$, and maximum variance function $d_{\max}$ are usually used to assess the statistical properties of the designs generated by the algorithm. The values for the design properties measured by the type I criteria for the resultant *D*-optimal designs are shown in **Figures 16** and **17**.

Step 2. For every value of N ($15 \leq N \leq 25$), at least one optimal experimental design ξ_{N^*} has been obtained by following the selected optimality criterion (here the *D*-optimality criterion). In this way, 14 possible *D*-optimal experimental designs have been generated and thus the question of what design or designs would be the best choice for experimentation must be answered. For this purpose, it should be considered a type II criterion such as the $d_{\max}$ over the region of interest. A representation of the evolution of this criterion is given in **Figure 18**.

It is clear that the experimental domain of interest is well represented by the 33 candidate design points. However, our objective is to find a reduced experimental design consisting of N runs ($N < 33$) that enables us to know the value of the property under study with an acceptable precision for the 33 candidate points. In this example, all the D-optimal experimental designs involving more than 17 points might be considered to know the value of the studied property with an acceptable precision. Then, which design should be chosen?

The spirit of any algorithm for selecting a subset of design points should be to help and not to dictate a design.[22] Among all the acceptable solutions, therefore, the final design will be chosen based on type III criteria, such as the number of experiments involved, the experimentation costs, and the easy feasibility.

Step 3. Given the objectives of the study and the assumed model for the response, we have a set of design points that allows us to generate useful information throughout the domain of interest with an acceptable quality. Remember that this is possible only if the model represents the studied response well. For validation of the model, however, some additional checkpoints are needed. It is evident that to detect lack of fit the additional points must not be the same that were used to estimate the model coefficients. These points are chosen so that useful information is provided to answer the following question: how well does the model represent the response behavior in the experimental domain of interest?

In the experimental domain of interest these points must be very far from the points belonging to ξ_{N^*}. Using the criteria for characterizing the distance between the points belonging to ξ_T (the candidate checkpoint set) and those belonging to ξ_{N^*}, let us choose the points located at the middle of the line joining the overall centroid to the vertices. Thus, there are 10 checkpoints possible, whose composition is as follows:

Checkpoints	*Length*	X_1	X_2	X_3	X_4
A	0.221	0.119	0.103	0.239	0.539
B	0.209	0.054	0.178	0.239	0.529
C	0.221	0.119	0.103	0.539	0.239
D	0.216	0.054	0.168	0.239	0.539
E	0.216	0.054	0.168	0.539	0.239
F	0.209	0.054	0.178	0.529	0.239
G	0.180	0.119	0.153	0.239	0.489
H	0.179	0.094	0.178	0.239	0.489
I	0.180	0.119	0.153	0.489	0.239
J	0.179	0.094	0.178	0.489	0.239

If we wish to reduce the number of checkpoints, the points with the smallest distance may be omitted. For instance, if to check the model lack of fit only five additional points are admitted, the following points should be chosen:

Checkpoints	X_1	X_2	X_3	X_4
A	0.119	0.103	0.239	0.539
B	0.054	0.178	0.239	0.529
C	0.119	0.103	0.539	0.239
D	0.054	0.168	0.239	0.539
E	0.054	0.168	0.539	0.239

Figure 19 illustrates the candidate design points used for generating D-optimal designs, along with the checkpoints for testing lack-of-fit model adequacy marked with a star symbol.

Table 10. Some optimality criteria for the *D*-optimal design solutions generated for the four-component system considered in Example 7: the determinant of the moment matrix ($|\mathbf{M}|$), the trace of the dispersion matrix tr $(X'X)^{-1}$, the maximum variance function (d_{max}), and *G*-efficiency (G_{eff})

N	$\|M\|^{1/14}$	$tr\,(X'X)^{-1}$	d_{max}	$\%G_{eff}$
15	1.220E–04	4.678E + 07	1.26	74
16	1.221E – 04	4.120E + 07	1.08	81
17	1.216E – 04	3.219E + 07	1.00	83
18	1.223E – 04	2.648E + 07	0.98	79
19	1.229E – 04	2.714E + 07	0.97	76
20	1.223E – 04	2.354E + 07	0.89	79
21	1.232E – 04	2.382E + 07	0.86	78
22	1.230E – 04	2.401E + 07	0.84	76
22	1.236E – 04	2.490E + 07	0.85	75
23	1.227E – 04	2.517E + 07	0.83	73
23	1.233E – 04	2.308E + 07	0.84	72
24	1.226E – 04	2.195E + 07	0.83	70
25	1.216E – 04	2.127E + 07	0.83	68
25	1.227E – 04	2.111E + 07	0.83	67

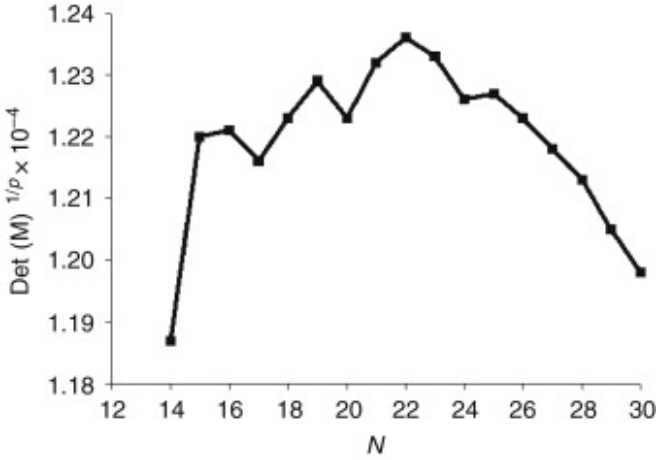

Figure 16. Trend of $|\mathbf{M}|^{1/14}$ criterion for the *D*-optimal designs generated by the algorithm.

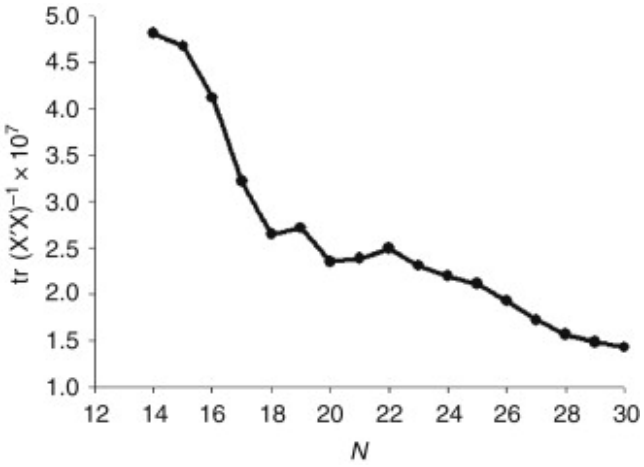

Figure 17. Trend of tr $(\mathbf{X'X})^{-1}$ criterion for the *D*-optimal designs generated by the algorithm.

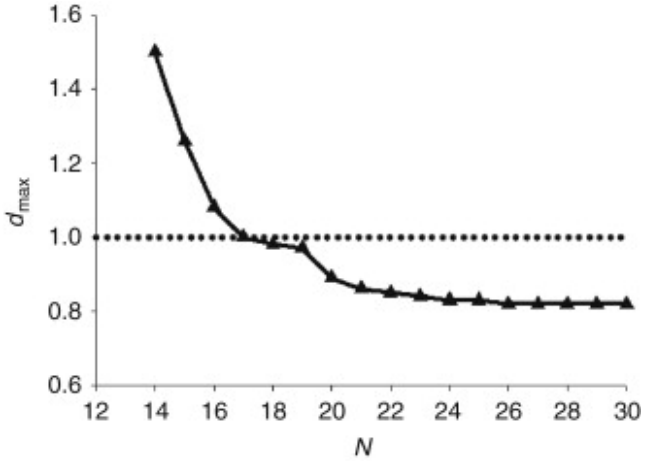

Figure 18. Trend of d_{max} criterion for the D-optimal designs generated by the algorithm.

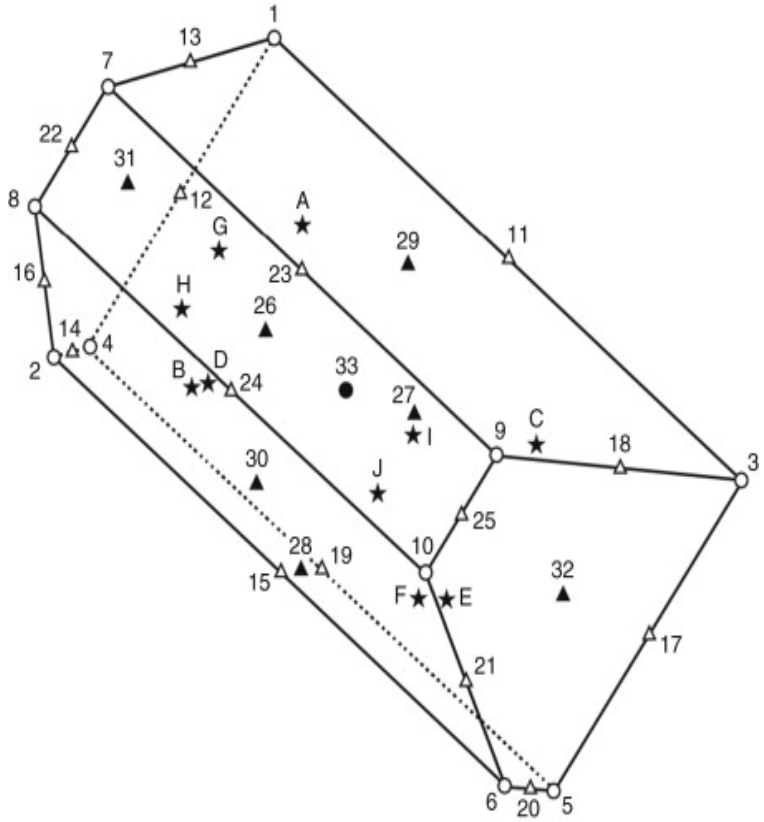

Figure 19. Design points in the constrained region for the four-component system (Example 7), along with the checkpoints for testing lack-of-fit model adequacy marked with the symbol ★.

Read full chapter

URL: https://www.sciencedirect.com/science/article/pii/B9780444527011000843

Complete, Balanced Factorial Experiments

Barry Kurt Moser, in Linear Models, 1996

Theorem 4.4.1

Let **Y** *be an* $n \times 1$ *random vector associated with the observations of a complete, balanced factorial experiment with an* $n \times 1$ *mean vector* $\mu = E(\mathbf{Y})$ *and* $n \times n$ *covariance* matrix $\Sigma = cov(\mathbf{Y})$. The expected mean square associated with the *sum of squares* $\mathbf{Y'AY}$ *is* $\mathbf{E}\{[1/tr(\mathbf{A}_s)]\mathbf{Y'AY}\} = [tr(\mathbf{A\Sigma}) + \mu'\mathbf{A}\mu]/tr(\mathbf{A})$ *where tr* (**A**) equals the *degrees of freedom* associated with $\mathbf{Y'AY}$.

Example 4.4.1

Consider the experiment described in Examples 4.3.1 and 4.3.3 in which a finite model was assumed. The sums of squares due to the random effect *B* and the fixed effect *T* are $\mathbf{Y'A}_2\mathbf{Y}$ and $\mathbf{Y'A}_3\mathbf{Y}$, respectively, where $\mathbf{A_2} = (1_b - \frac{1}{b}\mathbf{J}_b) \otimes \frac{1}{t}\mathbf{J}_t \otimes \frac{1}{r}\mathbf{J}_r$, $\mathbf{A_3} = \frac{1}{b}\mathbf{J}_b \otimes (\mathbf{I}_t - \frac{1}{t}\mathbf{J}_t) \otimes \frac{1}{r}\mathbf{J}_r$, and the $btr \times 1$ random vector $\mathbf{Y} = (\mathbf{Y}_{111}, \ldots, \mathbf{Y}_{11r}, \ldots, \mathbf{Y}_{btr})'$. The mean vector $\mu = \mathbf{E(Y)} = \mathbf{E}(\mathbf{Y}_{111}, \ldots, \mathbf{Y}_{11r}, \ldots, \mathbf{Y}_{bt1}, \ldots, \mathbf{Y}_{btr})' = 1_b \otimes (\mu_1, \ldots, \mu_t)' \otimes 1_r$. Note that $\mathbf{A_2\Sigma} = [tr\sigma_B^2 + \sigma_{R(BT)}^2]\mathbf{A}_2$ and $\mathbf{A_3\Sigma} = [r\sigma_{BT}^2 + \sigma_{R(BT)}^2]\mathbf{A}_3$. Therefore, by Theorem 4.4.1, the expected mean square of the random effect *B* equals

$$\begin{aligned}\mathbf{E}\left[\mathbf{Y}'\mathbf{A}_2\mathbf{Y}/tr\left(\mathbf{A}_2\right)\right] &= \left[r\left(\mathbf{A}_2\Sigma\right) + \mu'\mathbf{A}_2\mu\right]/tr\left(\mathbf{A}_2\right) = \left[tr\sigma_B^2 + \sigma_{R(BT)}^2\right] \\ &+ \left\{\left[1_b \otimes \left(\mu_1, \ldots, \mu_t\right)' \otimes 1_r\right]' \left[\left(\mathbf{I}_b - \tfrac{1}{b}\mathbf{J}_b\right) \otimes \tfrac{1}{t}\mathbf{J}_t \otimes\right.\right. \\ &\times \left.\left.\left[1_b \otimes \left(\mu_1, \ldots, \mu_t\right)' \otimes 1_r\right]/\left(b-1\right)\right\} \\ &= tr\sigma_B^2 + \sigma_{R(BT)}^2\end{aligned}$$

and the expected mean square of the fixed factor *T* equals

$$\begin{aligned}\mathbf{E}\left[\mathbf{Y}'\mathbf{A}_3\mathbf{Y}/tr\left(\mathbf{A}_3\right)\right] &= \left[tr\left(\mathbf{A}_3\Sigma\right) + \mu'\mathbf{A}_3\mu\right]/tr\left(\mathbf{A}_3\right) = \left[tr\sigma_B^2 + \sigma_{R(BT)}^2\right] \\ &+ \left\{\left[1_b \otimes \left(\mu_1, \ldots, \mu_t\right)' \otimes 1_r\right]' \left[\tfrac{1}{b}\mathbf{J}_b \otimes \left(\mathbf{I}_t - \tfrac{1}{t}\mathbf{J}_t\right) \otimes\right.\right. \\ &\times \left.\left.\left[1_b \otimes \left(\mu_1, \ldots, \mu_t\right)' \otimes 1_r\right]/\left(t-1\right)\right\} \\ &= \left[r\sigma_B^2 + \sigma_{R(BT)}^2\right] + br\textstyle\sum_{j=1}^{t}\left(\mu_j - \overline{\mu}\cdot\right)^2/\left(t-1\right)\cdot\end{aligned}$$

Thus, the expected mean square of the random effect *B* provides an unbiased estimate of $tr\sigma^2_B + \sigma^2_{R(BT)}$. Likewise, the expected mean square of the fixed factor *T* provides an unbiased estimate of $r\sigma_B^2 + \sigma_{R(BT)}^2 + br\Sigma_{j=1}^{t}(\mu_j - \overline{\mu}\cdot)^2/(t-1)$. The EMSs of the other effects can be calculated in a similar manner and are left to the reader.

Read full chapter

URL: https://www.sciencedirect.com/science/article/pii/B9780125084659500041

Chronometry of Mental Development

Arthur R. Jensen, in Clocking the Mind, 2006

Age Differences in the Effects of Procedural Conditions

Except for the overall relative slowness of RT for younger children, it is risky to generalize the details of any given paradigm or experimental procedure to others. Even rather subtle variations in these factors have effects on RT that are generally of greater magnitude in younger than in older children. This argues especially strongly for strict standardization of chronometric procedures in studies of preadolescent subjects if meaningful comparisons are to be made across different studies of a particular phenomenon.

Complex factorial experiments on the effects of varying several experimental conditions have been performed by Rogers Elliott (1970, 1972), using several age groups from 5 to 13 years and young adults (college students). In all studies, the RT task was SRT to an auditory stimulus. The five independent variables were: (1) *age* (years), (2) *preparatory interval* (PI = 1, 2, 4, 8, or 16 s); (3) *PI constant or varied* within a test session; *incentive* (monetary rewards for faster SRT); (4) *incentive-shift* (various combinations of shifting from a high to a low reward, e.g., HL, LH); and (5) *amount of practice* (1–10 sessions). Variation in all four of these conditions produced significant main effects, often surprisingly large. Within age groups most of the first-order interactions among the experimental variables were also significant. The results of such a multifactorial study with all its interactions are quite complex; they are most easily summarized graphically, as shown in Figure 5.10.

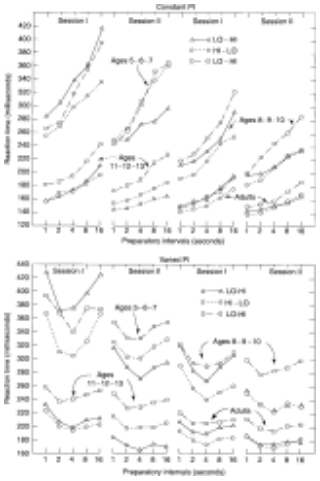

Figure 5.10. Auditory SRT as a function of five independent variables explained in the text.

(Reprinted from Elliott (1970, p. 94), with permission of Academic Press Inc.)

Read full chapter

URL: https://www.sciencedirect.com/science/article/pii/B9780080449395500069

Big Data Analytics

Saumyadipta Pyne, ... Madhav V. Marathe, in Handbook of Statistics, 2015

6.4 Decision Support Environments

The epidemiological modeling tools described above are capable of providing very detailed information on spatiotemporal disease dynamics. The size and scale of the data and the expertise required to use the simulations demand a user friendly

environment that provides an easy way to set up experiments and analyze the results. Recently, a number of visual analytics tools have been developed to support epidemiological research (see Livnat et al., 2010, 2012). We have built a tool called the SIBEL.[6] See http://isisdemo.vbi.vt.edu/didactic/isis.html for a demo version of SIBEL that allows a user to set up detailed factorial experiments (see Fig. 7). Using a simple interface to an underlying digital library, a user can choose from among many preconstructed instances: (i) a social contact network; (ii) a within-host disease progression model; and (iii) a set of interventions. Each intervention requires additional details such as compliance level, subpopulations to which the interventions are applied and intervention triggers. An experiment consists of sweeping one or more parameters across a user-specified range of values. After setting up the experiment, the user is provided access to the results of the simulations. A set of basic analyses are performed automatically and the results are displayed. The standard plots and epidemic curves provide very detailed information about the epidemic. Additional information such as the spatiotemporal dynamics and disease dendrogram (how the disease moved over the social network) is also available. A key aspect of this tool is its simplicity—we can train public health analysts to make effective use of the system in about 3 h. Several other groups are actively developing similar systems. They include: (i) The Biosurveillance Ecosystem (BSV) being developed by DTRA; (ii) The BARD model repository at the Los Alamos National Laboratory; (iii) The Texas Pandemic toolkit being developed at the University of Texas, Austin, http://flu.tacc.utexas.edu/; (iv) The MIDAS funded Apollo project at the University of Pittsburgh and the framework at RTI; (v) The FRED modeling framework at the University of Pittsburgh; and (vi) The EpiC framework being developed by MoBs laboratory at Northeastern University.

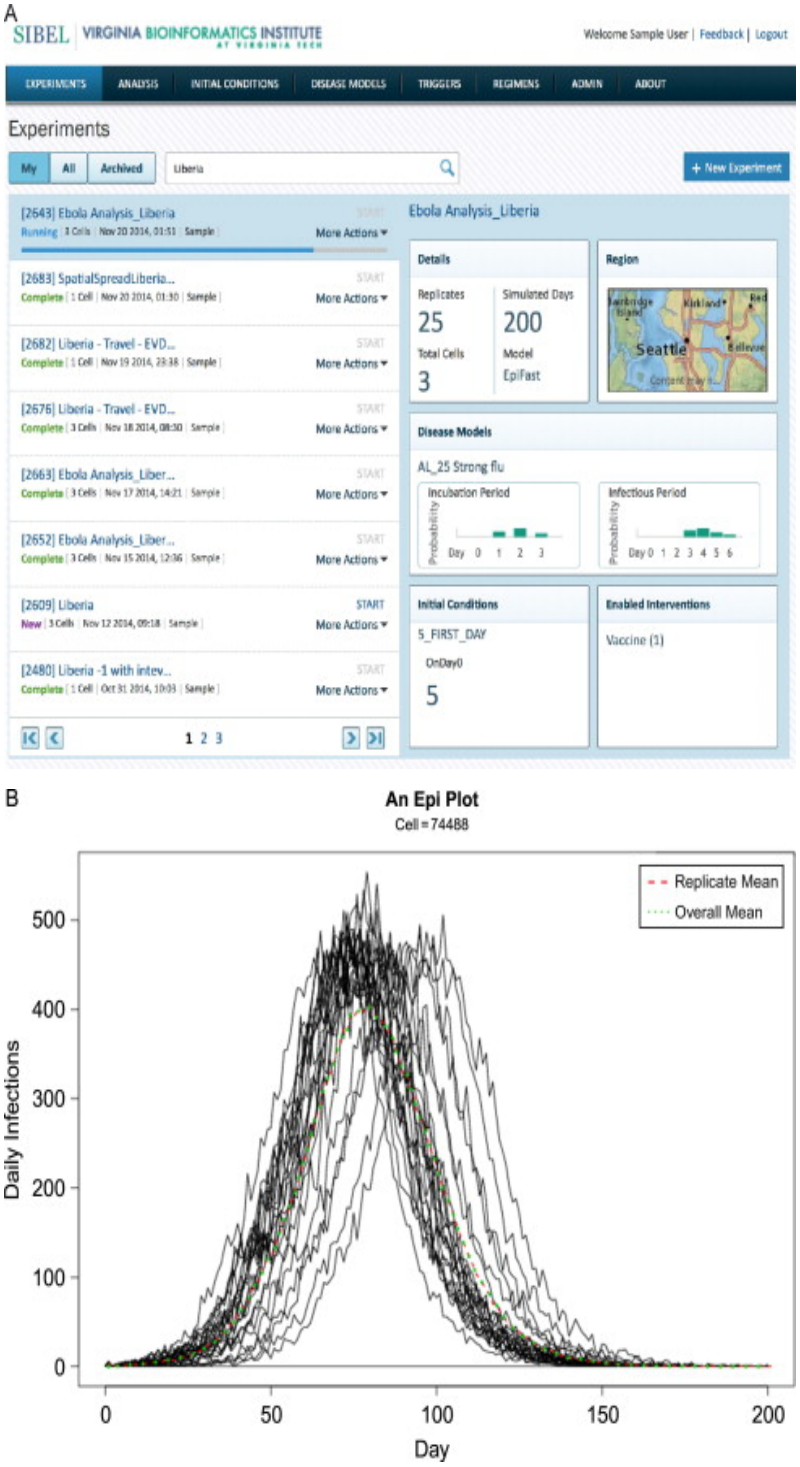

Figure 7. SIBEL interface (a). Example simulated epidemic curves (b).

Read full chapter

URL: https://www.sciencedirect.com/science/article/pii/B9780444634924000083