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Lecture 1

Experimental Design

Lesson 1: What is an Experiment?

- ◆ Experiment in *Statistics* is a scientific performance which is undertaken:
 - ★ to discover new facts,
 - ★ to test a hypothesis,
 - ★ to demonstrate a known fact.
- ◆ An experiment is a procedure carried out to support, refute, or validate a hypothesis.
- ◆ An experiment is a systematic investigation to advance our understanding of a phenomenon.
- ◆ Experiments vary greatly in goal and scale, but always rely on repeatable procedure and logical analysis of the results.
- ◆ An experiment is controlled tests to evaluate the factors that control the value of a parameter or group of parameters.

1.1 Random Experiment

Probability theory is based on the paradigm of a random experiment. A random experiment has the following properties:

- ◆ It has at least two outcomes,
- ◆ Whose outcome cannot be predicted with certainty, that depends on chance,
- ◆ It can be repeated arbitrarily often.

Lesson 2: Design of Experiment (DOE)

The process of **designing an experiment**, giving a detailed plan or strategy of conducting the experiment.

Design of Experiment is a branch of applied Statistics that deals with:

- ◆ planning (how to perform and design the experiment),
- ◆ conducting (how to conduct it),
- ◆ analyzing (data set to analyze), and
- ◆ interpreting (interpretation of outcomes from analysis)

All these steps are performed under the controlled tests to evaluate the factors that control the value of a parameter or group of parameters.

2.1 Main Concerns in Experimental Design

The main concerns in experimental design includes the establishment of:

- ◆ validity (valid results even if repeated),
- ◆ reliability (does results are reliable, i.e., less variability), and
- ◆ replicability (can be repeated again and again).

These concerns can be partially addressed by

- ◆ carefully choosing the independent variables
- ◆ reducing the risk of measurement error, and
- ◆ ensuring that the documentation of the method is sufficiently detailed
- ◆ achieving appropriate levels of statistical power and sensitivity.

Lesson 3: Objectives of an experiment

The main objectives of an experiment are as follows:

- ◆ To determine which variables are most important for the response,
- ◆ Different statistical tools are applied to quantify the importance of variables,
- ◆ To achieve desired response
For this we need suitable settings or levels of the influential variables are determined which may provide response in the desired range (within some limitation),
- ◆ To keep the variability of response small
It is achieved by determining the suitable settings of influential variables, the variability of response can be minimized which is also a desirable aspect,
- ◆ To make the system robust against outliers
For this we need to choose suitable levels of influential variables so that the effects of uncontrollable variables is minimized,
- ◆ To make the system robust against missing data
It is done by choosing suitable quantities of influential variables, the effects of missing observation on the analysis are minimized,
- ◆ Selection of design parameters to make the product robust to different variations in field conditions
- ◆ Determination of key product design parameters that impact product performance,
- ◆ Translate product design into a manufacturing system that operates effectively,
- ◆ To achieve the development objectives while using far fewer resources than traditional methods.

Read more on:

<https://itfeature.com/design-of-experiment-doe/design-of-experiments-overview>

Lecture 2

Application of Design of Experiments

Lesson 4: DOE in Agriculture

Many of the early applications of experimental design are in agriculture. Therefore, much of the terminology is derived from this heritage, like yield, split-plot, field trial, etc.

Many design types have been developed for field experiments. Any of several designs may be possible for a particular project, but each design has its own advantages and disadvantages.

Sir Ronald A. Fisher was the pioneer in the use of statistical methods in experimental design. For several years he had the responsibility of statistics and data analysis at Rothamsted Agriculture Experiment Station, London. He first used analysis of variance (ANOVA) technique in experimental design.

Commonly used designs in agriculture field are:

- ◆ Completely randomized design (CRD)
- ◆ Randomized complete block design (CRBD)
- ◆ Split-plot design
- ◆ Factorial designs
- ◆ Response surface designs (RSM)

The use of experimental design in agriculture can result in:

- ◆ Easier manufacturing
- ◆ Products with enhanced field performance
- ◆ More reliable products
- ◆ Lower product cost and time

Lesson 5: Some Agriculture Related Examples

◆ Example 1: Field trial

We want to compare 3 fertilizer treatments, denoted by A , B , and C assuming all other variables affecting the yield are uniform. We have 12 plots, and we decide to have four replications of each fertilizer.

This can be a completely randomized design (CRD).

◆ Example 2: Field trail

We want to compare 3 fertilizer treatments, denoted A , B , and C by applying them with 4

varieties α , β , γ and δ assuming all other variables affecting the yield are uniform. We have 12 plots.

This can be a randomized complete block design (CRBD) in which varieties can be used as 4 blocks.

◆ **Example 3: Optimization**

A farmer wants to optimize wheat yield. He considers seed, fertilizer, fertility and pesticide as potential factors contributing for the yield.

He may choose a factorial design to run his experiment. Experimental design will contain many trials based on different combinations of all four factors.

◆ **Example 4: Optimization**

A farm manager plans to optimize the use of a set of farm resources. He may think: "How can I get most net income from my limited land, labour, and capital?" or

"Would an extra bag of fertilizer per acre return a better net profit than, say a larger are of fodder crop, or more fencing?"

◆ **Example 5: Split-plot**

If irrigation is more difficult to vary on a small scale and fields are large enough to be split, a split plot design becomes appropriate. Irrigation levels are assigned to whole plots by CRD and fertilizer is assigned to subplots using RCBD (irrigation is the block).

Lesson 6: DOE in Engineering Design

Experimental designs play a major role in engineering design activities, which is a continuous process, where new products are developed and existing ones are improved.

6.1 Some Engineering Design Related Applications

- ◆ Evaluation and comparison of basic design configuration
- ◆ Evaluation of material alternatives
- ◆ Selection of design parameters to make the product robust to different variations in manufacturing/field conditions
- ◆ Determination of key product design parameters that impact product quality and quantity (performance)
- ◆ Translate this into a manufacturing system that operates effectively in a practicable manner
- ◆ To achieve the development objectives of optimization while using far fewer resources than traditional methods

The use of experimental design in these areas can result in:

- ◆ Easier manufacturing
- ◆ Products with enhanced field performance

- ◆ More reliable products
- ◆ Lower product cost and time

Lesson 7: Some Engineering Design Related Examples

Application of experimental design includes:

◆ Characterizing a process

Characterization, when used in materials science, refers to the broad and general process by which a material's structure and properties are probed and measured. It is a fundamental process, without which no scientific understanding of engineering materials could be ascertained. For example, a flow solder machine is used in the manufacturing process for printed circuit boards. An engineer wants to determine which factors affect the occurrence of defects on the printed circuit boards.

One can design an experiment that will enable him:

- ★ to estimate the magnitude and direction of factor effects, sometimes called a screening experiment
- ★ to use this information to identify the vital process factors
- ★ To determine direction of adjustments for these factors to reduce number of defects.
- ★ translate this into manufacturing system that operates effectively
- ★ to achieve the development objectives while using far fewer resources than traditional methods.

◆ Optimizing a process

After characterizing the process, it is natural to search for the region in important factors which leads to the best desirable response. If for example time and temperature are the vital factors for the response, it is necessary to vary both together, is called a factorial experimental design.

Experimental design method are often applied in the product design process. For example the engineers are designing a door hinge for an automobile. The latch design can be improved by varying the most influential factors on the latch check effort over certain ranges.

◆ Determining system and component tolerance

An engineer wants to design a circuit so that overall capability is good. An experimental design can be applied to determine which circuit components have the most critical tolerance and how much these can be tightened to produce adequate gauge capability.

Lesson 8: DOE in Life Sciences

In biology, data usually consist of a collection of observations or objects. These observations are usually sampling units (e.g., quadrats) or experimental units (e.g., individual organisms, and aquaria, etc.) and a set of these observations should represent a sample from a clearly defined population.

Some applications of DOE in life sciences include:

- ◆ Screening many factors which were initially considered important for a particular disease
- ◆ Identifying significant risk factors, for say, epidemiological diseases.
- ◆ Designing an efficient experiment for knowing the optimal combination of drugs.
- ◆ Designing experiments for clinical trials
- ◆ Designing experiments for follow-up studies

- ◆ Conducting Bayesian experimentation by using prior knowledge about a medical phenomenon
- ◆ Response surface designs are highly useful for laboratory experiments of life sciences where run-to-run variation is low and control of the experimenter is strong. These designs utilize all combinations of levels of each included factors and guide us to obtain an optimal response.

Lesson 9: Some Life Sciences Related Examples

◆ CRD Example:

A doctor wants to test the hypothesis that different treatment levels of a drug have same average effect upon the patients against the hypothesis that effects are different. He may run a completely randomized design to collect data from the patients. After performing analysis of variance, he could accept or reject the hypothesis.

◆ Split-plot Example:

A scientist wants to study different drugs, but these have different relative importance. He wants to apply the drugs on the experimental units of different size and importance. He may choose a split-plot design and apply the most important drug in subplots and less important in main plots.

◆ Central Composite Design:

In a clinical trial, a researcher wants to find the most suitable combination of drugs which optimize the response, i.e. response of the experimenter's choice. He may choose a central composite design and perform trial with different combination of selected drugs.

◆ Response Surface Design:

Response surface designs are highly useful for laboratory experiments where experimenter has strong control on the quantities of input variables. Drug manufacturing firms may use these designs to optimize the effectivity of their drugs.

Different designs are available in literature to handle different situations. For example, if experimental units are uniformly distributed then a completely randomized design can be used. If extraneous variables are in the study, then blocking can be done (that is randomized block design can be performed). After seeing the structure and properties of a design we can decide which design is useful for certain situation.

Lesson 10: DOE in Environmental Sciences

Environmental studies can be classified into baseline, monitoring and impact studies according to their objectives. Baseline studies are used to establish the "normal environment." Monitoring studies are used for detecting changes, and impact studies are designed to relate environmental changes to certain specific impact factors.

In an impact study, two controls, spatial and temporal, are needed to have an optimal impact design. An area-by-time factorial design provides evidence for impact effects in a significant area-by-time interaction.

The scope of the experiment is also defined by the objectives. For instance, a comparison of several varieties in several years in different locations, permits the researcher to make inferences about their behavior in different soil environments.

Thus the experimental design, in environmental sciences, is chosen to meet the following requirements:

- ◆ **The size of the study:**
Number of replications, and the size and shape of experimental units.
- ◆ **Environmental variables:**
The type of treatments, the levels of treatment, and the number of treatments.
- ◆ **Assignment of treatments to experimental units:**
Completely random, restricted Randomization, etc.
- ◆ **Error control:**
The error control can be accomplished by blocking techniques and the control of the environment using a growth chamber or greenhouse.

Types of DOE for environmental sciences

- ◆ Laboratory experiments
- ◆ Controlled environment
- ◆ Certain elements may not be included
- ◆ Missing factors and their interaction
- ◆ Simulation Experiments
- ◆ Randomization under defined model

Lesson 11: Some Environmental Sciences Related Examples

Some examples of experimental design in environmental studies

- ◆ **Randomized experimental design:**
In evaluating the environmental impact of the application of an herbicide, periodical soil data may have to be obtained from farms with herbicide application and farms without the herbicide application by using a randomized experimental design.
- ◆ **Completely randomized design:**
To study the environmental impact of fertilizers, 4 plots are selected at random for each fertilizer. This can be a completely randomized design. There are 4 replications for each treatment. If the experiment is run in succeeding years, then each year provides a different set of replications.
- ◆ **Repeated measures experimental design**
Same as the above example except the crop is a perennial. In this case the succeeding years are not replications. The fact that the crop is a perennial violates the independence requirement. This is a repeated measures experimental design.
- ◆ **Split-plot design:**
Same as above case except each of the 12 plots are further divided into three subplots. These subplots are not replications, they are subsamples. The randomization requirement above is violated. We may use split-plot design.
- ◆ **Split**

To optimize the ecosystem we may design the variables like:

- ◆ Wetland Depth
- ◆ Transfer Speed
- ◆ Water Table Use
- ◆ Pollution Levels

Under an efficient response surface design.

Lesson 12: DOE in Physical Sciences

The concepts and methods of DOE should be routine and essential part of the process of scientific investigation, and therefore of the education of scientists (Gunter and Matey, 1993).

Physical science is the systematic study of the inorganic world. Consisting of four broad areas:

- ◆ Astronomy,
- ◆ Physics,
- ◆ Chemistry, and
- ◆ Earth science.

Each is in turn divided into fields and subfields.

12.1 Major Physical Sciences Related Applications

- ◆ **Computer algorithms**
Computer software is now widely and economically available to automate the basic and most useful procedures.
Such as:
 - ★ Exchange algorithms for optimal designs
 - ★ Response surface (RS) designs
- ◆ **Response surface designs (RSM)**
Many RS design are available in literature and computer software which explore the experimental region of input variables like temperature, pressure, conductivity, thickness, etc. more efficiently, like:
 - ★ Central composite design
 - ★ Box-Behnken design
- ◆ **Mixtures experimentation**
New computational capabilities permit extension of experimental design to mixtures experiment in which the experimental factors include the proportions of ingredients of a mixture (e.g., paint, gasoline, steel, ceramics).

Lesson 13: Some Physical Sciences Related Examples

Following are some examples of DOE application in physical sciences:

- ◆ **Bayesian experimental design**
Consider a parameter inference problem. Its goal is to determine a substrate property from the behavior of a film deposited thereon. We design experiments to yield maximal information about the substrate property using only two measurements. A Bayesian experimental design approach is useful.
- ◆ **Response surface design**
An investigator is trying to develop a special plastic that acts as an electrical insulator in its normal state but can be made conductive by exposure to ultraviolet light. The controllable variables are:
 - ★ Forming speed

- ★ Fusion temperature
- ★ Cure time
- ★ Exposure intensity

An RS design may be employed in this case.

◆ **Balanced incomplete design**

An investigator wants to study three brands of batteries. He suspects that life of three brands is different. He wants to test 5 batteries from each brand. He may choose a completely randomized design and construct ANOVA table to test hypothesis of equal average life of all three brands.

- ◆ Seven different hardwood concentrations are to be studied to determine their effect on strength of paper. The pilot plant can only produce three runs each day, where the days can differ.

This experiment may be run using a balanced incomplete design.

Lesson 14: DOE in Management Sciences

Management science (MS), is the broad interdisciplinary study of problem solving and decision making in human organizations. It uses various scientific research-based principles, strategies and analytical methods.

Accurate management decisions are made by arriving at optimal or near optimal solutions to complex decision problems.

Planning is required in all types of organizations whether it is political, social, cultural, or business because it helps and directs various efforts towards a definite purpose.

Experimental research has been used extensively in the management sciences, e.g. experiments on business trends, identifying important factors, etc.

Incorporating a greater emphasis on designed experimental studies in management research is a route to similar advancements in that domain.

In management sciences following are the steps to follow when making use of statistical tools such as DOE:

- ◆ Organize projects and experiments
- ◆ Provide a uniform structure so that organization of experiments is possible
- ◆ Annotate the experiments so they can be cataloged and shared
- ◆ Annotate which resources are being used
- ◆ Annotate which results are produced by the experiment
- ◆ Provide information about the nature of the projects and experiments
- ◆ Provision resources to conduct the experiments
- ◆ Reproduce the experiment with the help of the recorded information

Lesson 15: Some Management Sciences Related Examples

Following are some examples showing application of DOE in management sciences:

- ◆ The management has to make a decision which products and how many units of each product should be produced.

The most frequent criteria of these models are profit (or revenue) maximization and cost minimization.

This kind of optimization can be achieved through proper design of experiment.

◆ **Product mix problems:**

Real situations in which some components are mixed to produce desired outputs are called blending problems, e.g. formulation of a paint.

Mixture experimental designs are most suitable for such experiments where input variables are the components forming a total product.

◆ **Consumer satisfaction:**

The goal of an enterprise is maximum consumer satisfaction by producing quality goods and at reasonable prices. This can be achieved by employing efficient experimental tools and making better use of scarce resources.

There are some steps to follow which are necessary in management sciences:

- ◆ Organize projects and experiments, e.g., project of solving transport issues
- ◆ Identify most vital market indicators/ decision variables
- ◆ Trying different models many managerial model are non-linear in nature, e.g., equilibrium and profit maximization models.

Lesson 16: DOE in Social Sciences

Social sciences are concerned with society and the relationships among individuals within a society, i.e., the social sciences consist of the scientific study of the human aspects of the world.

The social sciences include:

- ◆ Anthropology,
- ◆ Archaeology,
- ◆ Communication studies
- ◆ Economics
- ◆ History
- ◆ Human geography
- ◆ Linguistics
- ◆ Political science
- ◆ Psychology
- ◆ Sociology, etc.

Let we see which kind of social problems can be studied:

◆ **Comparing treatment with control:**

The effect of different treatments on the objects (experimental units) is compared with the effect when no treatment was applied.

A randomized design (blocked or unblocked) may be a suitable choice.

◆ **Repeated measures design-I:**

Changes in mean scores over three or more time points.

◆ **Repeated measures design-II**

Differences in mean scores under three or more different conditions.

Lesson 17: Some Social Sciences Related Examples

Here are examples of application of DOE in social sciences:

◆ **Randomized design (blocked or unblocked):**

A social scientist wants to obtain a clear evidence of the effects of various [policy] programs on education quality of the country.

He must use a randomized design, whether blocked or unblocked, to reach some conclusion.

◆ **Block design:**

If we are interested in understanding the effects of unemployment on three groups of individuals, people will be randomly allocated. All sorts of other personal and social characteristics can be separated by blocking.

A suitable blocked design is useful.

◆ **Repeated measures design:**

We might be investigating the effect of a psychological treatment for depression on a group of patients. We measure depression level at 3 separate time points.

A repeated measures design can be useful in this case.

Lecture 3

Basics of Design of Experiments

Lesson 18: Historical Perspective

The history of experimental design can be grouped into two era (i) Fisher's or before Fisher's era, and (ii) after Fisher's ear.

- ◆ Early applications in agriculture by R. A. Fisher at Rothamsted Experimental Station London in the 1920s and 1930s.
- ◆ **After Fisher**
- ◆ Some efficient designs for estimating several main effects were found by Raj Chandra Bose and K. Kishen in 1940 at the Indian Statistical Institute.
- ◆ Plackett–Burman designs and C. R. Rao's orthogonal arrays as experimental designs in 1940's.
- ◆ Experimental design for quality improvement in Japanese industry. The work of the Japanese quality consultant G. Taguchi on robust design for variation reduction, (see Taguchi, 1986; Nair, 1992).
- ◆ Developments of the theory of linear models- topics in algebra and combinatorics.
- ◆ The use of experimental design methods in the chemical industry was promoted in the 1950s by the extensive work of Box and his collaborators on response surface designs (Box and Draper, 1987).
- ◆ Frequentist to Bayesian approach
- ◆ Computer-aided design using simulation models, including applications in manufacturing (automobile and semiconductor industries), as well as in the nuclear industry. Sacks et al. (1989).
- ◆ Optimal designs (D-, A-, G-optimal, etc.)

Lesson 19: Definition of Basic Terms

Following are some definitions of terminologies used in DOE.

Definition 3.1

Treatment: A procedure or phenomenon whose effect on the experimental unit is observed, e.g., three varieties of wheat are three treatments.

Definition 3.2

Factor: A particular set of related treatments is called a factor, temperature is a factor that may be used in an experiment at different levels.

Definition 3.3

Level of Factor: The different states, quantities or intensities of a factor are called levels of a factor, e.g., different potencies of a drug.

Definition 3.4

Experimental Unit: A subset of experimental material to which treatment is applied is called experimental unit, e.g., a field, a patient, a machine, etc.

Definition 3.5

Block: A group of homogeneous experimental units is called a block, e.g., males or females, employed or unemployed, etc.

Definition 3.6

Response/Yield: The quantity which is measured as output from the experimental units after applying treatment.

Definition 3.7

Experimental Design: A set of rules or plan of applying treatment to the experimental units, e.g. one-factor-at-a-time design, factorial design, etc.

Definition 3.8

Run/Trial: The subset of an experiment, i.e., a single performance of an experiment is called a run.

Definition 3.9

Error: The variation among the responses observed from the experimental units treated alike is called experimental error.

- ◆ **Pure error**

Error measured from replication **Lack-of-fit error**

- ◆ Error produced from misfit of the assumed model

Basic Principles of DOE

There are basic principles to be used in DOE:

- ◆ Randomization
- ◆ Replication
- ◆ Local Control/ Blocking

Lesson 20: Basic Principles of DOE: Randomization

- ◆ The process of choosing experimental units randomly.
- ◆ We can also assign treatments randomly to the experimental units.
- ◆ Every object has a known probability of being sampled.
- ◆ Randomly decided which experimental trial is to be run.

How randomization is performed?

- ◆ By assigning random numbers from a random number table.
- ◆ Lottery method
- ◆ Using calculator or computer, etc.

Why it is necessary to do randomization?

Randomization guard against bias:

- ◆ Selection bias (where some groups are underrepresented) is eliminated
- ◆ Accidental bias (where chance imbalances happen) is minimized.
- ◆ Subjective bias (where personal liking or disliking) is minimized .

Statistical tests to check the randomness:

Testing a hypothesis if our sample is random, such as through run test.

Lesson 21: Examples of Randomization

Following are some examples of randomization:

- ◆ **Randomized block design:**
To study the effectiveness of 4 antibiotic medicines on 16 subjects. One may plan to divide them into 4 groups of 4 subjects each on the basis of 4 severity levels of disease. Using a randomized block design, the four members of each block are randomly assigned, one to each of the 4 medicine groups.
- ◆ **Split-plot design:**
Four varieties of wheat are to be compared, second variable affecting the production is fertilizers being applied at three levels. Since, both treatments have different importance for the experimenter, a split-plot design is chosen to randomly apply wheat varieties to sub-plots and the fertilizers to the main plots.
- ◆ **Central composite design:**
In a botanical experiment three quantitative variables temperature, volume and pH are contributing for the dye color. Experimenter decides to use a central composite design of three factors with 17 unique trials. Experimental trials are performed in random order.
- ◆ **Simplex-centroid design:**
A mixture experiment is planned to determine if an artificial sweetener could be developed for a soft drink that would minimize the aftertaste. Four different sweeteners are blended

through a simplex-centroid design of 4 components and 15 runs. The principle of randomization is applied to decide which trial is performed in which order.

Lesson 22: Basic Principles of DOE: Replication

The second most important basic principles of DOE. Replication is necessary because without replication we cannot know about the variation in response variable.

For example, if we need to compare grain yield of two varieties of wheat then each variety is applied to more than one experimental unit. The number of times these are applied on experimental units is called their number of replications.

Why Replication is necessary?

- ◆ Some variation exists because the experimental units, such as, individuals or plots of land, cannot be physically identical.
- ◆ Repeatedly produced results under same environment are more reliable

Statistical Importance of Replication

- ◆ It allows the experimenter to obtain an estimate of the experimental error (pure error).
- ◆ The more replication would provide the increased precision by reducing the standard error (SE) of mean.
- ◆ Researchers repeat the same studies on different experimental units to see if they produce the same statistically significant results each time.
- ◆ Replication provides some extra degrees of freedom to estimate random variation in response.

Therefore, without replication many aspects of analysis cannot be studied.

Lesson 23: Examples of Replication

Following are some examples of replication:

- ◆ Here's the production of four varieties (A, B, C, and D) and **4 replicates** of each, hence 16 experimental trials under a CRD.

D=25 1	D=27 2	B=35 3	C=38 4	D=29 5	C=36 6	A=22 7	A=24 8
C=33 9	B=37 10	A=21 11	B=34 12	C=38 13	B=37 14	A=29 15	D=30 16

- ◆ BP readings of 4 patients taking 4 different medicines, Each medicine is repeated twice on each patient, therefore a total of 16 experimental trials under a RCBD.

Medicine	Patient			
	1	2	3	4
1	135, 134	136, 137	133, 131	138, 140
2	136, 141	141, 140	141, 139	144, 142
3	134, 136	132, 130	135, 136	130, 133
4	129, 128	132, 132	135, 130	127, 129

- ◆ BP readings of 4 patients taking 4 different medicines. Each medicine is repeated twice on each patient under 4 diet plans *A, B, C*, and *D*, therefore, a total of 16 experimental trials under a Latin Squares Design. It is three-way Blocking, as there are 4 patients taking 4

Medicine	Patient			
	1	2	3	4
1	135, 134	136, 137	133, 131	138, 140
2	136, 141	141, 140	141, 139	144, 142
3	134, 136	132, 130	135, 136	130, 133
4	129, 128	132, 132	135, 130	127, 129

different medicines under 4 diet plans.

Lesson 24: Basic Principles of DOE: Local Control/Blocking

In the theory of the design of experiments, blocking is the arrangement of experimental units in groups (blocks) that are homogeneous internally and different from each other externally. Typically, a blocking factor is a source of variability that is not of primary interest to the experimenter.

Blocking Factors

A nuisance factor (extraneous variable) is used as a blocking factor. Blocks are constructed based on different levels/ quantities of blocking factor, e.g., in a cancer treatment experiment, the financial condition of patient can be blocking factor.

Blocking to “Remove” the Effect of Nuisance Factors

Since one block represents one level of blocking variable, response can be compared within a block.

Blocking used for nuisance factors that can be controlled

The basic concept is to create homogeneous blocks in which the nuisance factors are held constant (controlled at desirable level) and the factor of interest is allowed to vary.

Reducing Experimental Error

When we control nuisance factors, we reduce or eliminate the contribution of experimental error contributed by nuisance factors.

Block a few of the most important nuisance factors

The general rule is: “Block what you can; randomize what you cannot.”

Lesson 25: Examples of Local Control/ Blocking

- ◆ Clinical Trial
An experiment is designed to test a new drug on patients. There are two levels of the treatment, drug and placebo, administered to male and female patients. Since males and females respond the treatment differently, they are placed in two different blocks thus leading to greater precision.
- ◆ Elevation
Testing the effects of a new pesticide on a specific patch of grass. The grass area consists of two distinct regions- 'high elevation' and 'low elevation'. A treatment group (the new

pesticide) and a placebo group are applied to both regions of grass. In this instance the researcher is blocking the elevation factor.

◆ **Intervention**

Suppose a process is invented that intends to make the soles of shoes last longer, and a plan is formed to conduct a field trial. Given a group of n volunteers, one possible design would be to give $\frac{n}{2}$ of them shoes with the new soles and $\frac{n}{2}$ of them shoes with the ordinary soles, randomizing the assignment of the two kinds of soles. This is a CRD.

◆ **Scarcity of Resources**

Consider a factorial experiment designed to study the effects of three continuous two-level factors on a response. The full factorial plan has 8 runs but only 4 trials can be performed in one lab. We may run four trials in each of two labs as:

Lab 1	Lab 2
a	(1)
b	ab
c	ac
abc	bc

Lesson 26: Steps Involved in Designing of an Experiment

Following are steps involved in designing an experiment.

◆ **Recognizing the Problem**

- ★ Necessary to develop a solid understanding about the objectives of experiment.
- ★ A clear statement of the problem often contributes substantially to a better understanding of the phenomenon.

◆ **Choice of Factors and Levels**

- ★ Identifying suitable factors to be varied
- ★ Factor regions and number of levels of each factor
- ★ Practical experience and theoretical knowledge of the process helps a lot

◆ **Deciding About Response**

- ★ Which response really provides required information about process?
- ★ The form of response: average response, standard deviation or other transformation?
- ★ Single or multiple response?

◆ **Choosing Design**

Choice of design involves:

- ★ Which design? One-factor-at-a-time or factorial?
- ★ Size of design (number of trials)?
- ★ Blocking or not?
- ★ Fraction or Full?

◆ **Performing Experiment**

- ★ Careful execution of experiment is necessary
- ★ Random choice of experimental trials

◆ **Analysis**

- ★ Valid analyzing tools are necessary to get results in numeric form
- ★ Sometimes more than one analyzing tool is applied to have a clear picture

- ★ Graphical tools are helpful
- ★ Many statistical software are available like: Minitab, SPSS, R, etc.
- ◆ **Conclusion/Interpretation**
After analysis, experimenter must:
 - ★ Draw practical conclusions
 - ★ Recommend a course of action, e.g., follow-ups
 - ★ Give some future directions

Lesson 27: Some Practical Advises in DOE

- ◆ **Identify the Right Variables and Region**
When designing an experiment it is necessary to initially run some screening process to identify most suitable factors.
- ◆ **Spread Control Runs Evenly** By spacing center points evenly through the design, these observations serve as an indicator of the stability of your process during the experiment. The central run is an average of a variable and we expect that average response is being produced?
- ◆ **Improve Power of Design by Expanding the Range of Input Settings**
Test the largest range of input variable settings that is physically possible. This will allow you to use the experiment to understand your process so that you can find the optimal settings.
- ◆ **Fractionate to Save Runs-Resolution V designs**
In many cases, it's beneficial to choose a design with $\frac{1}{2}$ (half) or $\frac{1}{4}$ (quarter) of the runs of a full factorial. Resolution V design allows you to estimate all main effects and two-way interactions. Designs less than resolution V designs usually miss important estimates.
- ◆ **Improve Power with Replicates**
Power is the probability of detecting an effect on the response if that effect exists. To increase the chance that you will successfully identify the inputs that affect your response, add replicates to your experiment.
- ◆ **Improve Power by Using Quantitative Measures of Response**
Always try measuring a quantitative response. This will improve the power of your experiment with small number of runs.

Read more on

<https://itfeature.com/design-of-experiment-doe/basic-principles-of-experimental-design>

Lecture 4

Testing of Hypothesis-I

Lesson 28: Hypothesis Testing

Definition 4.1

A procedure of testing a hypothesis formulated about some population parameter, based on of sample information.

28.1 Steps Involved in Testing of Hypothesis

Step 1: Formulation of Hypothesis

A statement about some population parameter which is to be tested.

- ◆ Null hypothesis $H_0 : \mu = \mu_0$
- ◆ Alternate hypothesis $H_1 : \mu \neq \mu_0$ (two-tailed test)
 $H_1 : \mu > \mu_0$ OR $H_1 : \mu < \mu_0$ (one-tailed test)

Step 2: Level of significance (α)

- ◆ A suitable probability chosen to show the chances of rejecting H_0 when it was true. Also called type-I error.
- ◆ Usually kept at 1%, 5%, etc.

Step 3: Test Statistics

- ◆ A rule or formulae used for testing a hypothesis.
- ◆ For testing equality of means Z-statistic, t-statistic and F-statistics can be used.

$$Z = \frac{M(X) - \mu}{\frac{\sigma}{\sqrt{n}}},$$
$$Z = \frac{M(X) - \mu}{\frac{S(X)}{\sqrt{n}}},$$
$$t = \frac{M(X) - \mu}{\frac{s(X)}{\sqrt{n}}},$$

or $F = \frac{MSt}{MSe}$

where $S(X)$ is sample standard deviation, σ is population standard deviation, $M(X)$ is mean of the sample, μ is population mean assumed in formation of hypothesis.

If number of observations are large enough ($n > 30$) then we can use Z-statistics, otherwise t-statistics for testing the equality of means.

Step 4: **Critical Region**

- ◆ These are the set of values which lead the experimenter to reject H_0
- ◆ Also called rejection region
- For example, $|t| \geq t_{\frac{\alpha}{2}, d.f.}$ (two-tailed)
- $t > t_{\alpha, d.f.}$ (one-tailed)
- $t < -t_{\alpha, d.f.}$ (one-tailed)

Step 5: **Computation**

- ◆ In this step the formulae or test statistic is applied to obtain a numerical result

Step 6: **Conclusion**

- ◆ If the computed value of test statistic falls in the critical region, H_0 is rejected.
- ◆ Accepted otherwise.

Lesson 29: Testing Mean of Population

If we want to test mean of a population then there are some possible tests, such as:

- ◆ Most popular/common test
- ◆ Large sample(s) test: Z-test
- ◆ Small sample(s) test: t-test
- ◆ F-test (extension of t-test)

29.1 Large or Small Sample?

It is a relative term, and an experimenter decides either his sample is large or small.

- ◆ Interpretation varies
- ◆ Relative to population size
- ◆ t-test is more realistic and practical than z-test

29.2 Central Limit Theorem

- ◆ A random variable from a population has known mean and finite variance
- ◆ The sampling distribution of the sample from this population approaches normal distribution if sample size is large enough.

29.3 Z-test

- ◆ Population variance known, OR
- ◆ Sample size is large (sample is 5% or more than 5% of the population)

Lot of software (such as Minitab, SAS, SPSS, and R, etc.) are available to perform Z-test, t-test, and ANOVA test, etc.

Lesson 30: Testing Mean: A Numerical Example

Example 1: A report says that the average cost of rehabilitation for stroke victims is Rs. 124,672. From a random sample of 35 stroke victims at a hospital shows the average cost of Rs. 126,343.

The standard deviation of the population is Rs.3251. At a $\alpha = 0.01$, can it be concluded that the average cost of stroke rehabilitation at that hospital is significantly different?

Solution:

1.

$H_0 : \mu = Rs.124,672$ and $H_1 : \mu \neq Rs.124,672$ (claim)
2.

$\alpha = 0.01$
3.

$|Z| \geq |Z_{\frac{\alpha}{2}}|$ (two-tailed), i.e. $|Z| \geq 2.58$
4.

$Z = \frac{126343-124672}{\frac{3251}{\sqrt{35}}} = 3.04$
5.

Since calculated value of Z falls in rejection region, we reject the claim of Rs. 124,672 average expenditures.

□

Commonly used table Values of Z for Most common α

Level of Significance (α)	Two-Tailed Test	One-Tailed Test
0.01 (1%)	$Z_{\frac{\alpha}{2}} = \pm 1.645$	$Z_{\alpha} = \pm 2.33$
0.05 (5%)	$Z_{\frac{\alpha}{2}} = \pm 1.96$	$Z_{\alpha} = \pm 1.645$
0.10 (10%)	$Z_{\frac{\alpha}{2}} = \pm 2.58$	$Z_{\alpha} = \pm 1.28$

Example 2: A medical investigation claims that the average number of infections per week at a hospital in Lahore is 16.3. A random sample of 10 weeks had a mean number of 17.7 infections. The sample standard deviation is 1.8. Is there enough evidence to reject the investigator’s claim at a $\alpha = 0.05$?

Solution:

1.

$H_0 : \mu = 16.3$ and $H_1 : \mu \neq 16.3$
2.

$\alpha = 0.05$
3.

$|t| \geq |t_{\frac{\alpha}{2}(n-1)}|$ (two-tailed), i.e. $|t| \geq 2.262$
4.

$t = \frac{17.7-16.3}{\frac{1.8}{\sqrt{10}}} = 2.46$
5.

Since calculated value of t falls in rejection region, we reject H_0 .

□

Lesson 31: Testing Equality of Two Population Means

Here we learn how to population means are compared. We choose either Z-test or t-test on the bases of sample size.

- ◆

Z-test (Large samples)

★

Both populations are normal with known variances

★

Both populations are normal with unknown variances, large samples (following central limit theorem)

★

Both populations are non-normal with known/unknown variances, large samples (following central limit theorem)
- ◆

t-test (Small samples)

★

Both populations are normal with equal but unknown variances

★

Both populations are normal with unequal and unknown variances

★ Testing difference of two population means with paired observations

Lesson 32: Independent Samples When Population Variances are Equal

First we need to know what is meant by independent samples and equality of variances.

◆ Independent Samples

- ★ The samples that are selected randomly and independently from two normal populations.
- ★ Many statistical analyses are based on the assumption that samples are independent.

◆ Equal Variances

- ★ Independent samples t-test also assumes that the variance for population-1 is about the same as that of population-2, we can estimate the common variance by pooling information from samples from population-1 and population-2.

32.1 Procedures of Performing the Independent Sample t-Test

- Step 1: $H_0 : \mu_1 - \mu_2 = \Lambda_0$ VS
 $H_1 : \mu_1 - \mu_2 \neq \Lambda_0$ or
 $H_1 : \mu_1 - \mu_2 > \Lambda_0$ or
 $H_1 : \mu_1 - \mu_2 < \Lambda_0$

Step 2: Level of significance (α)

Step 3: Test statistic

$$t = \frac{(\bar{x}_1 - \bar{x}_2) - \Lambda_0}{s_p \sqrt{\frac{1}{n_1} + \frac{1}{n_2}}}$$

where

$$s_p^2 = \frac{(n_1 - 1)s_1^2 + (n_2 - 1)s_2^2}{n_1 + n_2 - 2} \text{ is pooled variance}$$

Step 4: Critical region

$$\begin{aligned} |t| &\geq t_{\frac{\alpha}{2}, d.f.} \text{ (two-tailed)} \\ t &> t_{\alpha, d.f.} \text{ (one-tailed)} \\ t &< -t_{\alpha, d.f.} \text{ (one-tailed)} \end{aligned}$$

Degree of freedom (d.f.) = $n_1 + n_2 - 2$

Step 5: Computation

Step 6: Conclusion

Lesson 33: Independent Samples t-test: Numerical Example

Example 3: A sample of 10 from a machine which packs cartons of jars shows mean time 42.14 min and S.D. 0.683 min. Another sample of 10 from a new machine shows mean time 43.23 min

with S.D. of 0.750 min. Test the hypothesis that second machine is faster, at $\alpha = 5\%$.

Solution:

- ◆ $H_0 : \mu_1 - \mu_2 = 0$
- ◆ $H_1 : \mu_1 - \mu_2 > 0$
- ◆ $\alpha = 0.05$
- ◆ $S_p^2 = \frac{(n_1-1)s_1^2 + (n_2-1)s_2^2}{n_1+n_2-2} \Rightarrow s_p = 0.717$
- ◆ $t = \frac{(\bar{X}_1 - \bar{X}_2) - \Delta_0}{s_p \sqrt{\frac{1}{n_1} + \frac{1}{n_2}}} = \frac{(42.14 - 43.23) - 0}{0.717 \sqrt{\frac{1}{10} + \frac{1}{10}}} = 3.40$
- ◆ $t > t_{0.05(18)} = 1.734$
- ◆ Reject H_0 at $\alpha = 0.05$

□

Lecture 5

Testing of Hypothesis-II

Lesson 34: Independent Samples When Population Variances are Unequal

It is assumed that

- ◆ The samples that are selected randomly and independently from two normal populations.
- ◆ Two populations are not known to have uniform variances.

34.1 Procedures of Performing the Independent Sample t-Test

- Step 1: $H_0 : \mu_1 - \mu_2 = \Lambda_0$
 $H_1 : \mu_1 - \mu_2 \neq \Lambda_0$ or
 $H_1 : \mu_1 - \mu_2 > \Lambda_0$ or
 $H_1 : \mu_1 - \mu_2 < \Lambda_0$
- Step 2: **Level of significance (α)**
- Step 3: **Test statistic**

$$t = \frac{(\bar{X}_1 - \bar{X}_2) - \Lambda_0}{\sqrt{\frac{s_1^2}{n_1} + \frac{s_2^2}{n_2}}}$$

- Step 4: **Critical region**

$$|t| \geq t_{\frac{\alpha}{2}, d.f.} \text{ (two-tailed)}$$

$$t > t_{\alpha, d.f.} \text{ (one-tailed)}$$

$$t < -t_{\alpha, d.f.} \text{ (one-tailed)}$$

Degree of freedom (d.f.):

$$d.f. = \frac{\left(\frac{s_1^2}{n_1} + \frac{s_2^2}{n_2}\right)^2}{\frac{1}{n_1-1} \left(\frac{s_1^2}{n_1}\right)^2 + \frac{1}{n_2-1} \left(\frac{s_2^2}{n_2}\right)^2}$$

- Step 5: **Computation**
- Step 6: **Conclusion**

Lesson 35: Independent Samples t-test: Numerical Example

Example 1: Independent random samples of 13 sophomores and 12 juniors attending a large university yield the following data on grade point averages

Sophomores: 3.04, 2.92, 2.86, 1.71, 3.60, 3.49, 3.30, 2.28, 3.11, 2.88, 2.82, 2.13, 2.11.

Juniors: 2.56, 3.47, 2.65, 2.77, 3.26, 3.00, 2.70, 3.20, 3.39, 3.00, 3.19, 2.58.

At the 5% significance level, do the data provide sufficient evidence to conclude that the mean GPAs of sophomores and juniors at the university differ?

Solution:

1. $H_0 : \mu_1 - \mu_2 = 0$
 $H_1 : \mu_1 - \mu_2 \neq 0$
2. $\alpha = 0.05$
3. $t = \frac{(\bar{X}_1 - \bar{X}_2) - \Delta_0}{\sqrt{\frac{s_1^2}{n_1} + \frac{s_2^2}{n_2}}} = -1.05$
4. $|t| \geq t_{0.025, df=19} = 2.093$
5. Accept H_0 at $\alpha = 0.05$.

□

Lesson 36: Testing Equality of Two Population Means: Paired Samples

Paired sample t-test is:

- ◆ If each data point in one sample is uniquely paired to a data point in the second sample.
- ◆ The information on one sample only is meaningless for the experimenter.

In **Paired Samples t-test**,

- ◆ The t-test assesses whether the mean scores from two experimental conditions are statistically different.
- ◆ A repeated-measures t-test (also known as the ‘related’ t-test)
- ◆ You should use in situations when your design is within participants.

Procedures of Performing the Paired Sample t-test

Step 1: $H_0 : \mu_d = 0$ vs $H_1 : \mu_d \neq 0$

Step 2: Level of significance (α)

Step 3: Test statistic

$$t = \frac{\bar{d} - \mu_d}{\frac{s_d}{\sqrt{n}}}$$

where from two samples X_1 and X_2 , $d_i = X_1 - X_2$

The S_d or S_d^2 can be computed as

$$S_d^2 = \frac{\sum (d_i - \bar{d})^2}{n-1}$$

Step 4: Critical Region

$$\begin{aligned}
 |t| &\geq t_{\frac{\alpha}{2}, d.f.} \quad (\text{two-tailed}) \\
 t &> t_{\alpha, d.f.} \quad (\text{one-tailed}) \\
 t &< -t_{\alpha, d.f.} \quad (\text{one-tailed}) \\
 d.f. &= n - 1 \text{ degrees of freedom}
 \end{aligned}$$

Step 5: Computation

Step 6: Conclusion

Lesson 37: Paired Sample t-test: Numerical Example

Example 2: Scores of a sample of 9 students which were given a diagnostic test before studying a particular module and after completing the module, are given as:

Pre-module: 18, 21, 16, 22, 19, 24, 17, 21, 23.

Post-module: 22, 25, 17, 24, 16, 29, 20, 23, 19.

We want to find out if, our teaching leads to significant improvements in students' test scores.

Solution:

1. $H_0 : \mu_d = 0$
 $H_1 : \mu_d \neq 0$
2. **Level of significance**
 $\alpha = 0.05$
3. **Test statistic**

$$t = \frac{\bar{d} - \mu_d}{\frac{s_d}{\sqrt{n}}}$$

where from two samples X_1 and X_2

$$\begin{aligned}
 \bar{d} &= -1.56 & S_d &= 3.1 \\
 t &= -1.50
 \end{aligned}$$

4. **Critical region**
 $|t| \geq t_{0.025(9)} = 2.262$
5. **Conclusion**

Since calculated value of test statistic does not fall in the critical region, therefore we accept H_0 , i.e. The group students did not improve their skills.

□

Lecture 6

Analysis of Variance

Analysis of Variance (ANOVA) is a statistical tool for comparing means of more than two populations.

Lesson 38: Analysis of variance (ANOVA)

Why ANOVA?

In real world, experimental data do not typically result in two groups being compared:

- ◆ Testing average production of three new varieties of wheat.
- ◆ Whether four different types of professionals have same purchasing power or not.
- ◆ Greater risk of a type-I error in case of t-test.
- ◆ ANOVA was developed by R. A. Fisher in 1920 at Rothamsted, London.
- ◆ ANOVA Suitable for comparing more than two population means.
- ◆ ANOVA allows us to see if there are differences between means with an OMNIBUS test.

F-statistic

Basic ANOVA measures two sources of variation:

- ◆ **Variation BETWEEN groups**
For each value look at the difference between its group mean and overall mean
- ◆ **Variation WITHIN groups**
Look at the difference between that value and the mean of that group

$$F = \frac{\text{Variability between groups}}{\text{Variability within groups}}$$

Critical Region

$$F \geq F_{\alpha, \text{between d.f., within d.f.}}$$

If F calculate value is greater than the F tabulated then we will reject the H_0 .

Lesson 39: Assumptions of ANOVA

The assumptions of ANOVA are:

◆ **Normality assumption**

The experimental errors of experimental data are normally distributed. For the validity of results and application of different inferential tools this assumption is necessary.

◆ **Homoscedasticity**

Equal variances between treatments, also called homogeneity of variances. It is assumed that each treatment is being drawn from same population or similar populations, that is, all treatments have equal variances.

◆ **Independence**

Each treatment is randomly and independently applied to the experimental units. There should be no biasedness in the selection of treatment for an experimental unit and one treatment does not depend on which other treatment at what level is being applied in the trial.

If all of these assumption follows then we can use ANOVA otherwise we need to choose some other statistical tool.

Lesson 40: Single Factor ANOVA

What Single Factor?

If only one variable is assumed to affect the response, then single factor ANOVA is applied.

The **Assumed Model** for single factor ANOVA will be

Let

$$y_{ij} = \mu + \tau_i + \varepsilon_{ij}$$

where

$$i = 1, 2, \dots, a, \quad j = 1, 2, \dots, n$$

a = types of a treatment

n = number of observations under each treatment

y_{ij} = j th observation under i th treatment level.

There are three terms in the model for single factor ANOVA. The model terms are

μ = overall mean

τ_i = i th treatment effect

ε_{ij} = random error

The data from single factor experiment

Treatment (Level)	1	2	...	n	Treatment	
1	y_{11}	y_{12}	$\vdots$	y_{1n}	$y_{1\cdot}$	$M(y_1)$
2	y_{21}	y_{22}	$\vdots$	y_{2n}	$y_{2\cdot}$	$M(y_2)$
$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$
a					$y_{\cdot\cdot}$	$M(y_{\cdot\cdot})$

Lesson 41: Definition of a Model and Types of Model

Definition 6.1

Model

A statistical model is a mathematical model that integrates a set of statistical assumptions concerning the generation of sample data.

Definition 6.2

Treatment Effect

The treatment effect is a measure used to compare treatments in randomized experiments. OR

It measures the difference in mean outcomes between units assigned to the treatment and units assigned to the control.

Treatment effect can be easily understand from following figure.

Definition 6.3

Types of Model

In experimental design studies, following types of models are considered:

- ◆ Fixed-effects model
- ◆ Random-effects model
- ◆ Mixed models

Lesson 42: Fixed Effect Models

Definition 6.4

If the experiment were to be repeated and same set of treatments would be included. The experimenter is interested in treatment means only. The model used is called a fixed effect model.

The structure of Fixed Effect Model for one treatment variable is,

$$y_{ij} = \mu + \tau_i + \varepsilon_{ij},$$

where y_{ij} = j th observation on i th treatment

μ = overall mean from all observations

τ_i = added effect of i th treatment measured as deviation from μ

ε_{ij} = random error associated with j th observation on i th treatment

The above model is one treatment variable model in which we can study only one variable.

The assumptions of Fixed Effect Model are:

- ◆ τ_i 's are fixed
- ◆ $\sum_{i=1}^a \tau_i = 0$ (Since τ_i are measured as deviation from μ)
- ◆ $\varepsilon_{ij} \sim N(0, \sigma^2)$

Lesson 43: Fixed Effect Model: Some Examples

- ◆ An experimenter develops three new pesticides and he is interested in the effect of these only. The model will be a fixed effect model.
- ◆ A researcher is interested to measure the rate of production of five machines. The model will be a fixed effect model.
- ◆ A scientist wants to study the working of four antibiotics. He repeatedly applies these drugs to some patients and observes their effect.
- ◆ To compare the IQ level of five students a series of tests is planned and IQ is computed on the basis of their results.

Lesson 44: Random Effect Models

Definition 6.5

If the treatments in a particular experiment are a random sample from a large population of similar treatments. Here the experimenter is interested in the variation among treatment means not the treatment means themselves.

The structure of random effect model for one treatment variable is,

$$y_{ij} = \mu + \tau_i + \varepsilon_{ij},$$

where y_{ij} = j th observation on i th treatment

μ = overall mean from all observations

τ_i = is random effect associated with i th treatment

ε_{ij} = is random error associated with j th observation on i th treatment

τ_i 's = are random samples from a population which is $\tau_i \sim N(0, \sigma_{\tau_i}^2)$

$\varepsilon_{ij} = NID(0, \sigma_{\varepsilon}^2)$

The above model is one treatment variable model in which we can study only one variable.

Lesson 45: Random Effect Model: Some Examples

Example 1: An experimenter is interested in the way how a particular class of pesticides works. He selects a random sample of pesticides from the group. The model will be a random effect model.

Example 2: A market analyst is interested to examine a particular brand of machines, he draws a random sample of the brand and examines the working of machines.

Example 3: To study how a particular group of antibiotics acts on the body, an experimenter takes a random sample from such antibiotics and observes their working.

Example 4: To study the IQ level of university graduates. A random sample of university students is selected and IQ is computed.

Lesson 46: Analysis of Fixed Effects Model

Let us assume one factor fixed effects model

$$y_{ij} = \mu + \tau_i + \varepsilon_{ij}$$

where $i = 1, 2, \dots, a$ $j = 1, 2, \dots, n$ (we have 'a' treatment and 'n' observations on each)

y_{ij} is j th observation on i th treatment

μ is overall mean

τ_i is effect of i th treatment

ε is random error.

Some terms will be used in the analysis:

$$i\text{th treatment total } y_{i.} = \sum_{j=1}^n y_{ij}$$

$$i\text{th treatment mean } \bar{y}_i = \frac{y_{i.}}{n}$$

$$\text{Grand Total } y_{..} = \sum_{i=1}^a \sum_{j=1}^n y_{ij}$$

To construct ANOVA Table we need compute the following:

Total sum of squares

$$SS_{total} = \sum_{i=1}^a \sum_{j=1}^n (y_{ij} - \bar{y}_{..})^2$$

The SS_{total} can be partitioned into its components:

$$SS_{total} = n \sum_{i=1}^a (\bar{y}_i - \bar{y}_{..})^2 + \sum_{i=1}^a \sum_{j=1}^n (y_{ij} - \bar{y}_i)^2$$

$$SS_{total} = SS_{(between)} + SS_{within} \quad \text{OR} \\ = SS_{treatment} + SS_{error}$$

Other alternative expressions

$$\begin{aligned}
 SS_{total} &= \sum_{i=1}^a \sum_{j=1}^n y_{ij}^2 + \frac{y_{..}^2}{an} \\
 SS_{treatment} &= \sum_{i=1}^a \frac{y_{i.}^2}{n} - \frac{y_{..}^2}{an} \\
 \Rightarrow SS_{error} &= SS_{total} - SS_{treatment}
 \end{aligned}$$

ANOVA table H_0 = All treatment levels have equal average effect

SOV	d.f.	S.O.S.	M.S.	F-ratio	p-value
Treatment	$a - 1$	$SS_{treatment}$	$MS_{treatment} = \frac{SS_{treatment}}{a-1}$	$F_{cal} = \frac{MS_{treatment}}{MS_{error}}$	$p(X > F)$
Error	$a(n - 1)$	S_{error}	$MS_{error} = \frac{SS_{error}}{a(n-1)}$		
Total	$an - 1$	SS_{total}			

H_1 : = At least one pair of treatment levels is different.

Critical Region $p < \alpha$

Decision will be on the basis of p-value. If p-value is smaller than level of significance then we will reject H_0 and accept H_1 .

Lecture 7

Components of Analysis

Cochran’s theorem is a base of Analysis of Variance technique.

Lesson 47: Cochran’s Theorem

Definition 7.1

Cochran’s theorem tells us about the distributions of partitioned sums of squares of normally distributed random variables.

The Theorem

- ◆ Let $Z_1, Z_2, \dots, Z_n$ be independently identically distributed as $N(\mu, 1)$
- ◆ Suppose that $\sum_{i=1}^n Z_i^2 = Q_1^2 + Q_2^2 + \dots + Q_s^2$, where Q_j has v_j degree of freedom.
- ◆ A necessary and sufficient condition for the Q_j to be independent of one another and for $Q_j \sim \chi^2(v_j)$ is that

$$\sum_{j=1}^s v_j = n$$

- ◆ Cochran’s theorem implies that $\frac{SS_E}{\sigma^2}$ and $\frac{SS_{treatment}}{\sigma^2}$ have independent χ^2 distributions with $n - a$ and $a - 1$ d.f., respectively.
- ◆ Recall: If X_1 and X_2 are two independent random variables, each with a χ^2 distribution, then

$$\frac{X_1/v_1}{X_2/v_2} \sim F(v_1, v_2)$$

Conclusion

The conclusion of Cochran’s theorem is that, under the assumption of normality, the various quadratic forms are independent and have χ^2 distribution.

Lesson 48: Decomposition of Total Sum of Squares

We partition total variability of experimental data into its components as:

- ◆ Sum of squares of treatment
- ◆ Sum of squares of error

$$\begin{aligned}
SS_{total} &= \sum_{i=1}^a \sum_{j=1}^n (y_{ij} - \bar{y}_{..})^2 \\
&= \sum_{i=1}^a \sum_{j=1}^n (y_{ij} - \bar{y}_{i.} + \bar{y}_{i.} - \bar{y}_{..})^2 \\
&= \sum_{i=1}^a \sum_{j=1}^n [(\bar{y}_{i.} - \bar{y}_{..}) + (y_{ij} - \bar{y}_{i.})]^2 \\
&= \sum_{i=1}^a \sum_{j=1}^n (\bar{y}_{i.} - \bar{y}_{..})^2 + \sum_{i=1}^a \sum_{j=1}^n (y_{ij} - \bar{y}_{i.})^2 + 2 \sum_{i=1}^a \sum_{j=1}^n (\bar{y}_{i.} - \bar{y}_{..})(y_{ij} - \bar{y}_{i.}) \\
&= n \sum_{i=1}^a (\bar{y}_{i.} - \bar{y}_{..})^2 + \sum_{i=1}^a \sum_{j=1}^n (y_{ij} - \bar{y}_{i.})^2 + 2 \sum_{i=1}^a (\bar{y}_{i.} - \bar{y}_{..}) \sum_{j=1}^n (y_{ij} - \bar{y}_{i.})
\end{aligned}$$

Now

$$\sum_{j=1}^n (y_{ij} - \bar{y}_{i.}) = \frac{n y_{i.}}{n} - n \bar{y}_{i.} = 0$$

Thus, total sum of squares

$$SS_{total} = n \sum_{i=1}^a (\bar{y}_{i.} - \bar{y}_{..})^2 + \sum_{i=1}^a \sum_{j=1}^n (y_{ij} - \bar{y}_{i.})^2$$

Now the two components are

$$n \sum_{i=1}^a (\bar{y}_{i.} - \bar{y}_{..})^2: \text{ between treatments sum of squares}$$

$$\sum_{i=1}^a \sum_{j=1}^n (y_{ij} - \bar{y}_{i.})^2: \text{ within treatments or error sum of squares, i.e.}$$

$$S_{total} = SS_{between} + SS_{within} \quad \text{OR}$$

$$SS_{total} = SS_{treatment} + SS_{error}$$

Lecture 8

Expected Values of Mean Square of Error and Treatment

Lesson 49: Expected Values of Mean Squares of Error

Before finding the expected values of mean Square of error, we need to define:

Degrees of freedom

There are 'a' treatments and 'n' replications of each.

So, $an = N$ total observations

d.f. of total = $N - 1$

d.f. for treatments = $a - 1$

d.f. for error = $(N - 1) - (a - 1)$
 $= N - a$

We known that **Mean squares of error** is the sum of squares of error divided by its degrees of freedom

$$MS_E = \frac{SS_E}{N - a}$$

$$= \frac{\sum_{i=1}^a \sum_{j=1}^n (y_{ij} - \bar{y}_{i.})^2}{N - a}$$

Therefore, the expected value of mean squares of error

$$E(MS_E) = \frac{1}{N - a} E \left[\sum_{i=1}^a \sum_{j=1}^n (y_{ij} - \bar{y}_{i.})^2 \right]$$

$$= \frac{1}{N - a} E \left[\sum_{i=1}^a \sum_{j=1}^n y_{ij}^2 - 2y_{ij}\bar{y}_{i.} + \bar{y}_{i.}^2 \right]$$

$$= \frac{1}{N - a} E \left[\sum_{i=1}^a \sum_{j=1}^n y_{ij}^2 - 2n \sum_{i=1}^a \bar{y}_{i.} + n \sum_{i=1}^a \bar{y}_{i.}^2 \right]$$

$$= \frac{1}{N - a} E \left[\sum_{i=1}^a \sum_{j=1}^n y_{ij}^2 - \frac{1}{n} \sum_{i=1}^a y_{i.}^2 \right]$$

After some algebra

$$\begin{aligned}
 E(MS_E) &= \frac{1}{N-a} \left[N\mu^2 + n \sum_{i=1}^a E(\tau_i^2) + \sum_{i=1}^a \sum_{j=1}^n E(\varepsilon_{ij}^2) + C.P. \right] - \frac{1}{n} E \left[\sum_{i=1}^a [n\mu + n\tau_i + \varepsilon_i]^2 \right] \\
 &= \frac{1}{N-a} \left[\left[N\mu^2 + n \sum_{i=1}^a E(\tau_i^2) + N\sigma^2 \right] - \frac{1}{n} \sum_{i=1}^a [n^2\mu^2 + n^2 E(\tau_i^2) + E(\varepsilon_i^2)] + C.P. \right] \\
 &= \frac{1}{N-a} \left[\left[N\mu^2 + n \sum_{i=1}^a E(\tau_i^2) + N\sigma^2 \right] - N\mu^2 - n \sum_{i=1}^a E(\tau_i^2) - \frac{a n \sigma^2}{n} \right] \\
 &= \frac{1}{N-a} [N\sigma^2 - a\sigma^2] = \frac{1}{N-a} (N-a)\sigma^2 \\
 E(MS_E) &= \sigma^2
 \end{aligned}$$

Lesson 50: Expected Values of Mean Squares of Treatment

Note the following

$$\begin{aligned}
 \sum_{i=1}^a \bar{y}_{i.} &= \frac{\sum_{i=1}^a \sum_{j=1}^n y_{ij}}{n} = \frac{y_{..}}{n} = \frac{ay_{..}}{an} = a\bar{y}_{..} \\
 E(\varepsilon_{ij}) &= 0, E(\varepsilon_{ij}^2) = \sigma^2, \text{ and } E(\varepsilon_{i.}^2) = n\sigma^2
 \end{aligned}$$

Also

$$\varepsilon_{..} = \sum_{i=1}^a \sum_{j=1}^n \varepsilon_{ij}$$

and

$$\begin{aligned}
 \varepsilon^2 &= \left(\sum_{i=1}^a \varepsilon_{i.} \right)^2 \\
 &= a\varepsilon_{i.}^2 \text{ as } \varepsilon_{i.} \text{ are independent} \\
 MS_{treat} &= \frac{SS_{treat}}{a-1} = \frac{n \sum_{i=1}^a (\bar{y}_{i.} - \bar{y}_{..})^2}{a-1} \\
 E(MS_{treat}) &= \frac{n}{a-1} E \left(\sum_{i=1}^a (\bar{y}_{i.}^2 + \bar{y}_{..}^2 - 2\bar{y}_{i.}\bar{y}_{..}) \right) \\
 &= \frac{n}{a-1} E \left(\sum_{i=1}^a \bar{y}_{i.}^2 + a\bar{y}_{..}^2 - 2\bar{y}_{..} \sum_{i=1}^a \bar{y}_{i.} \right) \\
 &= \frac{n}{a-1} E \left(\sum_{i=1}^a \bar{y}_{i.}^2 - N\bar{y}_{..}^2 \right) \quad \because an = N
 \end{aligned}$$

$$\begin{aligned}
&= \frac{1}{a-1} E \left(n \sum_{i=1}^a \left[\frac{\sum_{j=1}^n y_{ij}}{n} \right]^2 - N \left[\frac{\sum_{i=1}^a \sum_{j=1}^n y_{ij}}{N} \right]^2 \right) \\
&= \frac{1}{a-1} E \left(\frac{1}{n} \sum_{i=1}^a \left[\sum_{j=1}^n y_{ij} \right]^2 - \frac{1}{N} \left[\sum_{i=1}^a \sum_{j=1}^n y_{ij} \right]^2 \right) \\
&= \frac{1}{a-1} E \left(\frac{1}{n} \sum_{i=1}^a \left[\sum_{j=1}^n (\mu + \tau_i + \varepsilon_{ij}) \right]^2 - \frac{1}{N} \left[\sum_{i=1}^a \sum_{j=1}^n (\mu + \tau_i + \varepsilon_{ij}) \right]^2 \right) \\
&= \frac{1}{a-1} E \left(\frac{1}{n} \sum_{i=1}^a [n\mu + n\tau_i + \varepsilon_{i.}]^2 - \frac{1}{N} \left[N\mu + n \sum_{i=1}^a \tau_i + \varepsilon_{..} \right]^2 \right) \\
&= \frac{1}{a-1} E \left(\frac{1}{n} [an^2\mu^2 + n^2 \sum_{i=1}^a \tau_i^2 + \sum_{i=1}^a \varepsilon_{i.}^2] - \frac{1}{N} [N^2\mu^2 + \varepsilon_{..}^2] \right) \\
&= \frac{1}{a-1} E \left(N\mu^2 + n \sum_{i=1}^a \tau_i^2 + \frac{1}{n} \sum_{i=1}^a \varepsilon_{i.}^2 - N\mu^2 - \frac{1}{N} \varepsilon_{..}^2 \right) \\
&= \frac{1}{a-1} E \left(n \sum_{i=1}^a \tau_i^2 + \frac{1}{n} \sum_{i=1}^a \varepsilon_{i.}^2 - \frac{1}{N} \varepsilon_{..}^2 \right) = \frac{1}{a-1} E \left(n \sum_{i=1}^a \tau_i^2 + \frac{1}{n} \sum_{i=1}^a \varepsilon_{i.}^2 - \frac{1}{an} a \varepsilon_{i.}^2 \right) \\
&= \frac{1}{a-1} \left(n E \sum_{i=1}^a \tau_i^2 + \frac{1}{n} \sum_{i=1}^a E(\varepsilon_{i.}^2) - \frac{1}{n} E(\varepsilon_{i.}^2) \right) = \frac{1}{a-1} \left(n E \sum_{i=1}^a \tau_i^2 + \frac{1}{n} an \sigma^2 - \frac{1}{n} n \sigma^2 \right) \\
&= \frac{n \sum_{i=1}^a \tau_i^2}{a-1} + \frac{(a-1)\sigma^2}{a-1}, = \frac{n \sum_{i=1}^a \tau_i^2}{a-1} + \sigma^2 \quad \because E(\varepsilon_{ij}) = 0, E(\varepsilon_{ij}^2) = \sigma^2
\end{aligned}$$

Lecture 9

Model Adequacy Checking Tools

Lesson 51: Model Adequacy Checking

We will discuss here the model that we have consider is adequate or not.

Model Adequacy Assumptions are:

- ◆ The relationship between the response and explanatory variables is linear.
- ◆ The error term has zero mean.
- ◆ The error term has constant variance.
- ◆ The errors are uncorrelated.
- ◆ The errors are normally distributed.

The **Model adequacy tools** are:

- ◆ Residual Analysis,
- ◆ Residual plots,
- ◆ Detection of outliers,
- ◆ The PRESS statistic,
- ◆ Testing for lack-of-fit.

Some important graphs for **Model adequacy checking** are

- ◆ Histogram of residuals,
- ◆ Normal probability plot,
- ◆ Plot of residuals in time sequence,
- ◆ Plot of residuals vs fitted values

Some important numerical tools for **Model adequacy checking** are:

- ◆ Bartlett's test,
- ◆ Modified Levene's Test,
- ◆ Transformations,
- ◆ Kruskal-Wallis Test
(Non-parametric test)

Note that there are some parameter and some non-parameter tests as numerical tools for model adequacy checking.

Without model adequacy checking one cannot give solid conclusions.

Lesson 52: Coefficient of Determination

Definition 9.1

The coefficient of determination, R^2 is a measure used in statistical analysis that assesses how well a model explains and predicts future outcomes.

- ◆ It is indicative of the level of explained variability in the data set.
- ◆ Measure goodness of fit of the model
- ◆ R^2 used as a guideline to measure the accuracy of the model.
- ◆ So, if the $R^2 = 0.50$, then approximately half of the observed variation can be explained by the model.
- ◆ In a linear relation R^2 is equal to square of Pearson's correlation.

How to Measure R-Square

$$\begin{aligned}
 R^2 &= \frac{\text{Explained Variation}}{\text{Total Variation}} \\
 &= \frac{\sum(\hat{y} - \bar{y})^2}{\sum(y - \bar{y})^2} \\
 \text{since } SS_{res} + SS_{reg} &= SS_{total} \\
 R^2 &= \frac{SS_{reg}}{SS_{total}} \\
 \Rightarrow 0 &\leq R^2 \leq 1
 \end{aligned}$$

Adjusted R^2

- ◆ Adjusts for the number of explanatory terms in a model relative to the number of data points.
- ◆ Its value can be negative

Adjusted R^2 is computed as

$$\bar{R}^2 = 1 - \frac{SS_{reg}/d.f_{error}}{SS_{total}/d.f_{total}}$$

Lesson 53: Normality Assumption: Histogram of Residuals

Definition 9.2

Residuals are estimates of experimental error obtained by subtracting the observed responses from the predicted responses.

The predicted response is calculated from the chosen model, after all the unknown model parameters have been estimated from the experimental data.

Mathematically residuals can be computed as follows.

$$e_{ij} = y_{ij} - \hat{y}_{ij},$$

where

$$\begin{aligned} \hat{y}_{ij} &= \hat{\mu} + \hat{\tau}_i \\ &= \bar{y}_{..} + (\bar{y}_i - \bar{y}_{..}) \\ &= \bar{y}_i. \end{aligned}$$

Thus, the residuals

$$e_{ij} = y_{ij} - \bar{y}_i.$$

Discussion on Residuals

- ◆ Residuals as elements of variation unexplained by the fitted model.
- ◆ This is a form of error: one expects them to be (roughly) normal and (approximately) independently distributed with a mean of 0 and some constant variance.

Lesson 54: Normality Assumption: Normal Probability Plot

Definition 9.3

The normal probability plot is a graphical technique for assessing whether or not a data set is approximately normally distributed.

The data are plotted against a theoretical normal distribution in such a way that the points should form an approximate straight line.

Construction of plot

- ◆ Compute residuals $e_{ij} = y_{ij} - \bar{y}_i$.
- ◆ Arrange the N residuals in ascending order.
- ◆ Plot the k th of these residuals versus the cumulative probability point $p_k = \left(k - \frac{1}{2}\right) / N$ on normal probability paper.

Interpretation

- ◆ If the error distribution is normal the plot will resemble a straight line.
- ◆ Technique is also useful to detect outliers.

Lesson 55: Normality Assumption: Plot of Residuals in Time Series

Definition 9.4

One of the model assumptions is that the error terms are independent. The "residuals vs order plot" is a way of detecting a particular form of non-independence of the error terms, namely *serial correlation*.

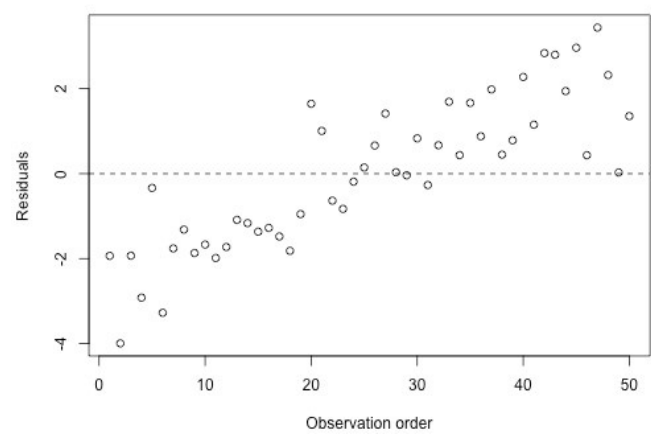
The plot is only appropriate if you know the order in which the data were collected. The above

plot exhibits no particular pattern

The above plot exhibits (positive) trend.

Interpretation of "Residuals vs order plot"

- ◆ Plots are helpful to detect correlation between residuals.
- ◆ If the spread of residuals is different on two ends of the plot then non-constant variance is suspected.
- ◆ If e_{ij} 's are correlated, the assumption of independence of error terms is violated.



Lesson 56: Normality Assumption: Plot of Residuals vs Fitted Values

A researcher wants to determine whether or not alcohol consumption was linearly related to muscle strength. He measured the total lifetime consumption of alcohol (x) on a random sample of $n = 50$ alcoholic men. They also measured the strength (y) of the deltoid muscle in each person’s non-dominant arm.

Note that, as defined, the residuals appear on the y axis and the fitted values appear on the x -axis. See how the data points there correspond to the data points in the residual versus fits plot here. Note that the predicted response of 5 men (whose alcohol consumption is around 40) is about 14.

Also, note the pattern. Now look at how and where these five data points appear in the residuals versus fits plot. Their fitted value is about 14 and their deviation from the residual = 0 line shares the same pattern as their deviation from the estimated regression line. Any data point that falls directly on the estimated regression line has a residual of 0. This plot is a classical example of a well-behaved residuals vs fits plot. Here are the characteristics of a well-behaved residual vs. fits plot and what they suggest about the appropriateness of the simple linear regression model.

Lecture 10

Barlett’s test and Nonparametric test in ANOVA

Lesson 57: Test the Equality of Variances

There are many tools for the testing of equality of variances: Some tests in the literature are:

- ◆ Bartlett’s test
- ◆ Goldfeld–Quandt test
- ◆ Levene’s test
- ◆ Brown–Forsythe test
- ◆ F-test for equality of two variance

57.1 The Bartlett’s Test

The Bartlett’s test: steps

- ◆ **Formulate the hypothesis**
 $H_0 : \sigma_1^2 = \sigma_2^2 = \dots = \sigma_a^2$
 $H_1 : \text{at least one pair of variances is not identical}$
- ◆ **Level of Significance**
 $\alpha = 1\%, 5\%, 10\%, \text{ etc}$
- ◆ **Test Statistic**

$$\chi_0^2 = 2.3026 \times \frac{q}{c} \sim \chi^2(a - 1),$$

where

$$q = (N - a) \log_{10} s_p^2 - \sum_{i=1}^a (n_i - 1) \log_{10} s_i^2$$
$$c = 1 + \frac{1}{3(a - 1)} \left(\sum_{i=1}^a (n_i - 1)^{-1} - (N - a)^{-1} \right)$$

and pooled variance

$$s_p^2 = \frac{\sum_{i=1}^a (n_i - 1) s_i^2}{N - a}$$

S_i^2 : sample variances from the i th population

◆ Critical Region

$$\chi_0^2 > \chi_{a,a-1}^2$$

Lesson 58: Other Plots Based on Residuals

There are other important graphical representations of residuals to check the different required assumptions.

Definition 10.1

The i th residual is computed by taking difference between the observed response and the average response of i th treatment.

$$e_{ij} = y_{ij} - \bar{y}_i.$$

Following is the plot between residuals and leverage values.

Following is the Normal Q-Q plot between theoretical Quantiles and Standardized residuals.

Following is another Normal Q-Q plot having data from non-linear distribution.

Linear and Non-Linear plots

Plot of Standardized Residuals VS Fitted values Plot between regression standardized predicted values and regression standardized residuals
A scatter plot with fitted line of the resulting data

Lesson 59: Violation of the Assumptions and Transformations

If assumptions does not fulfill then a question arose that what to do?.

- ◆ Carry out a different analysis which does not require the rejected assumptions:

- ★ Non-parametric tests (e.g. Durbin Test; Friedman RCBD Rank-Sum Test) Variance-
- ★ Weighted Welch's one-way ANOVA
- ◆ Transform the data
 - ★ The scale of measurement is arbitrary
 - ★ Transform a variable into a scale that best satisfies the assumptions of the analysis

59.1 Transformation

The commonly used linear (or arithmetic) scales are arbitrary:

- ◆ The logarithmic transformation
- ◆ The square root transformation
- ◆ The angular or arcsine transformation
- ◆ The power transformation

In Basic sciences **the common practice**

- ◆ Logarithms: pH values
- ◆ Square roots: Surface areas of organisms
- ◆ Reciprocals: Microbiological titrations

The following graph shows the violation of the assumption of independent residuals ($r = 0.89$). The following graph shows weak relationship ($r = 0.37$) after transformation and assumption of independence fulfill to some extent.

Lesson 60: Nonparametric Methods in ANOVA

Definition 10.2

Non-parametric (or distribution-free) inferential statistical methods are mathematical procedures for statistical hypothesis testing which, unlike parametric statistics, make no assumptions about the probability distributions of the variables being assessed.

The most frequently used nonparametric tests include:

- ◆ Friedman two-way analysis of variance
- ◆ Cochran's Q-test
- ◆ Kruskal–Wallis one-way analysis of variance
- ◆ Median test

60.1 Friedman two-way ANOVA

- ◆ This test is used to determine whether the M samples have been drawn from the same population.
- ◆ Cases are ranked and the mean rank is calculated for each sample.
- ◆ The test statistic is calculated as follows:

$$H = \frac{12R}{NM(M+1) - 3N(M+1)},$$

where N is the number of rows, M is the number of columns and R is the sum of squares of column rank totals.

- ◆ Finally, when N or M is large the probability distribution of H can be approximated by that of a chi-squared distribution, i.e. p-value is

$$P(\chi^2_{k-1} \geq H),$$

otherwise the p-value should be obtained from tables of H specially prepared for the Friedman test.

Lesson 61: The Kruskal-Wallis Test

Definition 10.3

The Kruskal–Wallis is a method for testing whether samples originate from the same distribution. It is used for comparing two or more independent samples of equal or different sample sizes. It extends the Mann–Whitney U test when there are only two groups.

The parametric equivalent of the Kruskal–Wallis test is the one-way analysis of variance (ANOVA), also called one-way ANOVA on ranks.

Steps of Computing the Kruskal-Wallis Test

- ◆ Rank all data from all groups together; i.e. rank the data from 1 to N ignoring group membership.
- ◆ Assign any tied values the average of the ranks they would have received had they not been tied.
- ◆ Set the ranks of the observations y_{ij} in ascending order.
- ◆ Replace each observation by its rank R_{ij} .
- ◆ The test statistic

$$H = \frac{1}{S^2} \left(\sum_{i=1}^a \frac{R_{i\cdot}^2}{n_i} - \frac{N(N+1)^2}{4} \right),$$

where
$$S^2 = \frac{1}{N-1} \left(\sum_{i=1}^n \sum_{j=1}^{n_i} R_{ij}^2 - \frac{N(N+1)^2}{4} \right)$$

If there is no ties then $S^2 = \frac{N(N+1)}{12}$

n_i is the number of observations in treatment
 R_{ij} is the rank of observation from treatment
 N is the total number of observations across all groups
 R_i sum of ranks of i th treatment

◆ Critical region

$$H > \chi^2_{\alpha, a-1}$$

◆ Conclusion

If the test is significant then at least one sample stochastically dominates another sample. Therefore, a researcher might use post-hoc tests like Dunn's test, etc.

Lesson 62: ANOVA on Ranks

One purpose for the ANOVA is to analyze differences in means between groups. The test statistic, F , assumes population normality.

ANOVA on ranks is a statistic designed for situations when the normality assumption has been violated.

This rank-based procedure has been recommended as being robust to non-normal errors, resistant to outliers, and highly efficient for many distributions.

Failure of ranking

◆ *Failure in the factorial ANOVA*

Monte Carlo studies and subsequent asymptotic studies found that the rank transformation is inappropriate for testing interaction effects in a factorial design, also there is an increase in Type-I error.

◆ *Failure in other complex layouts*

Similarly, it was found that the rank transformation increasingly fails in the two dependent samples layout as the correlation between pretest and posttest scores increase.

◆ *Variant of Rank Transformation: Failure in other Complex Situations*

A variant of rank-transformation is 'quantile normalization' in which a further transformation is applied to the ranks such that the resulting values have some defined distribution (often a normal distribution with a specified mean and variance).

However, two specific types of secondary transformations, the random normal scores and expected normal scores transformation, have been shown to greatly inflate Type-I errors and severely reduce statistical power.

Violating Homoscedasticity

The ANOVA on ranks has never been recommended when the underlying assumption of homogeneous variances has been violated, either by itself, or in conjunction with a violation of the assumption of population normality.

Lecture 11

Contrasts and Post-Hoc Tests

Lesson 63: Contrasts

Background

- 1. ANOVA can give us an indication that not all the treatments have the same mean response, but it does not tell us which treatments are different.
- 2. Need to look at the treatment means, or equivalently, at the treatment effects.
- 3. One method to examine treatment effects is called a contrast.

Definition 11.1

A linear combination of set of effects with coefficients summing to zero, i.e.,

$$\sum_{i=1}^a c_i \tau_i,$$

where

$$\sum_{i=1}^a c_i = 0$$

Contrasts of interest

A specific type of contrast which is usually of interest for the experimenter is the contrast of means, which is a linear combination of treatment means, i.e.

$$\begin{aligned} C &= \sum_{i=1}^a c_i \mu_i \\ &= c_1 \mu_1 + c_2 \mu_2 + \cdots + c_a \mu_a, \end{aligned}$$

where $c_1, c_2, \dots, c_a$ are contrast coefficients.

The i th treatment mean is

$$\mu_i = \mu + \tau_i,$$

where μ_i is estimated by $\bar{y}_i$.

Thus comparisons between treatment means are made using treatment total y_i . or treatment mean $\bar{y}_i$.

Lesson 64: Inference for Contrasts

We use contrasts in observed treatment means or effects to make inference about the corresponding contrasts in the true treatment means of effects.

The kinds of inference we work with point estimates, confidence intervals, and tests of significance.

Procedure

The procedures we use for contrasts are similar to the procedures we use when estimating or testing means.

The observed treatment mean $\bar{y}_i$ is an unbiased estimate of $\mu_i = \mu + \tau_i$, so any linear combination of observed is an unbiased estimate of corresponding combination of μ_i 's.

A contrast is the observed treatment means is an unbiased estimate of the corresponding contrast in the true treatment means.

The sum of squares for any contrast $SS_c = \frac{\left(\sum_{i=1}^a c_i y_i\right)^2}{n \sum_{i=1}^a c_i^2}$ has a single degree of freedom.

If the design is unbalanced the comparison requires $\sum_{i=1}^a n_i c_i = 0$ and the sum of squares equation becomes

$$SS_c = \frac{\left(\sum_{i=1}^a c_i y_i\right)^2}{\sum_{i=1}^a n_i c_i^2}$$

A contrast is tested by comparing its sum of squares (which is also its mean squares) to the error mean squares using ANOVA techniques. The resulting F -test would use degrees of freedom 1 and $N - a$.

Lesson 65: Orthogonal Contrasts

Let us define orthogonal contrasts. **Definition**

Definition 11.2

Two contrasts with coefficients c_i and d_i are orthogonal if

$$\sum_{i=1}^a c_i d_i = 0,$$

or for an unbalanced design

$$\sum_{i=1}^a n_i c_i d_i = 0,$$

where n_i : i th treatment size.

Note that

- 1. The coefficients form the basis to make contrasts meaningful in the context of experimental objectives.

- 2. Contrast coefficients must be chosen carefully prior to running the experiment.
- 3. There are many ways to choose sets of orthogonal contrasts.
- 4. The choice of contrasts is actually based on the nature of the experiment.
- 5. The choice of contrasts assessed that which orthogonal contrasts are of interest for the experimenter.
- 6. With ‘a’ treatments it is always possible to find ‘a – 1’ orthogonal contrasts.

Important features

- 1. Contrasts constructed according to rules are independent (as random variables).
- 2. Random error of one contrast is not correlated with the random error of other orthogonal contrast.
- 3. The contrasts partition the between groups sum of squares.

Lesson 66: Post-Hoc Tests in ANOVA

We need Post-Hoc Tests in ANOVA.

Definition 11.3

Post hoc (Latin, meaning “after this”) tests are designed for situations in which the researcher has already obtained a significant omnibus *F*-test with a factor that consists of three or more means, i.e. Null hypothesis of equal average effect of each treatment has been rejected through ANOVA.

Additional exploration of the differences among mean effects is needed to provide specific information on which means are significantly different from each other.

Post-Hoc tests are also known as multiple comparison tests.

66.1 Omnibus tests

Omnibus tests are a kind of statistical tests. They test whether the explained variance in a set of data is significantly greater than the unexplained variance, overall. One example is the *F*-test in the analysis of variance, i.e.

$$F = \frac{MS_{treat}}{MS_{error}}$$

66.2 Common Post-Hoc Tests

- 1. Fisher’s Least Significant Difference (LSD)
- 2. Duncan’s new multiple range test (MRT)
- 3. Newman-Keuls Test
- 4. Scheffé’s Method
- 5. Tukey’s Test (see also: Studentized Range Distribution)
- 6. Dunnett’s Correction
- 7. Bonferroni Procedure
- 8. Dunn’s Multiple Comparison Test
- 9. Holm-Bonferroni Procedure
- 10. Rodger’s Method
- 11. Benjamin-Hochberg (BH) Procedure

Note: if H_0 accepted then there is no need of any Post-Hoc test to conduct.

Lesson 67: Scheffé's Test

Definition 11.4

Scheffé's Test is a statistical test that is used to make unplanned comparisons, rather than pre-planned comparisons among the treatment means.

When to use

Scheffé's test can be used in situations where the results of an ANOVA experiment have yielded a significant F -statistic. This indicates that there is a meaningful difference in the means of the groups being compared. If the experimenter wishes to compare any set of contrasts this method is more useful.

Scheffé's Test Procedure

Let there are ' a ' contrasts in ' m ' treatments, i.e.

$$\Gamma_u = c_{1u}\mu_1 + c_{2u}\mu_2 + \cdots + c_{au}\mu_a,$$

where $u = 1, 2, \dots, m$.

μ 's are estimated by $\bar{y}_i$'s, so the constant

$$C_u = c_{1u}\bar{y}_1 + c_{2u}\bar{y}_2 + \cdots + c_{au}\bar{y}_a.$$

The standard error of u th contrast

$$S_{c_u} = \sqrt{MSE \sum_{i=1}^a \left(\frac{c_{iu}^2}{n_i} \right)},$$

where n_i is the number of observations in i th treatment.

To test

$$H_0 : \Gamma_u = 0 \quad \text{against}$$

$$H_1 : \Gamma_u \neq 0$$

Critical region

$$|C_u| > S_{\alpha, u},$$

where

$$S_{\alpha, u} = S_{c_u} \sqrt{(\alpha - 1) F_{\alpha, a-1, N-a}}$$

When to use

If we wish to compare only pairs of treatment means, i.e. we are interested only in

$$\Gamma = \mu_i - \mu_j, \quad \text{for } i \neq j,$$

the Scheffé's method is not most sensitive, we may choose other methods.

Lesson 68: Scheffé’s Test Examples

Tensile strength experiment

An engineer is interested in determining if varying the cotton content in a synthetic fiber affects the tensile strength.

%age of Cotton	Observed Tensile Strength					Total: Y_i	Average: $\bar{y}_i$
	1	2	3	4	5		
15	7	7	15	11	9	49	9.8
20	12	17	12	18	18	77	15.4
25	14	18	18	19	19	88	17.6
30	19	25	22	19	23	108	21.6
35	7	10	11	15	11	54	10.8
						$y_{..} = 376$	$\bar{y}_{..} = 15.06$

ANOVA

Response: Tensile strength.

	SOV	SS	df	MS	F	p-value
Between Groups		475.760	4	118.940	14.757	0.000
Within Groups		161.200	20	8.060		
Total		636.960	24			

Decision: Null hypothesis of equal average effect from all cotton percentages is rejected as p-value is quite low.

Since H_0 is rejected, suppose the contrasts of interest are:

$$\Gamma_1 = \mu_1 + \mu_3 - \mu_4 - \mu_5$$

and

$$\Gamma_2 = \mu_1 - \mu_4$$

The corresponding sample contrasts are:

$$\begin{aligned} C_1 &= \bar{y}_{1.} + \bar{y}_{3.} - \bar{y}_{4.} - \bar{y}_{5.} \\ &= 5.0 \end{aligned}$$

$$\begin{aligned} C_2 &= \bar{y}_{1.} - \bar{y}_{4.} \\ &= -11.80 \end{aligned}$$

$$\begin{aligned} S_{c_u} &= \sqrt{MSE \sum_{i=1}^a \left(\frac{c_{iu}^2}{n_i} \right)} \\ S_{C_1} &= \sqrt{8.06(1 + 1 + 1 + 1)/5} = 2.54 \\ S_{C_2} &= \sqrt{8.06(1 + 1)/5} = 1.80 \\ S_{\alpha,u} &= S_{c_u} \sqrt{(\alpha - 1)F_{\alpha,a-1,N-a}} \end{aligned}$$

With 1% critical values:

$$\begin{aligned} S_{0.01,1} &= 2.54 \sqrt{(5 - 1)F_{0.01,4,20}} = 10.69 \\ S_{0.01,2} &= 1.80 \sqrt{(5 - 1)F_{0.01,4,20}} = 7.58 \end{aligned}$$

Decision

Since $|C_1| < S_{0.01,1}$ we may not reject H_{01} that

$$\Gamma_1 = \mu_1 + \mu_3 - \mu_4 - \mu_5 = 0$$

However, since $|C_2| > S_{0.01,2}$ we may reject H_{02} that

$$\Gamma_2 = \mu_1 - \mu_4 = 0$$

Lecture 12

Least Significant Difference (LSD) Test and its Examples

Lesson 69: LSD Test

Least significant difference (LSD) is used when H_0 is rejected from ANOVA.

Definition 12.1

LSD test is one of the multiple comparison tests which are useful when we are interested in comparing all pairs of treatment means that is we wish to test

$$H_0 : \mu_i - \mu_j = 0 \quad \forall i \neq j$$

There will be $\binom{n}{2}$ pairs for comparison.

Steps

1. **Hypothesis**
 $H_0 : \mu_i - \mu_j = 0 \quad \forall i \neq j$
 $H_1 : \mu_i - \mu_j \neq 0$
2. **Level of significance**
 $\alpha = 1\%, 5\%, 10\%$, etc.
3. **Test statistics**

$$LSD = t_{\alpha/2, N-a} \sqrt{MSE \left(\frac{1}{n_i} + \frac{1}{n_j} \right)}$$

For a balanced design (if all treatments have same number of observations) $n_1 = n_2 = \dots = n_a = n$ The LSD formula for balanced design is, $LSD = t_{\alpha/2, N-a} \sqrt{\frac{2MSE}{n}}$

4. **Critical region**
 $|\bar{y}_i - \bar{y}_j| > LSD, \quad \forall i \neq j$

Lesson 70: LSD Test, Example

Tensile strength experiment

An engineer is interested in determining if varying the cotton content in a synthetic fiber affects the tensile strength. **ANOVA**

%age of Cotton	Observed Tensile Strenght					Total: $Y_{i.}$	Average: $\bar{y}_{i.}$
	1	2	3	4	5		
15	7	7	15	11	9	49	9.8
20	12	17	12	18	18	77	15.4
25	14	18	18	19	19	88	17.6
30	19	25	22	19	23	108	21.6
35	7	10	11	15	11	54	10.8
						$y_{..} = 376$	$\bar{y}_{..} = 15.06$

Response: Tensile strength.

	SOV	SS	df	MS	F	p-value
Between Groups		475.760	4	118.940	14.757	0.000
Within Groups		161.200	20	8.060		
Total		636.960	24			

Decision: Null hypothesis of equal average all cotton percentages is rejected as p-value is quite low. It means that all cotton contents do not put same affect on the response.

Computation of LSD value

LSD at 5% level of significance

$$LSD = t_{0.025,20} \sqrt{\frac{2MSE}{n}}$$
$$= 2.086 \sqrt{\frac{2(8.06)}{5}} = 3.75$$

The five treatment means are:

$\bar{y}_{1.} = 9.8, \bar{y}_{2.} = 15.4, \bar{y}_{3.} = 16.6, \bar{y}_{4.} = 21.6, \text{ and } \bar{y}_{5.} = 10.8$

Difference of means:

$$\begin{aligned} \bar{y}_{1.} - \bar{y}_{2.} &= -5.6^*, & \bar{y}_{1.} - \bar{y}_{3.} &= -7.8^* \\ \bar{y}_{1.} - \bar{y}_{4.} &= -11.8^*, & \bar{y}_{1.} - \bar{y}_{5.} &= -1.0 \\ \bar{y}_{2.} - \bar{y}_{3.} &= -2.2, & \bar{y}_{2.} - \bar{y}_{4.} &= -6.2^* \\ \bar{y}_{2.} - \bar{y}_{5.} &= 4.6^*, & \bar{y}_{3.} - \bar{y}_{4.} &= -4.0^* \\ \bar{y}_{3.} - \bar{y}_{5.} &= 6.8^*, & \bar{y}_{4.} - \bar{y}_{5.} &= 10.8^* \end{aligned}$$

Stars (*) on mean differences indicates these two treatments are different from each other.

Graph of significance

$\bar{y}_{1.}$	$\bar{y}_{5.}$	$\bar{y}_{2.}$	$\bar{y}_{3.}$	$\bar{y}_{4.}$
9.8	10.8	15.4	16.6	21.6

The underlined pairs of means do not differ significantly. The pair 1 & 5 and 2 & 3 are not statistically different from each other.

Lecture 13

Tukey’s Test and its Examples

Lesson 71: Tukey’s Test

Tukey’s test is widely used multiple comparison test.

Definition 13.1

One of the multiple comparison tests which deals with the pairs of treatment means regardless of how many means are in the group. The procedure is based on studentized range statistic.

Steps

- 1. **Hypothesis**
 $H_0 : \mu_i - \mu_j = 0 \quad \forall i \neq j$
 $H_1 : \mu_i - \mu_j \neq 0$
- 2. **Level of significance**
 $\alpha = 1\%, 5\%, 10\%, \text{ etc.}$
- 3. **Test statistic**

$$T_\alpha = q_\alpha(a, df_E) S_{\bar{y}_{i.}},$$

where df_E = Error degrees of freedom, a = number of treatments, and $q_\alpha(a, df_E)$ = percentage point of the studentized range statistic (presented in the table available in books). The standard error for a balanced design is

$$S_{\bar{y}_{i.}} = \sqrt{\frac{MSE}{n}}$$

The standard error for an unbalanced design, replace n with n_i

- 4. **Critical region**
 $|\bar{y}_{i.} - \bar{y}_{j.}| > T_\alpha$

Lesson 72: Tukey’s Test: Example

Tensile strength experiment

An engineer is interested in determining if varying the cotton content in a synthetic fiber affects the tensile strength.

%age of Cotton	Observed Tensile Strenght					Total: $Y_{i.}$	Average: $\bar{y}_{i.}$
	1	2	3	4	5		
15	7	7	15	11	9	49	9.8
20	12	17	12	18	18	77	15.4
25	14	18	18	19	19	88	17.6
30	19	25	22	19	23	108	21.6
35	7	10	11	15	11	54	10.8
						$y_{..} = 376$	$\bar{y}_{..} = 15.06$

ANOVA

Response: Tensile strength.

	SOV	SS	df	MS	F	p-value
Between Groups		475.760	4	118.940	14.757	0.000
Within Groups		161.200	20	8.060		
Total		636.960	24			

Decision: Null hypothesis of equal average all cotton percentages is rejected as p-value is quite low. Since H_0 is rejected, we need to use multiple comparison test such as Tukey's test.

Steps

1. Hypothesis

$$H_0 : \mu_i - \mu_j = 0 \quad i \neq j$$

$$H_1 : \mu_i - \mu_j \neq 0$$

2. Level of significance

$$\alpha = 5\%$$

3. Computations

At $\alpha = 5\%$ %age point of the studentized range statistic

$$q_{0.05}(5, 20) = 4.23$$

The standard error of treatment means is $S_{\bar{y}_{i.}} = \sqrt{\frac{8.06}{5}} = 1.27$

Now, the Tukey's value is

$$T_{0.05} = (4.23)(1.27) = 5.37$$

4. Critical region

$$|\bar{y}_{i.} - \bar{y}_{j.}| > 5.37$$

5. Decision

From the treatment means

$\bar{y}_{1.}$	$\bar{y}_{2.}$	$\bar{y}_{3.}$	$\bar{y}_{5.}$	$\bar{y}_{4.}$
9.8	15.4	16.6	21.6	10.8

we come to know 3rd and 4th treatment means do not differ significantly nor do 2nd and 3rd. Similarly the significance of other pairs can be observed.

Lecture 14

Duncan’s Multiple Range (DMR) Test and its Examples

Lesson 73: Duncan’s Multiple Range (DMR) Test

Definition 14.1

A widely used multiple comparison test developed by Duncan (1955). Test is used to compare all pairs of means.

Steps

- 1. **Hypothesis**
 $H_0 : \mu_i - \mu_j = 0 \quad \forall \quad i \neq j$
 $H_1 : \mu_i - \mu_j \neq 0$
- 2. **Level of significance**
 $\alpha = 1\%, 5\%, 10\%, \text{ etc.}$
- 3. **Test statistic**

$$R_p = r_\alpha(p, df_E) S_{\bar{y}_i},$$

where $p = 2, 3, \dots, a$
 a = number of treatments
 df_E = Error degrees of freedom
 $r_\alpha(p, df_E)$ is taken from Duncan’s table of significant ranges available for different α .
The standard error of the mean for a balanced is
 $S_{\bar{y}_i} \sqrt{\sqrt{MSE}n}$
The standard error of the mean for an unbalanced design replace n with n_i
$$n_h = \frac{a}{\sum_{i=1}^a \frac{1}{n_i}}$$

DMR Test Procedure

- 1. Arrange treatment means in ascending order.
- 2. Compute $a - 1$ least significant ranges R_p ’s.
- 3. Test the difference between pairs of means starting from difference of largest vs smallest means, then largest vs second smallest and so on, by comparing these differences with R_p .
- 4. The comparisons are continued until all means have been compared with the largest.

5. Take second largest and repeat the same process, and so on.
6. The process is done with all possible pairs of treatment means, i.e., $\binom{a}{2}$ pairs.

Lesson 74: DMR Test: An Example

Tensile strength experiment

An engineer is interested in determining if varying the cotton content in a synthetic fiber affects the tensile strength.

%age of Cotton	Observed Tensile Strenght					Total: $Y_{i\cdot}$	Average: $\bar{y}_{i\cdot}$
	1	2	3	4	5		
15	7	7	15	11	9	49	9.8
20	12	17	12	18	18	77	15.4
25	14	18	18	19	19	88	17.6
30	19	25	22	19	23	108	21.6
35	7	10	11	15	11	54	10.8
						$y_{\cdot\cdot} = 376$	$\bar{y}_{\cdot\cdot} = 15.06$

ANOVA

Response: Tensile strength.

	SOV	SS	df	MS	F	p-value
Between Groups		475.760	4	118.940	14.757	0.000
Within Groups		161.200	20	8.060		
Total		636.960	24			

Decision: Null hypothesis of equal average all cotton percentages is rejected as p-value is quite low.

Solution

The treatment means are

$$\begin{array}{ccccc} \bar{y}_{1\cdot} & \bar{y}_{2\cdot} & \bar{y}_{3\cdot} & \bar{y}_{4\cdot} & \bar{y}_{5\cdot} \\ 9.8 & 15.4 & 16.6 & 21.6 & 10.8 \end{array}$$

We have $S_{\bar{y}_{i\cdot}} = \sqrt{\frac{8.06}{5}} = 1.27$

From the table of significant ranges, the values of $r_{\alpha}(p, df_E)$ for $df_E = 20$, and $\alpha = 0.05$ are:

$$\begin{aligned} r_{0.05}(2, 20) &= 2.95, & r_{0.05}(3, 20) &= 3.10 \\ r_{0.05}(4, 20) &= 3.18, & r_{0.05}(5, 20) &= 3.25 \end{aligned}$$

The least significant ranges are computed as:

$$\begin{aligned} R_2 &= r_{0.05}(2, 20)S_{\bar{y}_{i\cdot}} = 2.95(1.27) = 3.75 \\ R_3 &= r_{0.05}(3, 20)S_{\bar{y}_{i\cdot}} = 3.10(1.27) = 3.94 \\ R_4 &= r_{0.05}(4, 20)S_{\bar{y}_{i\cdot}} = 3.18(1.27) = 4.04 \\ R_5 &= r_{0.05}(5, 20)S_{\bar{y}_{i\cdot}} = 3.25(1.27) = 4.13 \end{aligned}$$

Comparisons

$$\begin{aligned}
 4 \text{ vs } 1 & : 21.6 - 9.8 = 11.8 > 4.13(R_5) \\
 4 \text{ vs } 5 & : 21.6 - 10.8 = 10.8 > 4.04(R_4) \\
 4 \text{ vs } 2 & : 21.6 - 15.4 = 6.2 > 3.04(R_3) \\
 4 \text{ vs } 3 & : 21.6 - 17.6 = 4.0 > 3.75(R_2) \\
 3 \text{ vs } 1 & : 17.6 - 9.8 = 7.8 > 4.04(R_4) \\
 3 \text{ vs } 5 & : 17.6 - 10.8 = 6.8 > 3.95(R_3) \\
 3 \text{ vs } 2 & : 17.6 - 15.4 = 2.2 < 3.75(R_2)^* \\
 2 \text{ vs } 1 & : 15.4 - 9.8 = 5.6 > 3.94(R_3) \\
 2 \text{ vs } 5 & : 10.8 - 10.8 = 0.0 < 3.75(R_2) \\
 5 \text{ vs } 1 & : 10.8 - 9.8 = 1.0 < 3.75(R_2)^*
 \end{aligned}$$

The star (*) on each comparison indicates that the pair of treatment are not significantly different from each other.

Lecture 15

Dunnett's Test and its Example

Lesson 75: Dunnett's Test

Definition 15.1

In some experiments one of the treatment is *control* (e.g. a placebo in clinical trials). The analyst may be interested in comparing each of the remaining ' $a - 1$ ' treatments with the control. Dunnett (1964) presented a test to make such comparisons. This test is a modification of usual t -test.

Dunnett's Test Procedure

Suppose treatment is the control, then

1. **Hypothesis**

$$H_0 : \mu_i - \mu_a = 0$$

$$H_1 : \mu_i - \mu_a \neq 0$$

for all $i = 1, 2, \dots, a - 1$

2. **Test statistics**

For each hypothesis we compute the observed differences from the sample means and control treatment mean, i.e.

$$D_i = |\bar{y}_{i\cdot} - \bar{y}_{a\cdot}|$$

for all $i = 1, 2, \dots, a - 1$

3. **Critical region**

$$D_i > d \sqrt{MSE \left(\frac{1}{n_i} - \frac{1}{n_a} \right)},$$

where the value $d = d_\alpha(a - 1, df_E)$ comes from Dunnett's table constructed for different α values.

For a balanced design, when $n_i = n_a$ the critical region becomes

$$D_i > d \sqrt{\frac{2MSE}{n}}$$

where MSE is the mean squares of error.

Lesson 76: Dunnett’s Test: an Example

Tensile strength experiment

An engineer is interested in determining if varying the cotton content in a synthetic fiber affects the tensile strength.

%age of Cotton	Observed Tensile Strenght					Total: $Y_{i\cdot}$	Average: $\bar{y}_{i\cdot}$
	1	2	3	4	5		
15	7	7	15	11	9	49	9.8
20	12	17	12	18	18	77	15.4
25	14	18	18	19	19	88	17.6
30	19	25	22	19	23	108	21.6
35	7	10	11	15	11	54	10.8
						$y_{\cdot\cdot} = 376$	$\bar{y}_{\cdot\cdot} = 15.06$

ANOVA

Response: Tensile strength.

	SOV	SS	df	MS	F	p-value
Between Groups		475.760	4	118.940	14.757	0.000
Within Groups		161.200	20	8.060		
Total		636.960	24			

Decision: Null hypothesis of equal average all cotton percentages is rejected as p-value is quite low.

Illustration

In this example we have $a = 5, a - 1 = 4, df_E = 20, n_i = n_a = 5$ and $\alpha = 0.05$. We are considering ath treatment as control treatment.

We find the table value (from Dunnet’s table):

$d = d_{0.05}(4, 20) = 2.65$

The critical value is computed as

$$d\sqrt{\frac{2MSE}{n}} = 2.65\sqrt{\frac{2(8.06)}{5}} = 4.76$$

Thus any treatment whose mean differs from the control mean by more than 4.76 would be concluded significantly different from the control.

Difference of treatment means and the control mean:

$$\begin{aligned} 1 \text{ vs } 5 &: \bar{y}_{1\cdot} - \bar{y}_{5\cdot} = 9.8 - 10.8 = -1.0 \\ 2 \text{ vs } 5 &: \bar{y}_{2\cdot} - \bar{y}_{5\cdot} = 15.4 - 10.8 = 4.6 \\ 3 \text{ vs } 5 &: \bar{y}_{3\cdot} - \bar{y}_{5\cdot} = 17.6 - 10.8 = 6.8^* \\ 4 \text{ vs } 5 &: \bar{y}_{4\cdot} - \bar{y}_{5\cdot} = 21.6 - 10.8 = 10.8^* \end{aligned}$$

The 5th (ath) treatment is the control treatment.

Treatment 3 and treatment 4 are significantly different from control.

Lecture 16

The Neuman-Keul Test and its Example

Lesson 77: The Neuman-Keul Test

Definition 16.1

The Newman–Keuls or Student–Newman–Keuls (SNK) method is a stepwise multiple comparisons procedure used to identify sample means that are significantly different from each other. It was named after Student (1927), D. Newman (1939), and M. Keuls (1952).

Procedure

The Newman–Keuls method employs a stepwise approach when comparing sample means.

Steps

- 1. Prior to any mean comparison, all sample means are rank-ordered in ascending or descending order, thereby producing an ordered range (p) of sample means.
- 2. **Critical value**

$$q = \frac{\bar{y}_{max} - \bar{y}_{min}}{\sqrt{\frac{MSE}{2} \left(\frac{1}{n_{max}} + \frac{1}{n_{min}} \right)}}$$

is the studentized range value obtained by using the largest and smallest sample means.
For balanced design, $n_{max} = n_{min} = n$

$$q = \frac{\bar{y}_{max} - \bar{y}_{min}}{\sqrt{\frac{MSE}{n}}}$$

Procedure

- 1. First, we will compute

$$K_p = q_{\alpha}(p, df_E) S_{\bar{y}_{i.}} \quad \text{For } p = 2, 3, \dots, \alpha,$$

where $q_{\alpha}(p, df_E)$ is the percentage point of studentized range statistic for a specific α and error degree of freedom. α can be 1%, 5%, and 10%, etc.

- 2. Arrange treatment means in ascending order.
- 3. Test the difference between pairs of means starting from difference of largest vs smallest means, then largest vs second smallest and so on, by comparing these differences with K_p (for p in descending order).

Lesson 78: The Neuman-Keul: An Example

Tensile strength experiment

An engineer is interested in determining if varying the cotton content in a synthetic fiber affects the tensile strength.

%age of Cotton	Observed Tensile Strenght					Total: $Y_{i.}$	Average: $\bar{y}_{i.}$
	1	2	3	4	5		
15	7	7	15	11	9	49	9.8
20	12	17	12	18	18	77	15.4
25	14	18	18	19	19	88	17.6
30	19	25	22	19	23	108	21.6
35	7	10	11	15	11	54	10.8
						$y_{..} = 376$	$\bar{y}_{..} = 15.06$

ANOVA: Response: Tensile strength.

	SOV	SS	df	MS	F	p-value
Between Groups		475.760	4	118.940	14.757	0.000
Within Groups		161.200	20	8.060		
Total		636.960	24			

Decision: Null hypothesis of equal average all cotton percentages is rejected as p-value is quite low.

1. Critical value

$K_p = q_{\alpha}(p, df_E)S_{\bar{y}_{i.}}$, where $p = 2, 3, \dots, a$ with $S_{\bar{y}_{i.}} = \sqrt{8.06/5} = 1.27$ and $\alpha = 0.01$

$K_2 = q_{0.01}(2, 20) \times 1.27 = 4.02 \times 1.27 = 5.10$
 $K_3 = q_{0.01}(3, 20) \times 1.27 = 4.64 \times 1.27 = 5.89$
 $K_4 = q_{0.01}(4, 20) \times 1.27 = 5.02 \times 1.27 = 6.37$
 $K_5 = q_{0.01}(5, 20) \times 1.27 = 5.29 \times 1.27 = 6.72$

2. The treatment means $\bar{y}_{1.} = 9.8, \bar{y}_{2.} = 15.4, \bar{y}_{3.} = 16.6, \bar{y}_{4.} = 21.6, \bar{y}_{5.} = 10.8$
The treatments means (in ascending order) $\bar{y}_{4.} > \bar{y}_{3.} > \bar{y}_{2.} > \bar{y}_{5.} > \bar{y}_{1.}$

Comparisons

$4 \text{ vs } 1 : 21.6 - 9.8 = 11.8 > 6.72(K_5)$
 $4 \text{ vs } 5 : 21.6 - 10.8 = 10.8 > 6.37(K_4)$
 $4 \text{ vs } 2 : 21.6 - 15.4 = 6.2 > 5.89(K_3)$
 $4 \text{ vs } 3 : 21.6 - 17.6 = 4.0 < 5.10(K_2)^*$
 $3 \text{ vs } 1 : 17.6 - 9.8 = 7.8 > 6.37(K_4)$
 $3 \text{ vs } 5 : 17.6 - 10.8 = 6.8 > 5.89(K_3)$
 $3 \text{ vs } 2 : 17.6 - 15.4 = 2.2 < 5.10(K_2)^*$
 $2 \text{ vs } 1 : 15.4 - 9.8 = 5.6 > 5.89(K_3)^*$
 $2 \text{ vs } 5 : 15.4 - 10.8 = 4.6 > 5.10(K_2)^*$
 $5 \text{ vs } 1 : 10.8 - 9.8 = 1.0 > 5.10(K_2)^*$

Stars (*) indicates that the treatments means are significantly different from each other.

Lesson 79: Which Post-hoc Test should we Use

There are many multiple comparison methods or post-hoc tests available in the literature. These methods are employed when the hypothesis of equal treatment means is rejected through ANOVA. In the following we critically discuss the utility of some post-hoc tests and compare them for suitable use.

LSD test

Risk of type-I error (α) may be considerably inflated using LSD method, especially, when number of treatments increases. We may also occasionally find that overall F -test is significant, but LSD test fails to detect any pairwise significance. This is because F -test considers all possible comparisons not just pairwise comparisons.

Duncan's test

This test requires a greater observed differences to detect significantly different pairs of means as the number of means included in the groups increases. In case of small number of treatments this test resembles LSD test. Duncan's test is very powerful when real differences exist between the means.

The Newman-Keuls test

This test is more conservative than Duncan's test in that the Type-I error rate is smaller. Since α is generally low, the power of Newman-Keuls test is generally lower than Duncan's test.

Tukey's test

This test has a Type-I error rate of α for all pairwise comparisons on an experiment-wise basis. This is more conservative than either Newman-Keuls method and Duncan's method. Therefore, this test is less powerful than both of these tests.

Final words

There is no clear-cut answer to the question that which method (Post-hoc test) should we use? The professional statisticians have split opinion upon the choice. Cramer and Swanson (1973) have conducted Monte Carlo simulation studies of a number of multiple comparison methods. They report that LSD test is very effective when ANOVA shows significance at 5% α . They also reported good performance of Duncan's multiple range test for detecting true differences of means.

These and many other post-hoc tests are available in different statistical software packages like SPSS, Minitab, R, etc.

Lecture 17

One-Factor-at-a-Time Designs

Lesson 80: Basic Experimental Designs

Common types of basic experimental designs includes:

1. One-factor-at-a-time designs or One factor designs
2. Factorial designs

One Factor Design

Here we shall only discuss the designs where only one factor is under investigation, and the objective is to determine whether the response is significantly different at different factor levels. The factor can be qualitative or quantitative. We shall include **designs for main effects model** in this category.

Designs for Main Effects Model

1. **Completely Randomized Design (CRD)**
The model is $y_{ij} = \mu + \tau_i + \varepsilon_{ij}$
2. **Randomized Complete Block Design (RCBD)**
The model is $y_{ij} = \mu + \tau_i + \beta_j + \varepsilon_{ij}$
3. **Latin Squares Design**
The model is $y_{ijk} = \mu + \alpha_i + \tau_j + \beta_k + \varepsilon_{ijk}$
4. **Graeco Latin Squares Design**
The model is $y_{ijkl} = \mu + \theta_i + \tau_j + w_k + \psi_l + \varepsilon_{ijkl}$

There are many other designs for main effects model.

Lesson 81: Completely Randomized Design (CRD)- Layout and ANOVA

Definition 17.1

Suppose we have a number of treatments. If each experimental unit has equal chances of receiving a treatment and treatments are assigned randomly, the design is called a completely randomized design (CRD).

Layout

Given we have 4 treatments (A, B, C, and D) and 5 replicates of each treatment.

1	2	3	4	5	6	7	8	9	10
D	D	B	C	D	C	A	A	B	D
11	12	13	14	15	16	17	18	19	20
C	B	A	B	C	B	C	D	A	A

Note that there is no patterns in the allocation of treatments to experimental units.

How to analyze the CRD

We have a treatments and n replicates of each treatment.

$$SS_{total} = \sum_{i=1}^a \sum_{j=1}^n y_{ij}^2 - \frac{y_{..}^2}{an}$$
$$SS_{treatment} = \sum \frac{y_{i.}^2}{n} - \frac{y_{..}^2}{an}$$
$$SS_{error} = SS_{total} - S_{treatment}$$

Note that $\frac{y_{..}^2}{an}$ is called correction factor (CF).

ANOVA Table

We have a treatments and n replicates of each treatment. Thus total $an = N$ observation.

S.O.V	d.f.	S.O.S.	M.S.	F-value
Treatment	$a - 1$	$SS_{treatment}$	$MS_{treatment}$	$F = \frac{MS_{treatment}}{MS_{error}}$
Error	$N - a$	SS_{error}	MS_{error}	
Total	$N - 1$	SS_{total}		

Conclusion

$$F \geq F_{\alpha,a-1,N-a}$$

Lesson 82: Completely randomized design (CRD)- Advan-
tages and disadvantages

Advantages

1. Flexibility
- ◆ Any number of treatments and any number of replications may be used.

◆ Treatments may or may not be equally replicated.
2. Simplicity
- ◆ Statistical analysis is simple even with unequal replications or missing data.
3. Analysis
- ◆ The design provides maximum degrees of freedom to estimate error.

◆ Useful for the experiments when total number of experimental units are limited because it allocates enough degrees of freedom to error.
4. Precision

- ◆ The design is most precise if experimental units are uniform (homogeneous).
- ◆ It is useful if a large fraction of experimental units does not respond.

Disadvantages

1. Precision is low if experimental units are not uniform. Often units must group into blocks of homogeneous units.
2. CRD Not suited for large numbers of treatments.
3. Relatively low precision due to lack of restrictions which allows environmental variation to enter experimental error.

Lesson 83: Application of CRD

One should remember that appropriate use of completely randomized designs is under conditions where the experimental material is homogeneous.

Laboratory Experiments

1. Where a fraction of the experimental units is likely to be destroyed or fail to respond.
2. In small experiments where there is a small number of degrees of freedom.

Growth Chamber Experiments

1. The high cost of maintaining a controlled growth environment is often a limiting factor when determining experiment size and feasibility. Small scale experiments may be designed successfully.

Greenhouses and Seed Germinators

1. Environmental factors may be controlled by using such plans in greenhouse experiments or seed germinators in plant biology and agriculture sciences.

Computer-Based Experiments

1. In computer-based experiments the variation may be easily controlled through sophisticated software. Hence CRD may be successfully applied.

Small Experiments

1. Generally, in small experiments where there is a small number of degrees of freedom and small number of experimental units are required, CRD is quite useful.

Lesson 84: CRD: Examples

Example 1: Three chemists were asked to determine the percentage of methyl alcohol in a certain chemical compound. Each chemist makes three determinations. Results are as follows:

Chemist	Percentage of Methyl Alcohol			
1	84.99	84.04	84.38	85.15
2	85.13	84.88	84.72	84.88
3	85.16	84.20	84.10	85.55

Analyze the data.

Solution:

Solution

Hypothesis:

H_0 : All three chemists on the average make same determinations

H_1 : Not all have same determination

Test Statistics: F-test

Critical Region: $p < \alpha$

Source	DF	Adj. SS	Adj MS	F-value	p-value
Chemist	2	0.05542	0.02771	0.10	0.908
Error	9	2.56735	0.28526		
Total	11	2.62277			

Decision:

Since $p > \alpha$, therefore we accept H_0 and conclude that all three chemists on the average make same determinations. □

Example 2: Four catalysts that may affect the concentration of one component in a three component liquid mixture are being investigated. The following concentrations were observed: Test

Catalyst			
1	2	3	4
58.2	56.3	50.1	52.9
57.2	54.5	54.2	49.9
58.4	57	55.4	50.0
55.8	55.3		51.7
54.9			

whether the four catalysts have same effect on the concentration.

Solution:

- ◆ Null and alternative hypothesis
 H_0 : All four catalysts have same effect on the concentration
 H_1 : Not all four catalysts have same effect on the concentration
- ◆ Level of significance
 $\alpha = 5\%$
- ◆ Test Statistics
F-test
- ◆ Critical Region
 $p < \alpha$

Source	Df	Adj SS	Adj MS	F-value	P-value
Catalyst	3	85.68	28.559	9.92	0.001
Error	12	34.56	2.860		
Total	15	120.24			

◆ Conclusion

Since $p < \alpha$, we reject H_0 and conclude that all four catalysts do not have same effect on the concentration.

□

Lesson 85: Repeated Measures Designs (RMD)

Definition 17.2

In a repeated measures design, each group member in an experiment is tested for multiple conditions over time or under different conditions. This kind of experiments are usually conducted in social and behavioral sciences. Also known as **within-subjects** designs.

Types of Repeated Measures Designs

1. An **ordinary** repeated measures is where subjects are assigned a single treatment, and the results are measured over time (e.g. at 1, 4 and 8 weeks).
2. A **crossover** design is where subjects are assigned all treatments, and the results are measured over time.

Examples

- ◆ **Example 1:** A group of people with Type II diabetes might be given medications to see if it helps control their disease, and then they might be given nutritional counseling. A blood test to measure glucose levels is given to the patients after each treatment.
- ◆ **Example 2:** A study was performed to test two new cholesterol drugs against a control drug. Twenty patients with high cholesterol were randomly assigned to each of four treatments (two drugs, the control, and a placebo). For each, cholesterol was measured at six time periods. **Whether new drugs are effective at cholesterol and whether time and treatment interact.**

Lesson 86: Repeated Measures Design: Model and Layout

Model of RMD

Consider an experiment with a number of treatments and every treatment is to be used exactly once on each of n subjects.

$$y_{ij} = \mu\tau_i + \beta_j + \varepsilon_{ij},$$

where $i = 1, 2, \dots, a$, and $j = 1, 2, \dots, n$.

Model terms are:

1. y_{ij} represents the observed response of subject j to treatment i .
2. τ_i is the effect of i th treatment.
3. β_j is the parameter associated with j th subject.

RMD Model assumptions:

1. Treatments are fixed and effects are measured as deviation from mean, i.e.

$$\sum_{i=1}^a \tau_i = 0$$

2. Subjects are a random sample from a large population and we assume:

$$E(\beta_j) = 0, V(\beta_j) = \sigma_\beta^2$$

Layout of data from RMD

Data for a single factor repeated measure experiment.

Treatment	Subjects				Treatment Total
	1	2	...	n	
1	y_{11}	y_{12}	$\vdots$	y_{1n}	$y_{1\cdot}$
2	y_{21}	y_{22}	$\vdots$	y_{2n}	$y_{2\cdot}$
$\vdots$	$\vdots$	$\vdots$		$\vdots$	$\vdots$
a	y_{a1}	y_{a2}		y_{an}	$y_{a\cdot}$
Subject Total	$y_{\cdot 1}$	$y_{\cdot 2}$	$y_{\cdot 2}$	$y_{\cdot n}$	$y_{\cdot \cdot}$

Lesson 87: Repeated Measures Design: ANOVA

Definition 17.3

Repeated measures ANOVA is the equivalent of the one-way ANOVA, but for related, not independent groups, and is the extension of the dependent t -test. A repeated measures ANOVA is also referred to as a within-subjects ANOVA or ANOVA for correlated samples.

We can analyze data using a repeated measures ANOVA for two types of study design:

1. Studies that investigate changes in mean scores over three or more time points,
2. Differences in mean scores under three or more different conditions.

ANOVA test

1. **Hypothesis**
 $H_0 : \mu_1 = \mu_2 \cdots = \mu_k$
 $H_1 : \text{At least one pair is different}$
2. **Level of significance** $\alpha = 1\%, 5\%, 10\%, \text{etc.}$
3. **Test statistic** $F = \frac{MS_{conditions}}{MS_{error}}$
4. **Critical region** $F \geq F_{\alpha, df_{condition}, df_{error}}$

ANOVA Table

We can analyze data using a repeated measures design.

S.O.V.	d.f.	S.o.S	M.S.	F
Conditions	$k - 1$	$SS_{conditions}$	$MS_{conditions}$	$F_c = \frac{MS_{conditions}}{MS_{error}}$
Subjects	$n - 1$	$SS_{subjects}$	$MS_{subjects}$	$F_s = \frac{MS_{subjects}}{ME_{error}}$
Error	$(k - 1)(n - 1)$	SS_{error}	MS_{error}	
Total	$nk - 1$	SS_{total}		

Lesson 88: Repeated Measures Design: Real Life Example

Example 3: Consider the example of a 6-month exercise-training intervention where six subjects had their fitness level measured on three occasions: pre-, 3 months, and post-intervention. Their data is shown below along with some initial calculations:

Exercise Intervention				
Subjects	Pre-	3 Months	6 Months	Subject Means:
1	45	50	55	50
2	42	42	45	43
3	36	41	43	40
4	39	35	40	38
5	51	55	59	55
6	44	49	56	49.7
Monthly Means	42.8	45.3	49.7	
Grand Mean			45.9	

Analyze data.

Solution: The sums of squares

$$SS_{time} = SS_b = \sum_{i=1}^k n_i(\bar{x}_i - \bar{x})^2$$
$$= 6[(42.8 - 45.9)^2 + (45.3 - 45.9)^2 + (49.7 - 45.9)^2]$$
$$= 6[9.61 + 0.36 + 14.44] = 143.44$$
$$SS_w = \sum_i (x_{i1} - \bar{1})^2 + \sum_2 (x_{i2} - \bar{2})^2 + \sum_3 (x_{i3} - \bar{3})^2$$
$$= [(45 - 42.8)^2 + (42 - 42.8)^2 + (36 - 42.8)^2 + (39 - 42.8)^2 + (51 - 42.8)^2 + (44 - 42.8)^2]$$
$$+ [(50 - 45.3)^2 + (42 - 45.3)^2 + (41 - 45.3)^2 + (35 - 45.3)^2 + (55 - 45.3)^2 + (49 - 45.3)^2]$$
$$+ [(55 - 49.7)^2 + (45 - 49.7)^2 + (43 - 49.7)^2 + (40 - 49.7)^2 + (59 - 49.7)^2 + (56 - 49.7)^2]$$
$$= 715.5$$
$$SS_{subjects} = k \cdot \sum (\bar{i} - \bar{x})^2$$
$$= 3[(50 - 45.9)^2 + (43 - 45.9)^2 + (40 - 45.9)^2 + (38 - 45.9)^2 + (55 - 45.9)^2 + (49.7 - 45.9)^2]$$
$$= 658.3$$
$$SS_{error} = SS_w - SS_{subjects} = 715.5 - 658.3 = 57.2$$

Critical region

$$F \geq F_{\alpha, df_{time}, df_{error}}$$
$$F_{0.05, 2, 10} = 4.10, \quad F_{calculated} = 12.53$$

Decision: Since calculated value of F is greater than tabulated value therefore we reject H_0 . $\square$

Lecture 18

Randomized Complete Block Design and its Application

Lesson 89: RCBD: Basics of Blocking

Definition 18.1

Blocking

In the statistical theory of the design of experiments, blocking is the arrangement of experimental units in groups (blocks), each block contains similar experimental units.

Basics of Blocking

1. Blocking to “remove” the effect of nuisance factors.
2. Blocking is used for nuisance factors that can be controlled.
3. Blocking reduces unexplained variability.
4. In field experiments, neighboring plot usually have same fertility level. They can be included in the same block.
5. In animal experiments, the animal of the same breed or sex tend to have similar characteristics.
6. In some experiments the time of treatment application may form a block.
7. In general, the blocking factors might include, time, proximity, genetic background, etc.

Examples of Blocking

1. Male and Female

An experiment is designed to test a new drug on patients. There are two levels of the treatment, drug, and placebo, administered to male and female patients in a double blind trial. The sex of the patient is a blocking factor accounting for treatment variability between males and females.

2. Elevation

An experiment is designed to test the production of a new variety of wheat on a specific land. The land area contains - 'high elevation' and 'low elevation' regions. The new and the old variety are applied to both the high elevation and low elevation areas of land. In this instance the researcher is blocking the elevation factor.

Lesson 90: Randomized Complete Block Design - Precautions

◆ Structure of Experimental Units

When employing an RCBD, the experimenter must know the complete structure of experimental units so that it could be decided whether the units remain consistent or not.

◆ Size of Experimental Units

Large size experiments also have a risk to change their behavior unevenly during the progress of experiment.

◆ Nature of Experimental Units

In the experiments of life sciences, the experimental units change their response unexpectedly under the influence of extraneous variables.

◆ More than one Extraneous Source

In case of more than one extraneous sources of variability, especially when experimenter does not know about it, experimental error inflates.

Lesson 91: RCBD - Model and Assumptions

The model of an RCBD

The model of an RCBD includes two variable terms a treatments and b blocks along with overall mean and random error

$$y_{ij} = \mu + \tau_i + \beta_j + \varepsilon_{ij}$$

For $i = 1, 2, \dots, a$, and $j = 1, 2, \dots, b$

Model terms

1. μ : overall mean
2. τ_i : i th treatment effect
3. β_j : j th block effect
4. ε_{ij} : random error

The RCBD Model Assumptions

The model of an RCBD is based on following underlying assumptions:

1. Normality

- ◆ Random error is normally and independently distributed with mean 0 and fixed variance

$$\varepsilon_{ij} \sim NID(0, \sigma_\varepsilon^2)$$

2. Additivity

- ◆ Treatment effects τ_i 's are constant over different blocks.
 - ◆ Block effects β_j 's are constant for all plots within a block.
3. τ_i 's are taken as deviation from overall mean. Therefore,

$$\sum_{i=1}^a \tau_i = 0$$

4. β_j 's are taken as deviation from overall mean. Therefore,

$$\sum_{j=1}^b \beta_j = 0$$

There will be two F -test, one for treatment and other for blocks.

Lesson 92: Layout of RCBD

Consider the sample **Sample layout**.

Different colors represent different treatments; each horizontal row represents a block. There are 4 blocks (I–IV) and 4 treatments (A–D) in this example.

Treatments are randomly allocated and every block includes all available treatments.

Another way of RCBD layout

Block I	A	B	C	D
Block II	D	A	B	C
Block III	B	D	C	A
Block IV	C	A	B	D

Another example of **RCBD with four treatments in five blocks**

Single Replicate RCBD: Complete (every treatment occurs in every block) block layout with each treatment replicated once in each block (balanced).

The general structure (layout) of RCBD for t treatments and b blocks.

Treatment	Blocks				
	1	2	3	...	b
1	y_{11}	y_{12}	y_{13}	...	y_{1b}
2	y_{21}	y_{22}	y_{23}	...	y_{2b}
$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$
t	y_{t1}	y_{t2}	y_{t3}	...	y_{tb}

Lesson 93: RCBD - Advantages

In randomized complete block design, each treatment is applied in each block in equal number. There many advantages of such arrangement.

1. Precision

In RCBD blocking blocks the effect of one source of variation and that source is naturally an extraneous source of variation. Hence blocking can improve the precision of the experiment by decreasing experimental error.

2. Flexibility

In RCBD there is no restriction of number of blocks or size of a block. Any number of blocks and any number of treatment can be used given that each treatment is replicated the same number of times in each block.

3. Randomization

In RCBD treatments in a block are randomly assigned to the experimental units and blocks are randomly run. This approves a basic principle of design of experiment.

4. Simplicity

The analysis of the data from an RCBD is relatively simple when compared to other designs with complex blocking.

5. Validity

If experimental error is heterogeneous, valid comparisons can still be made.

Lesson 94: RCBD - Disadvantages

Along with many advantages there are also some disadvantages of using an RCBD.

1. Missing data

We may be confronted with a situation in which some observations are lost or unavailable due to some accident or cost constraints. In case of an RCBD missing data can cause more difficulty in analysis as compared to CRD.

2. Loss of precision

A careful allocation of treatments in a block are required in an RCBD. A wrong assignment of treatments can cause a loss of precision.

3. More extraneous sources

In case of more than one extraneous sources of variation, the design is less efficient than some other blocked designs.

- 4. **Block size**
The efficiency of design decreases when the block size increases.
- 5. **Homogeneous units**
If the experimental units are homogeneous, then CRD is more efficient than RCBD.
- 6. **Error degree of freedom**
Error degree of freedom is smaller than that for the CRD (problem with a small number of treatments).

Lesson 95: Application of RCBD

Definition 18.2

Randomized complete block design (RCBD)

A blocked design in which each treatment is present in each block and each treatment is replicated equally.

- ◆ **Agriculture**
The RCBD is the standard design for agricultural experiments where similar experimental units are grouped into blocks or replicates.
It is used to control variation in an experiment by accounting for spatial effects in field or greenhouse. For example, variation in fertility or drainage differences in a field.
- ◆ **Clinical trials**
When experimenter is working on clinical trials, the subject or experimental units are the patients. Patients having different diseases other than the disease under study may form different blocks.
- ◆ **Balance**
The defining feature of the randomized complete block design is that each block sees each treatment exactly once

Lesson 96: Attention

RCBD - A Popular Design

RCBD is a commonly used design in agriculture, behavioral and social sciences and many areas of physical and life sciences.

When choosing an RCBD many cares should be taken:

- 1. **Basis of Blocks**
In an RCBD blocks are constructed based on an extraneous source of variation. Different blocks represent different levels of that extraneous variable. For example, if different seed varieties are to be compared and plots are of three fertility levels, experiment is run in three blocks.
- 2. **Homogeneity within Blocks**
In an RCBD, homogeneity within blocks is of key importance. Careful selection of experimental units for a block is necessary, otherwise blocking may decrease design efficiency.
- 3. **Block Size** This is not necessary to have same size of each block in the experiment. Block size depends on the number of experimental units of similar characteristic related to the extraneous variable.

4. **Complete Blocks** In RCBD each block is a complete replicate, i.e. each block contains all the treatments of the experiment.
5. **Randomness** When running the experiment, which block is to be run when? Is decided purely at random. Also, when running experiments within a block, a random selection of trials is made.
6. **Avoid Blocking** If all the experimental units are homogeneous, there is need of blocking or choosing an RCBD. In such situation a CRD may be more efficient as it allocates maximum degrees of freedom to error.

Lesson 97: Partitioning Total Sum of Squares (TSS) into Component Parts in an RCBD

Decomposition

We partition total sum of squares of experimental data into its components as:

1. Sum of squares of treatment
2. Sum of squares of blocks
3. Sum of squares of error

We note that model

$$\begin{aligned}
 y_{ij} &= \mu + \tau_i + \beta_j + \varepsilon_{ij}; \quad \text{where } \begin{matrix} i=1,2,\dots,a \\ j=1,2,\dots,b \end{matrix} \\
 \text{also } \sum_{i=1}^a \tau_i &= 0, \quad \sum_{j=1}^b \beta_j = 0 \\
 y_{\cdot j} &= \sum_{i=1}^a y_{ij}, \quad \bar{y}_{\cdot j} = \frac{y_{\cdot j}}{a} \\
 y_{i \cdot} &= \sum_{j=1}^b y_{ij}, \quad \bar{y}_{i \cdot} = \frac{y_{i \cdot}}{b}, \quad y_{\cdot \cdot} = \sum_{i=1}^a \sum_{j=1}^b y_{ij}, \quad \bar{y}_{\cdot \cdot} = \frac{y_{\cdot \cdot}}{N}, \quad \text{where } N = ab \\
 SS_{total} &= \sum_{i=1}^a \sum_{j=1}^b (y_{ij} - \bar{y}_{\cdot \cdot})^2 \\
 &= \sum_{i=1}^a \sum_{j=1}^b \left((y_{ij} - \bar{y}_{\cdot \cdot}) + (\bar{y}_{\cdot j} - \bar{y}_{\cdot \cdot}) + (y_{ij} - \bar{y}_{i \cdot} + \bar{y}_{\cdot j} - \bar{y}_{\cdot \cdot}) \right)^2 \\
 &= b \sum_{i=1}^a (\bar{y}_{i \cdot} - \bar{y}_{\cdot \cdot})^2 + a \sum_{j=1}^b (\bar{y}_{\cdot j} - \bar{y}_{\cdot \cdot})^2 + \sum_{i=1}^a \sum_{j=1}^b (y_{ij} - \bar{y}_{i \cdot} + \bar{y}_{\cdot j} - \bar{y}_{\cdot \cdot})^2 + 0(CP) \\
 SS_{total} &= SS_{treatment} + SS_{blocks} + SS_{error}
 \end{aligned}$$

OR

$$SS_{error} = SS_{total} - SS_{treatment} - SS_{blocks}$$

Alternative expressions

$$SS_{total} = \sum_{i=1}^a \sum_{j=1}^b y_{ij}^2 - C.F.$$

$$SS_{treat} = \frac{1}{b} \sum_{i=1}^a y_{i.}^2 - C.F.$$

$$SS_{block} = \frac{1}{a} \sum_{j=1}^b y_{.j}^2 - C.F.$$

where $C.F. = \frac{y_{..}^2}{N}$

We can obtain Sum of Squares of Error as:

$$SS_{error} = SS_{total} - SS_{treatment} - SS_{blocks}$$

Lesson 98: Expected Values of Mean Squares of Treatment

Sum of squares and mean squares of treatments in RCBD

$$SS_{treat} = b \sum_{i=1}^a (\bar{y}_{i.} - \bar{y}_{..})^2$$

$$MS_{treat} = \frac{b \sum_{i=1}^a (\bar{y}_{i.} - \bar{y}_{..})^2}{a - 1}$$

Expected value of mean squares

$$\begin{aligned} E(MS_{treat}) &= \frac{b}{a-1} E \left(\sum_{i=1}^a (\bar{y}_{i.}^2 + \bar{y}_{..}^2 - 2\bar{y}_{i.}\bar{y}_{..}) \right) \\ &= \frac{b}{a-1} E \left(\sum_{i=1}^a \bar{y}_{i.}^2 + a\bar{y}_{..}^2 - 2\bar{y}_{..} \sum_{i=1}^a \bar{y}_{i.} \right) = \frac{b}{a-1} E \left(\sum_{i=1}^a \bar{y}_{i.}^2 - a\bar{y}_{..}^2 \right) \\ &= \frac{1}{a-1} E \left(b \sum_{i=1}^a \left(\frac{\sum_{j=1}^b y_{ij}}{b} \right)^2 - ab \left(\frac{\sum_{i=1}^a \sum_{j=1}^b y_{ij}}{ab} \right)^2 \right) \end{aligned}$$

as we have $\bar{y}_{i.} = \frac{y_{i.}}{b}$, $y_{..} = \sum_{i=1}^a y_{i.}$, $\bar{y}_{..} = \frac{y_{..}}{ab}$, $a\bar{y}_{..} = \frac{y_{..}}{b}$

$$\begin{aligned} E(MS_{treat}) &= \frac{1}{a-1} E \left(\frac{1}{b} \sum_{i=1}^a \left(\sum_{j=1}^b y_{ij} \right)^2 - \frac{1}{ab} \left(\sum_{i=1}^a \sum_{j=1}^b y_{ij} \right)^2 \right) \\ &= \frac{1}{a-1} E \left(\frac{1}{b} \sum_{i=1}^a \left(b\mu + b\tau_i + \sum_{j=1}^a \beta_j + \varepsilon_{i.} \right)^2 - \frac{a}{ab} \left(ab\mu + b \sum_{i=1}^a \tau_i + a \sum_{j=1}^b \beta_j + \varepsilon_{..} \right)^2 \right) \\ &= \frac{1}{a-1} E \left(\frac{1}{b} \left(ab^2\mu^2 + b^2 \sum_{i=1}^a \tau_i^2 + \sum_{i=1}^a \varepsilon_{i.}^2 \right) - \frac{1}{ab} (a^2b^2\mu^2 + \varepsilon_{..}^2) \right) \end{aligned}$$

$$\begin{aligned}
E(MS_{treat}) &= \frac{1}{a-1} E \left(ab\mu^2 + b \sum_{i=1}^a \tau_i^2 + \frac{1}{b} \sum_{i=1}^a \varepsilon_{i.}^2 - ab\mu^2 + \frac{1}{ab} \varepsilon_{..}^2 \right) \\
&= \frac{1}{a-1} E \left(b \sum_{i=1}^a \tau_i^2 + \frac{1}{b} \sum_{i=1}^a \varepsilon_{i.}^2 + \frac{1}{ab} \varepsilon_{..}^2 \right) \\
&= \frac{1}{a-1} E \left(b \sum_{i=1}^a \tau_i^2 + \frac{1}{b} \sum_{i=1}^a \varepsilon_{i.}^2 + \frac{1}{ab} a \varepsilon_{i.}^2 \right) \\
&= \frac{1}{a-1} \left(b E \sum_{i=1}^a \tau_i^2 + \frac{1}{b} \sum_{i=1}^a E(\varepsilon_{i.}^2) - \frac{1}{b} E(\varepsilon_{..}^2) \right) \\
E(MS_{reat}) &= \frac{1}{a-1} \left(b E \sum_{i=1}^a \tau_i^2 + \frac{1}{b} ab\sigma^2 - \frac{1}{b} b\sigma^2 \right) \\
&= \frac{b \sum_{i=1}^a \tau_i^2}{a-1} + \frac{(a-1)\sigma^2}{a-1}, \quad \text{where } E(\varepsilon_{ij}) = 0, \quad E(\varepsilon_{ij}^2) = \sigma^2 \\
E(MS_{treat}) &= \frac{b \sum_{i=1}^a \tau_i^2}{a-1} + \sigma^2
\end{aligned}$$

Lesson 99: Expected Values of Mean Squares of Error

First we need to know the **degrees of freedom**. There are 'a' treatments and 'b' blocks in the experiment. So ab total observations.

d.f. of total = $ab - 1$

d.f. for treatments = $a - 1$

d.f. for error = $(ab - 1) - (a - 1) = a(b - 1)$

Some of squares of error and its mean

$$\begin{aligned}
SS_E &= \sum_{i=1}^a \sum_{j=1}^b (y_{ij} - \bar{y}_{i.})^2 \\
MS_E &= \frac{SS_E}{a(b-1)} = \frac{\sum_{i=1}^a \sum_{j=1}^b (y_{ij} - \bar{y}_{i.})^2}{a(b-1)} \\
E(MS_E) &= \frac{1}{a(b-1)} E \left(\sum_{i=1}^a \sum_{j=1}^b (y_{ij} - \bar{y}_{i.})^2 \right)
\end{aligned}$$

Applying Expectations

$$\begin{aligned}
&= \frac{1}{a(b-1)} E \left(\sum_{i=1}^a \sum_{j=1}^b (y_{ij}^2 - 2y_{ij}\bar{y}_{i.} + \bar{y}_{i.}^2) \right) \\
&= \frac{1}{ab-1} E \left(\sum_{i=1}^a \sum_{j=1}^b y_{ij}^2 - 2n \sum_{i=1}^a \bar{y}_{i.} + n \sum_{i=1}^a \bar{y}_{i.}^2 \right)
\end{aligned}$$

$$\begin{aligned}
&= \frac{1}{a(b-1)} E \left(\sum_{i=1}^a \sum_{j=1}^b y_{ij}^2 - \frac{1}{n} \sum_{i=1}^a y_i^2 \right) \\
&= \frac{1}{a(b-1)} \left(ab\mu^2 + n \sum_{i=1}^a E(\tau_i^2) + \sum_{i=1}^a \sum_{j=1}^b E(\varepsilon_{ij}^2) + C.P. - \frac{1}{n} E \sum_{i=1}^a (b\mu^2 + n\tau_i + \varepsilon_i)^2 \right) \\
&= \frac{1}{a(b-1)} \left(ab\mu^2 + b \sum_{i=1}^a E(\tau_i^2) + ab\sigma^2 - \frac{1}{b} \sum_{i=1}^a (b^2\mu^2 + b^2 E(\tau_i^2) + E(\varepsilon_i^2) + C.P.) \right) \\
&= \frac{1}{a(b-1)} \left(ab\mu^2 + b \sum_{i=1}^a E(\tau_i^2) + ab\sigma^2 - ab\mu^2 - b \sum_{i=1}^a E(\tau_i^2) - \frac{ab\sigma^2}{b} \right) \\
&= \frac{1}{a(b-1)} (ab\sigma^2 - a\sigma^2) \\
E(MS_E) &= \sigma^2
\end{aligned}$$

Lesson 100: Expected Values of Mean Squares of Blocks

Sum of squares and mean squares of blocks in RCBD

$$\begin{aligned}
SS_{blocks} &= a \sum_{j=1}^b (\bar{y}_{.j} - \bar{y}_{..})^2 \\
MS_{blocks} &= \frac{a \sum_{j=1}^b (\bar{y}_{.j} - \bar{y}_{..})^2}{b-1}
\end{aligned}$$

Expected value of mean squares of blocks in RCBD

$$\begin{aligned}
E(MS_{break}) &= \frac{a}{b-1} E \left(\sum_{j=1}^b (\bar{y}_{.j}^2 + \bar{y}_{..}^2 - 2\bar{y}_{.j}\bar{y}_{..}) \right) \\
&= \frac{a}{b-1} E \left(\sum_{j=1}^b \bar{y}_{.j}^2 + b\bar{y}_{..}^2 - 2\bar{y}_{..} \sum_{j=1}^b \bar{y}_{.j} \right) = \frac{a}{b-1} E \left(\sum_{j=1}^b \bar{y}_{.j}^2 - ab\bar{y}_{..}^2 \right) \\
E(MS_{block}) &= \frac{1}{b-1} E \left(a \sum_{j=1}^b \left(\frac{\sum_{i=1}^a y_{ij}}{a} \right)^2 - ab \left(\frac{\sum_{i=1}^a \sum_{j=1}^b y_{ij}}{ab} \right)^2 \right) \\
&= \frac{1}{b-1} E \left(\frac{1}{a} \sum_{j=1}^b \left(\sum_{i=1}^a y_{ij} \right)^2 - \frac{1}{ab} \left(\sum_{i=1}^a \sum_{j=1}^b y_{ij} \right)^2 \right) \\
&= \frac{1}{b-1} \left(\frac{1}{a} \sum_{j=1}^b \left(a\mu + \sum_{i=1}^a \tau_i + a\beta_j + \varepsilon_{.j} \right)^2 - \frac{1}{ab} \left(ab\mu + b \sum_{i=1}^a \tau_i + a \sum_{j=1}^b \beta_j + \varepsilon_{..} \right)^2 \right)
\end{aligned}$$

$$\begin{aligned}
E(MS_{block}) &= \frac{1}{b-1} E \left(\frac{1}{a} (a^2 b \mu^2 + a^2 \sum_{j=1}^b \beta_j^2 + \sum_{j=1}^b \varepsilon_{.j}^2) - \frac{1}{ab} (a^2 b^2 \mu^2 + \varepsilon_{..}^2) \right) \\
&= \frac{1}{b-1} E \left(ab \mu^2 + a \sum_{j=1}^b \beta_j^2 + \frac{1}{a} \sum_{j=1}^b \varepsilon_{.j}^2 - ab \mu^2 + \frac{1}{ab} \varepsilon_{..}^2 \right) \\
&= \frac{1}{b-1} E \left(a \sum_{j=1}^b \beta_j^2 + \frac{1}{a} \sum_{j=1}^b \varepsilon_{.j}^2 + \frac{a}{ab} \varepsilon_{..}^2 \right) \\
E(MS_{blocks}) &= \frac{1}{b-1} E \left(a \sum_{j=1}^b \beta_j^2 + \frac{1}{a} \sum_{j=1}^b \varepsilon_{.j}^2 + \frac{1}{ab} b \varepsilon_{.j}^2 \right) \\
&= \frac{1}{b-1} \left(a E \left(\sum_{j=1}^b \beta_j^2 \right) + \frac{1}{a} \sum_{j=1}^b E(\varepsilon_{.j}^2) - \frac{1}{a} E(\varepsilon_{.j}^2) \right) \\
&= \frac{1}{b-1} \left(a E \left(\sum_{j=1}^b \beta_j^2 \right) + \frac{1}{a} ab \sigma^2 - \frac{1}{a} a \sigma^2 \right) \\
&= \frac{a \sum_{j=1}^b \beta_j^2}{b-1} + \frac{(b-1) \sigma^2}{b-1} \quad \text{where } E(\varepsilon_{ij}) = 0, E(\varepsilon_{ij}^2) = \sigma^2 \\
E(MS_{blocks}) &= \frac{a \sum_{j=1}^b \beta_j^2}{b-1} + \sigma^2
\end{aligned}$$

Lecture 19

Estimation of Missing Observation in RCBD

Lesson 101: ANOVA of an RCBD

The model of an RCBD includes two variable terms along with overall mean and random error

$$y_{ij} = \mu\tau_i + \beta_j + \varepsilon_{ij}, \quad \begin{matrix} i=1,2,\dots,a \\ j=1,2,\dots,b \end{matrix}$$

where

μ = overall mean, τ_i = i th treatment effect, β_j = j th block effect, and ε_{ij} = random error

- 1. Hypothesis
 H_{0T} : $\mu_1 = \mu_2 = \dots = \mu_a$ All treatment means are equal
 H_{1T} : At least one pair of treatment means is not equal

 H_{0B} : $\mu_1 = \mu_2 = \dots = \mu_b$ All block means are equal
 H_{1B} : At least one pair of block means is not equal
- 2. Level of significance: $\alpha = 0.01, 0.05, \text{etc.}$
- 3. Test statistics
 $F_T = \frac{MS_{treat}}{MS_{error}},$
 $F_B = \frac{MS_{block}}{MS_{error}}$
- 4. Critical region
 $F_T \geq F_{\alpha,a-1,(a-1)(b-1)},$
 $F_B \geq F_{\alpha,b-1,(a-1)(b-1)}$
- 5. Computation

$$\begin{aligned} SS_{total} &= \sum_{i=1}^a \sum_{j=1}^b y_{ij}^2 - \frac{y_{..}^2}{ab} \\ SS_{treat} &= \frac{1}{b} \sum_{i=1}^a y_{i.}^2 - \frac{y_{..}^2}{ab} \\ SS_{block} &= \frac{1}{a} \sum_{j=1}^b y_{.j}^2 - \frac{y_{..}^2}{ab} \\ SS_{error} &= SS_{total} - SS_{treat} - SS_{block} \end{aligned}$$

ANOVA table

S.O.V	d.f.	S.o.S.	M.S.	F
Treatment	$a - 1$	SS_{treat}	$MS_{treat} = \frac{SS_{treat}}{a-1}$	$F_T = \frac{MS_{treat}}{MS_{error}}$
Block	$b - 1$	SS_{block}	$MS_{block} = \frac{SS_{block}}{b-1}$	
Error	$(a - 1)(b - 1)$	SS_{error}	$MS_{error} = \frac{SS_{error}}{(a-1)(b-1)}$	
Total	$ab - 1$	SS_{total}		

6. **Conclusion**
If calculated value of F_T or F_B falls in the critical region, we shall reject H_0 , accept otherwise.

Lesson 102: Estimation of One Missing Observation in RCBD

Missing observations are unavoidable.
We wish to estimate a missing observation x_{ij} , so that x_{ij} will have minimum contribution to error sum of squares SS_E .
Choosing x_{ij} to minimize SS_E require to take partial derivative of SS_E with respect to x_{ij} , i.e.,

$$\frac{\partial SS_E}{\partial x_{ij}} = 0$$

Solution:

$$\begin{aligned} SS_E &= \sum_{i=1}^a \sum_{j=1}^b (y_{ij} - \bar{y}_{i.} - \bar{y}_{.j} + \bar{y}_{..})^2 \\ &= \sum_{i=1}^a \sum_{j=1}^b y_{ij}^2 - \frac{1}{b} \sum_{i=1}^a \left(\sum_{j=1}^b y_{ij} \right)^2 - \frac{1}{a} \sum_{j=1}^b \left(\sum_{i=1}^a y_{ij} \right)^2 + \frac{1}{ab} \left(\sum_{i=1}^a \sum_{j=1}^b y_{ij} \right)^2 \\ SS_E &= \sum_{i=1}^a \sum_{j=1}^b y_{ij}^2 - \frac{1}{b} \sum_{i=1}^a y_{i.}^2 - \frac{1}{a} \sum_{j=1}^b y_{.j}^2 + \frac{1}{ab} y_{..}^2 \\ &= x_{ij}^2 - \frac{1}{b} (y'_{i.} + x_{ij})^2 - \frac{1}{a} (y'_{.j} + x_{ij})^2 + \frac{1}{ab} (y'_{..} + x_{ij})^2 + R \text{ where } x_{ij} \text{ is missing observation} \end{aligned}$$

R includes all terms which do not include x_{ij} . In further solution we shall use x in place of x_{ij} .

$$\frac{\partial SS_E}{\partial x_{ij}} = 2x - 2\frac{1}{b}(y'_{i.} + x) - 2\frac{1}{a}(y'_{.j} + x) + 2\frac{1}{ab}(y'_{..} + x) = 0$$

After simplification we get the expression for estimating the missing observation from the data of RCBD,

$$x = \frac{a \cdot y'_{i.} + b \cdot y'_{.j} - y'_{..}}{(a - 1)(b - 1)}$$

Lesson 103: Estimation of More Than one Missing Observation in RCBD

In case of one missing observation substitute x_{ij} in place of missing value and perform ANOVA. However, one degree of freedom is reduced from total degree of freedom.

$$x_{ij} = \frac{a \cdot y'_{i.} + b \cdot y'_{.j} - y'_{..}}{(a - 1)(b - 1)}$$

For more than one missing observations in RCBD

Assume x_1, x_2 and x_3 are missing.

Follow the steps:

- ◆ Use arbitrary (guessed) values in place of x_2 and x_3 .
- ◆ Approximate x_1 using:
$$x_1 = \frac{a \cdot y'_{i.} + b \cdot y'_{.j} - y'_{..}}{(a - 1)(b - 1)}$$
- ◆ With the approximated value of x_1 and the guessed value of x_3 solve the above relation to find x_2 .
- ◆ Now with approximated values of x_1 and x_2 solve the relation to find x_3 .
- ◆ Repeat the cycle until the approximated values are converged (not much different) to the original data.
- ◆ Finally, ANOVA is performed and one degree of freedom is reduced from total degree of freedom as well as from error degree of freedom for each approximated value.

Note that if there are many values missing and they are in the same block or treatment simply exclude this block or treatment.

Lesson 104: Relative Efficiency of RCBD Compared to CRD

We are interested to know how much precision is gained by using an RCBD or whether blocking has been effective or not? There are two ways to answer this question:

1. Test the significance of blocking through ANOVA.
2. Compute relative efficiency.

To compute relative efficiency we need some preliminary Computations.

In an experiment with a treatments and b blocks, we have

$$\begin{aligned} SS_{total} &= \sum_{i=1}^a \sum_{j=1}^b y_{ij}^2 - \frac{y_{..}^2}{ab} \\ SS_{treat} &= \frac{1}{b} \sum_{i=1}^a y_{i.}^2 - \frac{y_{..}^2}{ab} \\ SS_{block} &= \frac{1}{a} \sum_{j=1}^b y_{.j}^2 - \frac{y_{..}^2}{ab} \\ SS_{error} &= SS_{total} - SS_{treat} - SS_{block} \\ MS_{blocks} &= \frac{SS_{blocks}}{b - 1} \\ MS_{error} &= \frac{SS_{error}}{(a - 1)(b - 1)} \end{aligned}$$

Therefore, the Relative Efficiency is,

$$R.E. = \frac{(b - 1)MS_{blocks} + b(a - 1)MS_{error}}{(ab - 1)MS_{error}}$$

If blocking increases the precision of the data, then R.E. will be greater than 1.

Note that: The quantity $(R.E. - 1)100\%$ measures the percentage increase in precision due to blocking.

Lesson 105: RCBD - Practical Example

Example 1: A chemist wishes to test the effect of four chemical agents on the tensile strength of four types of fiber rope. There might be variability from one rope to another, the chemists consider rope types as blocks. The resulting tensile strength is given as:

Type of Chemical	Fiber Rope			
	1	2	3	4
1	9.3	9.4	9.6	10.0
2	9.4	9.3	9.8	9.9
3	9.2	9.4	9.5	9.7
4	9.7	9.6	10.0	10.2

Solution:

1. **Hypothesis**

H_{0c} : All four chemicals have same average effect on the tensile strength.

H_{1c} : At least one chemical has different average effect.

H_{0R} : All four ropes types have same average tensile strength.

H_{0R} : At least one rope type has different average tensile strength.

2. **Level of significance:** $\alpha = 0.05$

3. **Test statistics**

$$F_C = \frac{MS_C}{MS_E}, \quad F_R = \frac{MS_R}{MS_E}$$

4. **Critical region**

$$F_C \geq F_{0.05,3,9} = 3.86, \quad F_R \geq F_{0.05,3,9} = 3.86$$

5. **Computations**

$$SS_{total} = \sum_{i=1}^4 \sum_{j=1}^4 y_{ij}^2 - \frac{y_{..}^2}{4 \times 4} = 154 - \frac{(20)^2}{16} = 129.00$$

$$SS_{treat} = \frac{1}{4} \sum_{i=1}^4 y_{i.}^2 - \frac{y_{..}^2}{4 \times 4} = \frac{254}{4} - \frac{(20)^2}{16} = 38.50$$

$$SS_{blocks} = \frac{1}{4} \sum_{j=1}^4 y_{.j}^2 - \frac{y_{..}^2}{4 \times 4} = \frac{430}{4} - \frac{(20)^2}{16} = 82.50$$

$$SS_E = SS_{total} - SS_{treat} - SS_{blocks} = 8.00$$

ANOVA Table

S.O.V.	d.f.	S.O.S.	M.S.	F-value	p-value
Chemical	3	38.50	12.83	14.44	0.001
Rope	3	82.50	27.50	30.89	0.000
Error	9	8.00	0.89		
Total	15	129.00			

6. **Conclusion** Since the F -values of both sources of variation lie in the rejection region, therefore we reject both H_0 .

□

Lecture 20

Latin Square Design and its Application

Lesson 106: Latin Squares (LS) Design - Definition and Model

Definition 20.1

A Latin square design is used when we want to control the variation of two nuisance factors or two extraneous variables. Thus, a Latin square design allows blocking in two directions, row-wise and column-wise. The rows and columns actually represent two checks on randomization.

A Latin square design is applied when two sources of variation are used in same number of levels which is also equal to the number of levels of main treatment. Therefore, a Latin square design for p factors is also called a $p \times p$ Latin square design or a double grouping design.

The **Model** for Latin square design is,

$$y_{ijk} = \mu + \alpha_i + \tau_j + \beta_k + \varepsilon_{ijk}, \quad \begin{matrix} i=1,2,\dots,p \\ j=1,2,\dots,p \\ k=1,2,\dots,p \end{matrix}$$

where

y_{ijk} : Yield from the experimental unit under i th row variable, j th treatment subjected to the k th column variable.

μ : Overall mean.

α_i : i th row variable effect.

τ_j : j th treatment effect.

β_k : k th column variable effect.

ε_{ijk} : Random error.

The assumption of Latin square model are:

1. Additive model with no interactions.
2. Row effect $\alpha_i \sim NID(0, \sigma_\alpha^2)$
3. Column effect $\beta_k \sim NID(0, \sigma_k^2)$
4. Treatment effect $\tau_i \sim NID(0, \sigma_\tau^2)$
5. Error $\varepsilon_{ijk} \sim N(0, \sigma_\varepsilon^2)$

Lesson 107: Layout of 3×3 and 4×4 LS Design, Properties

3×3 Latin Square Design: A 3×3 Latin square design contains three rows, three columns, and three treatments.

A	C	B
B	A	C
C	B	A

4×4 Latin Square Design: A 4×4 Latin square design contains four rows, four columns, and four treatments.

A	D	C	B
B	A	D	C
C	B	A	D
D	C	B	A

Properties of a Latin Square Design

- 1. **Double Grouping**
Latin Square designs are similar to randomized block designs, except that instead of the removal of one blocking variable, these designs are carefully constructed to allow the removal of two blocking factors.
- 2. **Reduced Design**
This design uses less number of experimental units as compared to a CRD, e.g., in a 4×4 (16 run) design letters are arranged so that each letter occurs only once within each row and each column. Notice that a simple random design would require $4 \times 4 \times 4 \times 4 = 64$ experimental units.
- 3. **Orthogonal Array Representation** If each entry of an $n \times n$ Latin square is written as a triple (r, c, s) , where r is the row, c is the column, and s is the symbol, we obtain a set of triples called the orthogonal array representation of the square. For example,

A	C	B
B	A	C
C	B	A

Latin square design has following orthogonal array representation:
 $\{(1, 1, 1), (1, 2, 3), (1, 3, 2), (2, 1, 2), (2, 2, 1), (2, 3, 3), (3, 1, 3), (3, 2, 2), (3, 3, 1)\}$.

- 4. **Equivalence classes of Latin Square** Many operations on a Latin square produce another Latin square. For example, permute the rows, permute the columns, and permute the names of the symbols of a Latin square, we obtain a new Latin square said to be isotopic to the first. **Isotopism is an equivalence relation and all isotopic Latin squares make isotopy class.**

Lesson 108: ANOVA of a LS Design

The step by step procedure is,

- 1. **Three Hypothesis**
 H_{0T} : All treatments have same effect on the response.

H_{1T} : At least two treatments have different effect.
 H_{0R} : All row variables have same effect on response.
 H_{1R} : At least two row variables have different effect. H_{0C} : All col. variables have same effect on response.
 H_{1C} : At least two col. variables have different effect.

2. **Level of Significance**

$\alpha = 1\%, 5\%, 10\%$, etc.

3. **Computations**

$$SS_{treat} = \frac{\sum_{j=1}^p y_{.j}^2}{p} - \frac{y_{..}^2}{N}$$
$$SS_{row} = \frac{\sum_{i=1}^p y_{i.}^2}{p} - \frac{y_{..}^2}{N}$$
$$SS_{col.} = \frac{\sum_{j=1}^p y_{.j}^2}{p} - \frac{y_{..}^2}{N}$$
$$SS_{total} = \sum_{i=1}^p \sum_{j=1}^p \sum_{k=1}^p y_{ijk}^2 - \frac{y_{..}^2}{N}$$
$$S_{error} = SS_{total} - (SS_{treat} + SS_{row} + SS_{col.})$$

4. **ANOVA table**

S.O.V	d.f.	S.O.S.	M.S.	F-value
Treat	$p - 1$	SS_{treat}	$\frac{SS_{treat}}{(p-1)}$	$F_{treat} = \frac{MS_{treat}}{MS_{error}}$
Row	$p - 1$	SS_{row}	$\frac{SS_{row}}{(p-1)}$	$F_{row} = \frac{MS_{row}}{MS_{error}}$
Column	$p - 1$	SS_{column}	$\frac{SS_{column}}{(p-1)}$	$F_{column} = \frac{MS_{column}}{MS_{error}}$
Error	$(p - 1)(p - 2)$	SS_{error}		
Total	$p^2 - 1$			

5. **Conclusion** If calculated values of F -statistic lie in the following rejection region:

$$F_{cal} \geq F_{\alpha,p-1,(p-1)(p-2)}$$

then reject H_0 , accept otherwise.

Lesson 109: Replication of Latin Squares

First we will see Why want to replicate a Latin Square Design.

Consider the following examples:

We can see that small Latin squares provide small number of error degrees of freedom in the ANOVA table.

Therefore,

- 1. When using small Latin squares, it is highly desirable to replicate the Latin squares to have enough degrees of freedom to estimate error.
- 2. A single Latin square does not allow the analysis of interaction in any case.

S.O.V	3×3	4×4	5×5
	Latin Square	Latin Square	Latin Square
	df	df	df
Treat	$3-1=2$	$4-1=3$	$5-1=4$
Row	$3-1=2$	$4-1=3$	$5-1=4$
Column	$3-1=2$	$4-1=3$	$5-1=4$
Error	$(3-1)(3-2)=2$	$(4-1)(4-2)=6$	$(5-1)(5-2)=12$
Total	$9-1=8$	$16-1=15$	$25-1=24$

How to Replicate

There are several ways to replicate Latin squares. Some are as follows: **In each replicate**

1. Use same rows and same columns.
2. Use same rows but different columns.
3. Use same columns but different rows.
4. Use different rows and different columns.

Analysis of Replicated Latin Square

The structure of ANOVA table of the replicated Latin squares in these different scenarios are different with respect to sums of squares and degrees of freedom. Therefore, the resultant F values also changes.

Lesson 110: ANOVA of Replicated LS Design: Case-I

Same Rows and Same Columns: When the same levels of the row factor and same levels of the column factor are used in each replicate.

Consider y_{ijkl} the response produced from i th level of row factor, j th treatment, k th level of column factor, and l th replicate. There are $N = np^2$ total observations.

Test Steps are:

1. **Hypothesis**
 H_{0T} : All treatments have same effect on the response.
 H_{1T} : At least two treatments have different effect.
 H_{0R} : All row variables have same effect on response.
 H_{1R} : At least two row variables have different effect.
 H_{0C} : All col. variables have same effect on response.
 H_{1C} : At least two col. variables have different effect.
 H_{0Re} : All row variables have same effect on response.
 H_{1Re} : At least two row variables have different effect.
2. **Level of Significance**
 $\alpha = 1\%, 5\%, 10\%$, etc.
3. **Computations**

$$SS_{treat} = \frac{1}{np} \sum_{j=1}^p y_{.j..}^2 - \frac{y_{....}^2}{N}$$
$$SS_{row} = \frac{1}{np} \sum_{i=1}^p y_{i...}^2 - \frac{y_{....}^2}{N}$$
$$SS_{col} = \frac{1}{np} \sum_{k=1}^p y_{..k.}^2 - \frac{y_{....}^2}{N}$$
$$SS_{repl} = \frac{1}{p^2} \sum_{l=1}^n y_{...l}^2 - \frac{y_{....}^2}{N}$$
$$SS_{total} = \sum_{i=1}^p \sum_{j=1}^p \sum_{k=1}^p \sum_{l=1}^n y_{ijkl}^2 - \frac{y_{....}^2}{N}$$
$$SS_{error} = SS_{total} - (SS_{treat} + SS_{row} + SS_{col} + SS_{repl})$$

ANOVA table

S.O.V	d.f.	S.O.S.	M.S.	F-Value
Treat	$p - 1$	SS_{treat}	$\frac{SS_{treat}}{(p-1)}$	$F_{treat} = \frac{MS_{treat}}{MS_{error}}$
Row	$p - 1$	SS_{row}	$\frac{SS_{row}}{(p-1)}$	$MS_{row} = \frac{MS_{row}}{MS_{error}}$
Column	$p - 1$	SS_{column}	$\frac{SS_{column}}{p-1}$	$MS_{col} = \frac{MS_{col}}{MS_{error}}$
Replicate	$n - 1$	$SS_{replicate}$	$\frac{SS_{replicate}}{(n-1)}$	$MS_{repl} = \frac{MS_{repl}}{MS_{error}}$
Error	$(p - 1)[n(p + 1) - 3]$	SS_{error}	$\frac{SS_{error}}{(p-1)[n(p+1)-3]}$	
Total	$np^2 - 1$			

4. Conclusion

If calculated values of F -statistic lie in the following rejection region:

$$F_{cal} \geq F_{\alpha,p-1,(p-1)[n(p+1)-3]}$$

then reject H_0 , accept otherwise.

Note: To test replication the two degrees of freedom are: $n - 1, (p - 1)[n(p + 1) - 3]$.

Lesson 111: ANOVA of Replicated LS Design: Case-II

Different Rows and Same Columns: When different levels of the row factor and same levels of the column factor are used in each replicate. Thus there are p new rows within each replicate.

The source of variation for the rows measures the variation between rows within the n replicates. Thus total observations: $N = np^2$

Test Steps

1. Hypothesis

- H_{0T} :

All treatments have same effect on the response.
- H_{1T} :

At least two treatments have different effect.
- H_{0R} :

All row variables have same effect on response.
- H_{1R} :

At least two row variables have different effect.
- H_{0C} :

All col. variables have same effect on response.

H_{1C} : At least two col. variables have different effect.

H_{0Re} : All row variables have same effect on response.

H_{1Re} : At least two row variables have different effect.

2. Level of Significance

$\alpha = 1\%, 5\%, 10\%$, etc.

3. Computations

$$SS_{treat} = \frac{1}{np} \sum_{j=1}^p y_{.j..}^2 - \frac{y_{...}^2}{N}$$

$$SS_{row} = \frac{1}{p} \sum_{i=1}^p \sum_{l=1}^n y_{i..l}^2 - \frac{y_{...}^2}{p^2}$$

$$SS_{col} = \frac{1}{np} \sum_{k=1}^p y_{..k.}^2 - \frac{y_{...}^2}{N}$$

$$SS_{repl} = \frac{1}{p^2} \sum_{l=1}^n y_{...l}^2 - \frac{y_{...}^2}{N}$$

$$SS_{total} = \sum_{i=1}^p \sum_{j=1}^p \sum_{k=1}^p \sum_{l=1}^n y_{ijkl}^2 - \frac{y_{...}^2}{N}$$

$$SS_{error} = SS_{total} - (SS_{treat} + SS_{row} + SS_{col} + SS_{repl})$$

ANOVA Table

S.O.V.	d.f.	S.O.S.	M.S.	F-value
Treat	$p - 1$	SS_{treat}	$\frac{SS_{treat}}{(p-1)}$	$F_{treat} = \frac{MS_{treat}}{MS_{error}}$
Row	$n(p - 1)$	SS_{row}	$\frac{SS_{row}}{n(p-1)}$	$F_{row} = \frac{MS_{row}}{MS_{error}}$
Column	$p - 1$	SS_{column}	$\frac{SS_{column}}{(p-1)}$	$F_{col} = \frac{MS_{col}}{MS_{error}}$
Replicate	$n - 1$	$SS_{replicate}$	$\frac{SS_{replicate}}{(n-1)}$	$F_{replicate} = \frac{MS_{replicate}}{MS_{error}}$
Error	$(p - 1)(np - 1)$	SS_{error}	$\frac{SS_{error}}{(p-1)(np-1)}$	
total	$np^2 - 1$			

4. Conclusion

If calculated values of F -statistic lie in the following rejection region:

$$F_{cal} \geq F_{\alpha, df_{source}, df_{error}}$$

then reject H_0 , accept otherwise.

Lesson 112: ANOVA of Replicated LS Design: Case-III

Different Rows and Different Columns: When different levels of the row factor and different levels of the column factor are used in each replicate.

The source of variation for the rows and columns measures the variation resulting from these factors within the n replicates. Thus, total observation are $N = np^2$

Test Steps

1. Hypothesis

H_{0T} : All treatments have same effect on the response.

H_{1T} : At least two treatments have different effect.

H_{0R} : All row variables have same effect on response.

H_{1R} : At least two row variables have different effect.

H_{0C} : All col. variables have same effect on response.

H_{1C} : At least two col. variables have different effect.

H_{0Re} : All row variables have same effect on response.

H_{1Re} : At least two row variables have different effect.

2. Level of Significance

$\alpha = 1\%, 5\%, 10\%$, etc.

3. Computations

$$SS_{treat} = \frac{1}{np} \sum_{j=1}^p y_{j..}^2 - \frac{y_{...}^2}{N}$$

$$SS_{row} = \frac{1}{p} \sum_{i=1}^p \sum_{l=1}^n y_{i..l}^2 - \sum_{l=1}^n \frac{y_{...l}^2}{p^2}$$

$$SS_{col} = \frac{1}{np} \sum_{k=1}^p \sum_{l=1}^n y_{..kl}^2 - \frac{y_{...}^2}{p^2}$$

$$SS_{repl} = \frac{1}{p^2} \sum_{l=1}^n y_{...l}^2 - \frac{y_{...}^2}{N}$$

$$SS_{total} = \sum_{i=1}^p \sum_{j=1}^p \sum_{k=1}^p \sum_{l=1}^n y_{ijkl}^2 - \frac{y_{...}^2}{N}$$

$$SS_{error} = SS_{total} - (SS_{treat} + SS_{row} + SS_{col} + SS_{repl})$$

ANOVA table

S.O.V.	d.f.	S.O.S.	M.S.	F-value
Treat	$p - 1$	SS_{treat}	$\frac{SS_{treat}}{(p-1)}$	$F_{treat} = \frac{MS_{treat}}{MS_{error}}$
Row	$n(p - 1)$	SS_{row}	$\frac{SS_{row}}{n(p-1)}$	$F_{row} = \frac{MS_{row}}{MS_{error}}$
Column	$n(p - 1)$	SS_{column}	$\frac{SS_{column}}{n(p-1)}$	$F_{col} = \frac{MS_{col}}{MS_{error}}$
Replicate	$n - 1$	$SS_{replicate}$	$\frac{SS_{replicate}}{(n-1)}$	$F_{replicate} = \frac{MS_{replicate}}{MS_{error}}$
Error	$(p - 1)[n(p - 1) - 1]$	SS_{error}	$\frac{SS_{error}}{(p-1)[n(p-1)-1]}$	
Total	$np^2 - 1$			

4. Conclusion

If calculated values of F-statistic lie in the following rejection region:

$$F_{cal} \geq F_{\alpha, df_{source}, df_{error}}$$

then reject H_0 , accept otherwise.

Lecture 21

Estimation of Missing Observation in LSD

Lesson 113: Estimation of Missing Observation

The model for LSD is

$$y_{ijk} = \mu + \alpha_i + \tau_j + \beta_k + \varepsilon_{ijk}$$

where

$$i = 1, 2, \dots, p, \quad j = 1, 2, \dots, p, \quad k = 1, 2, \dots, p$$

y_{ijk} is response of the experimental unit under i th row variable, j th treatment subjected to the k th. column variable.

Following are terms used for estimating the missing observation.

- 1. **Total response at i th levels of row variable:**

$$y_{i..} = \sum_{j=1}^p \sum_{k=1}^p y_{ijk}$$

$y'_{i..}$ = Total response with one missing observation.

- 2. **Total response of j th treatment:**

$$y_{.j.} = \sum_{i=1}^p \sum_{k=1}^p y_{ijk}$$

$y'_{.j.}$ = Total response with one missing observation.

- 3. **Total response at k th levels of column variable:**

$$y_{..k} = \sum_{i=1}^p \sum_{j=1}^p y_{ijk}$$

$y'_{..k}$ = Total response with one missing observation.

- 4. **Grand total of response:**

$$y_{...} = \sum_{i=1}^p \sum_{j=1}^p \sum_{k=1}^p y_{ijk}$$

$y'_{...}$ = Grand total with one missing observation.

Let the missing response is from i th row, k th column under j th treatment

$$x_{ijk} = \frac{p(y'_{i..} + y'_{.j.} + y'_{..k}) - 2y'_{...}}{(p-2)(p-1)}$$

Estimation of more than one Missing Observations

Note that for more than one missing observation, an iterative procedure is adopted by assuming arbitrary values against the missing observations except one that is estimated with the above formulae. Continue the iteration process till the estimated values converge.

Lesson 114: Relative Efficiency of LS Design

Definition 21.1

Efficiency measures the estimation power or capacity of a design. We may measure the efficiency of a Latin squares design relative to other popularly used designs. The effectiveness of either row or column grouping may be assessed by computing relative efficiency with either considering rows or columns as blocks.

Column Blocking: Relative efficiency with rows omitted and considered columns as blocks:

$$R.E = \frac{MS_R + (p-1)MS_E}{p \times MS_E}$$

MS_R = Mean squares of rows
 MS_E = Mean squares of error

Row Blocking: Relative efficiency with columns omitted and considered rows as blocks:

$$R.E. = \frac{MS_c + (p-1)MS_E}{p \times MS_E}$$

MS_C = Mean squares of rows
 MS_E = Mean squares of error

Comparing Efficiency With CRD

$$R.E. = \frac{MS_R + MS_c + (p-1)MS_E}{(p+1) \times MS_E}$$

MS_R = Mean squares of rows
 MS_C = Mean squares of rows
 MS_E = Mean squares of error

In all cases (Row Blocking, column blocking, or in comparison with CRD) if $R.E. > 1$ the blocking has improved efficiency.

Lesson 115: Practical Example of LS Design

Example 1: An industrial engineer is investigating the effect of four assembly methods (A, B, C, D) on the assembly time for a color television component. Four operators are selected for

the study. Furthermore, the engineer knows that each assembly method produces such fatigue that the time required for the last assembly may be greater than the time required for the first, regardless of the method. That is, a trend develops in the required assembly time. To account for this source of variability, the engineer uses the Latin square design shown below. Analyze the data from this experiment ($\alpha = 0.05$) draw appropriate conclusions.

Order of Assembly	Operator			
	1	2	3	4
1	$C = 10$	$D = 14$	$A = 7$	$B = 8$
2	$B = 7$	$C = 18$	$D = 11$	$A = 8$
3	$A = 5$	$B = 10$	$C = 11$	$D = 9$
4	$D = 10$	$A = 10$	$B = 12$	$C = 14$

Solution:

- Hypothesis
 H_{0T} : Each assembly method has same average effect.
 H_{1T} : At least two methods have different effects.
 H_{0R} : Order of assembly does not have significant effect.
 H_{1R} : Order of assembly is significant.
 H_{0C} : All operators same average effect on response.
 H_{1C} : At least two operators have different effect.

- Level of Significance

$$\alpha = 5\%$$

- Solution

ANOVA table

S.O.V.	DF	Adj. SOS	Adj MS	F	p
Method	3	72.50	24.17	13.81	0.004
Order	3	18.50	6.17	3.52	0.089
Operator	3	51.50	17.17	9.81	0.010
Error	6	10.50	1.75		
Total	15	153.50			

- Conclusion** Since the p -value of assembly method and operator is lower than 5% ($=0.05$) therefore we conclude that assembly methods and operators have significantly different effect on the response at different levels. Whereas, order of assembly is significant at 10% level of significant and insignificant at 5% level of significance.

□

Lecture 22

Crossover Design

Lesson 116: Crossover Design

We need to define **Parallel Design** before defining the **Crossover Design**.

Definition 22.1

Parallel Design

In parallel design the units are randomized to a treatment and remain on that treatment throughout the trial duration. For example, RCBD, Latin Square design, and Graceo-Latin Square design etc. are examples of parallel design.

Definition 22.2

Crossover Design

A crossover design is a repeated/ longitudinal measurements design. The experimental units cross over from one treatment to another during the trial course. This is in contrast to a parallel design The order of treatment in a crossover experiment is called a **sequence**.

Advantages of Crossover design

- 1. The influence of confounding covariates is reduced because each experimental unit serves as its own control.
- 2. Optimal crossover designs are statistically efficient and require fewer subjects than do non-crossover designs or other repeated measures designs.

Disadvantages of Crossover design

- 1. Carryover effects (the effects from previous period to current period) may be confounded with direct treatment effects, i.e., these effects cannot be estimated separately.
- 2. We have to choose designs where treatment and carryover are not aliased with each other.

Usage of Crossover design

Used in experiments in which experimental units receive more than one factor-level combination in a preassigned time sequence. Many biological and medical experiments use crossover designs so that each subject or patient can act as its own control. This type of design is a block design in which each experimental unit (subject, patient) is a block. Especially useful when there is

considerable variation among experimental units. If excessive variation exists among experimental units, comparisons of factor effects could be confounded by the effects of the groups of experimental units that receive the respective factor levels.

Examples of Crossover design

1. 2-period, 2-treatment crossover design ($AB|BA$)

Sequence	Period-I	Period-II
AB	A	B
BA	B	A

2. 3-period, 3-treatment, crossover design ($ABC|BCA|CAB$)

Sequence	Period-I	Period-II	Period-III
ABC	A	B	C
BCA	B	C	A
CAB	C	A	B

Analysis of Crossover design

To compare the two sequences, the null and alternative hypothesis will be

$$H_0 : \mu_{AB} - \mu_{BA} = 0$$

$$H_1 : \mu_{AB} - \mu_{BA} \neq 0$$

We can use

- ◆ Two-sample t test
- ◆ Wilcoxon rank-sum test (Mann-Whitney-Wilcoxon rank-sum test)

If response from a crossover trial is binary and that there are no period effects, then we can use

- ◆ logistic regression

Lecture 23

Graeco-Latin Square Design and its Applications

Lesson 117: Graeco-Latin Square Design - Definition and Layout

Definition 23.1

A Graeco Latin square (GLS) design is used to control three sources of variation other than treatment. The experimental units are grouped in three different ways, by rows, by columns and by Greek letters. Design is also called **Triple Grouping Design**.

How to Construct a Graeco=Latin Square Design.

The design is constructed by considering a $p \times p$ Latin square with treatments denoted by Latin letters and superimposing on it a second $p \times p$ Latin square which variable levels are denoted by Greek letters. The Greek letters are usually assigned in a way that each Greek letters occurs once and only once in a row and column.

A **Layout** of a 3×3 Graeco Latin Square design is, A **Layout** of a 4×4 Graeco Latin Square

A α	B γ	C β
B β	C α	A γ
C γ	A β	B α

Design is, A **Layout** of a 5×5 Graeco Latin square design is, Note that two separate Latin square

A α	B γ	C δ	D β
B β	A δ	D γ	C α
C δ	D α	A β	B δ
D δ	C β	B α	A γ

designs are super-imposed and combined to make a Graeco Latin Square design.

The Latin square letter and Graeco Latin letter appear only once in the design.

A α	B δ	C β	D ε	E γ
B β	C ε	D γ	E α	A δ
C γ	D α	E δ	A β	B ε
D δ	E β	A ε	B β	C α
E ε	A γ	B α	C δ	D β

Lesson 118: Statistical Model for GLS Design

The Model for Graeco Latin Square design

$$y_{ijkl} = \mu + \theta_i + \tau_j + \omega_k + \psi_l + \varepsilon_{ijkl}$$

where the variations:

$$\begin{aligned} i &= 1, 2, \dots, p(\text{rows}) \\ j &= 1, 2, \dots, p(\text{Latin letters}) \\ k &= 1, 2, \dots, p(\text{Greek letters}) \\ l &= 1, 2, \dots, p(\text{columns}) \end{aligned}$$

The model terms are:

- y_{ijkl} :The observed response
- μ :Overall mean
- θ_i : i th row variable effect
- τ_j : j th Latin letter treatment effect
- ω_k :Effect of k th level of Greek letter effect
- ψ_j : j th Latin letter treatment effect
- ε_{ijkl} : Random error

The **Model Assumptions** of Graeco Latin Square design are:

1. The random error
$$\varepsilon_{ijkl} \sim NID(0, \sigma_{\varepsilon}^2)$$
2. Effects are measured as deviation from overall mean.
3. Sum of effects is equal to zero.
4. The commonly used model is fixed effects model.

Lesson 119: ANOVA of GLS Design

Consider the being used for Graeco Latin Square design,

$$y_{ijkl} = \mu + \theta_i + \tau_j + \omega_k + \psi_l + \varepsilon_{ijkl}$$

Where the variations:

$$\begin{aligned} i &= 1, 2, \dots, p(\text{rows}) \\ j &= 1, 2, \dots, p(\text{Latin letters}) \\ k &= 1, 2, \dots, p(\text{Greek letters}) \\ l &= 1, 2, \dots, p(\text{columns}) \end{aligned}$$

The model terms are:

- y_{ijkl} :The observed response
- μ :Overall mean
- θ_i : i th row variable effect
- τ_j : j th Latin letter treatment effect
- ω_k :Effect of k th level of Greek letter effect ψ_j : j th Latin letter treatment effect
- ε_{ijkl} : Random error

The computations we need are:

Sums of squares

$C.F. = \frac{y_{...}^2}{p^2}$	(Correction factor)
$SS_L = \frac{1}{p} \sum_{j=1}^p y_{.j..}^2 - C.F.$	(Latin letters treatment sum of squares)
$SS_G = \frac{1}{p} \sum_{k=1}^p y_{..k.}^2 - C.F.$	(Greek letters treatment sum of squares)
$SS_R = \frac{1}{p} \sum_{i=1}^p y_{i...}^2 - C.F.$	(Rows sum of squares)
$SS_c = \frac{1}{p} \sum_{l=1}^p y_{...l}^2 - C.F.$	(Columns sum of squares)
$SS_{total} = \sum_{i=1}^p \sum_{j=1}^p \sum_{k=1}^p \sum_{l=1}^p y_{ijkl}^2 - C.F.$	(Total sum of squares)

The sum of square of error is,

$$SS_E = SS_{total} - (SS_L + SS_G + SS_R + SS_C)$$

Anova Table will be

S.O.V	d.f.	S.O.S.	M.S.	F-value
Lattin letters	$p - 1$	SS_L	MS_L	$F_L = \frac{MS_L}{MS_E}$
Greek letters	$p - 1$	SS_G	MS_G	$F_G = \frac{MS_G}{MS_E}$
Rows	$p - 1$	SS_R	MS_R	$F_R = \frac{MS_R}{MS_E}$
Columns	$p - 1$	SS_C	MS_C	$F_C = \frac{MS_C}{MS_E}$
Error	$(p - 1)(p - 3)$	SS_E	MS_E	
Total	$p^2 - 1$			

Conclusion

If calculated values of F-statistic of the treatment lies in the following rejection region:

$$F_{cal} \geq F_{\alpha,p-1,(p-1)(p-3)}$$

then that treatment is significant, insignificant otherwise.

Lesson 120: Advantages of GLS Design

Let define a GLS design first.

Definition 23.2

A design in which three sources of variation are controlled through blocking, also called Triple Grouping Design.

1. **Controls more variation**

Controls more variation than CR or RCB designs because of 2-way stratification. This results in a smaller mean square for error.

2. **Simple Analysis**

The analysis of data from a GLS design is simple. All sources of variation have equal degree of freedom, sums of squares are easily computed.

3. **Missing observation**

The analysis of data from a GLS design when some observation is missing is simple. The design does not lose its efficiency a lot in case of missing data.

Lesson 121: Disadvantages and Limitations of GLS Design

1. **More resources**

The required number of experimental units increase rapidly as the number of treatments increase, as the design size changes in squares. For example, in a 4 treatment design size there are $4 \times 4 = 16$ trials, and in a 5 treatment design size $5 \times 5 = 25$ trials. It means we need more resources when increase the number of treatments for a applying a Graeco Latin Square design.

2. **Error degree of freedom**

The degree of freedom of error is small if the number of treatments is small as for a p treatment GLS design, the error degree of freedom is just $(p - 1)(p - 3)$.

3. **Balance**

Since there is three way blocking, the balance is sometime quite difficult. Since we have to do three way blocking and we have to balance the design with respect to Greek letter, Latin letter, row-wise, and column-wise, that is why, the balancing becomes difficult.

4. **Restrictions**

- ◆ GLS designs are constructed for all number of treatments from 3–12 except 10. The 10 treatment GLS design cannot be constructed.
- ◆ When $p = 3$, error degree of freedom is zero.

Lesson 122: Practical Example of GLS Design

Example 1: An industrial engineer is investigating the effect of four assembly methods (A, B, C, D) on the assembly time for a color television component. Four operators are selected for the study. Furthermore, the engineer knows that each assembly method produces such fatigue that the time required for the last assembly may be greater than the time required for the first, regardless of the method. That is, a trend develops in the required assembly time. The engineer also suspects that the workplace used by the four operators may represent an additional source of variation. To account for this source of variability, the engineer uses the Graeco Latin square design. The data is shown below: Analyze the data from this experiment ($\alpha = 0.05$) draw appropriate conclusions.

Solution:

Order of Assembly	Operator			
	1	2	3	4
1	$C\beta = 11$	$B\gamma = 10$	$D\delta = 14$	$A\alpha = 8$
2	$B\alpha = 8$	$C\delta = 12$	$A\gamma = 10$	$D\beta = 12$
3	$A\delta = 9$	$D\alpha = 11$	$B\beta = 7$	$C\gamma = 15$
4	$D\gamma = 9$	$A\beta = 8$	$C\alpha = 18$	$B\delta = 6$

1. Hypothesis

H_{0L} : Latin letter treatments have same average effect.

H_{1L} : At least two Latin letters have different effects.

H_{0G} : Greek letter treatments have same average effect.

H_{1G} : At least two Greek letters have different effects.

H_{0R} : All row treatment same average effect on response.

H_{1R} : At least two rows have different effect.

H_{0C} : All column treatments have same average effect.

H_{1C} : At least two columns have different effects.

2. Level of Significance

$\alpha = 5\%$.

3. ANOVA table

Source	DF	Adj SS	Adj MS	F-value	p-value
L	3	98.315	32.7718	3.11	0.188
G	3	7.190	2.3968	0.23	0.873
R	3	1.690	0.5635	0.05	0.981
C	3	14.857	4.9524	0.47	0.725
Error	3	31.643	10.5476		
Total	15	150.00			

4. Conclusion

Since the p -value of all sources of variations is greater than all values of commonly used level of significance, therefore we conclude that all sources of variation are insignificant at all α values.

□

Lecture 24

Incomplete Block Design

We known that in literature there are many complete block design such as Randomize Complete Block Design (RCBD), Latin Square Design (LSD), and Graeco Latin Square Design (GLSD). In this lecture we will discuss about the incomplete block designs.

Lesson 123: Incomplete Block Design (IBD)

In case of complete block design all treatments are introduced in each block. In some situations complete block design is not possible to implement because:

1. (physical) block size is too small,
2. too expensive,
3. not advisable in some situations,

Definition 24.1

A randomized block design in which every treatment is not present in every block is called an **incomplete block design**.

Different **Types** of incomplete block designs:

1. **Balanced Incomplete Design (BIBD)**
If the incomplete block design contains each pair of treatments in equal number of times.
2. **Partially Balanced Incomplete Design (PBIBD)**
This design lacks the symmetry of balanced incomplete block designs.
3. **Youden Squared Design (YSD)**
Blocking on two sources of variation using incomplete blocks.
4. **Cyclic Design (CD)**
Cyclic designs structure includes some balanced incomplete and partially balanced incomplete block designs.
5. **Lattice Design (LD)**
Lattice design is used in the situation when there are a large number of treatment combinations. In order to reduce the design size partially balance lattices are considered.

Lesson 124: Balanced Incomplete Block Design (BIBD)

Definition 24.2

The incomplete design in which each pair of treatments (τ_i, τ_j) occurs together same number of times, say λ . The balance means that all differences between treatments are measured with equal precision, i.e. $Var(\tau_i - \tau_j)$ is constant.

BIBD Example:

Following is an example of how four treatments are assigned to blocks with a natural size of three experimental units. Four blocks are required for this BIBD.

Blocks	Treatments
1	ABC
2	ABD
3	ACD
4	BCD

It can be seen that all pair of treatments are occurring equal number of times.

Basic Properties of Balance Incomplete Block Design.

Box, Hunter, and Hunter (1978) point out the following rules when using BIBD.

1. Randomly assign the numbers to the blocks.
2. Randomly assign the letters to the treatments.
3. Randomly assign the treatments within the blocks.
4. Randomly group blocks as replicates. A replicate is a complete set of all treatments.

Limitations of balance incomplete block design The following table shows what block sizes are available for each number of treatments:

Number of Treatment	Block Size Available
4	2, 3
5	2, 3, 4
6	2, 3, 4, 5
7	2, 3, 4, 6
8	2, 4, 7
9	2, 4, 5, 6, 8
10	2, 3, 4, 5, 6, 9

Lesson 125: Layout and Notations of BIBD**Notations** for a BIBD:

Following are different notations which are commonly used in the construction of a BIBD:

t : No. of treatments.

b : No. of blocks.

r : No. of replicates.

k : No. of treatments per block.

Using above notation we will compute λ as

$$\lambda = \frac{r(k-1)}{t-1}$$

λ is no. of times each pair of treatments appears together. $kb = tr = N$ is total number of observations.

125.1 Examples of BIBD

Example 1: BIB Design

A balanced incomplete block design for $b = 4, k = 3, t = 4, r = 3, \lambda = 2$.

Treatment	Block			
	1	2	3	4
A	Y_{11}	Y_{12}	Y_{13}	–
B	Y_{21}	Y_{22}	–	Y_{24}
C	Y_{32}	–	Y_{33}	Y_{34}
D	–	Y_{41}	Y_{43}	Y_{44}

Example 2: BIB Design

A balanced incomplete block design for $b = 15, k = 4, t = 6, r = 10, \lambda = 6$

Block		Block		Block	
1	1 2 3 4	6	3 4 5 6	11	1 3 5 6
2	1 4 5 6	7	1 2 3 6	12	2 3 4 6
3	2 3 4 6	8	1 3 4 5	13	1 2 5 6
4	1 2 3 5	9	2 4 5 6	14	1 3 4 6
5	1 2 4 6	10	1 2 4 5	12	2 3 4 5

Example 3: BIB Design A balanced incomplete block design for $b = 4, k = 3, t = 4, r = 3$ and $\lambda = 2$.

	Block			
	1	2	3	4
A	A	A	A	B
B	B	B	C	C
C	C	D	D	D

Lesson 126: The Model and ANOVA of BIBD

The model of a BIBD includes two variable terms along with overall mean and random error

$$y_{ij} = \mu + \tau_i + \beta_j + \varepsilon_{ij} \qquad , \text{ for } \begin{matrix} i=1,2,\dots,t \\ j=1,2,\dots,b \end{matrix}$$

- 1. μ : overall mean.

2. τ_i : i th treatment effect.
3. β_j : j th block effect.
4. ε_{ij} : random error

To apply **ANOVA Test** for BIBD, we need to follow these steps:

1. **Hypothesis** $H_{0T} : \mu_1 = \mu_2 = \dots = \mu_t$
 H_{1T} : At least one pair of treatment means is not equal
 $H_{0B} : \mu_1 = \mu_2 = \dots = \mu_b$
 H_{1B} : At least one pair of block means is not equal
2. **Level of significance**
 $\alpha = 0.01, 0.05, 0.1$, etc.
3. The required **Computations**

Total sum of squares

$$SS_{total} = \sum_{i=1}^t \sum_{j=1}^b y_{ij}^2 - \frac{y_{..}^2}{N}$$

Blocks sum of squares

$$SS_{block} = \frac{1}{k} \sum_{j=1}^b y_{.j}^2 - \frac{y_{..}^2}{N}$$

Sum of squares of treatments needs adjustments for incompleteness

$$SS_{treat(adj)} = \left(\frac{k}{\lambda t} \right) \sum_{i=1}^t Q_i^2,$$

where

$Q_i = y_{i.} - \left(\frac{1}{k} \right) \sum_{j=1}^b n_{ij} y_{.j}$ is the block average containing treatment i .

$$n_{ij} = \begin{cases} 1 & \text{if } i\text{th observation appears in } j\text{th block} \\ 0 & \text{if } i\text{th observation does not appear in } j\text{th block} \end{cases}$$

$\sum_{i=1}^t Q_i = 0$, that is, adjusted treatment total sums to zero.

4. ANOVA Table

S.O.v.	d.f.	S.o.S.	M.S.	F
Treatment	$t - 1$	$SS_{treat(adj)}$	$MS_{treat} = \frac{SS_{treat(adj)}}{t-1}$	$F_t = \frac{MS_{treat}}{MS_{error}}$
Block	$b - 1$	SS_{block}	$MS_{block} = \frac{SS_{block}}{b-1}$	$F_B = \frac{MS_{block}}{MS_{error}}$
Error	$N - t - b + 1$	SS_{error}	MS_{error}	
Total	$N - 1$	SS_{total}		

5. Critical Region

$$F_T \geq F_{\alpha, t-1, N-t-b+1}, F_B \geq F_{\alpha, b-1, N-t-b+1}$$

Treatment (Catalyst)	Block (Batch of Raw Material)				Treatment Total Y_i
	1	2	3	4	
1	73	74	–	71	218
2	–	75	67	72	214
3	73	75	68	–	216
4	75	–	72	75	222
(block total) $Y_{.j}$	221	224	207	218	870= $Y_{..}$

Lesson 127: Real Life Example of BIBD

BIBD for Catalyst Experiment, Time of Reaction is Response.

Example 1: Solution:

1. Hypothesis
- $H_0 : \mu_1 = \mu_2 = \mu_3 = \mu_4$ (all catalysts have same reaction time)
- $H_1 :$ At least two of them have different reaction time.
2. Level of Significance
- $\alpha = 5\%$
3. Test Statistic
- $F = \frac{MS_{cat}}{MS_E}$
4. Critical Region
- $F_{cat} \geq F_{0.05,3,5} = 5.41$
5. Computations
- From the data table we can see:
- $t = 4, b = 4, k = 3, r = 3, \lambda = 2,$ and $N = 12.$

$$C.F. = \frac{y_{..}^2}{N} = \frac{870^2}{12}$$

$$SS_{total} = \sum_{i=1}^t \sum_{j=1}^b y_{ij}^2 - C.F. = 63156 - 63075 = 81.00$$

$$SS_{block} = \frac{1}{k} \sum_{j=1}^b y_{.j}^2 - C.F.$$

$$= \frac{221^2 + 207^2 + 224^2 + 218^2}{3} - 63075 = 55.00$$

To compute sum of squares of treatment adjusted for blocks, we proceed as:

$$Q_1 = 218 - \frac{1}{3}(221 + 224 + 218) = -\frac{9}{3}$$

$$Q_2 = 214 - \frac{1}{3}(207 + 224 + 218) = -\frac{7}{3}$$

$$Q_3 = 216 - \frac{1}{3}(221 + 207 + 224) = -\frac{4}{3}$$

$$Q_4 = 222 - \frac{1}{3}(221 + 207 + 218) = \frac{20}{3}$$

$$SS_{treat(adj)} = \frac{3 \left[\left(-\frac{9}{3}\right)^2 + \left(-\frac{7}{3}\right)^2 + \left(-\frac{4}{3}\right)^2 + \left(\frac{20}{3}\right)^2 \right]}{2 \times 4} = 22.75$$

$$SS_E = SS_{total} - SS_{treat(adj)} - SS_{block} = 81.00 - 22.75 - 55.00 = 3.25$$

6. ANOVA Table

Source	DF	AdjSS	AdjMS	F-Value
Catalyst (adjusted)	3	22.75	7.58	11.66
Blocks	3	55.00	—	
Error	5	3.25	0.65	
Total	11	81.00		

7. **Conclusion** Since calculated value of F_{cal} falls in the critical region, So we reject H_0 .

□

Lesson 128: Estimation of Treatment Effects of a BIBD

The model of a BIBD includes two variable terms along with overall mean and random error,

$$y_{ij} = \mu + \tau_i + \beta_j + \varepsilon_{ij}, \quad \text{for } \begin{matrix} i=1,2,\dots,t \\ j=1,2,\dots,b \end{matrix}$$

1. μ : overall mean
2. τ_i : i th treatment effect
3. β_j : j th block effect
4. ε_{ij} : random error

Estimation of Effects

1. **Interblock Analysis**
2. **Intrablock Analysis**

In this module we shall discuss Interblock Analysis.

128.1 Interblock Analysis

Random effects analysis is known as interblock analysis or Recovery of Interblock Information. If blocks are random, we can obtain additional information about τ_i 's by considering the information between block totals.

From the above model, we can write the block totals as

$$y_{.j} = k\mu + \sum_{i=1}^t n_{ij}\tau_i + \text{error}$$

and compute the least squares estimates of τ_i and μ .

According to Yates (1940), if block effects are uncorrelated random variables with zero mean and fixed variance σ_β^2 then the least square estimates are

$$\hat{\mu} = \bar{y}_{..}$$

$$\hat{\tau}_i = \frac{\sum_{j=1}^b n_{ij}y_{.j} - kr\bar{y}_{..}}{r - \lambda}$$

Lesson 129: IntraBlock Analysis of BIBD

The model of a BIBD includes two variable terms along with overall mean and random error,

$$y_{ij} = \mu + \tau_i + \beta_j + \varepsilon_{ij}, \quad \text{for } \begin{matrix} i=1,2,\dots,t \\ j=1,2,\dots,b \end{matrix}$$

1. μ : overall mean
2. τ_i : i th treatment effect
3. β_j : j th block effect
4. ε_{ij} : random error

Estimates of the model effects are:

By constructing normal equations using method of least squares, we find the estimates of model effects as:

$$\begin{aligned} \hat{\mu} &= \bar{y}_{..} \\ \hat{\tau}_i &= \frac{kQ_i}{\lambda t} \\ \hat{\beta}_j &= \frac{rQ_j}{\lambda b} \end{aligned}$$

where

$$\begin{aligned} Q_i &= y_{i.} - \frac{1}{k} \sum_{j=1}^b n_{ij} y_{.j} \\ Q_j &= y_{.j} - \frac{1}{r} \sum_{i=1}^t n_{ij} y_{i.} \end{aligned}$$

and

$$\begin{aligned} Var(Q_i) &= \frac{(k-1)r}{k} \times \sigma^2 \\ Var(\hat{\tau}_i) &= \frac{(t-1)k}{\lambda t^2} \times \sigma^2 \end{aligned}$$

Sum of Squares

Block sum of squares adjusted for incompleteness

$$SS_{blocks(adj)} = \frac{r \sum_{j=1}^b Q_j^2}{\lambda b}$$

Lecture 25

Partially Balanced Incomplete Block Designs

Lesson 130: Partially Balanced Incomplete Block Design (PBIBD)

Why PBIBD

Sometimes the smallest possible BIBD for a given number of treatments (t) and block size (k) is too big to be practical.

Example of a BIBD

For a design for $t = 12$ and $k = 7$, to be a BIBD require

$$\lambda = \frac{r(k-1)}{t-1} = \frac{6r}{11}$$

1. that must be a whole number
2. r must be some multiple of 11
3. also for a balance incomplete block design,

$$\begin{aligned} kb &= tr \\ \Rightarrow b &= \frac{tr}{k} = \frac{12(11 \times m)}{7} \\ \Rightarrow b &= \frac{12 \times 11 \times m}{7} \end{aligned}$$

4. b must be whole number that is possible only if b is multiple of $12 \times 11 = 132$.
5. We need large number of blocks for BIBD.

Important Aspects of PBIBD

1. A **PBIBD** allows us to run an incomplete design with fewer number of blocks than may be required in BIBD.
2. This design does not requires that each pair of treatments occurs together equal number of times.
3. We may say all differences in estimated treatment effects do not have same variance in PBIBD.

Lesson 131: Layout of PBIBD

Why PBIBD

We see that sometimes the smallest possible BIBD for a given number of treatments (t) and block size (k) is too big to be practical. The incomplete block design which lacks full balance and possesses some properties of symmetry is called Partially Balanced Incomplete Block Design (PBIBD).

Notations of PBIBD

- t : Number of treatments
- b : Number of blocks (total number of blocks)
- k : Number of treatments in each blocks (block size)
- r : Number of times each treatment appears in the design (also called number of replication)

Layout: A PBIBD with $t = 9, k = 3, r = 3, b = 9$ is, The each pair of treatments does not

Block	Replicate I		
(1)	1	2	3
(2)	4	5	6
(3)	7	8	9
	Replicate II		
(4)	1	4	7
(5)	2	5	8
(6)	3	6	9
	Replicate III		
(7)	1	5	9
(8)	7	2	6
(9)	4	8	3

appear equal number of times. However, some symmetry exists such as block size, replication of treatment, total number of block are same.

Layout: A PBIBD with $t = 12, k = 7, r = 7$, and $b = 12$

Lesson 132: Properties of PBIBD

Properties of PBIBD

Although a PBIBD lack balance of a BIBD still the design has certain aspects of symmetry, as:

- 1. **Same Block Size**
Every block in a PBIBD contains equal number of units, say k .
- 2. **Equal Replication**
Every treatment appears r times in the design.
- 3. **Replication of Treatment in a Block**
No treatment appears more than once in a block.
- 4. **Replication of Treatment in a Block**
No treatment appears more than once in a block.
- 5. **Pair of Treatments**
Every pair of treatments appears together in either λ_1 or λ_2 blocks. (in BIBD every pair of treatment appear equal number of time (λ times). In PBIBD there are more than one λ)
- 6. **Any Two Treatments**
Given any two treatments which appear together λ_1 times, the number of treatments that appear λ_2 times with the first treatment and λ_3 times with the second treatment is the same.

Lesson 133: Association Scheme of PBIBD

Association scheme is very important for PBIBD. The association scheme helps us to compared different PBIBD.

Consider a PBIBD with $t = 9, k = 3, r = 3, b = 9$ We explain association scheme through above

Block	Replicate I		
(1)	1	2	3
(2)	4	5	6
(3)	7	8	9
	Replicate II		
(4)	1	4	7
(5)	2	5	8
(6)	3	6	9
	Replicate III		
(7)	1	5	9
(8)	7	2	6
(9)	4	8	3

design:

- 1. **Consider treatment 1**
The other treatments that appear together with treatment 1 are treatment 2 and 3 (block 1), treatment 4 and 7 (block 4) and treatment 5 and 9 (block 7). The two treatments that do not appear with treatment 1 are 6 and 8.
- 2. **Consider Any other Treatment** Similarly, if we start with any other treatment, we find six treatments which appear together with this treatment in different blocks and two treatments that do not appear together with this treatment.
- 3. **First Associates** Pairs of treatments that appear in the same block are called first associates, i.e. pair of treatments occur together in λ_1 blocks.
- 4. **Second Associates** The treatments that do not appear in the same block are second associates, i.e. pair of treatments occur together in λ_2 blocks.

5. Thus the above design has two associate classes with $\lambda_1 = 1$ and $\lambda_2 = 0$.

Lesson 134: Example of PBIBD

Consider a PBIBD with two association classes

In this design $a = 6, b = 6, k = 3, r = 3, \lambda_2 = 2, \lambda_1 = 1, n_1 = 1, n_2 = 4$.

Block	Treatment Combination		
1	1	2	3
2	3	4	5
3	2	5	6
4	1	2	4
5	3	4	6
6	1	5	6

We can see that

- 1. 6 treatments are arranged in 6 blocks.
- 2. Each block contains 3 runs.
- 3. Each treatment appears in 3 blocks.
- 4. Each treatment has 1 first associate ($n_1 = 1$) and 4 second associate ($n_2 = 4$).

Association Scheme in 2×2 Matrix

If two treatments are i th associates then the number of treatments that are j th associate of one treatment and k th associate of the other can be expressed as 2×2 matrix,

$$\rho^i_{jk}, \quad (i, j, k = 1, 2)$$

Explanation

We have to determine ρ^1_{jk} and ρ^2_{jk} for the above example.

- 1. For ρ^1_{jk}
Consider any two treatments that are first associates, say 1 and 2.

Treatment 1	Treatment 2	
	1st Associate	2nd Associate
1 Associate	3, 4, 5, 6	
2nd Associate		

$$\rho^1_{jk} = \begin{bmatrix} 0 & 0 \\ 0 & 4 \end{bmatrix}$$

- 2. For ρ^2_{jk}
Now consider any two treatments that are second associates, say 2 and 5.

$$\rho^2_{jk} = \begin{bmatrix} 0 & 1 \\ 1 & 2 \end{bmatrix}$$

Treatment 1	Treatment 2	
	1st Associate	2nd Associate
1 Associate		6
2nd Associate	1	3, 4

Lesson 135: Model and Assumptions of PBIBD

The linear statistical model for the PBIBD with two associate classes:

$$y_{ij} = \mu + \tau_i + \beta_j + \varepsilon_{ij}, \quad \begin{matrix} i=1,2,\dots,a \\ j=1,2,\dots,b \end{matrix}$$

where the model terms

1. μ : overall mean,
2. τ_i : i th treatment effect,
3. β_j : j th block effect,
4. ε_{ij} : random error.

Assumptions of PBIBD

1. Treatment effects measured as deviations

$$\sum_{i=1}^n \tau_i = 0$$

2. Block effects measured as deviations

$$\sum_{j=1}^n \beta_j = 0$$

Lesson 136: Analysis of PBIBD

Intrablock Analysis of PBIBD

Consider a PBIBD under two associate scheme. The parameters of this scheme are:

$$b, a, r, k, \lambda_1, \lambda_2, n_1, n_2, \rho_{11}^1, \rho_{22}^1, \rho_{12}^1, \rho_{11}^2, \rho_{22}^2, \text{ and } \rho_{12}^2$$

$$n_{ij} = 0 \text{ or } 1, k_i = k, \quad \text{for all } i = 1, 2, \dots, a$$

$$\text{and } r_j = r, \quad \text{for all } j = 1, 2, \dots, b$$

Estimation of Treatment Effect

1. Sum of Squares of Residuals

$$\sum_{i=1}^a \sum_{j=1}^b (y_{ij} - \mu - \beta_j - \tau_i)^2$$

2. Through normal equations we get the estimate of i th treatment effect

$$\hat{\tau}_i = \frac{(k - c_2)Q_i + (c_1 - c_2)S_1(Q_i)}{r(k - 1)}$$

We have
Adjusted Total for the i th Treatment

$$Q_i = y_{i\cdot} - \left(\frac{1}{k}\right) \sum_{j=1}^b n_{ij} y_{\cdot j}$$

Also we have

$$\begin{aligned} S_1(Q_i) &= \sum_s Q_s \\ \Delta &= k^{-2} \left[\{ (rk - r - \lambda_1)(rk - r - \lambda_2) + (\lambda_1 - \lambda_2) \} \times \left(r(k-1)(\rho_{12}^1 - \rho_{12}^2) + \lambda_2 \rho_{22}^1 - \lambda_2 \rho_{12}^2 \right) \right] \\ c_1 &= (k\Delta)^{-1} \{ \lambda_1(rk - r - \lambda_2) + (\lambda_1 - \lambda_2)(\lambda_2 \rho_{12}^1 - \lambda_1 \rho_{12}^2) \} \\ c_2 &= (k\Delta)^{-1} \{ \lambda_2(rk - r - \lambda_1) + (\lambda_1 - \lambda_2)(\lambda_2 \rho_{12}^1 - \lambda_1 \rho_{12}^2) \} \end{aligned}$$

3. Variance of Contrast

We may show that variance of any treatment contrast of the form $\hat{\tau}_u \hat{\tau}_v$ is

$$Var(\hat{\tau}_u \hat{\tau}_v) = \frac{2(k - c_i)\sigma^2}{r(k - 1)},$$

where treatments u and v are i th associates ($i = 1, 2$).

4. Hence the comparisons between treatments are not estimated with the same precision. This is due to partial balance of the design.

Lesson 137: ANOVA of PBIBD

The linear statistical model for the PBIBD with two associate classes:

$$y_{ij} = \mu + \tau_i + \beta_j + \varepsilon_{ij}, \quad \begin{matrix} i=1,2,\dots,a \\ j=1,2,\dots,b \end{matrix}$$

ANOVA Test for PBIBD

Steps for computing the ANOVA test for PBIBD

- 1. Hypothesis
 $H_0 : \tau_1 = \tau_2 = \dots = \tau_a$
 H_1 : At least one pair of treatments is different
- 2. Level of significance: $\alpha = 0.05, 0.01$, etc
- 3. Test Statistic: $F_0 = \frac{MS_{Treat}}{MS_{Error}}$
- 4. Critical Region: $F_0 \geq F_{\alpha,a-1,N-a-b+1}$
- 5. Computation

$$\begin{aligned} SS_{total} &= \sum_{i=1}^a \sum_{j=1}^b y_{ij}^2 - \frac{y_{..}^2}{N} \\ SS_{Treat(Adj)} &= \sum_{i=1}^a \hat{\tau}_i Q_i \\ SS_{Block(Unadj)} &= \left(\frac{1}{k}\right) \left(\sum_{j=1}^b \beta_j\right)^2 - \frac{y_{..}^2}{N} \\ SS_{Error} &= SS_{total} - SS_{Treat(Adj)} - SS_{Block(Unadj)} \end{aligned}$$

- 6. ANOVA Table
- 7. Decision If the computed value of F -Statistic falls in the critical region reject H_0 , accept otherwise.

S.O.V.	d.f.	S.o.S.	M.S.	F ₀
Treatment (Adjusted)	$a - 1$	$SS_{treat(adj)}$	$MS_{treat} = \frac{SS_{treat_{adj}}}{a-1}$	$F_t = \frac{MS_{treat}}{MS_{error}}$
Block (Unadj)	$b - 1$	$SS_{block(Unadj)}$	$MS_{block} = \frac{SS_{block}}{b-1}$	
Error	$N - t - b + 1$	SS_{error}	$MS_{error} = \frac{SS_{error}}{N-t-b+1}$	
Total	$N - 1$	S_{total}		

Lecture 26

Youden Squares Design

Lesson 138: Youden Squares Design: Introduction

Definition 26.1

We use Latin square (LS) design when we want to control two sources of variation in complete blocks, i.e., we use two-way blocking. We can use a Youden Square design when need to block on two sources of variation but can not set up complete blocks as were in case of LS design.

A Youden Square design for 4 treatments in 3 blocks is We considered rows as blocks and columns

A	B	C	D
B	A	D	C
C	D	A	B

as treatment. Note that the above design is not Latin Square design.

A symmetric BIBD with $b = a = 7$ and $r = k = 3$ forms a Youden Square as: Note that none of

A	B	C	D	E	F	G
B	C	D	E	F	G	A
C	E	E	G	A	B	C

the block contains all treatments.

Model for Youden Square Design

The Linear model for a Youden square design is

$$y_{ijm} = \mu + \alpha_i + \beta_j + \gamma_m + \varepsilon_{ijm}$$

The model terms are,

- μ : Overall mean
- α_i : i th block effect
- β_j : j th treatment effect
- γ_m : m th position effect
- $\varepsilon_{ijm} \sim NID(0, \sigma_i^2)$: is random error

Lesson 139: Construction of a Youden Squares Design

The simplest example of a Youden Square design is with a LS design by deleting

- 1. One of its row or
- 2. One of its column or
- 3. Diagonal entries

Let us perform these actions one-by-one.

- 1. Deleting One Row (from 4×4 Latin Square Design)

A	B	C	D
C	D	A	B
D	C	B	A
B	A	D	C

- 2. Deleting One Column (from 4×4 Latin Square Design)

A	B	C	D
C	D	A	B
D	C	B	A
B	A	D	C

- 3. Deleting Diagonal Entries (from 4×4 Latin Square Design)

A	B	C	D
C	D	A	B
D	C	B	A
B	A	D	C

Note that deleted rows, columns, or diagonal elements are in gray colour.

Note That:

- 1. A BIBD with *Number of blocks* = *Number of treatments* (i.e., $b = a$), forms a Youden Square Design
- 2. It is not true that every LS design with one row/one column or diagonal missing is a Youden Square design.
- 3. In some cases deleting more than one row or column destroys balance.

Lesson 140: The Design Rules for a Youden Squares Design

A Youden Square design follows the following decision rules:

- 1. There are ‘ a ’ treatments.
- 2. Each treatment is replicated ‘ r ’ times.
- 3. There are ‘ b ’ blocks of size k . The size of each block must be same.
- 4. $k < a$. If $k = a$ then Youden square design becomes complete block design.
- 5. Since $bk = ar$, no treatment occurs more than once in a block.

6. There are ‘ m ’ associate classes (pairs of treatments), i.e. i th associates appear together in λ_i blocks.
7. We usually arrange λ_i ’s in decreasing order, so that first associates appear together most number of times.
8. A design with λ_i with $i = 1, 2, \dots, m$, is said to have m -associate classes.
9. All treatments have same number of i th associates.

Lesson 141: Analysis of a Youden Squares Design

An industrial engineer wants to study the effect of illumination levels on the occurrence of defects in an assembly operation. The experiment is run in five days(blocks) on four work stations. The coded data is presented below:

days	Work Station				$y_{i..}$	$y_{.j.}$
	1	2	3	4		
1	$A = 3$	$B = 1$	$C = -2$	$D = 0$	2	$12(A)$
2	$B = 0$	$C = 0$	$D = -1$	$E = 7$	6	$2(B)$
3	$C = -1$	$D = 0$	$E = 5$	$A = 3$	7	$-4(C)$
4	$D = -1$	$E = 6$	$A = 4$	$B = 0$	9	$-2(D)$
5	$E = 5$	$A = 2$	$B = 1$	$C = -1$	7	$23(E)$
$y_{..m}$	6	9	7	9	$y_{...} = 31$	

The Linear model for a Youden square design:

$$y_{ijm} = \mu + \alpha_i + \beta_j + \gamma_m + \varepsilon_{ijm}$$

where, μ : Overall mean, α_i : i th block effect, β_j : j th treatment effect
 γ_m : m th position effect, $\varepsilon_{ijm} \sim NID(0, \sigma_i^2)$ random error.

Analysis of Youden Square Design

The design has $a = b = 5, r = k = 4, \lambda = 3$. The required computation are:

$$SS_{total} = \sum_{i=1}^b \sum_{j=1}^a \sum_{m=1}^k y_{ijm}^2 - \frac{y_{...}^2}{N}$$

$$Q_j = y_{.j.} - \frac{1}{m} \sum_{i=1}^b \sum_{i=1}^b y_{i..} = \frac{23}{4}, -\frac{16}{4}, -\frac{32}{4}, \frac{63}{4}$$

$y_{i..}$: blocks totals containing j th treatment

$$SS_{treat(adj)} = \frac{\sum_{j=1}^b Q_j^2}{\lambda a} = 12.37$$

$$SS_{days} = \sum_{i=1}^b \frac{y_{i..}^2}{k} - \frac{y_{...}^2}{N} = 6.70$$

$$SS_{station} = \sum_{m=1}^k \frac{y_{..m}^2}{b} - \frac{y_{...}^2}{N} = 1.35$$

$$SS_E = SS_{total} - SS_{treat(adj)} - SS_{days} - SS_{station} = 6.53$$

The adjusted block (day) S.O.S may be computed as:

$$Q'_j = y_{i..} - \frac{1}{m} \sum_{j=1}^a y_{..} = \frac{0}{4}, \frac{5}{4}, -\frac{1}{4}, \frac{1}{4}, -\frac{5}{4}$$

$y_{.j.}$: treatment totals belong to i th block

$$SS_{days(adj)} = \frac{k \sum_{j=1}^b Q_j'^2}{\lambda b} = 0.87$$

The ANOVA Table

S.O.V.	d.f.	S.O.S.	M.S.S.	F_0	
Illumination Level (Adj.)	4	120.37	30.09	36.87	Sig.
Days, Unadj.	4	6.70	—		
Days, Adj.	(4)	(0.87)	0.22		Insig
Work Station	3	1.35	0.45		Insig
Error	8	6.53	0.82		
Total	19	134.95			

Lecture 27

Factorial Experiments

Lesson 142: Factorial Experiments

Definition 27.1

A factorial experiment is an experiment whose design consists of two or more factors, each with discrete possible values (the “levels”).

The experiment allows to estimate the effect of each factor and the interaction effect of factors on the response.

There are two **Types** of factorial experiments

- 1. **Full factorial experiment**
The experimental units of such experiment take on all possible combinations of all levels across all the factors. Therefore, a full factorial design is also called a fully crossed design.
- 2. **Fractional factorial experiment**
If the full factorial design includes too many combinations (runs) to be logically feasible, a fractional factorial may be used. The fractional factorial design may include half, one third, etc. runs of full factorial experiment.

Beginning of Factorial Design

Factorial design was initially used in 19th century at Rothamsted Experimental Station (one of the oldest research station in UK). Ronal Fisher and Frank Yates are the pioneers of factorial design.

Lesson 143: Advantages of Factorial Experiments

Advantages of Factorial Experiment to One-Factor-at-a-time Experiment.

- 1. **Required Less Number of Observations**
Let A and B be two factors. The information on a factor can be obtained by varying that factor and keeping the other factor fixed. Effect of changing factor $A = A_2B_1 - A_1B_1$
Effect of changing factor $B = A_1B_2 - A_1B_1$
Three treatment combinations are used for two effects, for error estimation we need two replicates so six observations are needed.

		Factor B	
		B_1	B_2
Factor A	A_1	A_1B_1	A_1B_2
	A_2	A_2B_1	A_2B_2

In case of factorial experiments one more combination A_2B_2 is utilized and we get:
Two estimates of A as

$$= A_2B_1 - A_1B_1 \qquad \text{and} \qquad = A_2B_2 - A_1B_2$$

Two estimates of B are

$$= A_1B_2 - A_1B_1 \qquad \text{and} \qquad = A_2B_2 - A_2B_1$$

Thus, by using four observations we can get the estimates of same precision under a factorial experiment.

2. **More Relative Efficiency**

In case of two factors the relative efficiency of factorial design to one-factor-at-a-time experimental design is $\frac{6}{4} = 1.5$
This relative efficiency increases with the increase of number of factors.

3. **Necessary When Interaction is Present**

When using one-factor-at-a-time design and the response of A_1B_2 and A_2B_1 is better than A_1B_1 , an experimenter logically concludes that the response of A_2B_2 would be even better than A_1B_1 . Whereas, A_2B_2 is available in factorial design.

4. **Versatility**

Factorial designs are more versatile in computing effects. These designs provide a chance to estimate the effect of a factor at several levels of the other factor.

Lesson 144: Factor Effects - Main and Interaction Effect of 2^2 Design

Definition 27.2

Effect of a Factor

Change in the quantity of response due to the change in level of a factor is called effect of that factor. Here we mean average effect.

Example

Consider a two factor factorial experiment

		Factor B	
		B_1	B_2
Factor A	A_1	20	35
	A_2	45	60

Main Effects:

Main effect of A = Average response at high level of A – Average response at low level of A

$$= \frac{45 + 60}{2} - \frac{20 + 35}{2} = 25$$

Interpretation

Increase in factor A from first level to the second level brings an average increase of 25 units in response.

$$\begin{aligned}\text{Main effect of } B &= \text{Average response at high level of } B - \text{Average response at low level of } B \\ &= \frac{35 + 60}{2} - \frac{20 + 45}{2} = 15\end{aligned}$$

Effect of AB Interaction:

If the change in response between the levels of a factor is not the same at all levels of the other factor/s, then there is an interaction between the factors. Consider

		Factor B	
		B_1	B_2
Factor A	A_1	20	40
	A_2	50	15

Effect of AB Interaction

= Average difference between effect of A at high level of B and the effect of A at low level of B .

OR

= Average difference between effect of B at high level of A and the effect of B at low level of A .

Lecture 28

2² Factorial Experiments

Lesson 145: Layout of 2² Factorial Experiment

The geometrical structure of two factors, Factor *A* and *B*, each factor has two levels, low (−) and high (+). Response 1 is at low level of *A* and low level of *B*, similarly, response 2 is produced at high level of *A* and low level of *B*. Third response is at low level of *A* and high level of *B*, similarly, the 4th response is at high level of *A* and high level of *B*..

Layout for Two Factor Two Level in *n* Replicates *y*₁₁₁ is the response from first factor

		Factor B			
		1	2	...	b
Factor A	1	<i>y</i> ₁₁₁ , <i>y</i> ₁₁₂ , ... <i>y</i> _{11<i>n</i>}	<i>y</i> ₁₂₁ , <i>y</i> ₁₂₂ , ..., <i>y</i> _{12<i>n</i>}	...	<i>y</i> _{1<i>b</i>1} , <i>y</i> _{1<i>b</i>2} , ..., <i>y</i> _{1<i>b</i><i>n</i>}
	2	<i>y</i> ₂₁₁ , <i>y</i> ₂₁₂ , ... <i>y</i> _{21<i>n</i>}	<i>y</i> ₂₂₁ , <i>y</i> ₂₂₂ , ..., <i>y</i> _{22<i>n</i>}	...	<i>y</i> _{2<i>b</i>1} , <i>y</i> _{2<i>b</i>2} , ..., <i>y</i> _{2<i>b</i><i>n</i>}
	...	⋮	⋮	⋮	⋮
	<i>a</i>	<i>y</i> _{<i>a</i>11} , <i>y</i> _{<i>a</i>12} , ... <i>y</i> _{<i>a</i>1<i>n</i>}	<i>y</i> _{<i>a</i>21} , <i>y</i> _{<i>a</i>22} , ..., <i>y</i> _{<i>a</i>2<i>n</i>}	...	<i>y</i> _{<i>a</i><i>b</i>1} , <i>y</i> _{<i>a</i><i>b</i>2} , ..., <i>y</i> _{<i>a</i><i>b</i><i>n</i>}

at low level, second factor at low level and first replicate of trial. Similarly, *y*₁₁₂ represents the second replicate of the same trial and upto *n*th observation is *n*th trial at the same level of *A* and *B*.

Real Life Example

The concentration of reactant vs the amount of the catalyst produces some response, experiment has three replicates.

Geometrical Structure of the above example

Factor		Treatment Combination	Replicate			
A	B		I	II	III	Total
–	–	A low, B low	28	25	27	80
+	–	A high, B low	36	32	32	100
–	+	A low, B high	18	19	23	60
+	+	A high, B high	31	30	29	90

Figure 28.1: Treatment Combination in 2² Design

Factor Effects

$$A = \frac{(a + ab) - ((I) + b)}{2} = \frac{100 + 90 - 80 - 60}{2} = 25$$
$$B = \frac{(b + ab) - ((I) + a)}{2} = \frac{60 + 90 - 80 - 100}{2} = -15$$
$$AB = \frac{((I) + ab) - (a + b)}{2} = \frac{80 + 90 - 100 - 60}{2} = 5$$

Minus 15 (–15) is the effect of *B* shows the change in factor level from low to high brings on the average –15 decrease in the response.

Objectives of Factorial Experiments

- 1. Want to understand how factors interact.
- 2. Want to estimate each factor effect. independent of the existence of other factor effects.
- 3. Want to estimate factor effects well; this implies estimating effects from averages.
- 4. Want to obtain the most information in the fewest number of runs.

Lesson 146: Statistical Analysis of 2² Factorial Experiment
- Model and Assumptions

The Model assuming two factors *A* and *B*

$$y_{ijk} = \mu + \tau_i + \beta_j + (\tau\beta)_{ij} + \varepsilon_{ijk}$$

for

- $i = 1, 2, \dots, a$ (Levels of Factor A)
- $j = 1, 2, \dots, b$ (Levels of Factor B)
- $k = 1, 2, \dots, n$ (Number of replicates)

where the terms in the model are

- μ : Overall mean
- τ_i : Effect of i th level of A β_j : Effect of j th level of B $(\tau\beta)_{ij}$: Interaction effect, effect of i th level of A and j th level of B
- ε_{ijk} : Random error

Assumptions of the Model

- 1. The effect of factor A and B is fixed and measured as deviation from overall mean, therefore $\sum_{i=1}^n \tau_i = 0$ $\sum_{j=1}^b \beta_j = 0$ and $\sum_{i=1}^a (\tau\beta)_{ij} = 0$ and $\sum_{j=1}^b (\tau\beta)_{ij} = 0$
The factorial analysis has several assumptions:
- 2. **Interval data of the dependent variable,**
- 3. **Normality: Data is normally distributed,**
- 4. **Homoscedasticity,** and
- 5. **No multicollinearity.**

Lesson 147: Statistical Analysis of 2² Factorial Experiment - Model Estimates

The Model, assuming two factors A and B

$$y_{ijk} = \mu + \tau_i + \beta_j + (\tau\beta)_{ij} + \varepsilon_{ijk}$$

The estimated model is

$$\hat{y}_{ijk} = \hat{\mu} + \hat{\tau}_i + \hat{\beta}_j + (\hat{\tau}\hat{\beta})_{ij}$$

The sum of squared deviations from mean

$$\begin{aligned} S &= \sum_{i=1}^a \sum_{j=1}^b \sum_{k=1}^n (\hat{y}_{ijk} - \bar{y}_{...})^2 \\ &= \sum_{i=1}^a \sum_{j=1}^b \sum_{k=1}^n (\hat{\mu} + \hat{\tau}_i + \hat{\beta}_j + (\hat{\tau}\hat{\beta})_{ij} - \bar{y}_{...})^2 \end{aligned}$$

◆ To estimate μ , put $\frac{\partial S}{\partial \mu} = 0$, we get

$$abn\hat{\mu} + bn \sum_{i=1}^a \hat{\tau}_i + an \sum_{j=1}^b \hat{\beta}_j + n \sum_{i=1}^a \sum_{j=1}^b (\hat{\tau}\hat{\beta})_{ij} - abn\bar{y}_{...} = 0$$

Since $\sum_{i=1}^a \hat{\tau}_i = 0, \sum_{j=1}^b \hat{\beta}_j = 0, \sum_{i=1}^a \sum_{j=1}^b (\hat{\tau}\hat{\beta})_{ij} = 0$

We get estimate of μ as

$$\hat{\mu} = \bar{y}_{..}$$

- ◆ To estimate τ_i , put $\frac{\partial S}{\partial \tau_i} = 0$, ignoring $\sum_{i=1}^a$ as τ_i is to estimate, we get

$$bn\hat{\mu} + bn\hat{\tau}_i + n\sum_{j=1}^b\hat{\beta}_j + n\sum_{j=1}^b(\hat{\tau}\hat{\beta})_{ij} - abn\bar{y}_{...} - bn\frac{y_{i..}}{bn} = 0$$

Since $\sum_{j=1}^b\hat{\beta}_j = 0, \sum_{j=1}^b(\hat{\tau}\hat{\beta})_{ij} = 0$

We get estimate of τ_i as

$$\hat{\tau}_i = \bar{y}_{i..} - \bar{y}_{...}$$

- ◆ Similarly we get the estimates of β_j and $(\tau\beta)_{ij}$ as:

$$\hat{\beta}_j = \bar{y}_{.j.} - \bar{y}_{...}$$

and

$$(\hat{\tau}\hat{\beta})_{ij} = \bar{y}_{ij.} - \bar{y}_{i..} - \bar{y}_{.j.} + \bar{y}_{...}$$

Lesson 148: Statistical Analysis of Factorial Experiment - ANOVA of a 2² Design

To perform **ANOVA Test**, the step by step procedure is.

1. **Hypothesis**

- ◆ For *A*
 $H_0 : \tau_1 = \tau_2 = \dots = \tau_a = 0$
 $H_1 =$ at least one $\tau_{\tau_i} \neq 0$
- ◆ For *B*
 $H_{00} : \beta_1 = \beta_2 = \dots = \beta_b = 0$
 $H_{11} :$ at least one $\beta_j \neq 0$
- ◆ For *AB* interaction
 $H_{000} : (\tau\beta)_{ij} = 0$
 $H_{111} :$ at least one $(\tau\beta)_{ij} \neq 0$

2. **Level of Significance**

$\alpha = 1\%, 5\%, 10\%$, etc.

3. **Test Statistic**

$$F_{0A} = \frac{MS_A}{MS_E}$$
$$F_{0B} = \frac{MS_B}{MS_E}$$
$$F_{0AB} = \frac{MS_{AB}}{MS_E}$$

4. **Critical Region**

$$F_0 \geq F_{\alpha,a-1,N-a-b+1}$$
$$F_0 \geq F_{\alpha,b-1,N-a-b+1}$$
$$F_0 \geq F_{\alpha,(a-1)(b-1),N-a-b+1}$$

S.O.V.	d.f.	S.S.	M.S.S	F_0
A	$a - 1$	SS_A	MS_A	$F_A = \frac{MS_A}{MS_{error}}$
B	$b - 1$	SS_B	MS_B	$F_B = \frac{MS_B}{MS_{error}}$
AB	$(a - 1)(b - 1)$	SS_{AB}	MS_{AB}	$F_{AB} = \frac{MS_{AB}}{MS_{error}}$
Error	$ab(n - 1)$	SS_{error}	MS_{error}	
Total	$abn - 1$	SS_{total}		

5. ANOVA Table

6. Conclusion

If the calculated value of F falls in critical region reject H_0 . accept otherwise.

Lesson 149: 2-level Factorial Experiments: Assumptions

The factorial Analysis has a several assumptions that need to be fulfilled:

1. Interval data of the dependent variable,
2. Normality,
3. Homoscedasticity, and
4. No multicollinearity.

Let us see the detail of each assumption.

1. Measurement Scale

- ◆ The factorial model requires the dependent variable to be of metric measurement level (that is ratio or interval data).
- ◆ The independent variables can be nominal. If not nominal or ordinal they need to be grouped first before the factorial analysis can be done.

2. Normality

- ◆ We assume that the dependent variable approximates a multivariate normal distribution.
- ◆ It can be checked graphically (either a histogram with normal distribution curve, or with a Q-Q-Plot) or with a goodness of fit test (Kolmogorov-Smirnov test is preferable for interval or ratio scaled data).
- ◆ Some statisticians argue that the Central Limit Theorem implies that large random samples automatically approximate normal distribution.
- ◆ Small, non-normal samples can be increased in size by boot-strapping.
- ◆ In some situations transformations work better.

3. Homoscedasticity

- ◆ The factorial model assumes that the error variances of all data points of the dependent variable are equal throughout the sample, i.e. the variability in the measurement error should be stable along the scale.
- ◆ The Levene's Test addresses this assumption.

4. No Multidisciplinary

- ◆ The factorial analysis requires the observations to be mutually independent (e.g., no repeated measurements)
- ◆ Also, the independent variables are independent from each other, i.e. no multidisciplinary between them.

Lesson 150: Notations and Coding of 2-level Factorial Design

The notations used to denote factorial experiments conveys a lot of information.

- 1. A two level factorial design is generally denoted by 2^k .
 - ◆ k denotes number of factors in the experiment.
 - ◆ 2 represents number of levels of each factor.
- 2. A 2^5 design has five factors, each with two levels, and $2^5 = 32$ experimental conditions or trial or runs.
- 3. Factorial experiments can involve factors with different numbers of levels. A 2^43 design has five factors, four with two levels and one with three levels, and has $16 \times 3 = 48$ runs.

Coding

- 1. The points in a two-level factorial design are often abbreviated with plus and minus signs. conventionally, $-$ for the first (or low) level, and $+$ for the second (or high) level.
- 2. The factorial points of two factor design can also be abbreviated by control (I), a, b , and ab , the presence of a letter indicates that the specified factor is at its high level and the absence of a letter indicates that the specified factor is at its low level. (I) is called control, used to indicate all factors at their lowest values.
- 3. Sometimes 4 runs of a two factor, two level design can be represented as
 - ◆ 00, 10, 01, 11 or
 - ◆ $a_0b_0, a_1b_0, a_0b_1, a_1b_1$

Lesson 151: Sign Table of 2^2 Factorial

Sign Table

Sign table is used to represent a design. Different signs represent different levels of a factor.

A design is usually presented in the form of a matrix, called **design matrix**. The sign table is usually presented in matrix form called design matrix.

Design Matrix

- 1. Different columns of the design matrix represent factors in the experiment.
- 2. Each row of the design matrix represents an experimental trial or run.

Sign Table: $+$ and $-$ signs Factor A and B both are measured at two levels (low and high).

A	B
-	-
+	-
-	+
+	+

There are four different combination of these factors.

0 and 1 digit signs

Treatment Combinations

A	B
0	0
1	0
0	1
1	1

(I)	a_0b_0
a	a_1b_0
b	a_0b_1
ab	a_1b_1

Lesson 152: Geometrical View of 2-level Factorial Design

Experimental Region

The sequential experimentation is performed within a practicable space of the set of independent variables. The range of factor levels in which an experiment can possibly be performed is commonly known as **operability region**.

After the first phase when an experimenter has completed the screening of factors and he thinks that he has reached the point which is near optimum, he makes his approach narrower and more focused.

In the second phase of the experiment he defines a more accurate and smaller region for his experiment which is called experimental region or region of interest. Typically, region of experimentation is a **cuboidal** or a **spherical** region.

The experimental region of a two level factorial is cuboidal.

Geometry of 2² Design

Lesson 153: Estimation of Effects of a 2² Factorial Experiment

Definition 28.1

Factor Effect

Average change in response due to the changes in level of a factor.

Data of 2² Factorial Experiment

Runs	Treatment	A	B	Response (Y)
	Combination			
1	(I)	–	–	Y_1
2	a	+	–	Y_2
3	b	–	+	Y_3
4	ab	+	+	Y_4

Factor Effects of 2² Factorial for *n* Replicates

Average Effect of *A*

= Average effect of *A* at high level of *A* – Average effect of *A* at low level of *A*

$$B = \frac{1}{2n}(ab + a) - \frac{1}{2n}(b + (I))$$
$$= \overline{Y}_{A+} - \overline{Y}_{A-}$$

Average Effect of *B*

= Average effect of *B* at high level of *B* – Average effect of *B* at low level of *B*

$$B = \frac{1}{2n}(ab + b) - \frac{1}{2n}(a + (I))$$
$$= \overline{Y}_{B+} - \overline{Y}_{B-}$$

Interaction Effect of *AB*

= Average difference b/w effect of *A* at high level of *B* and the effect of *A* at low level of *B*

$$AB = \frac{1}{2n}\{(ab - b) - (a - (I))\}$$
$$= \frac{1}{2n}\{(ab + (I)) - (a - b)\}$$

Lesson 154: Sums of Squares of a 2² Experiment

The Model for two factors: assuming two factors *A* and *B*

$$y_{ijk} = \mu + \tau_i + \beta_j + (\tau\beta)_{ij} + \varepsilon_{ijk}$$

We can see

$$y_{i..} = \sum_{j=1}^b \sum_{k=1}^n y_{ijk}, \quad \overline{y}_{i..} = \frac{y_{i..}}{bn}$$
$$y_{..} = \sum_{i=1}^a \sum_{k=1}^n y_{ijk}, \quad \overline{y}_{..} = \frac{y_{..}}{an}$$
$$y_{ij.} = \sum_{k=1}^n y_{ijk}, \quad \overline{y}_{ij.} = \frac{y_{ij.}}{n}$$
$$y_{...} = \sum_{i=1}^a \sum_{j=1}^b \sum_{k=1}^n y_{ijk}, \quad \overline{y}_{...} = \frac{y_{...}}{abn}$$

Partitioning Total Sum of Squares: assuming two factors *A* and *B*

1. Correction Factor

$$C.F. = \frac{y_{...}^2}{abn}$$

2. Total Sum of Squares

$$SS_{total} = \sum_{i=1}^a \sum_{j=1}^b \sum_{k=1}^n y_{ijk}^2 - C.F.$$

3. Sum of Squares of Factor A

$$SS_A = \frac{1}{bn} \sum_{i=1}^a y_{i..}^2 - C.F.$$

4. Sum of Squares of Factor B

$$SS_B = \frac{1}{an} \sum_{j=1}^b y_{.j.}^2 - C.F.$$

5. Sum of Squares of Interaction AB

$$SS_{AB} = SS_{subtotal(AB)} - SS_A - SS_B$$

$$SS_{subtotal(AB)} = \frac{1}{n} \sum_{i=1}^a \sum_{j=1}^b y_{ij.}^2 - C.F.$$

$$SS_{error} = SS_{total} - SS_{subtotal(AB)}$$

Lesson 155: Use of Contrasts in the Analysis of 2^2 Factorial Experiment

Definition 28.2

Contrast: A linear combination of set of effects with coefficients summing to zero.

The contrast of an effect is computed by adding all responses with the corresponding sign (+ or -) in the sign table.

1. Contrast of A

$$= ab + a - b - (I)$$

2. Contrast of B

$$= ab + b - a - (I)$$

3. Contrast of AB

$$= ab + (I) - a - b$$

Uses of Contrast

1. A contrast may be used to know the magnitude or direction of a factor effect to determine which factors are important.
2. Contrast can be used to compute effects.
3. Contrast can be used to compute sums of squares for analysis.

General Formulas

Contrast is generally represented by

$$= \sum_{i=1}^a c_i y_i \quad \text{with} \quad \sum_{i=1}^a c_i = 0$$

where c_i is contrast coefficients, and y_i is response

Sum of Squares of a Contrast

$$SS_c = \frac{(\sum_{i=1}^a c_i y_i)^2}{n \sum_{i=1}^a c_i^2}$$

Computing Average **Effects** from contrast

1. Average effect of A for n replicates

$$A = \frac{\text{contrast } A}{2n}$$

2. Average effect of B for n replicates

$$B = \frac{\text{contrast } B}{2n}$$

3. Average effect of AB for n replicates

$$AB = \frac{\text{contrast } AB}{2n}$$

Sums of Squares

1. S.O.S of A for n replicates

$$SS_A = \frac{(\text{contrast } A)^2}{4n}$$

2. S.O.S of B for n replicates

$$SS_B = \frac{(\text{contrast } B)^2}{4n}$$

3. S.O.S of AB for n replicates

$$SS_{AB} = \frac{(\text{contrast } AB)^2}{4n}$$

Lecture 29

2^3 Factorial Experiments

Lesson 156: Sign Table of 2^3 Factorial Design

Sign table is used to represent a factorial design.

A two level three factor design is presented in the form of a 3-column matrix, called design matrix. Each row of the design matrix represents an experimental trial or run, showing level (quantity) of each factor.

Sign Table of 2^3 Design

- ◆ +1 and -1 signs [h]

Factors		
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

- ◆ 0 and 1 digit signs

A	B	C
0	0	0
1	0	0
0	1	0
1	1	0
0	0	1
1	0	1
0	1	1
1	1	1

Lesson 157: Layout of 2³ Factorial Design

The Model for two factors is

$$y_{ijk} = \mu + \tau_i\beta_j + (\tau\beta)_{ij} + \varepsilon_{ijk}$$
$$i = 1, 2, \dots, a(\text{levels of factor } A)$$
$$j = 1, 2, \dots, b(\text{levels of factor } B)$$
$$k = 1, 2, \dots, n(\text{Numbers of replicates})$$

General Structure of Layout for $k = 3$

Factor B		Factor A												
		1	2	...	a	1	2	...	a	...	1	2	...	a
		1				2				b				
Factor C	1	y_{111}	Y_{211}	...	y_{a11}	y_{121}	y_{221}	...	y_{a21}	...	y_{1b1}	y_{2b1}	...	y_{ab1}
	2	y_{112}	Y_{212}	...	y_{a12}	y_{122}	y_{222}	...	y_{a22}	...	y_{1b2}	y_{2b2}	...	y_{ab2}
	⋮	⋮		⋮		⋮				⋮			⋮	
	c	y_{11c}	Y_{21c}	...	y_{a1c}	y_{12c}	y_{22c}	...	y_{a2c}	...	y_{1bc}	y_{2bc}	...	y_{abc}

Layout for 2³ Design in Coded Form

Factor B	Factor C	Factor A	
		-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

Lesson 158: Factor Effects of 2³ Factorial Experiment

Sign Table for 2³ factorial design.

Runs	Treatment Combination	A	B	C	AB	AC	BC	ABC	Response (Y)
1	(I)	-	-	-	+	+	+	-	Y_1
2	a	+	-	-	-	-	+	+	Y_2
3	b	-	+	-	-	+	-	+	Y_3
4	ab	+	+	-	+	-	-	-	Y_4
5	c	-	-	+	+	-	-	+	Y_5
6	ac	+	-	+	-	+	-	-	Y_6
7	bc	-	+	+	-	-	+	-	Y_7
8	abc	+	+	+	+	+	+	+	Y_8

Computing the Effects

1. Main Effects

$$A = \frac{a + ab + ac + abc}{2n} - \frac{(I) + b + c + bc}{2n}$$

$$B = \frac{b + ab + bc + abc}{2n} - \frac{(I)a + c + ac}{2n}$$

$$C = \frac{c + ac + bc + abc}{2n} - \frac{(I) + a + b + ab}{2n}$$

2. Two Factor Interaction Effects

$$AB = \frac{(I) + ab + c + abc}{2n} - \frac{a + b + ac + bc}{2n}$$

$$AC = \frac{(I) + b + ac + abc}{2n} - \frac{a + ab + c + bc}{2n}$$

$$BC = \frac{(I) + a + bc + abc}{2n} - \frac{b + ab + c + ac}{2n}$$

3. Three Factor Interaction Effect

$$ABC = \frac{a + b + c + abc}{2n} - \frac{(I) + ab + ac + bc}{2n}$$

Note that treatment combinations actually represent corresponding value in the response column as:

$$\begin{aligned} (I) &: y_1, & a &: y_2, \\ b &: y_3, & ab &: y_4, \\ c &: y_5, & ac &: y_6, \\ bc &: y_7, & abc &: y_8, \end{aligned}$$

Lesson 159: Geometrical View of 2^3 Factorial Design

(a) 3-Dimensions

(b) A point in 3-Dimensions

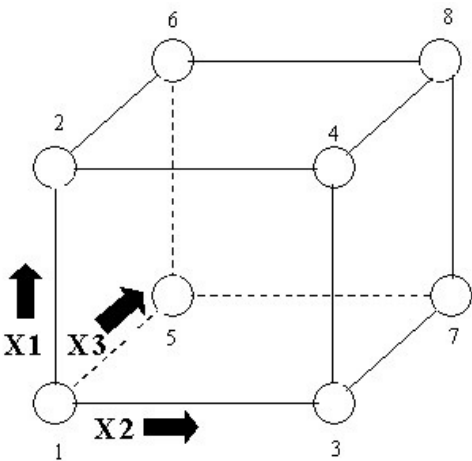
Figure 29.1: Geometrical View of 2^3 Factorial Design

3-Dimensional Cube

Sign Table

run	X_1	X_2	X_3
1	-1	-1	-1
2	1	-1	-1
3	-1	1	-1
4	1	1	-1
5	-1	-1	1
6	1	-1	1
7	-1	1	1
8	1	1	1

3-D View of Design



Lesson 160: Yate’s Algorithm for S.O.S. in 2² Factorial Experiment

Steps for Yate’s Algorithm are:

1. List treatment combinations in standard order in first column.
2. In the second column put total response of each treatment combination from all replications.
3. Create k new columns:
4. The first 2^{k-1} entries of col-1 are obtained by adding pairs of adjacent response values.
5. The remaining 2^{k-1} entries are obtained by subtracting first entry in each pair from the second entry.
6. The col-2 is obtained by performing same steps on col-1.
7. Process continues till the k th column is obtained from the $(k-1)$ th column.
8. The first entry in the k th column (corresponding to (I)) is the grand total and remaining entries are the totals of the effects corresponding to the treatment combination.
9. Average effects are obtained by dividing each total to ' $n2^{k-1}$ ' where n is number of replicates.
10. The sums of squares of the effects are obtained by squaring k th column and dividing by ' $n2^k$ '.

Sums of Squares and Effects.

Total Response	Col-1	Col-2	Effects	S.O.S.
(I)	(I)+a	$(I) + a + b + ab = [I]$	$[I]/n2^{k-1}$	$[I]^2/n2^k$
a	b+ab	$ab - b + a - (I) = [A]$	$[A]/n2^{k-1}$	$[A]^2/n2^k$
b	$a - (I)$	$b + ab - (I) - a = [B]$	$[B]/n2^{k-1}$	$[B]^2/n2^k$
ab	$ab - b$	$ab - b - a + (I) = [AB]$	$[AB]/n2^{k-1}$	$[AB]^2/n2^k$

Lecture 30

Blocking and Confounding in Factorial Experiments

Lesson 161: Blocking and Confounding

Definition 30.1

Blocking: Blocking is the strategy of running an experiments in parts. These systematically formed parts are called blocks. There can be two, four, and eight, etc., number of blocks of a 2^k and three, nine, etc., blocks of a 3^k factorial experiment.

Why we need Blocking?

- ◆ **Extraneous Factors**
If we want to eliminate the influence of extraneous factors when running an experiment. We do this by **blocking**.
- ◆ **Design Size**
Sometimes the design or experiment size large enough that it becomes difficult to run all the experiment runs at a time. For example, following table list how many trials we need to run for different factor levels.

k	2^k	3^k
2	4	9
3	8	27
4	16	81
5	32	243
6	64	729

It means with increase of number of factors the number of trials increases.

Definition 30.2

Confounding: A technique which arranges a full factorial experiment in blocks. A situation which occurs as a result of blocking when certain treatment effects become indistinguishable from blocks, is called confounding.

Note that,

- ◆ A block size is smaller than the number of treatment combinations in a single replicate.
- ◆ The order of running treatment combinations within a block is random.
- ◆ Each block is also run randomly.

Lesson 162: Methods of Confounding: Geometrical Concept

Confounding 2² experiment

The design of 2² factorial experiment,

Treatment Name	Factors	
	A	B
(I)	−1	−1
a	1	−1
b	−1	1
ab	1	1

Blocking 2² Experiment: We can allocate treatment combination in to two blocks. The geometrical view of 2² factorial experiment.

Note that treatment combinations on a diagonal form "Block 1" and the treatment combinations on the other diagonal form "Block 2".

The design 2³ factorial experiment: There are 8 experimental trials.

Blocking 2³ Experiment: We need three dimension diagram. We can allocate treatment combination in to two blocks. The geometrical view of 2³ factorial experiment.

Note that the design points on a diagonal of one face and the opposite diagonal of the other face form “Block 1”. The remaining design points form “Block 2”.

Treatment Combination	A B C		
	A	B	C
(I)	−	−	−
a	+	−	−
b	−	+	−
ab	+	+	−
c	−	−	+
ac	+	−	+
bc	−	+	+
abc	+	+	+

Lesson 163: Methods of Confounding: Sign Table Method

Confounding 2² Factorial Experiment

Treatment Combination	Effects			
	<i>I</i>	<i>A</i>	<i>B</i>	<i>AB</i>
(<i>I</i>)	+	−	−	+
<i>a</i>	+	+	−	−
<i>b</i>	+	−	+	−
<i>ab</i>	+	+	+	+

Confounding 2² Experiment through sign table method:

Block 1	Block 2
<i>AB</i>	<i>AB</i>
+	−
(<i>I</i>)	<i>a</i>
<i>ab</i>	<i>b</i>

AB effect is confounded with block effect. Both effects are indistinguishable. We choose *AB* because are less interested in *AB* effect as compared to main effects *a* and *b*. *AB* will be confounding in blocks.

Confounding 2³ Factorial Experiment

The main effects (*a*, *b*, and *c*) are most important factors, then two factor interaction (*AB*, *AC*, and *BC*) and least important in this experiment are *ABC* three factor interaction effect. To do blocking or confounding, our wish will be to do on the basis of less important effect *ABC*.

Effect of *ABC* and block effect are confounded with each other.

Lesson 164: Method of Confounding: Defining Contrast Method

Definition 30.3

Definition Contrast

A linear combination

$$L = \alpha_1x_1 + \alpha_2x_2 + \cdots + \alpha_kx_k$$

is called defining contrast, with

α_i is the exponent (power) of the *i*th factor

Treatment Combination	Effects							
	(I)	A	B	C	AB	AC	BC	ABC
(I)	+	−	−	−	+	+	+	−
a	+	+	−	−	−	−	+	+
b	+	−	+	−	−	+	−	+
ab	+	+	+	−	+	−	−	−
c	+	−	−	+	+	−	−	+
ac	+	+	−	+	−	+	−	−
bc	+	−	+	+	−	−	+	−
abc	+	+	+	+	+	+	+	+

Block 1	Block 2
ABC	ABC
+	−
a	(I)
b	ab
c	ac
abc	bc

x_i is the level of the i th factor appearing in a particular treatment combination, where levels are denoted by 0, 1, $\dots$ coding. 0 shows the low level and 1 is for high level.

Blocking:

The treatment combinations with same value of defining contrast $L(Mod2)$ are assigned to same block. The levels are denoted by 0, 1, $\dots$ coding.

Confounding 2^2 factorial experiment

$(I) : \quad 1(0) + 1(0) = 0 \mod 2 = 0$

$a : \quad 1(1) + 1(0) = 1 \mod 2 = 1$

$b : \quad 1(0) + 1(1) = 1 \mod 2 = 1$

$ab : \quad 1(1) + 1(1) = 2 \mod 2 = 0$

These four treatment combination results in two values 0 and 1 in defining contrast. Two treatment combination results in 0 and two results in value of 1. We will put treatment combinations in “Block 1” that results in 0 and the other treatment combinations that results in value of 1 will be in “Block 2”. That is,

Block 1	Block 2
$L = 0$	$L = 1$
(I) ab	a b

Lesson 165: 2^k Factorial Design in Four Blocks: Sign Table Method

Four Blocks of 2^k Design

2^k design may be run in 4 blocks of size 2^{k-2} each. Designs are quite useful for $k \geq 4$. Two defining contrasts are required for 4 blocks.

Defining Contrast: Example

Defining contrast of ABC

$$ABC = -, +$$

Defining contrast of BCD

$$BCD = -, +$$

Two signs of each column form four different pairs of combinations.

Sing Table

Treat. comb.	(I)	Effects						Treat. comb.	(I)	Effects					
		A	B	C	D	ABC	BCD			A	B	C	D	ABC	BCD
(I)	+	-	-	-	-	-	-	d	+	-	-	-	+	-	+
a	+	+	-	-	-	+	-	ad	+	+	-	-	+	+	+
b	+	-	+	-	-	+	+	bd	+	-	+	-	+	+	-
ab	+	+	+	-	-	-	+	abd	+	+	+	-	+	-	-
c	+	-	-	+	-	+	+	cd	+	-	-	+	+	+	-
ac	+	+	-	+	-	-	+	acd	+	-	+	+	+	-	-
bc	+	-	+	+	-	-	-	bcd	+	-	+	+	+	-	+
abc	+	+	+	+	-	+	-	abcd	+	+	+	+	+	+	+

We can see from ABC and BCD columns that there are four pairs of $-$ and $+$ signs.

$$(ABC, BCD) = \{(-, -), (-, +), (+, -), (+, +)\}$$

Blocks

Treatment combinations against each pair of signs forms a block.

Block 1	Block 2	Block 3	Block 4
$-, -$	$-, +$	$+, -$	$+, +$
(I)	ab	a	b
bc	ac	abc	c
abd	d	bd	ad
acd	bcd	cd	abcd

Lecture 31

Complete and Partial Confounding

Lesson 166: 2^k Factorial Experiment in 4 Blocks - Defining Contrast Method

Four Blocks of 2^k Design

2^k design may be run in 4 blocks of size 2^{k-2} each. We have to choose two basic generators to be confounded with blocks.

Example: Five Factor Design

- ◆ **Basic Generators**
We choose ABC and BDE as basic generators.
- ◆ **Generalized Interaction**
 $ABC \times BDE = ACDE$
- ◆ **Total confounded Effects**
 ABC, BDE , and $ACDE$

Defining Contrasts of Basic Generators

- ◆ For ABC
$$L_1 = X_1 + X_2 + X_3 = 0, 1, \text{ Mod } 2$$
- ◆ For BDE
$$L_2 = X_2 + X_4 + X_5 = 0, 1, \text{ Mod } 2$$
- ◆ Possible Pairs
$$(L_1, L_2) = \{(0, 0), (0, 1), (1, 0), (1, 1)\}$$

Sign Table

For some treating combinations the L_1 and L_2 pairs are zero and zero, respectively, and for some zero and one, and for others one and one, etc.

Blocks

We converted the $2^5 = 32$ runs factorial design into blocks by using Defining Contrasts.

Treat. Comb.	Effects							Treat. Comb.	Effects						
	A	B	C	D	E	L ₁	L ₂		A	B	C	D	E	L ₁	L ₂
(I)	0	0	0	0	0	0	0	e	0	0	0	0	1	0	1
a	1	0	0	0	0	1	0	ae	1	0	0	0	1	1	1
b	0	1	0	0	0	1	1	be	0	1	0	0	1	1	0
ab	1	1	0	0	0	0	1	abe	1	1	0	0	1	0	0
c	0	0	1	0	0	1	0	ce	0	0	1	0	1	1	1
ac	1	0	1	0	0	0	0	ace	1	0	1	0	1	0	1
bc	0	1	1	0	0	0	1	bce	0	1	1	0	1	0	0
abc	1	1	1	0	0	1	1	abce	1	1	1	0	1	1	0
d	1	0	0	1	0	0	1	de	0	0	0	1	1	0	0
ad	1	0	0	1	0	1	1	ade	1	0	0	1	1	1	0
bd	0	1	0	1	0	1	0	bde	0	1	0	1	1	1	1
abd	1	1	0	1	0	0	0	abde	1	1	0	1	1	0	1
cd	0	0	1	1	0	1	1	cde	0	0	1	1	1	1	0
acd	1	0	1	1	0	0	1	acde	1	0	1	1	1	0	0
bcd	0	1	1	1	0	0	0	bcde	0	1	1	1	1	0	1
abcd	1	1	1	1	0	0	0	abcde	1	1	1	1	1	1	1

Block 1		Block 2		Block 3		Block 4
0, 0		0, 1		1, 0		1, 1
(I)		ab		a		b
ac		bc		c		abc
abd		d		bd		ad
bcd		acd		abcd		cd
abe		e		be		ae
bce		ace		abce		ce
de		abde		ade		bde
acde		bcde		cde		abcde

Lesson 167: 2^k Design in 2^p Blocks of Size 2^{k−p}

Important terms

- ◆ **Generators**
The basic effects which are chosen to confound with blocks, some times called 'words'.
- ◆ **Generalized Interactions**
The effects which are obtained by multiplying the generators Mod 2 are called generalized interactions. A generalized interaction may be obtained by multiplying an effect with other generalized interaction.
- ◆ **Independent Effect**
An effect is called independent if it is not a generalized interaction of any other effects.

Steps Involved

- ◆ **Independent Effect**
Select *p* independent effects to be confounded with blocks
- ◆ **Method of Blocking**
Choose any method of blocking from:
 - ★ Sign Table Method

- ★ Defining Contrast Method
- ★ Geometrical Method, etc.

Lesson 168: Complete and Partial Confounding in Two Level Design

Definition 31.1

Complete Confounding

In a blocked design when some effects are completely confounded with blocks (in all replicates), i.e., their effects are identical to block effects, this refers to complete confounding.

Completely confounded effects can be estimated.

Definition 31.2

partial Confounding

In a blocked replicated design if one effect is confounded in one replicate and some other effect is confounded in other replicate, this refers to partial confounding.

Partially confounded effects can be estimated from the replicates where these are not confounded.

Example: ABC is completely confounded with blocks First block is of minus sign while second

ABC Confounded							
Replicate I		Replicate II		Replicate III		Replicate IV	
(I)	a	(I)	a	(I)	a	(I)	a
ab	b	ab	b	ab	b	ab	b
ac	c	ac	c	ac	c	ac	c
bc	abc	bc	abc	bc	abc	bc	abc

block is of positive sign. All four replicates have same type of blocking. Same effect being confounded in blocks. Therefore, it is complete confounded.

Example: Different effects are Partially Confounded with Blocks in each Replicate. First block

ABC Confounded		AB Confounded		AC Confounded		BC Confounded	
Replicate I		Replicate II		Replicate III		Replicate IV	
(I)	a	(I)	a	(I)	a	(I)	b
ab	b	ab	b	b	ab	a	c
ac	c	c	ac	ac	c	bc	ab
bc	abc	abc	bc	abc	bc	bc	ac

is of minus sign while second block is of positive sign on the bases of signs of ABC . Different effects are being confounded in all four replicates. If we want to estimate ABC using remaining three replicates after skipping first replicate. Similarly, we can do with AB , AC , and BC too.

Lesson 169: Analysis in Case of Complete and Partial Con-
founding

General Structure of ANOVA with four replicates and two blocks.

Complete Confounding		Partial Confounding	
SOV	df	SOV	df
Replicates	3	Replicates	3
Blocks (<i>ABC</i>)	1	Block with Repl.	1+1+1+1
		<i>ABC</i> (Rep I) + <i>AB</i> (Rep II) + <i>AC</i> (Rep III) + <i>BC</i> (Rep IV)	=4
Error for <i>ABC</i> (Rep. × Blocks)	3	<i>A</i>	1
<i>A</i>	1	<i>B</i>	1
<i>B</i>	1	<i>C</i>	1
<i>AB</i>	1	<i>AB</i> (Rep I, III & IV)	1
<i>C</i>	1	<i>AC</i> (Rep I, II, & IV)	1
<i>AC</i>	1	<i>BC</i> (Rep I, II & III)	1
<i>BC</i>	1	<i>ABC</i> (Rep II, III & IV)	1
Error	18	Error	17
(Rep × Effects)	(= 6 × 3)		
Total	31	Total	31
	(= <i>nabc</i> − 1)		(= <i>nabc</i> − 1)

Example 1: A study was conducted to determine the effect of percent carbonation (*A*), operating pressure (*B*), and line speed (*C*) on the fill height (response) of a carbon beverage. Suppose each batch can conduct only four trials. Thus each replicate of 2³ design must be run in two blocks of size four each. Different effects are confounded in each replicate as data shows:

Replicate I		Replicate II	
<i>ABC</i> Confounded		<i>AB</i> Confounded	
Block 1	Block 2	Block 3	Block 4
(<i>I</i>) = −3	<i>a</i> = 0	(<i>I</i>) = −1	<i>a</i> = 1
<i>ab</i> = 2	<i>b</i> = −1	<i>c</i> = 0	<i>b</i> = 0
<i>ac</i> = 2	<i>c</i> = −1	<i>ab</i> = 3	<i>ac</i> = 1
<i>bc</i> = 1	<i>abc</i> = 6	<i>abc</i> = 5	<i>bc</i> = 1
Block Total	2	4	3

Solution: All sums of squares can be calculated using Yate’s method except S.O.S. of *ABC* is computed from Rep-II and S.O.S. of *AB* from Rep-II following the sign table as:

$$SS_{ABC} = \frac{[a + b + c + abc - ab - ac - bc - (I)]^2}{n2^3 = 8} = 0.50$$
$$SS_{AB} = \frac{[(I) + ab + c + abc - a - b - ac - bc]^2}{n2^3 = 8} = 0.50$$
$$SS_{rep} = \sum_{i=1}^2 \frac{R_i^2}{2^3} - \frac{y_{..}^2}{N} = \frac{(6)^2 + (10)^2}{8} - \frac{(16)^2}{16} = 1.00$$

ANOVA Table All three main effects are statistically significant. □

S.O.V.	d.f.	S.O.S.	M.S.	F_0
Replicates	1	1.00	1.00	—
Block within Repl. ABC (Rep I), AB (Rep II)	1+1 =2	2.50	1.25	—
A	1	36.00	36.00	48.00*
B	1	20.25	20.25	27.00*
C	1	12.25	12.25	16.33*
AB (Rep I)	1	0.50	0.50	0.67
AC	1	0.25	0.25	0.33
BC	1	1.00	1.00	1.33
ABC (Rep II)	1	0.50	0.50	0.67
Error	5	3.75	0.75	—
Total	15	78	—	—

Lesson 170: 2^4 Factorial Design in Four Blocks

Four Blocks of 2^4 Design

2^4 design may be run in 4 blocks of size 2^{4-2} each. Two defining contrast are required for 4 blocks.

Example: Consider the two defining contrast

Defining contrast of ABC

$$ABC = -, +$$

Defining contrast of BCD

$$BCD = -, +$$

Two signs of each column form four different pairs of combinations.

Sign Table of 2^4 factorial experiment,

Treat. comb.	(I)	Effects						Treat. comb.	(I)	Effects					
		A	B	C	D	ABC	BCD			A	B	C	D	ABC	BCD
(I)	+	—	—	—	—	—	—	d	+	—	—	—	+	—	+
a	+	+	—	—	—	+	—	ad	+	+	—	—	+	+	+
b	+	—	+	—	—	+	+	bd	+	—	+	—	+	+	—
ab	+	+	+	—	—	—	+	abd	+	+	+	—	+	—	—
c	+	—	—	+	—	+	+	cd	+	—	—	+	+	+	—
ac	+	+	—	+	—	—	+	acd	+	—	+	+	+	—	—
bc	+	—	+	+	—	—	—	bcd	+	—	+	+	+	—	+
abc	+	+	+	+	—	+	—	abcd	+	+	+	+	+	+	+

We can see from ABC and BCD columns that there are four pairs of $-$ and $+$ signs.

$$(ABC, BCD) = \{(-, -), (-, +), (+, -), (+, +)\}$$

Blocks: Treatment combinations against each pair of signs forms a block.

Block 1	Block 2	Block 3	Block 4
−, −	−, +	+, −	+, +
(I)	ab	a	b
bc	ac	abc	c
abd	d	bd	ad
acd	bcd	cd	abcd

Lesson 171: 2⁴ Factorial Design in Eight Blocks

Four Blocks of 2⁴ Design

2⁴ design may be run in 8 blocks of size 2⁴⁻³ each. Three defining contrasts are required for 8 blocks.

Example: Three defining contrasts,

Defining contrast of AC

AC = −, +

Defining contrast of BD

BD = − +

Defining contrast of BC

BC = −, +

Generalized interactions

AC × BD = ABCD
AC × BC = AB
BD × BC = CD
AC × CD = AD

ABC² Mod 2 = AB
B²CD Mod 2 = CD
AC²D Mod 2 = AD

Discussion:

- ◆ All two-factor interactions confounded with blocks
- ◆ Two-factor interactions are usually important for the experimenter
- ◆ Poor design with estimation point of view

Lesson 172: Two Level Factorial Experiment in more than Eight Blocks

Prerequisite for running an experiment in more than eight blocks

In order to construct a design in more than 8 blocks, the experiment should contain large number of factors, usually more than six factors. So that effects of vital interest may not confounded with blocks.

Example: 2⁸ design contains 256 runs.

- ◆ Experimenter decides to run the experiment in 16 blocks of 16 runs each.
- ◆ The experimenter selects 4 independent effects to be confounded with blocks.
- ◆ In addition to these 4 independent effects other 2⁴ − 4 − 1 = 11 effect will be confounded with blocks as generalized interactions.

The four independent effects are $BCDE$, $ACDF$, $ABCG$, and $ABDH$.

The eleven generalized interactions are: $ABEF$, $ADEG$, $BDFG$, $CEFG$, $ACEH$, $BCFH$, $DEFH$, $CDGH$, $BEGH$, $AFGH$, and $ABCDEFGH$.

Therefore, fifteen effects will be confounded if design is run in 16 blocks.

Lecture 32

Fractional Factorial Design

Lesson 173: Fractional Factorial Design (FFD)

Why Fraction

When number of factors increase, the number of runs in regular factorial design increase more rapidly. And most of the times resources become scarce to run the whole experiment.

Runs in Regular Factorial

k	2^k	3^k
2	4	9
3	8	27
4	16	81
5	32	243
6	64	729
7	128	2187
8	256	6561

Regular Fractions

1. **From 2^k Factorial**

From regular 2^k factorial we can have one-half fraction, one-fourth fraction, one-eighth fraction, etc., that is, fraction in any power of $\frac{1}{2}$.

2. **From 3^k Factorial**

From regular 3^k factorial we can have one-third fraction, one-ninth fraction, one-twenty seventh fraction, etc., that is, fraction in any power of $\frac{1}{3}$.

3. **Irregular Fractions**

For higher number of factors, sometimes, an irregular fraction can be quite useful. For example, three-fourth fraction of 2^5 design, that is, $\frac{3}{4}2^5 = 24$, seven-eighth fraction of 2^5 , i.e., $\frac{7}{8}2^5 = 28$, three-eighth fraction of 2^6 , i.e., $\frac{3}{8}2^6 = 24$, seven-sixteenth fraction of design 2^6 , etc.

Lesson 174: Motivation of using a Fractional Factorial Design

There are three basic concepts which motivate an experimenter to use a fractional factorial in place of full factorial design.

1. The Sparsity-of Effects Principal

- ◆ A system is usually dominated by main effects and lower-order interactions. This is most likely that order three and higher order interactions are rare.
- ◆ Also referred as **Hierarchical Ordering Principle**.

2. The Projection Property

- ◆ A fractional factorial design may be projected into stronger designs of the subsets of significance factors. In other words, every fractional factorial contains full factorials in fewer factors.

3. Sequential Experimentation

- ◆ The fractional factorial design may be sequentially constructed by adding (augmenting) portions. OR
- ◆ The runs of two or more fractional factorial designs may be combined to assemble sequentially a larger design to estimate the effects of vital interest.

Lesson 175: 2-level Fractional Factorial Design

Why Fraction of Two Level Factorial

In two level factorial design number of runs increase in more rapidly than the number of factors, number of runs increase in power of 2. In case of large number of factors most resources are wasted in unnecessary experimentation.

Example: Consider $2^6 = 64$ runs design

- ◆ There are $64 - 1 = 63$ degrees of freedom available during analysis.
- ◆ $\binom{6}{1} = 6$ degrees of freedom are available for the estimation of main effects.
- ◆ $\binom{6}{2} = 15$ degrees of freedom are available for the estimation of two-factor interactions.
- ◆ Remaining 42 degrees of freedom are for three-factor and higher-order interactions, which are usually not of interest for the experimenter.

Remarks

If some higher-order interactions are negligible for the experimenter, he may run only a fraction of the whole experiment and still manage to obtain estimates of main effects and lower-order interactions.

Lesson 176: One-half Fraction of 2-level Fractional Factorial Design

Basis of Fraction

Fraction of a full factorial design is usually constructed on the basis of some higher-order interaction(s). According to ‘**Hierarchical Ordering Principle**’ lower-order effects are more important than higher-order effects.

Example 1: Consider a 2^3 design. Assume that the experimenter can afford to run only 4 experimental trials. He decides to run 2^{3-1} , i.e., one-half fraction of 2^3 design.

Solution: **Table of Signs for 2^3 design** We can choose any one fraction due to sign of ABC .

Treat.		Factorial Effects						
Comb.	I	A	B	C	AB	AC	BC	ABC
a	+	+	–	–	–	–	+	+
b	+	–	+	–	–	+	–	+
c	+	–	–	+	+	–	–	+
abc	+	+	+	+	+	+	+	+
(I)	+	–	–	–	+	+	+	–
ab	+	+	+	–	+	–	–	–
ac	+	+	–	+	–	+	–	–
bc	+	–	+	+	–	–	+	–

The design will be of four runs.

The fraction with ‘+’ signs in ABC column is called **principal fraction** and is denoted by $I = ABC$. The fraction with ‘–’ signs in ABC column is called **alternate fraction** denoted by $I = -ABC$. The effect used to identify fraction is called a **generator** or a **word**. Number of letters in a word are called word-length. $\square$

Lesson 177: One-quarter Fraction of 2-level Fractional Factorial Design

Basis of Fraction

Fraction of a full factorial design is usually constructed on the basis of some higher-order interaction(s), i.e., by following the ‘**Hierarchical Ordering Principle**’.

According to ‘**Hierarchical Ordering Principle**’ lower-order effects are more important than higher-order effects.

Example 2: Consider a 2^4 design. Assume that the experimenter can afford to run only 4 experimental trials. He decides to run quarter fraction, i.e., 2^{4-2} design.

Solution:

Table of Signs for 2^4 design Quarter-fraction of design is formed by taking treatment combinations that have ‘–, –’, ‘–, +’, ‘+, –’ or ‘+, +’ pair of signs in from ABC and BCD columns.

$\square$

Treat. Effects								Treat. Effects							
comb.	I	A	B	C	D	ABC	BCD	comb.	I	A	B	C	D	ABC	BCD
(I)	+	-	-	-	-	-	-	ab	+	+	+	-	-	-	+
bc	+	-	+	+	-	-	-	ac	+	+	-	+	-	-	+
abd	+	+	+	-	+	-	-	d	+	-	-	-	+	-	+
acd	+	+	-	+	+	-	-	bcd	+	-	+	+	+	-	+
a	+	+	-	-	-	+	-	b	+	-	+	-	-	+	+
abc	+	+	+	+	-	+	-	c	+	-	-	+	-	+	+
bd	+	-	+	-	+	+	-	ad	+	+	-	-	+	+	+
cd	+	-	-	+	+	+	-	ac	+	+	+	+	+	+	+

Lesson 178: Aliasing in Fractional Factorial Experiment

Definition 32.1

Pair of Aliases

The pair of effects whose estimates can not be differentiated is called pair of aliases. OR

Two effects having same linear combination is called pair of aliases.

Example: Consider 2^{3-1} design with $I = ABC$.

The alias structure of a fractional factorial design is obtained by multiplying columns of different effects by I (defining relation) Mod 2.

The of **Pairs of Aliases**:

$$A = I \cdot A = ABC \cdot A = A^2BC \text{ MOD } 2 = BC$$

$$B = I \cdot B = ABC \cdot B = AB^2C \text{ MOD } 2 = AC$$

$$C = I \cdot C = ABC \cdot C = ABC^2 \text{ MOD } 2 = AB$$

where $A^2 = B^2 = C^2 = I \text{ MOD } 2$

Remarks

Thus, A and BC , B and AC & C and AB are pairs of aliases. The effects of these pairs can not be differentiated.

De-aliasing

If we run both principal and alternate fractions, all the runs associated with the full factorial design are available, i.e. we may de-alias the effect estimates.

Lecture 33

Design Resolutions

Lesson 179: Confounding in Fractional Replications

Blocking Fractional Factorial

1. Sometimes a fractional factorial design consists of so many experimental trials.
2. All trials may not be conducted under homogeneous conditions.
3. A fractional factorial may be performed in blocks.

Example 1: Consider 2^{6-2} resolution-IV design (2_{IV}^{6-2}) with $I = ABCE = BCDF = ADEF$. The $ADEF$ is generalized interaction and $ABCE$ & $BCDF$ are basic generators. Therefore, there are three effects are being confound here.

Solution:

1. The fractional factorial design contains 16 runs.
2. The experimenter wants to run the experiment in two blocks of size 8 each.
3. To select an effect to be confounded with blocks we need alias structure of the design.

$$\begin{aligned}
 A &= BCE = DEF, & B &= ACE = CDF, \\
 C &= ABE = BDF, & D &= BCF = AEF, \\
 E &= ABC = ADF, & F &= BCD = ADE, \\
 AB &= CE, AC = BE, & AD &= EF, \\
 AE &= BC = DF, & AF &= DE, \\
 BD &= CDF, & BF &= CD, \\
 ABD &= CDE = ACF = BEF \\
 ACD &= BDE = ABF = CEF
 \end{aligned}$$

Alias structure suggests to choose ABD or ACD to be confounded with blocks. We choose ABD .

The defining contrast:

$$L = x_1 + x_2 + x_4 = 0, 1 \text{ MOD } 2$$

□

$L = 0$	$L = 1$
Block 1	Block 2
(I)	ae
abf	acf
cef	bef
abce	bc
adef	df
bde	abd
acd	cde
bcd	abcde

Lesson 180: Design Resolution

A 2^{k-p} fractional factorial design is uniquely determined by a set of independent defining relations. The group generated by these independent defining relations is called defining contrast subgroup. Length of the shortest word in the defining contrast subgroup of a fractional factorial design is called its resolution.

A roman numeric subscript III, IV, V, etc. is usually employed to denote resolution of a design. Design resolution is the classification of fractional factorial designs. Designs are classified on the basis of their power to estimate the effects under **Hierarchical Ordering Principle**. Fractional factorial designs with same estimation power are ranked in one class of resolution.

Lesson 181: Resolution III Designs

A 2^{k-p} fractional factorial design in which

- ◆ No main effect is aliased (or confound) with any other main effect,
- ◆ Main effects are aliased with two-factor interactions.
- ◆ A two-factor interaction may be aliased with some other two-factor interaction.

Example

Consider 2^{5-2}_{III} with defining relations $I = ABD = ACE = BCDE$. ABC and ACE are basic generators, while $BCDE$ is generalized interaction. The defining relation consist of three words (ABD , ACE , and $BCDE$). On the basis of shortest word, it is called Resolution III Designs.

The alias structure

$$\begin{aligned} A \cdot I &= A^2BD = A^2CE = ABCDE \\ A &= BD = CE = ABCDE \text{ MOD } 2 \\ B \cdot I &= AB^2D = ABCE = B^2CDE \\ B &= AD = ABCE = CDE \text{ Mod } 2 \\ C \cdot I &= ABCD = AC^2E = BC^2DE \\ C &= ABCD = AE = BDE \text{ MOD } 2 \\ \\ D \cdot I &= ABD^2 = ACDE = BCD^2E \\ D &= AB = ACDE = BCE \text{ MOD } 2 \\ E \cdot I &= ABDE = ACE^2 = BCDE^2 \\ E &= ABDE = AC = BCD \text{ MOD } 2 \end{aligned}$$

Lesson 182: Resolution IV Designs

A 2^{k-p} fractional factorial design in which

- ◆ No main effect is aliased with any other main effect,
- ◆ Main effects are not aliased with two-factor interactions.
- ◆ Two-factor interactions are aliased with each other.

Example: Consider 2^{6-2} design with defining relations $I = ABCE = BCDF = ADEF$. The alias structure

$$\begin{aligned} A &= BCE = DEF \\ B &= ACE = CDF \\ C &= ABE = BDF \\ D &= BCF = AEF \\ E &= ABC = ADF \\ F &= BCD = ADE \\ AB &= CE \\ AC &= BE \\ AD &= EF \\ AE &= BC = DF \\ AF &= DE \\ BD &= CF \\ BF &= CD \\ ABD &= CDE = ACF = BEF \\ ACD &= BDE = ABF = CEF \end{aligned}$$

Lesson 183: Resolution V Designs

A 2^{k-p} fractional factorial design in which

- 1. No main effect is aliased with any other main effect.
- 2. No main effect is aliased with any two-factor interaction.
- 3. No main effect is aliased with any three-factor interaction.
- 4. Two-factor interactions are not aliased with each other.
- 5. Two-factor interactions are aliased with three-factor interactions.

Example: Consider 2^{5-1}_V with $I = ABCDE$. Length of word is 5. It is half fraction of five factor full factorial.

The alias structure

$$\begin{aligned} A \cdot I &= A^2BCDE = BCDE \text{ MOD } 2 \\ B \cdot I &= AB^2CDE = ACDE \text{ MOD } 2 \\ C \cdot I &= ABC^2DE = ABDE \text{ MOD } 2 \\ D \cdot I &= ABCD^2E = ABCE \text{ MOD } 2 \\ E \cdot I &= ABCDE^2 = ABCD \text{ MOD } 2 \\ AB \cdot I &= IA^2B^2CDE = CDE \text{ MOD } 2 \\ AC \cdot I &= IA^2BC^2DE = BDE \text{ MOD } 2 \\ AD \cdot I &= IA^2BCD^2E = BCE \text{ MOD } 2 \\ AE \cdot I &= IA^2BCDE^2 = BCD \text{ MOD } 2 \\ BC \cdot I &= IAB^2C^2DE = ADE \text{ MOD } 2 \\ BD \cdot I &= IAB^2CD^2E = ACE \text{ MOD } 2 \\ BE \cdot I &= IAB^2CDE^2 = ACD \text{ MOD } 2 \\ CD \cdot I &= IABC^2D^2E = ABE \text{ MOD } 2 \\ CE \cdot I &= IABC^2DE^2 = ABD \text{ MOD } 2 \\ DE \cdot I &= IABCD^2E^2 = ABC \text{ MOD } 2 \end{aligned}$$

Lesson 184: Design Resolution and Minimum Aberration

Design Resolution is the classification of 2^{k-p} fractional factorial designs with respect to their estimation capability. Designs with same resolution have same length of the shortest word in the defining relation. Designs with same resolution are usually considered to have same estimation power.

Minimum Aberration Design

Let $W_i(D)$ be the number of words of length i in the defining contrast subgroup of design D . For any two 2^{k-p} fractional factorial designs D_1 and D_2 , if j is the smallest positive integer and $W_j(D_1) < W_j(D_2)$ the D_1 will be called minimum aberration design.

Example: Consider two designs

D_1 : resolution III design

$$\begin{aligned} 2^{6-2}_{III}, I &= ABE = ACDE = BCDEF \\ WLP_{D_1} &= (1 \ 1 \ 1 \ 1 \ 0 \ 0) \end{aligned}$$

D_2 : resolution III design

$$\begin{aligned} 2^{6-2}_{III}, I &= ABE = CDF = ABCDEF \\ WLP_{D_1} &= (2 \ 0 \ 0 \ 1 \ 0) \end{aligned}$$

D_1 minimum aberration design

Remarks: Designs with same resolution can further be classified on the basis of **word length pattern**.

Lesson 185: Fold-over Design (Mirror Image Fold-over Design)

Definition 33.1

An experimental design technique used when a fractional factorial design produces ambiguous results. A fold-over design is achieved by reversing the signs of the values assigned to all factors and running additional experiments, i.e., providing more data on potential combinations of factors.

Augmenting a fractional factorial design of resolution III with another fraction by fold-over techniques produces a design with higher resolution and one more factor, i.e. folding over 2_{III}^{k-p} design produces 2_{IV}^{k+1-p} .

Remarks

- ◆ A fold-over design breaks the alias links of the initial fraction.
- ◆ The combined design is able to estimate all main effects clear of two-factor interactions.
- ◆ We could study one more factor after fold-over.
- ◆ Fold-over techniques motivates for sequential building of factorial designs.

Lesson 186: Example of a Fold-over Design

Example: Consider 2_{III}^{3-1} design, consisting of principal fraction, i.e. $I = ABC$.

Treatment combination I					Initial Fraction $I = ABC$
	A	B	C	$C = AB$	
a	+	−	−	+	
b	+	+	−	−	
c	+	−	+	−	
abc	+	+	+	+	
(I)	−	+	+	−	Alternate Fraction $I = ABC$
ab	−	−	+	+	
ac	−	+	−	+	
bc	−	−	−	−	

Example: 2_{IV}^{4-1} design, with $I = ABCD$, after fold-over.

Remarks

- ◆ A fold-over design breaks the alias links of 2_{III}^{3-1} initial fraction.
- ◆ The combined design is able to estimate all main effects clear of two-factor interactions as the fold-over design is of resolution IV.
- ◆ After fold-over we can study four factors.

Treatment Combination	$D = I$	A	B	C	$ABCD$
cd	+	-	-	+	+
ad	+	+	-	-	+
bd	+	-	+	-	+
$abcd$	+	+	+	+	+
ab	-	+	+	-	+
bc	-	-	+	+	+
ac	-	+	-	+	+
(I)	-	-	-	-	+

Lecture 34

Split Plot Design

Lesson 187: Split Plot Designs

Why Split-plot

- 1. There are some situations when the experiment involving two or more factors require different sizes of experimental units.
- 2. It is used when some factors are harder (or more expensive) to vary than others.

Definition 34.1

design which could have some factors to be applied at large units which are made up of small units. The other factors can be applied at small units.

A split-plot experiment is a blocked experiment in which blocks serve as experimental units. After blocking the levels of other factor are randomly applied to large units within blocks, often called **whole plots** or **main plots**.

The large units are then divided into small units called **subplots** or **split plots**.

Example: Consider the following factorial problem:

- ◆ 3 different irrigation levels
- ◆ 4 different corn varieties
- ◆ Response: biomass
- ◆ Available resources: 6 plots of land
- ◆ We can not vary the irrigation level on a too small scale.
- ◆ We are “forced” to use “large” experimental units for the irrigation level factor.
- ◆ Randomly assign each irrigation level to 2 of the plots (the so called whole plots or main plots).
- ◆ In every of the plots, randomly assign the 4 different corn varieties to the so called split plots.

Lesson 188: Layout of a Split Plot Design

Example: Consider two types of seeds B_1 and B_2 are to be applied in four plots. Two plots have irrigation system and two have A_2 .

The Layout

split Plot	Whole Plots			
	A ₂	A ₂	A ₁	A ₁
	A ₂ B ₁	A ₂ B ₂	A ₁ B ₂	A ₁ B ₁
	A ₂ B ₂	A ₂ B ₁	A ₁ B ₁	A ₁ B ₂

General Layout: Consider three factors

Factor B (Whole Plot Treatment)			1				2				...				a					
			1	2	...	b	1	2	...	b	...	1	2	...	b	...	1	2	...	b
Factor C (Sub Plot Treatment)	1		Y ₁₁₁	Y ₁₂₁	...	Y _{1b1}	Y ₂₁₁	Y ₂₂₁	...	Y _{2b1}	...	Y _{a11}	Y _{a21}	...	Y _{ab1}					
	1		Y ₁₁₂	Y ₁₂₂	...	Y _{1b2}	Y ₂₁₂	Y ₂₂₂	...	Y _{2b2}	...	Y _{a12}	Y _{a22}	...	Y _{ab2}					
	.		.	.		.	.	.		.		.	.		.					
	.		.	.		.	.	.		.		.	.		.					
	.		.	.		.	.	.		.		.	.		.					
	c		Y _{11c}	Y _{12c}	...	Y _{1bc}	Y _{21c}	Y _{22c}	...	Y _{2bc}	...	Y _{a1c}	Y _{a2c}	...	Y _{abc}					

Lesson 189: Model of a Split Plot Design

The Model

$$y_{ijk} = \mu + tau_i + \beta_j + (\tau\beta)_{ij} + \gamma_k + (\tau\gamma)_{ik} + (\beta\gamma)_{jk} + (\tau\beta\gamma)_{ijk} + \varepsilon_{ijk}$$

$$i = 1, 2, \dots, a \text{ levels of factor } A$$

$$j = 1, 2, \dots, b \text{ levels of factor } B$$

$$k = 1, 2, \dots, c \text{ levels of factor } C$$

Model Terms

- ◆ **Linear**
 - μ: Overall mean
 - τ_i: Effect of *i*th level of *A*

β_j : Effect of j th level of B

γ_k : Effect of k th level of C

◆ **Interactions** $(\tau\beta)_{ij}$: Interaction effect of A and B

$(\tau\gamma)_{ik}$: Interaction effect of A and C

$(\beta\gamma)_{jk}$: Interaction effect of B and C

$(\tau\beta\gamma)_{ijk}$: Interaction effect of A , B and C

◆ **Error** ε_{ijk} : Random error at i th level of A , j th level of B and k th level of C
 $\varepsilon_{ijk} \sim NID(0, \sigma_\varepsilon^2)$

◆ **Response**

y_{ijk} : Response of i th level of A , j th level of B and k th level of C

Lesson 190: Sums of Squares of a Split Plot Design

The Model for three factor split design

$$y_{ijk} = \mu + \tau\alpha_i + \beta_j + (\tau\beta)_{ij} + \gamma_k + (\tau\gamma)_{ik} + (\beta\gamma)_{jk} + (\tau\beta\gamma)_{ijk} + \varepsilon_{ijk}$$

$i = 1, 2, \dots, a$ levels of factor A

$j = 1, 2, \dots, b$ levels of factor B

$k = 1, 2, \dots, c$ levels of factor C

Sums of Squares for three factor split design

Sums of squares of a split-plot design are computed as in the three way analysis of variance without replication.

$$\text{Correction factor (C.F.)} = \frac{y_{...}^2}{abc}$$

$$SS_{total} = \sum_{i=1}^a \sum_{j=1}^b \sum_{k=1}^c y_{ijk}^2 - C.F.$$

$$SS_A = \frac{1}{bc} \sum_{i=1}^a y_{i..}^2 - C.F.$$

$$SS_B = \frac{1}{ac} \sum_{j=1}^b y_{.j.}^2 - C.F.$$

Whole plot sum of squares (S.O.S. of subtotal of AB)

$$SS_w = \frac{1}{c} \sum_{i=1}^a \sum_{j=1}^b y_{ij.}^2 - C.F.$$

Whole plot error sum of squares

$$\begin{aligned}
 SS_{E(AB)} &= SS_w - SS_A - SS_B \\
 SS_C &= \frac{1}{ab} \sum_{k=1}^c y_{..k}^2 - C.F. \\
 SS_{AC} &= SS_{subtotal(AC)} - SS_A - SS_C \\
 SS_{subtotal(AC)} &= \frac{1}{b} \sum_{i=1}^a \sum_{k=1}^c y_{i.k}^2 - C.F. \\
 SS_{BC} &= SS_{subtotal(BC)} - SS_B - SS_C \\
 SS_{subtotal(BC)} &= \frac{1}{a} \sum_{j=1}^b \sum_{k=1}^c y_{.jk}^2 - C.F. \\
 SS_{subploterror} &= SS_{total} - SS_1 - SS_B - SS_{E(AB)} - SS_C - SS_{AC} - SS_{BC}
 \end{aligned}$$

Lesson 191: ANOVA of Split Plot Design

The three factor **The Model**

$$\begin{aligned}
 y_{ijk} &= \mu + \tau\alpha_i + \beta_j + (\tau\beta)_{ij} + \gamma_k + (\tau\gamma)_{ik} + (\beta\gamma)_{jk} + (\tau\beta\gamma)_{ijk} + \varepsilon_{ijk} \\
 i &= 1, 2, \dots, a \text{ levels of factor } A \\
 j &= 1, 2, \dots, b \text{ levels of factor } B \\
 k &= 1, 2, \dots, c \text{ levels of factor } C
 \end{aligned}$$

The Model Assumptions

- ◆ The errors ε_{ijk} are independently sampled from a normal distribution with mean 0 and variance σ_ε^2 .
- ◆ The individual effects are also independently sampled from a normal distribution with mean 0 and fixed variance.
- ◆ The effects are independent to each other.

ANOVA Table

S.O.V	d.f.	S.O.S.	M.S.	F ₀
Block (Factor A)	$a - 1$	SS_A	$MS_A = \frac{SS_A}{a-1}$	
Whole Plot (Factor B)	$(b - 1)$	SS_B	$MS_B = \frac{SS_B}{(b-1)}$	$F_B = \frac{MS_B}{MS_{AB}}$
Whole Plot Error (AB)	$(a - 1)(b - 1)$	SS_{AB}	$MS_{AB} = \frac{SS_{AB}}{(a-1)(b-1)}$	
Subplot (Factor C)	$c - 1$	SS_C	$MS_C = \frac{SS_C}{c-1}$	$F_C = \frac{MS_C}{MS_{ABC}}$
AC	$(a - 1)(c - 1)$	SS_{AC}	$MS_{AC} = \frac{SS_{AC}}{(a-1)(c-1)}$	$F_{AC} = \frac{MS_{AC}}{MS_{ABC}}$
BC	$(b - 1)(c - 1)$	SS_{BC}	$MS_{BC} = \frac{SS_{BC}}{(b-1)(c-1)}$	$F_{BC} = \frac{MS_{BC}}{MS_{ABC}}$
Subplot Error (ABC)	$(a - 1)(b - 1)(c - 1)$	SS_{ABC}	$MS_{ABC} = \frac{SS_{ABC}}{(a-1)(b-1)(c-1)}$	
Total	$abc - 1$	SS_{total}		

Lesson 192: Advantages of Split Plot Design

- ◆ **More Practical**
Randomizing hard-to-change factors in groups, rather, than randomizing every run, is much less labor and time intensive.
- ◆ **Pliable**
Factors that naturally have large experimental units can be easily combined with factors having smaller experimental units.
- ◆ **More powerful**
Tests for the subplot effects from the easy-to-change factors generally have higher power due to partitioning the variance sources.
- ◆ **Adaptable**
New treatments can be introduced to experiments that are already in progress.
- ◆ **Cheaper to Run**
In case of a CRD, implementing a new irrigation method for each subplot would be extremely expensive.
- ◆ **More Efficient**
Changing the hard-to-change factors causes more error (increased variance) than changing the easy-to-change factors a split-plot design is more precise (than a completely randomized run order) for the subplot factors, subplot by subplot interactions and subplot by whole-plot interactions.

Example 1: Suppose we want to study the effects of two irrigation methods (factor 1) and two different fertilizer types (factor 2) on four different fields (“whole plots”). While a field can easily be split into two for the two different fertilizers, the field cannot easily be split into two for irrigation: One irrigation system normally covers a whole field and the systems are expensive to replace.

Lesson 193: Disadvantages of Split Plot Design

- ◆ **Less powerful**
Tests for the hard-to-change factors are less powerful, having a larger variance to test against and fewer changes to help overcome the larger error.
- ◆ **Unfamiliar**
Analysis requires specialized methods to cope with partitioned variance sources.
- ◆ **Different**
Hard-to-change (whole-plot) and easy-to-change (subplot) factor effects are tested against different estimated noise. This can result in large whole-plot effects not being statistically

significant, whereas small subplot effects are significant even though they may not be practically important.

Lesson 194: Points to be Noted About a Split Plot Design

◆ Reduced Effort

The reason split-plot designs are used is to reduce effort making it easier to run a DOE.

◆ Risk of Confounding

Not randomizing the groups increases the risk of confounding the group effects with a lurking (ambiguous, hidden) variable.

◆ Factor Reset

When a group change occurs, factors that are not changing should be reset. If factors are not reset, then it is another restriction on the randomization.

◆ Careful Consideration

Carefully consider the cost savings of the split-plot design vs. the loss of power to detect hard-to-change factor effects.

◆ Appropriate use

- ★ When the practical limit for plot size is much larger for one factor compared with the other, be assigned to the main plots while other factor should be assigned to the subplots.
- ★ When greater precision is desired in one factor relative to the other e.g., if several varieties are being compared at different fertilizer levels and the factor of primary interest is the varieties, then it should be assigned to the subplots and fertilizer levels assigned to the main plots.

Lesson 195: Difference Between Split Plot Experiment and Factorial Experiment

◆ Experimental Units

The main idea in the split plot is that the experimental unit has been “split” into sub units, and another treatment has been applied to those sub units. Most people would probably think of a split-plot as a sub-type of factorial designs, but of course, non-factorial split-plot designs are quite possible.

◆ Blocked Factorial

Don't confuse a split-plot design with a blocked factorial design. In a blocked design the “pile” of potential experimental units under study is split into homogeneous blocks in order to reduce experimental error – the units themselves remain whole. In a split-plot the experimental unit itself is split.

◆ Error

Split plot experiment produces two types of errors, whole plot error and subplot error. Whereas, factorial experiment has only one experimental error.

◆ Sums of Squares

The sums of squares of three factor split plot experiment are calculated exactly the same way as a three-factor factorial design. What is different is that no tests exist for the effects involving Replicate because of the restrictions on randomization.

◆ Split-Plot With Factorial

- ★ Split-plot With Factorial Main Plot

Combinations of levels of factors A and B are assigned to main plots, levels of factor C to subplots within each main plot.

★ **Split-plot with factorial subplot**

Levels of factor A are assigned to main plots, combinations of levels of factors B and C are assigned to subplots.

★ **Split-split plot**

Levels of factor A are assigned to main plots, levels of factor B to subplots within each main plot, and levels of factor C to sub-subplots within each subplot.

Lecture 35

Three Level Factorial Design

Lesson 196: 3-level Factorial Design

Definition 35.1

These designs are a generalization of the 2^k factorial designs. Design includes two or more factors. Each factor is varied at three equally-spaced levels.

Nature of Factors

We will be assuming in the 3^k designs that the factors are all quantitative. With 2^k designs we weren't as strict about this because we could have either qualitative or quantitative factors.

Response Function

With 3^k designs we are moving from screening factors to analyzing them to understand what their actual response function looks like. With three level of each factor we now have points at the middle so we will be able to fit curved response functions, i.e., quadratic response functions.

Lesson 197: Design Matrix of 3-level Factorial Experiment

Example: 3^2 Design.

-1, 0 + 1		0, 1, 2	
Coding Scheme (Rare)		Coding Scheme (More Common)	
A	B	A	B
-1	-1	0	0
0	-1	1	0
1	-1	2	0
-1	0	0	1
0	0	1	1
1	0	2	1
-1	1	0	2
0	1	1	2
1	1	2	2

Example: 3^3 Design. 0, 1, 2 Coding Scheme

<i>A</i>	<i>B</i>	<i>C</i>	<i>A</i>	<i>B</i>	<i>C</i>	<i>A</i>	<i>B</i>	<i>C</i>
0	0	0	0	1	0	0	2	0
1	0	0	1	1	0	1	2	0
2	0	0	2	1	0	2	2	0
0	0	1	0	1	1	0	2	1
1	0	1	1	1	1	1	2	1
2	0	1	2	1	1	2	2	1
0	0	2	0	1	2	0	2	2
1	0	2	1	1	2	1	2	2
2	0	2	2	1	2	2	2	2

Lesson 198: Geometry of 3² Factorial Design

There are many advantages of showing a design geometrically. It tells us how experimental design is using experimental space or experimental region.

(a) Two-Dimensional Space 1 (b) Points in Two-Dimensional Plane 2

Figure 35.1: Geometry of 3² Factorial Design

Example: 3² Design

<i>Run</i>	<i>A</i>	<i>B</i>
1	0	0
2	1	0
3	2	0
4	0	1
5	1	1
6	2	1
7	0	2
8	1	2
9	2	2

Lesson 199: Effects and Their Components in 3-level Factorial Experiment

In 3^k factorial we can compute two kinds of **Effects**

- ◆ **Main Effects**
- ◆ **Interaction Effects**

Example: Consider 3^3 Factorial Design.

◆ Main Effects

Main effects may be partitioned into **linear** and **quadratic** components, 2 d.f. for each main effect, i.e.,

$$A : A_L, A_Q$$

$$B : B_L, B_Q$$

$$C : C_L, C_Q$$

◆ Interaction Effects

★ Two-factor Interactions

Two-factor interactions may be partitioned, with 4 d.f., as:

$$AB : AB_{L \times L},$$

$$AB_{L \times Q},$$

$$AB_{Q \times L},$$

$$AB_{Q \times Q}$$

★ Three-factor Interactions

Three-factor interactions may be partitioned, with 8 d.f., as:

$$ABC : ABC_{L \times L \times L}, ABC_{L \times L \times Q},$$

$$: ABC_{L \times Q \times L}, ABC_{Q \times L \times L},$$

$$: ABC_{Q \times Q \times L}, ABC_{Q \times L \times Q},$$

$$: ABC_{L \times Q \times Q}, ABC_{Q \times Q \times Q},$$

Note That

When considering interaction effects, it is a convention that only exponent allowed on the first letter is 1. If it is not then entire expression is squared and then reduced to modulus 3, e.g.

$$\begin{aligned} A^2BC &= (A^2BC)^2 \\ &= A^4B^2C^2 \text{ Mod } 3 = AB^2C^2 \end{aligned}$$

We can replace A^2BC with AB^2C^2 .

Lesson 200: Geometry of 3³ Factorial Design

Consider the 3-Dimensional Space



Figure 35.2: Geometry of 3³ Factorial Design

Example: Consider 3³ Design with 0, 1, 2 Coding Scheme.

A	B	C	A	B	C	A	B	C
0	0	0	0	1	0	0	2	0
1	0	0	1	1	0	1	2	0
2	0	0	2	1	0	2	2	0
0	0	1	0	1	1	0	2	1
1	0	1	1	1	1	1	2	1
2	0	1	2	1	1	2	2	1
0	0	2	0	1	2	0	2	2
1	0	2	1	1	2	1	2	2
2	0	2	2	1	2	2	2	2

3³ Design Geometrical View This geometry represents the 27 runs of the design in 3-Dimensional plane. This geometrical diagram shows that how allocation of design points of 3³ factorial design with different design points is done. It has corner points, edge points, faces' center.

Lesson 201: Analysis of 3^k Factorial Experiment

- ◆ When there is a curvilinear relation between the response and a quantitative factor like temperature. It is not possible to detect such a curvature effect with two levels.
- ◆ A qualitative factor may have three levels (e.g., three types of machines or three suppliers).
- ◆ It is common to study the effect of a factor on the response at its current setting x₀ and two settings around x₀.

Consider 3² Design: We consider a simplified version of the seat-belt experiment as a 3³ full factorial experiment with factors A, B, C. Each trial is repeated three times.

Factor	Level		
	0	1	2
A. pressure (psi)	1100	1400	1700
B. die flat (mm)	10.0	10.2	10.4
C. crimp length (mm)	18	23	27

- ◆ For ANOVA, we can compute the sum of squares for main effects A , B , C , interactions $A \times B$, $A \times C$, $B \times C$, and $A \times B \times C$ and the residual sum of squares.
- ◆ The break-up of the degrees of freedom will be as follows:
 - ★ Each main effect has 2 degrees of freedom because each factor has three levels.
 - ★ Each two-factor interaction has $(3 - 1) \times (3 - 1) = 4$ degrees of freedom.
 - ★ The $A \times B \times C$ interaction has $(3 - 1) \times (3 - 1) \times (3 - 1) = 8$ degrees of freedom.
 - ★ The residual degrees of freedom is $54 (= 27 \times (3 - 1))$, since there are three replicates.

ANOVA Table

SOV	df	SOS	MS	F	p-value
$A(A_L, A_Q)$	2	3462746	17310873	85.58	0.000
$B(B_L, B_Q)$	2	938539	469270	2.32	0.108
$C(C_L, C_Q)$	2	9549481	4774741	23.61	0.000
$A \times B$ ($A_L \times B_L, A_L \times B_Q, A_Q \times B_L, A_Q \times B_Q$)	4	3298246	824561	4.08	0.006
$A \times C$ ($A_L \times C_L, A_L \times C_Q, A_Q \times C_L, A_Q \times C_Q$)	4	3872179	968045	4.79	0.002
$B \times C$ ($B_L \times C_L, B_L \times C_Q, B_Q \times C_L, B_Q \times C_Q$)	4	448348	112087	0.55	0.697
$A \times B \times C$ ($A_L \times B_L \times C_L, A_L \times B_L \times C_Q, A_L \times B_Q \times C_L,$ $A_Q \times B_L \times C_L, A_Q \times B_Q \times C_L, A_Q \times B_L \times C_Q,$ $A_L \times B_Q \times C_Q, A_Q \times B_Q \times C_Q$)	8	5206919	6508665	3.22	0.005
Error	54	10922599	202270		
Total	80	68858056			

Lesson 202: Yate's Algorithm for Computing Sums of Squares in 3^k Factorial Experiment

Steps

1. Write down the design in standard order by introducing all levels of one factor with one level of the other then with the second level and so on.
2. In the next column put total response from all replicates.
3. Introduce k -columns as:
 - ◆ The first 3^{rd} entries of col-1 are produced by summing all three sets of three values in the response column.
 - ◆ The second 3^{rd} entries are produced by subtracting the 1^{st} entry from the 3^{rd} entry in each set of three values.
 - ◆ The last 3^{rd} entries of col-1 are computed by adding 1^{st} and 3^{rd} value and subtracting twice of the middle value from each set of three.
 - ◆ Col-2 is produced in similar way from col-1 and so on.

Effects

k^{th} column represents effects corresponding to the treatment combination, i.e.

10 : A_L , 20 : A_Q ,

11 : $A_L B_L$,

12 : $A_L B_Q$,

22 : $A_Q B_Q$

Sums of Squares

Sums of squares are computed by squaring k^{th} column and dividing by $2^r 3^t n$, where

r : number of non-zero entries in a design point.

t : number of factors in the experiment – number of linear terms in the design point.

n : number of replicates

Lecture 36

Blocking in 3-level Factorial Experiment

Lesson 203: Blocking in 3-level Factorial Experiment

Blocking

- ◆ Blocking is the strategy of running an experiment in parts.
- ◆ These systematically formed parts are called blocks.
- ◆ There can be three, nine, twenty seven, etc., number of blocks of 3^k factorial experiment.

Why Blocking

- ◆ **Nuisance Factors**
If we want to eliminate the influence of extraneous factors when running an experiment. We do this by "blocking".
- ◆ **Large Experiment**

k	4^k
2	9
3	27
4	81
5	243
6	729
7	2187
8	6561
9	19683
10	59049

Note That

- ◆ **Block Size:** A block size is smaller than the number of treatment combinations in a single replicate.
- ◆ **Randomness:** The order of running treatment combinations within a block is random. Each block is also run randomly.

Fro blocking we can use **Defining Contrast Method of Blocking**

A linear combination

$$L = \alpha_1x_1 + \alpha_2x_2 + \cdots + \alpha_kx_k$$

is called defining contrast,

with

- ◆ α_i : the exponent (power) of the i th factor
- ◆ x_i : level of the i th factor appearing in a particular treatment combination, where levels are denoted by $0, 1, \dots$ coding.

Blocks

1. The treatment combinations with same value of defining contrast $L(Mod3)$ are assigned to same block.
2. The levels of variables must be denoted by $0, 1, 2$ coding.

Lesson 204: 3-level Factorial Design in 3 blocks

Defining Contrast

- ◆ For three blocks of a 3^k factorial experiment we need one defining contrast.
- ◆ Common practice is to choose a highest order interaction as defining contrast.
- ◆ For two factors highest order interaction is **AB**.
- ◆ AB has two components: AB and AB^2 .
- ◆ Any component of highest order interaction may be chosen as defining contrast.
- ◆ Let L be the defining contrast corresponding to AB^2

$$L = x_1 + 2x_2$$
$$= 0, 1, 2 \text{ Mod } 3$$

Consider the 3^2 Factorial Design

<i>Trial</i>	<i>A</i>	<i>B</i>	<i>L</i>
1	0	0	0
2	0	1	2
3	0	2	1
4	1	0	1
5	1	1	0
6	1	2	2
7	2	0	2
8	2	1	1
9	2	2	0

Blocks

Block I		Block II		Block III	
L=0		L=1		L=2	
0	0	0	2	0	1
1	1	1	0	1	2
2	2	1	1	2	0

Lesson 205: 3-level Factorial Design in 9 Blocks

Defining Contrast

- ◆ For nine blocks of a 3^k factorial experiment we need two defining contrasts.
- ◆ Common practice is to choose high order interactions as defining contrast.

Design

- ◆ Consider 3^4 design.
- ◆ The design has 81 runs.

Defining Contrast ...

- ◆ We carefully choose two defining contrasts to be confounded with blocks, as ABC and AB^2D^2 .

$$L_1 = x_1 + x_2 + x_3 = 0, 1, 2 \text{ Mod } 3$$
$$L_2 = x_1 + 2x_2 + 2x_4 = 0, 1, 2 \text{ Mod } 3$$

- ◆ Treatment combination corresponding to the following 9 pairs of (L_1, L_2) form 9 blocks

$$(L_1, L_2) = (0, 0), (0, 1), (0, 2), (1, 0), (1, 1), (1, 2), (2, 0), (2, 1), (2, 2)$$

Blocks Following are 9 blocks confounded with ABC and AB^2D^2 , and with AC^2D and BC^2D^2 as generalized interactions.

(0,0)	(0,1)	(0,2)	(1,0)	(1,1)	(1,2)	(2,0)	(2,1)	(2,2)
Block 1	Block 2	Block 3	Block 4	Block 5	Block 6	Block 7	Block 8	Block 9
0000	0001	0002	0100	1000	0010	0200	0020	2000
0122	0120	0121	0222	1122	0102	0022	0112	2122
0211	0212	0210	0011	1211	0221	0111	0201	2211
1021	1022	1020	1121	2021	1001	0221	1011	0021
1110	1111	1112	1210	2110	1120	1010	1100	0110
1201	1200	1201	1002	2202	1212	1102	1222	0202
2012	2010	2011	2112	0012	2022	2212	2002	1012
2101	2012	2100	2201	0101	2111	2001	2121	1101
2220	2221	2222	2020	0220	2200	2120	2210	1220

Lesson 206: 3-level Factorial Design in 3^p Blocks

Steps

- ◆ 3^k design may be constructed in 3^p blocks of size 3^{k-p} each, where $P < k$.
- ◆ Effects
Choose p independent effects to be confounded with block
- ◆ **Effects to Confound**
Choose p independent effects to be confounded with block.
- ◆ Following the ‘Hierarchical Ordering Principle’, a common practice is to choose higher order interactions.

Generalized Interactions

- ◆ In addition to p independent effects other $(3^p - 2p - 1)/2$ effects will automatically be confounded with the blocks.
- ◆ These effects are the generalized interactions of p independent effects.

Example

- ◆ Consider 3^4 design to be confounded in 9 blocks.
- ◆ We choose ABC and AB^2D^2 as independent effects.
- ◆ The generalized interactions are computed as
 $(ABC)(AB^2D^2) = (A^2B^3CD^2)^2 = A^4B^6C^2D^4 \text{ Mod } 3 = AC^2D$
and
 $(ABC)(AB^2D^2)^2 = A^3B^5CD^4 \text{ Mod } 3 = (B^2CD)^2 \text{ Mod } 3 = BC^2D^2$
- ◆ Thus along with ABC and AB^2D^2 , AC^2D and BC^2D^2 are also confounded with blocks.

Lesson 207: Three-level Fractional Factorial Design

Why Fraction

Total number of trials in a 3^k factorial design increase rapidly as the number of factors increase.

Fractional Factorial

We can run one-third, one-ninth, one-twenty seventh, etc., fraction of a 3^k factorial design. Any fraction can be chosen.

Defining Contrast

- ◆ A defining contrast is the linear combination of set of effects.
- ◆ Defining contrast for a 3-level design

$$L = x_1 + \alpha_2x_2 + \cdots + \alpha_kx_k = 0, 1, 2, \text{ Mod } 3,$$

where $\alpha_i = 1, 2$.

- ◆ Higher order interaction(s) are chosen as defining contrast(s) to generate fraction(s).
- ◆ Any component of the chosen effect can be used as defining contrast.

Alias Structure

We use I to represent the defining contrast(s):

- ◆ Each main effect has two aliases obtained by multiplying it with I and $I^2 \text{ Mod } 3$.
- ◆ Component of any interaction also has two aliases obtained by multiplying it I and $I^2 \text{ Mod } 3$

Lesson 208: The One-third Fraction of the 3^k Design

Why Fraction

- ◆ Total number of trials in a 3^k factorial design become too large with the increase of factors.
- ◆ Sometime a fraction of full factorial can estimate the effects of vital interest.
- ◆ Experimenter is ready to use higher order interactions.

Construction of 3^{k-1} Design

- ◆ First, write down the basic design, i.e. three level full factorial in $k - 1$ factors.
- ◆ Denote factor labels by $x_1, x_2, \cdots, x_k$.

- ◆ Introduce k th factor by assigning levels corresponding to each treatment combination, i.e.

$$x_k = \beta_1 x_1 + \beta_2 x_2 + \cdots + \beta_{k-1} x_{k-1},$$

where $\beta_i = (3 - \alpha_k)\alpha_i \text{ Mod } 3$ and $1 \leq i \leq k - 1$

- ◆ α_k : Exponent of k th factor in the defining relation
- ◆ α_i : Exponent of i th factor in the defining relation

Remarks

Following this procedure we can get three level fractional factorial with highest possible resolution.

Lesson 209: Other 3^{k-p} Fractional Factorial Designs

There are Different Three-Level Fractional Factorial Designs

- ◆ **One-Third Fractions:** 3^{3-1} , 3^{4-1} , 3^{5-1} , etc. of 9, 27, 81 runs, respectively.
- ◆ **One-Ninth Fraction:** 3^{4-2} , 3^{5-2} , 3^{6-2} , etc. of 9, 27, 81 runs, respectively.
- ◆ **One-Twenty Seventh Fraction:** 3^{5-3} , 3^{6-3} , etc. and so on.

Design Construction

Consider 3^{3-1} Design with $I = AB^2C$. Defining Contrast

$$x_3 = \beta_1 x_1 + \beta_2 x_2$$

$$\beta_i = (3 - \alpha_3)\alpha_i \text{ Mod } 3, 1 \leq i \leq 2$$

x_3 is label of third factor.

where

α_3 = Exponent of 3rd factor in $I = 1$

α_i = Exponent of i th factor in I

Now

$$\beta_1 = (3 - 1)1 = 2 \text{ Mod } 3 = 2$$

$$\beta_2 = (3 - 1)2 = 4 \text{ Mod } 3 = 1$$

So $x_3 = 2x_1 + x_2$

Design Matrix

X_1	X_2	X_3
0	0	$2(0) + 1(0) = 0$
1	0	$2(1) + 1(0) = 2$
2	0	$2(2) + 1(0) = 4 \text{ Mod } 3 = 1$
0	1	$2(0) + 1(1) = 1$
1	1	$2(1) + 1(1) = 3 \text{ Mod } 3 = 0$
2	1	$2(2) + 1(1) = 5 \text{ Mod } 3 = 2$
0	2	$2(0) + 1(2) = 2$
1	2	$2(1) + 1(2) = 4 \text{ Mod } 3 = 1$
2	2	$2(2) + 1(2) = 6 \text{ Mod } 3 = 0$

Lecture 37

Mixed Level Factorial Designs and Response Surface Methodology

Lesson 210: Mixed Level Factorial Designs

Why Mixed Level

We believe that the two level full factorial and fractional factorial are the cornerstone of industrial experimentation. There are, however, some situations which require that some factors are applied at different levels, i.e., at three or four levels or so.

Mixed level designs can also be considered due to following reasons:

- ◆ Factors include both quantitative and categorical variables.
- ◆ Polynomial models can be modified during analysis to accommodate different variables at different levels.

Fractional Factorial Mixed Level Design

- ◆ The full factorial mixed-level design could be very large in terms of run number, depending on the number of factors and the factor levels. For example, with a three-level factor, a five-level factor, and a seven-level factor the full factorial design contains a total of 105 runs.
- ◆ Therefore, it may be desirable to use fractional factorial mixed-level designs instead of the full factorial. Some mixed-level designs are available in the literature. Orthogonal and near orthogonal mixed-level designs are discussed by Sloane (2006) and Xu (2002).

References

- ◆ Sloane, N. J. A. (2006). A Library of Orthogonal Designs, www.research.att.com/~njas/oadir/index.html
- ◆ Xu, H. (2002). "An Algorithm for Constructing Orthogonal and Nearly-Orthogonal Designs with Mixed Levels and Small Runs". Technometrics 44, pp. 356-368.

Lesson 211: Factorials With Factors at Two and Three Levels

Design Construction

Mixed level design in which some factors are at two levels and other at three levels can be constructed using sign table of usual 2^k factorial design.

Consider two variables, A at two levels and X at three levels. Consider the following table:

Run#	A	X_L	X_L	$A \times X_L$	$A \times X_L$	X_Q	$A \times X_Q$	Actual	
	A	B	C	BC	AC	BC	ABC	A	X
1	—	—	—	+	+	+	—	Low	Low
2	+	—	—	—	—	+	+	High	Low
3	—	+	—	—	+	—	+	Low	Med
4	+	+	—	+	—	—	—	High	Med
5	—	—	+	+	—	—	+	Low	Med
6	+	—	+	—	+	—	—	Low	Low
7	—	+	+	—	—	+	—	Low	Low
8	+	+	+	+	+	+	+	Low	Low

The signs in column B and C have following pattern:

Two Level Factors		Three Level Factor
B	C	X
—	—	Low
+	—	Med
—	+	Med
+	+	High

Note that A can be estimated from low levels of X or high levels of X . Runs 3 and 5 & 4 and 6 are replicates giving 2 degrees of freedom to error.

ANOVA Table

SOV	df	SOS	MS	F-Ratio
A	1	SS_A	MS_A	$F_A = \frac{MS_A}{MS_E}$
$X(X_L + X_Q)$	2	SS_X	MS_X	$F_X = \frac{MS_X}{MS_E}$
$AX(A \times X_L + A \times X_Q)$	2	SS_{AX}	MS_{AX}	$F_{AX} = \frac{MS_{AX}}{MS_E}$
Error (from run 3, 5 and 4, 6)	2	SS_E	MS_E	
Total	7	SS_T		

Lesson 212: Factorials With Factors at Two and Four Levels

Design Construction

Mixed level design in which some factors are at two levels and other at four levels can be easily accommodated in a 2^k factorial design.

Design Construction: Mixed level design

Pattern of A and B column The effects A and B are orthogonal to each other and correspond to 3 degrees of freedom for X .

Run#	(A	B)	X	C	D	AB	AC	BC	ABC	AD	BD	ABD	CD	ACD	BCD	ABCD
1	–	–	X ₁	–	–	+	+	+	–	+	+	–	+	–	–	+
2	+	–	X ₂	–	–	–	–	+	+	–	+	+	+	+	–	–
3	–	+	X ₃	–	–	–	+	–	+	+	–	+	+	–	+	–
4	+	+	X ₄	–	–	+	–	–	–	–	–	–	+	+	+	+
5	–	–	X ₁	+	–	+	–	–	+	+	+	–	–	+	+	–
6	+	–	X ₂	+	–	–	+	–	–	–	+	+	–	–	+	+
7	–	+	X ₃	+	–	–	–	+	–	+	–	+	–	+	–	+
8	+	+	X ₄	+	–	+	+	+	+	–	–	–	–	–	–	–
9	–	–	X ₁	–	+	+	+	+	–	–	–	+	–	+	+	–
10	+	–	X ₂	–	+	–	–	+	+	+	–	–	–	–	+	+
11	–	+	X ₃	–	+	–	+	–	+	–	+	–	–	+	–	+
12	+	+	X ₄	–	+	+	–	–	–	+	+	+	–	–	–	–
13	–	–	X ₁	+	+	+	–	–	+	–	–	+	+	–	–	+
14	+	–	X ₂	+	+	–	+	–	–	+	–	–	+	+	–	–
15	–	+	X ₃	+	+	–	–	+	–	–	+	–	+	–	+	–
16	+	+	X ₄	+	+	+	+	+	+	+	+	+	+	+	+	+

Two Level Factors		Three Level Factor
A	B	X
–	–	X ₁
+	–	X ₂
–	+	X ₃
+	+	X ₄

For further analysis we need **Sums of Squares**. The sum of squares for mixed level design can be computed as

$$SS_X = SS_A + SS_B + SS_{AB} \qquad (3 \text{ degrees of freedom})$$
$$SS_C = SS_C \qquad (1 \text{ degrees of freedom})$$
$$SS_D = SS_D \qquad (1 \text{ degrees of freedom})$$
$$SS_{CD} = SS_{CD} \qquad (1 \text{ degrees of freedom})$$
$$SS_{XC} = SS_{AC} + SS_{BC} + SS_{ABC} \qquad (3 \text{ degrees of freedom})$$
$$SS_{XD} = SS_{AD} + SS_{BD} + SS_{ABD} \qquad (3 \text{ degrees of freedom})$$
$$SS_{XCD} = SS_{ACD} + SS_{BCD} + SS_{ABCD} \qquad (3 \text{ degrees of freedom})$$

Lesson 213: Response surface methodology (RSM)

The response surface methodology is the further extension factorial experiment.

Definition 37.1

Response Surface Methodology (RSM) is a set of mathematical and statistical tools used to explore the relationships between several explanatory variables and one or more response variables.

The method was initially introduced by Box and Wilson in 1951.

Nature of Variables

RSM is an efficient tool of modern statistics which is used to study the relationship among one or more responses and a number of quantitative treatment factors.

Response Function

- ◆ The experimenter is interested in the response y that depends on the k controllable variables, i.e.,

$$E(y) = f(\xi_1, \xi_2, \dots, \xi_k)$$

- ◆ The form of the response function is usually unknown that needs to be estimated.
- ◆ The variables ξ_1, ξ_2, ξ_k are usually called natural variables. Because they are expressed in natural units of measurements such as kg, cm, and minutes, etc.

True Response Function

The true response in terms of coded variables is

$$\eta = f(x_1, x_2, \dots, x_k)$$

Coded Variables

- ◆ This is common in RSM that natural variables are transformed in coded variables

$$x_1, x_2, \dots, x_k$$

- ◆ Coded variables are dimensionless with mean 0 and equal spread, and

$$x_i = \frac{\frac{\xi_i - (\xi_{i(Max)} + \xi_{i(Min)})}{2}}{\frac{(\xi_{i(Max)} - \xi_{i(Min)})}{2}}$$

where ξ_i is the value of the i th factor, $\xi_{i(Max)}$ is the maximum value of that factor, and $\xi_{i(Min)}$ is the minimum value of the i th factor.

Lesson 214: Sequential Nature of RSM

Definition 37.2

When the cost of running an experiment is of particular concern, one of the major objectives of RSM is to find, in smallest possible number of runs, the point within the experimental region R at which response is maximum or minimum (as wished by the experimenter).

There may be many design choices to accomplish these tasks. The experimenter usually likes to conduct his experiment sequentially, in stages, so that each stage may be designed keeping in view the knowledge gained by the previous stage.

By successive use of sequential approach, and by using knowledge obtained from one sub-region to the next, an optimal response should be reached (See, Box and Wilson 1951).

Sequential Stages: There are two stages.

- ◆ **Phase I**

An experimental program may begin with a screening stage, in which we identify the important factors from among many candidate factors. A subsequent experimental effort, if needed, can be focused on those factors that appear to be of current practical importance.

◆ Phase II

This phase may include many sequential steps:

- ★ We incorporate a more efficient design to explore the experimental region.
- ★ We make the model adequate using a suitable stepwise method.
- ★ A Bayesian strategy can be quite useful which allows to use previous knowledge.

Lecture 38

Variance optimal designs

Lesson 215: First Order RS Model and its Matrix Structure

RS Model
Multiple regression includes statistical techniques used to build empirical models required in RSM. Also called polynomial models.

First Order Response Model
A multiple linear regression or first order model for response y in k predictors/ regressors,

$$x_1, x_2, \dots, x_k$$

and linear (unknown) parameters

$$\beta_0, \beta_1, \beta_2, \dots, \beta_k$$

with random error ε is:

$$y = \beta_0 + \beta_1x_1 + \dots + \beta_kx_k + \varepsilon$$

Matrix Structure
A first order model in matrix form can be represented as

$$y = \mathbf{X}\beta + \varepsilon$$

where

$$y = \begin{bmatrix} y_1 \\ y_2 \\ \vdots \\ y_n \end{bmatrix}, \quad \beta = \begin{bmatrix} \beta_1 \\ \beta_2 \\ \vdots \\ \beta_k \end{bmatrix}, \quad \varepsilon = \begin{bmatrix} \varepsilon_1 \\ \varepsilon_2 \\ \vdots \\ \varepsilon_n \end{bmatrix}$$
$$X = \begin{bmatrix} 1 & x_{11} & x_{12} & \cdots & x_{1k} \\ 1 & x_{21} & x_{22} & \cdots & x_{2k} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 1 & x_{n1} & x_{n2} & \cdots & x_{nk} \end{bmatrix}$$

The **Estimated Model** is,

$$\hat{y} = X\beta$$

where the least squares estimator of β is

$$b = (X^T X)^{-1}y$$

Lesson 216: First Order Response Surface (RS) Designs

First Order Response Model

A first order model for response y and k treatment variables $x_1, x_2, \dots, x_l$ and linear (unknown) parameters $\beta_0, \beta_1, \beta_2, \dots, \beta_k$ with random error ε is:

$$y = \beta_0 + \beta_1x_1 + \dots + \beta_kx_k + \varepsilon$$

Estimation of First Order Model

To estimate a first order model a design require to have:

- ◆ at least two levels of each factor.
- ◆ at least as many number of experimental trials as the number of terms in the model.

First Order Design

Response surface design used to estimate the first order polynomial model are called first order RS designs.

Some common first order response surface design:

- ◆ 2^k factorial designs
- ◆ 2^{k-p} fractional factorial designs
- ◆ Plackett-Burman designs
- ◆ Design based on orthogonal arrays

Lesson 217: First Order Orthogonal RS Designs

Orthogonal Matrix

Definition 38.1

A symmetric matrix (matrix with equal number of columns and rows) is orthogonal if all its entries other than diagonal are equal to 0. For example,

$$A = \begin{bmatrix} \mathbf{A}_1 & 0 & \cdots & 0 \\ 0 & \mathbf{A}_2 & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & \mathbf{A}_n \end{bmatrix}$$

Description

First order design is orthogonal if $X^T X$ is a diagonal matrix, i.e., columns of model matrix X are mutually orthogonal, where

$$X = \begin{bmatrix} 1 & x_1 & x_2 & \cdots & x_k \end{bmatrix}$$

- ◆ Orthogonality further implies that:

$$\begin{aligned} \mathbf{x}_i^T \mathbf{x}_j &= 0 \\ \mathbf{1}^T \mathbf{x}_j &= 0, \quad i \neq j \end{aligned}$$

where x_i and x_j are i^{th} and j^{th} columns of X .

- ◆ The levels of two corresponding variables are linearly independent, i.e. there roles are independently assessed.

Lesson 218: Variance-optimal First Order Designs

A first order design to be variance optimal require that:

- ◆ Design should be orthogonal.
- ◆ Levels of input variables are taken at two extremes.

Variance-Optimal design

- ◆ A design is called variance optimal if it produces minimum variance of regression coefficients, i.e. variance optimal design minimizes $Var(\beta_i)$.
Variance optimal design minimizes $Var(\beta_o)$ on a per observation basis, i.e., for the first order model, the design with fixed size N in which

$$x_j \in [-1, 1], \quad j = 1, 2, \dots, k$$

then

$$var(b_i)/\sigma^2 \text{ for } i = 1, 2, \dots, k$$

is minimized if design is orthogonal.

- ◆ The diagonal elements of $(X^T X)^{-1}$ are minimized by making the off-diagonal elements zero, i.e. forcing the diagonal of $X^T X$ to be as large as possible.
- ◆ Note that diagonal of $(X^T X)^{-1}$ are variances and off-diagonals are covariances of regression coefficients.

Lesson 219: Variance-optimal First Order Designs-Situation-I

Situation-I

Half fraction of resolution IV: Consider 2^{4-1} (half fraction of four factor full factorial) with defining relation $I = ABCD$.

$$X = \begin{bmatrix} & x_1 & x_2 & x_3 & x_4 \\ 1 & -1 & -1 & -1 & -1 \\ 1 & 1 & 1 & -1 & -1 \\ 1 & 1 & -1 & 1 & -1 \\ 1 & 1 & -1 & -1 & 1 \\ 1 & -1 & 1 & 1 & -1 \\ 1 & -1 & 1 & -1 & 1 \\ 1 & -1 & -1 & 1 & 1 \\ 1 & 1 & 1 & 1 & 1 \end{bmatrix}$$

Information Matrix

$$X^T X = 8 \times \begin{bmatrix} 1 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 1 \end{bmatrix} = 8I_5$$

Variance Covariance Matrix

$$\begin{aligned} (X^T X)^{-1} &= \begin{bmatrix} 1/8 & 0 & 0 & 0 & 0 \\ 0 & 1/8 & 0 & 0 & 0 \\ 0 & 0 & 1/8 & 0 & 0 \\ 0 & 0 & 0 & 1/8 & 0 \\ 0 & 0 & 0 & 0 & 1/8 \end{bmatrix} \\ &= \frac{1}{8} I_5 \\ \text{Var}(\beta_i) &= \sigma^2 (X^T X)^{-1} = \frac{1}{8} \sigma^2 \end{aligned}$$

Comments:

- ◆ It is to be noted that no other design with 8 runs could result in variance of regression coefficients smaller than $\frac{\sigma^2}{8}$ on per observation basis.
- ◆ For the 2^4 full factorial design the variance is $\frac{\sigma^2}{16}$, i.e., if the design size is doubled the variances of coefficients are halved. However, both designs are variance optimal on per observation basis.

Lesson 220: Variance-optimal First Order Designs-Situation-II

Situation-II

Half fraction of resolution III: Consider 2^{3-1} with defining relation $I = ABC$ and each design point is replicated twice.

Design Matrix

$$X = \begin{bmatrix} & x_1 & x_2 & x_3 \\ 1 & 1 & -1 & -1 \\ 1 & 1 & -1 & -1 \\ 1 & -1 & 1 & -1 \\ 1 & -1 & 1 & -1 \\ 1 & -1 & -1 & 1 \\ 1 & -1 & -1 & 1 \\ 1 & 1 & 1 & 1 \\ 1 & 1 & 1 & 1 \end{bmatrix}$$

Information and Precision Matrices (Variance-Covariance matrix)

$$\begin{aligned} X^T X &= 8 \times \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix} = 8 I_4 \\ (X^T X)^{-1} &= (1/8) \times \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix} = 1/8 I_4 \end{aligned}$$

This is orthogonal design with extreme levels of each variable. This is a variance-optimal design with

$$\text{Var}(\beta_i) = \sigma^2 (X^T X)^{-1} = \sigma^2 8$$

Lesson 221: Variance-optimal First Order Designs-Comparison of Two Situations

There are two **Two Situations** and we have to compare them.

- ◆ **First Situation**
 2^3 Full Factorial Design
- ◆ **Second Situation**
 2_{III}^{3-1} Design with $I = ABC$, replicated twice

Comparison

- ◆ **Same Variance Covariance**
 It is noted that both designs result in the same $(X^T X)^{-1}$ matrix, i.e., same variances of regression coefficients, $Var(b)$.
- ◆ **Different Variance Covariance**
 Designs are quite different with some other respects.
 - ★ **Lack-of-Fit**
 We consider first-order model which contains 4 terms to be estimated:
 - * In case of 2_{III}^{3-1} design replicated twice, there is no degree of freedom for lack-of-fit, because design has only 4 unique trials.
 - * In case of 2^3 design, there are four degrees of freedom for lack-of-fit attributed to x_1x_2 , x_1x_3 , x_2x_3 , $x_1x_2x_3$ model terms.
 - ★ **Pure Error**
 Pure error can be estimated through replicated trials.
 - * In case of 2_{III}^{3-1} design replicated twice, there is 4 degree of freedom for the estimation of pure error.
 - * 2^3 design allocates no degree of freedom for pure error.

Comments

Both designs are variance equivalent but they are chosen in different circumstances.

Lesson 222: Prediction Variance

First Order Response Model

A multiple linear regression or first order model for response y in k predictors/ regressors,

$$x_1, x_2, \dots, x_k$$

and linear (unknown) parameters

$$\beta_0, \beta_1, \beta_2, \dots, \beta_k$$

with random error ε is:

$$y = \beta_0 + \beta_1 x_1 + \dots + \beta_k x_k + \varepsilon$$

Matrix Structure

A first order model in matrix form can be represented as

$$y = \mathbf{X}\beta + \varepsilon$$

where

$$y = \begin{bmatrix} y_1 \\ y_2 \\ \vdots \\ y_n \end{bmatrix}, \quad \beta = \begin{bmatrix} \beta_1 \\ \beta_2 \\ \vdots \\ \beta_k \end{bmatrix}, \quad \varepsilon = \begin{bmatrix} \varepsilon_1 \\ \varepsilon_2 \\ \vdots \\ \varepsilon_n \end{bmatrix}$$

$$X = \begin{bmatrix} 1 & x_{11} & x_{12} & \cdots & x_{1k} \\ 1 & x_{21} & x_{22} & \cdots & x_{2k} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 1 & x_{n1} & x_{n2} & \cdots & x_{nk} \end{bmatrix}$$

The **Estimated Model** is,

$$\hat{y} = X\beta$$

where the least squares estimator of β is

$$b = (X^T X)^{-1} y$$

Prediction Variance

For the first order model, variance of the predicted response is

$$\text{Var}[\hat{y}(x)] = \sigma^2 \cdot x^{(m)'} (X^T X)^{-1} X^{(m)}$$

$x^{(m)}$ is the function of location in the design variables at which one wants to predict. It is also a function of model, m stands for model.

For the k -factor first order model

$$x^{(1)'} = [1 \quad x_1 \quad x_2 \quad \cdots \quad x_k]$$

$\text{Var}[y(\hat{x})]$ varies from location to location (point to point).

$\text{Var}[y(\hat{x})]$ reflects how well one can predict with the estimated model.

Lecture 39

Scaled Prediction Variance

Lesson 223: Scaled Prediction Variance

First of all we define prediction variance. We can write

$$\frac{1}{\sigma^2} \text{Var}[\hat{y}(x)] = x^{(m)'} (X^T X)^{-1} x^{(m)}$$

Why we need to scale prediction variance?

We know that larger sized variance-optimal design has smaller variance of regression coefficients. For the comparison of designs of different size on the basis of prediction variance, it is better to scale the prediction variance.

The Scaled Prediction Variance (SPV) is defined as

$$\frac{N}{\sigma^2} \text{Var}[\hat{y}(x)] = N x^{(m)'} (X^T X)^{-1} x^{(m)}$$

SPV for Variance-Optimal First Order Design

$$\frac{N}{\sigma^2} \text{Var}[\hat{y}(x)] = N x^{(1)'} (X^T X)^{-1} x^{(1)}$$

$$x^{(1)} = \begin{bmatrix} 1 & x_1 & x_2 & \cdots & x_k \end{bmatrix} \text{ and } (X^T X)^{-1} = \frac{1}{I_p}$$

So

$$\frac{N}{\sigma^2} \text{Var}[\hat{y}(x)] = \begin{bmatrix} 1 & x_1 & x_2 & \cdots & x_k \end{bmatrix} \times \begin{bmatrix} 1 \\ x_1 \\ x_2 \\ \vdots \\ x_k \end{bmatrix} = 1 + \sum_{i=1}^k x_i^2 = 1 + \rho_x^2$$

ρ_x is the distance of the points $x^{(1)} = \begin{bmatrix} 1 & x_1 & x_2 & \cdots & x_k \end{bmatrix}$ from the design center. SPV is 1 at the design center and increases as the point moves towards the design perimeter.

Lesson 224: Example: Scaled Prediction Variance

The formula of scaled prediction variance is

$$\frac{N}{\sigma^2}Var[\hat{y}(x)] = Nx^{(m)'}(X^TX)^{-1}x^{(m)}$$

Consider 2^{3-1}_{III} (resolution III design with three factors that have half fraction of full factorial) augmented with 4 center runs. The model matrix is

$$X = \begin{bmatrix} 1 & 1 & -1 & -1 \\ 1 & -1 & 1 & -1 \\ 1 & -1 & -1 & 1 \\ 1 & 1 & 1 & 1 \\ 1 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 \end{bmatrix}$$

$$X^TX = \begin{bmatrix} 8 & 0 & 0 & 0 \\ 0 & 4 & 0 & 0 \\ 0 & 0 & 4 & 0 \\ 0 & 0 & 0 & 4 \end{bmatrix}$$

and

$$(X^TX)^{-1} = \begin{bmatrix} \frac{1}{8} & 0 & 0 & 0 \\ 0 & \frac{1}{4} & 0 & 0 \\ 0 & 0 & \frac{1}{4} & 0 \\ 0 & 0 & 0 & \frac{1}{4} \end{bmatrix}$$

where

$$x^{(m)} = \begin{bmatrix} 1 & x_1 & x_2 & x_3 \end{bmatrix}$$

Now the SPV

$$\begin{aligned} \frac{NVar[\hat{y}(x)]}{\sigma^2} &= 8x^{(m)'}(X^TX)^{-1}x^{(m)} \\ &= 1 + 2(x_1^2 + x_2^2 + x_3^2) \\ &= 1 + 2\sum_{i=1}^3 x_i^2 = 1 + 2\rho_x^2 \end{aligned}$$

ρ_x is the distance of design point from the center. SPV increases fast when away from center.

Lesson 225: Second Order RS Model

Let us first define the **Response Surface Model**

The model relates the response variable y to the function of input variable treatments $f(x)$, i.e. ,

$$y = f'(x)\beta + \varepsilon$$

Now we define **Second Order RS Model**. This is the Polynomial Model

$$y = \beta_0 + \sum_{i=1}^k \beta_i x_i + \sum_{i=1}^k \beta_{ii} x_i^2 + \sum_{i=1}^{k-1} \sum_{j=i+1}^k \beta_{ij} x_i x_j + \varepsilon$$

Total Number of Parameters in the Model $1 + k + k + \binom{k}{2} = \binom{k+2}{2}$.

The Model Terms are:

- ◆ β_0 : Response intercept-Value of response when all inputs are Null.
- ◆ $\beta_i x_i$: Linear model terms-Terms include main effects of the input variables.
- ◆ $\beta_{ii} x_i^2$: Quadratic terms-Terms include quadratic effects of the input variables.
- ◆ $\beta_{ij} x_i x_j$: Bi-linear or interaction terms, Terms include two factor interactions of the input variables.
- ◆ ε : Random error terms.

Uses of second order models,

- ◆ Second order response surface model is used when the first order model becomes inadequate in the screening stage.
- ◆ When the system shows curvature.
- ◆ When experimenter is near the optimum point and wants to explore the response surface in more details.

Lesson 226: Models and Least Squares

Model in Matrix Form of response surface model.

Consider first order model in matrix form can be represented as

$$y = X\beta + \varepsilon$$

where

$$y = \begin{bmatrix} y_1 \\ y_2 \\ \vdots \\ y_n \end{bmatrix}, \quad \beta = \begin{bmatrix} \beta_1 \\ \beta_2 \\ \vdots \\ \beta_k \end{bmatrix}, \quad \varepsilon = \begin{bmatrix} \varepsilon_1 \\ \varepsilon_2 \\ \vdots \\ \varepsilon_n \end{bmatrix}$$
$$X = \begin{bmatrix} 1 & x_{11} & x_{12} & \cdots & x_{1k} \\ 1 & x_{21} & x_{22} & \cdots & x_{2k} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 1 & x_{n1} & x_{n2} & \cdots & x_{nk} \end{bmatrix}$$

To use method of least square, we need Residuals

$$e = y - Xb$$

b is the estimate of β .

Sum of Squares of Residuals

$$\begin{aligned} SS_e &= \sum_{i=1}^n e_i^2 = e'e \\ &= (y - Xb)'(y - Xb) \\ &= y'y - y'Xb - b'X'y + b'X'Xb \end{aligned}$$

Derivation of Least Squares

◆ Minimizing sum of squares of Residuals

$$\begin{aligned}\frac{\partial SS_e}{\partial b} &= -2X'y + 2X'Xb = 0 \\ \Rightarrow X'Xb &= X'y \\ \Rightarrow b &= (X'X)^{-1}X'y\end{aligned}$$

★ Second Derivative

$$\frac{\partial^2 SS_e}{\partial b \partial b'} = 2X'X$$

which is positive definite

Summary of Computations

In the **Least squares estimation** we will

- ◆ Choose the variable to be explained (y) and the explanatory variables ($x_1, \dots, x_k$).
- ◆ Collect n observations of y and of the related values of $x_1, \dots, x_k$.
- ◆ Compute the least squares estimates by the OLS method.

Lesson 227: Simple Regression in Matrix Notations

Linear Regression Model can be of two types,

- ◆ Simple Linear Regression Model
- ◆ Multiple Linear Regression Model

Simple Linear Regression Model

A simple linear regression model for response y in predictor/ regressor x , linear (unknown) parameter β and random error ε is:

$$y = \beta_0 + \beta x + \varepsilon$$

A simple linear regression model contains:

- ◆ Single variable (y) as response.
- ◆ Response values are being received by applying predictor (x) at different levels.
- ◆ Contribution of predictor is measure by linear (unknown) parameter β .

Multiple Linear Regression Model

If we represent the linear regression models (Multiple Predictors), the First order model for k variables is,

$$y_i = \beta_0 + \sum_{i=1}^k \beta_i x_i + \varepsilon_i$$

This **Model includes**,

- ◆ Response intercept
- ◆ Linear terms
- ◆ Random error

Model for k variables in Matrix Form

First order model in matrix form can be represented as

$$y = X\beta + \varepsilon$$

where

$$y = \begin{bmatrix} y_1 \\ y_2 \\ \vdots \\ y_n \end{bmatrix}, \quad \beta = \begin{bmatrix} \beta_1 \\ \beta_2 \\ \vdots \\ \beta_k \end{bmatrix}, \quad \varepsilon = \begin{bmatrix} \varepsilon_1 \\ \varepsilon_2 \\ \vdots \\ \varepsilon_n \end{bmatrix}$$
$$X = \begin{bmatrix} 1 & x_{11} & x_{12} & \cdots & x_{1k} \\ 1 & x_{21} & x_{22} & \cdots & x_{2k} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 1 & x_{n1} & x_{n2} & \cdots & x_{nk} \end{bmatrix}$$

A multiple linear regression model for response y in k predictors/ regressors $x_1, x_2, \dots, x_k$ and linear (unknown) parameters $\beta_0, \beta_1, \beta_2, \dots, \beta_k$, and random error ε is: $y = \beta_0 + \beta_1x_1 + \cdots + \beta_kx_k + \varepsilon$

Lesson 228: Quadratic Regression in Matrix Notations

Quadratic Regression Model: A polynomial regression model which contains,

- ◆ Linear terms,
- ◆ Quadratic terms,
- ◆ Bi-linear/two-variable-interaction terms.

A polynomial regression model:

$$y = \beta_0 + \sum_{i=1}^k \beta_i x_i + \sum_{i=1}^k \beta_{ii} x_i^2 + \sum_{i=1}^{k-1} \sum_{j=i+1}^k \beta_{ij} x_i x_j + \varepsilon$$

Model contains $1 + k + k + \binom{k}{2} = \binom{k+2}{2}$ terms.

Matrix Form of a polynomial regression model in matrix is,

$$y = X\beta + \varepsilon$$

- ◆ **Model Matrix**

$$X = \begin{bmatrix} 1 & x_{11} & \cdots & x_{1k} & x_{11}^2 & \cdots & x_{1k}^2 & x_{11}x_{12} & \cdots & x_{1,k-1}x_{1k} \\ 1 & x_{21} & \cdots & x_{2k} & x_{21}^2 & \cdots & x_{2k}^2 & x_{21}x_{22} & \cdots & x_{2,k-1}x_{2k} \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\ 1 & x_{n1} & \cdots & x_{nk} & x_{n1}^2 & \cdots & x_{nk}^2 & x_{n1}x_{n2} & \cdots & x_{n,k-1}x_{nk} \end{bmatrix}$$

- ◆ **Regression Coefficients**

$$\beta' = [\beta_0 \quad \beta_1 \quad \cdots \quad \beta_k \quad \beta_{11} \quad \cdots \quad \beta_{kk} \quad \beta_{12} \quad \cdots \quad \beta_{k-1,k}]$$

- ◆ **Random Errors**

$$\varepsilon' = [\varepsilon_1 \quad \varepsilon_2 \quad \cdots \quad \varepsilon_n]$$

- ◆ **Responses**

$$y' = [y_1 \quad y_2 \quad \cdots \quad y_n]$$

Lesson 229: Second Order RS Designs

Second Order Response Model are used to estimate the second order polynomial models.

$$y = \beta_0 + \sum_{i=1}^k \beta_i x_i + \sum_{i=1}^k \beta_{ii} x_i^2 + \sum_{i=1}^{k-1} \sum_{j=i+1}^k \beta_{ij} x_i x_j + \varepsilon$$

These models are required when in screening stage the first order model is inadequate. To estimate the first order model we choose a screening (or first order) design that have 2 levels most of the time.

Model contains $1 + k + k + \binom{k}{2} = \binom{k+2}{2}$ terms.

Second Order Response Design

- ◆ A factorial design which contains at least $\binom{k+2}{2}$ runs.
- ◆ All factors are applied at more than two levels.
- ◆ 3^k designs,
- ◆ Central Composite designs.
- ◆ Box-Behnken designs.
- ◆ Subset Designs.
- ◆ Augmented Pairs Designs
- ◆ Etc.

Lecture 40

Screening Stage of Response Surface Methodology

Lesson 230: Screening Stage of RSM

WHICH Stage

There could be a long list of natural input variables which could be of importance for response:

List Reduction

- ◆ Sit down with the investigator (biologist, chemist, physical scientist, etc.).
- ◆ Employ a preliminary screening design.

HOW Stage

The form of the true response is unknown at least initially. Iterative nature of RSM ensures, as the investigation proceeds, it's possible to learn about the:

- ◆ Amount of replication,
- ◆ Location of experimental region,
- ◆ Appropriate scaling and transformation,
- ◆ Designs needed.

WHY Stage

- ◆ Since the form of the true response function is unknown, we have to approximate it by a graduating function.
- ◆ We hope to achieve a working mechanistic model, which at least, takes into account the principal features of mechanism.

In **WHY Stage** a mechanistic model has following advantages:

- ◆ It contributes to the scientific understanding of the phenomenon.
- ◆ It provides a better basis for extrapolation.
- ◆ It helps to provide better estimates of the response.

Lesson 231: Different Screening Strategies

- ◆ Design Strategy

- ★ Factorial Designs
- ★ General Full Factorial Designs
- ★ Two Level Full Factorial Designs
- ★ Two Level Fractional Factorial Design
- ★ Plackett-Burman Design
- ★ Taguchi's Orthogonal Arrays
- ◆ **ANOVA Test**
By applying ANOVA test we shall come to know which effects (predictors) are significant for the response.
- ◆ **Regression Analysis**
Estimated regression model tells the individual contribution of each predictor for the response.
- ◆ **Model Validation**
After estimating the regression model we could check the validity of overall model through different statistical tools like coefficient of determination, residual analysis, etc.
- ◆ **Graphical Techniques**
Different graphical techniques are also available to assess the relationship between response and input variable/s, like scatter plot, normal probability plot, etc.

Lesson 232: Some Screening Designs

- ◆ **Factorial Designs**
 - ★ **General Full Factorial Designs**
In general, in full factorial designs the factors can have different number of levels, and they can be quantitative or qualitative.
 - ★ **Two Level Full Factorial Designs**
With these designs, all factors must have only two levels. Restricting the levels to two and running a full factorial experiment reduces the number of treatment combinations.
 - ★ **Two Level Fractional Factorial Design**
This is a special category of two level designs, where not all factor level combinations are considered, and the experimenter can choose which combinations are to be excluded.
 - ★ **Plackett-Burman Design**
A special category of two level fractional factorial designs, proposed by R. L. Plackett and J. P. Burman (1946), where only a few specifically chosen runs are performed to investigate just the main effects.
 - ★ **Taguchi's Orthogonal Arrays**
Taguchi's orthogonal arrays are highly fractional designs, used to estimate main effects using only a few experimental runs. Designs are also available to investigate main effects for certain mixed level experiments.

Lesson 233: Selection of Best Screening Design

Definition 40.1

Screening Design

Screening designs are useful for situations where a large number of factors is examined but

only few of these are expected to be important. It is of practical interest for a given k to know best projection of the design into the k dimensions.

Two level orthogonal arrays, when used in factorial experiments, permit orthogonal estimation of all the main effects and therefore, are often called orthogonal main effects plans.

Best Screening Design ...

Hall, M. J. (1961, 1965) generated Hadamard matrices for order 16 and 20. A rich and readily available class of orthogonal designs can be constructed by choosing columns from Hadamard matrices.

- ◆ Plackett-Burman designs as well as regular factorials are the special cases of orthogonal designs.
- ◆ Designs based on Hadamard matrices are useful screening designs, and fill the gaps between the run sizes available from regular designs.
- ◆ Hedayat and Wallis (1978) investigated the existence of Hadamard matrices for different sizes (n) and many of their applications.
- ◆ Deng and Tang (1999) proposed generalized resolution and generalized minimum aberration and their use as systematic criteria to compare and assess the goodness of non-regular factorials.
- ◆ Ma and Fang (2001) extended the idea of word-length pattern and minimum aberration for non-regular designs. They proposed new concepts like the generalized word-length pattern and minimum G2-aberration.
- ◆ Steinberg and Lin (2006) developed a construction method for orthogonal Latin hypercube designs. These designs are popular choice when computer simulation is used.
- ◆ Jacroux (2009) discussed industrial experiments which have hard to change and easy to change levels of experimental factors. Usually, fractional factorial split plot designs are used in such situations.

Lesson 234: Region of Experimentation, Region of Interest, Operability region

Region of Experimentation

The sequential experimentation is performed within a practicable space of the set of independent variables.

After the first phase when an experimenter has completed the screening of factors and he thinks that he has reached the point which is near optimum, he makes his approach more narrow and focused.

In the second phase of the experiment he defines a more accurate and smaller region for his experiment which is called region of experimentation or region of interest ($\mathcal{R}$).

Note That

In many practical situations the region of interest is not very clear. It is often difficult enough to get a commitment from a scientist or engineer on what are of interest and permissible ranges of the factors. Mistakes are often made and adjustments adopted in future experiments.

Lesson 235: Cuboidal Region

A design which resides its points on or inside the lines of a square, cube or hypercube is called a cuboidal design, e.g., a face-centered central composite design is a second order response surface design whose factorial points reside on the corners and axial points on the center of the faces of a cube or hypercube.

Cuboidal Region Geometry: 3-Factor (Box-Behnken) Design constructed in Cuboidal Region

3-Factor, 3-Level Design in Cuboidal Region

Note That

- ◆ In case of cuboidal region most of design points lie on corners and/ or edges of cube or hypercube.
- ◆ All the design points are at equal distance from the design center in case of a BBD.
- ◆ All design points are not at the same distance in case of 3-level factorial design.

Lesson 236: Spherical Region

Definition 40.2

A sphere is a perfectly round geometrical object in three-dimensional space that is the surface of a completely round ball.

Definition 40.3

Spherical Region

The situations may suggest the use of spherical region for the construction of designs.

Myers and Montgomery (2000) discuss the ranges on the factors which may define the corners where the factorial points should reside. Then the question regarding the design region should hinge on whether some design points outside the ranges are scientifically permissible and should be included in the region of interest.

Let us define spherical region in **Two situations**

Spherical Central Composite Design

Note That

Confusion regarding type of design should never be an excuse for not using designed experiments. Using a spherical region when it is more naturally cuboidal, for example, will still provide important information. This will, among other things, lead to more educated selection of regions for future experiments.

Lecture 41

Contour Plot and Central Composite Design

Lesson 237: Rotatability

In many response surface situations the experimenter is interested in predicting the response or estimating the mean response at a particular point in the experimental region.

The variance of the prediction at point x_0

$$\text{Var}[\hat{y}(x_0)] = \sigma^2 x_0' (X'X)^{-1} x_0$$

is important, it is direct measure of error associated with the point estimate produced by the model. Thus, a reasonably stable scaled prediction variance $N \frac{\text{var}[\hat{y}(x_0)]}{\sigma^2}$ insures roughly the same quality of $\hat{y}(x_0)$ throughout the region of interest.

Definition 41.1

Rotatability

A design is called a rotatable design if it has same value of scaled prediction variance at the points which are equidistant from the design center, i.e., scaled prediction variance is constant on spheres.

Rationale: The rationale of rotatability is that at two locations x_1 and x_2 in the design space which are at equal distance from the design center $(0, 0, \dots, 0)$, i.e., $\sqrt{x_1'x_1} = \sqrt{x_2'x_2}$ the predicted values $\hat{y}(x_1)$ and $\hat{y}(x_2)$ are equally good as having equal variance.

Lesson 238: Design Moments

Definition 41.2

Many important properties of a design are quantified through design moments. Consider the

design matrix of first order design,

$$\begin{bmatrix} x_{11} & x_{21} & \cdots & x_{k1} \\ x_{12} & x_{22} & \cdots & x_{k2} \\ \cdots & \cdots & \ddots & \vdots \\ x_{1N} & x_{2N} & \cdots & x_{kN} \end{bmatrix}$$

The relevant design moments are

- (i) $\frac{1}{N} \sum_{m=1}^N x_{im},$
- (ii) $\frac{1}{N} \sum_{m=1}^N x_{im}^2,$
- (iii) $\frac{1}{N} \sum_{m=1}^N x_{im}x_{jm},$
- (iv) $\frac{1}{N} \sum_{m=1}^N x_{im}^3,$
- (v) $\frac{1}{N} \sum_{m=1}^N x_{im}^2x_{jm}^2,$
- (vi) $\frac{1}{N} \sum_{m=1}^N x_{im}^4,$ etc.

Importance of studying the design moments:
The idea of design moments is to simplify the important property of **orthogonality** for a first order design.

The first order design is orthogonal if $X'X$ is diagonal, i.e.

$$\frac{1}{N}(X'X) = \begin{bmatrix} 1 & 0 & \cdots & \cdots & 0 \\ 0 & [11] & 0 & \cdots & 0 \\ 0 & 0 & [22] & \cdots & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & 0 & \cdots & [kk] \end{bmatrix}$$

Note That

- ◆ The moment matrix contains the moments through order 2.
- ◆ Design is orthogonal if all odd order moments are 0, i.e. $[i] = [ij] = 0,$ etc.
- ◆ By odd moment, we mean any moment for which at least one design variable possesses a power that is odd.

Lesson 239: Properties of a Good RS Design

Desirable Properties

- ◆ It should generate a satisfactory distribution of information throughout the design region.
- ◆ It should ensure that the fitted value $\hat{y}(x)$ be as close to the true value at x .
- ◆ It should provide an estimate of the pure experimental error.
- ◆ It should give good detectability of model lack-of-fit.
- ◆ It should allow for designs of increasing order to be constructed sequentially.
- ◆ It should be efficient with respect to the number of experimental runs.
- ◆ It should provide a check of the homogeneity of variance assumption.

- ◆ It should provide a good distribution of the scaled prediction variance $N \text{var}[\hat{y}(x)]/\sigma^2$ throughout the design region.
- ◆ It should be robust to the presence of outliers in the data.

Lesson 240: Contour Plot

Definition 41.3

contour plot is a graphical technique for representing a 3-dimensional surface by plotting constant z (response variable) slices, called contours, on a 2-dimensional format.

Given a value for z (response), lines are drawn for connecting the x and y (two input variables) coordinates where that z value occurs.

Thus contour plot is suitable to represent a relation like $z = f(x, y)$

Contour Plot: Example

- ◆ Role of two predictors x_1 and x_2 for different responses

- ◆ Role of $MgSO_4$ and $FeSO_4$ for a particular compound

- ◆ Contour Plot of Mixture Experiment

Lesson 241: 3-D Response Surface Plot

Definition 41.4

A three dimensional plot which shows behavior of response by varying two variables (other variables, if there, are held at fixed level). The plot is a companion plot to the contour plot.

The 3D surface is constructed using the averaged values, it does not show the variation at each grid point.

3D Response Plot: Examples

- ◆ A RS plot showing Enzyme Activity by varying Sorbitol and Yeast Extract, maximum is optimum

- ◆ 3D RS plot showing yield at different combinations of temperature and time
- ◆ Optimization Through 3D Response Plot
- ◆ Complex Functions 3D Plot

Lesson 242: Central Composite Design (CCD)

This is the second Order Polynomial Model. It can estimate the second order polynomial models. Response y depends upon k input variables.

$$y = \beta_0 + \sum_{i=1}^n \beta_i x_i + \sum_{i=1}^k \beta_{ii} x_i^2 + \sum_{i=1}^{k-1} \sum_{j=i+1}^k \beta_{ij} x_i x_j + \varepsilon$$

Model contains

β_0 : Response Intercept,

$$\sum_{i=1}^k \beta_i X_i : k \text{ linear terms,}$$
$$\sum_{i=1}^k \beta_{ii} X_i^2 : k \text{ quadratic terms,}$$
$$\sum_{i=1}^{k-1} \sum_{j=i+1}^k \beta_{ij} x_i x_j : k(k-1)/2 \text{ interaction (bilinear) terms}$$

Definition 41.5

CCD is presented by Box and Wilson (1951). A second order RS design with each factor at three or five levels. Design may be used to estimate up to fourth order model terms.

Design Points

- ◆ A k -factor CCD consists of three types of design points:
- ◆ Two level full factorial (2^k) or fractional factorial (2^{k-p}) of resolution at least V .
- ◆ $2k$ axial (star) points.
- ◆ Some center runs.

Discussion

- ◆ Factorial points of a CCD are the only points which contribute to the estimation of interaction terms.
- ◆ **Axial points** contribute to estimate the quadratic terms, without axial points only the sum of the quadratic terms could be estimated.
- ◆ **Center runs** provide degree of freedom to estimate pure error and also contribute to estimate quadratic terms.

Lesson 243: Geometrical Structure of a CCD

Why Geometric Structure

- ◆ Geometric structure of a design can be pretty useful to know how the design utilizes the experimental region.
- ◆ Which locations of experimental region are still needed to be explored?
- ◆ Geometry can be useful to compare to designs.

Different Examples:

◆ Two Factor CCD

	x_1	x_2
	-1	-1
	1	-1
	-1	1
	1	1
	$-\alpha$	0
$D=$	α	0
	0	$-\alpha$
	0	α
	0	0
	0	0
	0	0

◆ Two Factor Spherical CCD

◆ Three Factor-Centered CCD: $\alpha = 1$

◆ Three Factor Spherical CCD: $\alpha = \sqrt{k} = \sqrt{3}$

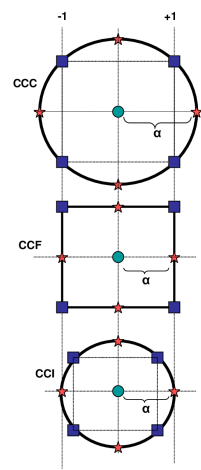
◆ Three Factor Hybrid CCD

Lesson 244: Types of CCD

General Types

- ◆ **Circumscribed:** All the design points lies on a sphere or hypersphere
- ◆ **Face Centered:** All the design points lie on a cube or hypercube.
- ◆ **Inscribed:** Axial points lies on the sphere, factorial points lie at distance less than spherical distance.

See the geometric structure of general types of CCD.



Augmented CCD

CCD may also be constructed by adding design points at some other locations to the experimental region. For example some edge points.

Example 1: Three Factor CCD, Design Matrix

x_1	x_2	x_3
-1	-1	-1
1	-1	-1
-1	1	-1
1	1	-1
-1	-1	1
1	-1	1
-1	1	1
1	1	1
$-\alpha$	0	0
α	0	0
0	$-\alpha$	0
0	α	0
0	0	$-\alpha$
0	0	α
0	0	0
0	0	0
0	0	0

- ◆ To construct cuboidal CCD put $\alpha = 1$
- ◆ To construct spherical CCD put $\alpha = \sqrt{k} = \sqrt{3}$

Lesson 245: Design Moments of CCD

Definition 41.6

For a second-order model, the model matrix will include columns for the intercept, first-order terms, squared terms, and cross-product terms.

In addition to the first-order model moments, the relevant design moments for the second order model are also present.

For $k = 3$ CCD

Model Matrix

$$X = [1 | X_L | X_Q | X_B]$$
$$X_L = \begin{bmatrix} x_{11} & x_{21} & x_{31} \\ x_{12} & x_{22} & x_{32} \\ \vdots & \vdots & \vdots \\ x_{1N} & x_{2N} & x_{3N} \end{bmatrix}$$
$$X_Q = \begin{bmatrix} x_{11}^2 & x_{21}^2 & x_{31}^2 \\ x_{12}^2 & x_{22}^2 & x_{32}^2 \\ \vdots & \vdots & \vdots \\ x_{1N}^2 & x_{2N}^2 & x_{3N}^2 \end{bmatrix}$$
$$1 = \begin{bmatrix} 1 \\ 1 \\ \dots \\ 1 \end{bmatrix}, \quad X_B = \begin{bmatrix} x_{11}x_{21} & x_{11}x_{31} & x_{21}x_{31} \\ x_{12}x_{22} & x_{12}x_{32} & x_{22}x_{32} \\ \vdots & \vdots & \vdots \\ x_{1N}x_{2N} & x_{1N}x_{3N} & x_{2N}x_{3N} \end{bmatrix}$$

Moment Matrix

$$\frac{X'X}{N} = \begin{bmatrix} 1 & [1] & [2] & [3] & [11] & [22] & [33] & [12] & [13] & [23] \\ & [11] & [12] & [13] & [111] & [122] & [133] & [112] & [113] & [123] \\ & & [22] & [23] & [112] & [222] & [233] & [122] & [123] & [223] \\ & & & [33] & [113] & [223] & [333] & [123] & [133] & [233] \\ & & & & [1111] & [1122] & [1133] & [1112] & [1113] & [1123] \\ & & & & & [2222] & [2233] & [1222] & [1223] & [2223] \\ & & & & & & [3333] & [1233] & [1333] & [2333] \\ & & & & & & & [1122] & [1123] & [1223] \\ & & & & & & & & [1133] & [1233] \\ & & & & & & & & & [2233] \end{bmatrix}$$

Rotatable Second Order Design-Partitioned Matrix

$$\frac{X'X}{N} = \begin{bmatrix} 1 & 0_{1 \times k} & 0_{1 \times k^*} & \lambda_2 J_K^T \\ 0_{k \times 1} & \lambda_2 I_k & 0_{k \times k^*} & 0_{k \times k} \\ 0_{k^* \times 1} & 0_{k^* \times k} & \lambda_4 I_{k^*} & 0_{k^* \times k} \\ \lambda_2 J_k & 0_{k \times k^*} & 0_{k \times k^*} & \lambda_4 (2I_k + J_k^T) \end{bmatrix}$$

Design to be Rotatable

- ◆ All odd order moments are zero.
- ◆ The quantities λ_2 and λ_4 are determined by the scaling of the design variables.
- ◆ $\frac{[iiii]}{[iijj]} = 3$ for $i \neq j$.

Lesson 246: Rotatability of CCD:

- ◆ For any CCD, all odd moments are zero due to the orthogonality among the x_i , x_ix_j and x_i^2 columns.
- ◆ Non-orthogonality occurs
 - ★ Between the column of ones and the x_i^2 columns and
 - ★ Between the x_i^2 and x_j^2 columns ($i \neq j$).
- ◆ To make a rotatable CCD, we must find the appropriate choice of α so that $\frac{X'X}{N}$ satisfies the rotatability criterion $\frac{[iiii]}{[iijj]} = 3$ where $[iiii]$ and $[iijj]$ are the moments corresponding to the products among the x_i^2 columns.
- ◆ For any CCD to be rotatable $\frac{[iiii]}{[iijj]} = \frac{n_f+2\alpha^4}{n_f} = 3$, where n_f is the number of factorial points. Solving we get $\alpha = (n_f)^{\frac{1}{n}}$

The Model matrix of Rotatable Two Factor CCD

$$x = \begin{bmatrix} & x_1 & x_2 & x_1^2 & x_2^2 & x_1x_2 \\ 1 & -1 & -1 & 1 & 1 & 1 \\ 1 & 1 & -1 & 1 & 1 & 1 \\ 1 & -1 & 1 & 1 & 1 & 1 \\ 1 & 1 & 1 & 1 & 1 & 1 \\ 1 & -\sqrt{2} & 0 & 2 & 0 & 0 \\ 1 & \sqrt{2} & 0 & 2 & 0 & 0 \\ 1 & 0 & -\sqrt{2} & 0 & 2 & 0 \\ 1 & 0 & \sqrt{2} & 0 & 2 & 0 \\ 1 & 0 & 0 & 0 & 0 & 0 \end{bmatrix} \Rightarrow X'X = \begin{bmatrix} 9 & 0 & 0 & 9 & 8 & 0 \\ 0 & 8 & 0 & 0 & 0 & 0 \\ 0 & 0 & 8 & 0 & 0 & 0 \\ 8 & 0 & 0 & 12 & 4 & 0 \\ 8 & 0 & 0 & 4 & 12 & 0 \\ 0 & 0 & 0 & 0 & 0 & 4 \end{bmatrix}$$

Moment Matrix

$$\frac{X'X}{N} = \frac{X'X}{9} = \begin{bmatrix} 1 & 0 & 0 & 8/9 & 8/9 & 0 \\ 0 & 8/9 & 0 & 0 & 0 & 0 \\ 0 & 0 & 8/9 & 0 & 0 & 0 \\ 8/9 & 0 & 0 & 4/9(3) & 4/9 & 0 \\ 8/9 & 0 & 0 & 4/9 & 4/9(3) & 0 \\ 0 & 0 & 0 & 0 & 0 & 4/9 \end{bmatrix}$$

Dividing $\frac{4/9(3)}{4/9}$ results in 3.

Lesson 247: Application of a CCD

Utility of CCD

- ◆ CCDs are used in almost all areas of process optimization.
- ◆ Design is successfully applied in the second stage of process development when the experimenter wishes to explore the experimental region in more detail usually through second order modeling.

Some Selected Applications

From the numerous applications of CCD we have chosen some applications as real examples from major fields like:

- ◆ **Energy Sector**
Marcin Dutka, Mario Ditaranto and Terese Løvås (2014) used a four factor rotatable CCD to study nitrogen oxide (NO₂) emissions of a low NO₂ burner. Factors involved in the experiment were:
 - ★ Hydrogen fraction
 - ★ Air/fuel equivalence ratio
 - ★ Lance position
 - ★ Secondary fuel fraction
- ◆ **Biotechnology and Food Technology**
 - ★ Tran Hong Thang, et al. (2010) applied three factor CCD for the optimization activity interaction of enzyme invertase including three factors: pH, temperature (t °C), ratio enzyme/substrate (E/S).
- ◆ **Chemical industry**
 - ★ Wan Salwanis Wan Md. Zain, et al. (2006) used two factor rotatable CCD for Optimization of the (Carbon/Nitrogen) C/N ratio in the feed stream.
- ◆ **Environmental sciences**
 - ★ Cho and Zoh (2006) applied CCD in the optimization of photocatalytic degradation of azo dye. The reactions were described as the function of parameters such as amount of T_iO₂, dye concentration and UV intensity.

Lesson 248: Choosing Number of Center Runs in CCD

Definition 41.7

Center Runs

Standard CCD includes each factor at three or five levels.
Center run represents the middle quantities of each variable (factor).
Since replication is a basic principle of DOE, replication at center is quite straight forward.
We can use any number of replications at design center which is not possible at other locations.

Why Center Runs?

- ◆ Center runs provide a kind of stability to the prediction variance of a design.
- ◆ In a spherical region of experimentation we can not computer determinant of information matrix without a center run.
- ◆ 3-6 center runs provide a reasonable distribution of scaled prediction variance in spherical region.
- ◆ In a cuboidal region of experimentation one or two center runs are sufficient to produce

reasonable stability to prediction variance.

Estimation of Pure Error

- ◆ In order to estimate pure error, we need extra degree of freedom which should come from replication.
- ◆ Multiple center runs may provide degree of freedom to estimate pure error in spherical as well as cuboidal region.

Lecture 42

Box-Behnken Design

Lesson 249: Box-Behnken Design (BBD)

Definition 42.1

Three level response surface designs developed by Box and Behnken (1960). Designs can be used to estimate models up to second order.

Design Construction

- ◆ BBD is constructed on the basic structure of Balanced incomplete Block Design (BIBD) in which not all treatments are applied in each block.
- ◆ For six factors the design uses the structure of Partially Balanced Incomplete Block Design (PBIBD).

General Structure: For three factors Two treatments are paired together in a 2^2 factorial.

Three Factor BBD

$$D = \begin{bmatrix} -1 & -1 & 0 \\ 1 & -1 & 0 \\ -1 & 1 & 0 \\ 1 & 1 & 0 \\ -1 & 0 & -1 \\ 1 & 0 & -1 \\ -1 & 0 & 1 \\ 1 & 0 & 1 \\ 0 & -1 & -1 \\ 0 & 1 & -1 \\ 0 & -1 & 1 \\ 0 & 1 & 1 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix} = 12 + n_c$$

Design is constructed by $2^3 = 8$ factorial runs.

$$D = \begin{bmatrix} \pm 1 & \pm 1 & 0 & \pm 1 & 0 & 0 \\ 0 & \pm 1 & \pm 1 & 0 & \pm 1 & 0 \\ 0 & 0 & \pm 1 & \pm 1 & 0 & \pm 1 \\ \pm 1 & 0 & 0 & \pm 1 & \pm 1 & 0 \\ 0 & \pm 1 & 0 & 0 & \pm 1 & \pm 1 \\ \pm 1 & 0 & \pm 1 & 0 & 0 & \pm 1 \\ 0 & 0 & 0 & 0 & 0 & 0 \end{bmatrix} \Rightarrow 48 + n_c$$

Different BBDs

Factors	Design Size	Coefficients in Quadratic Model
3	$12 + n_c$	10
4	$24 + n_c$	15
5	$40 + n_c$	21
6	$48 + n_c$	28
7	$56 + n_c$	36
9	$96 + n_c$	55
10	$160 + n_c$	66
11	$176 + n_c$	78
12	$384 + n_c$	91

Lesson 250: Geometrical Structure of a BBD

- ◆ General Structure:
For three factors

Two treatments are paired together in a 2^2 factorial.

- ◆ Design Matrix and Axis

- ◆ Second Order Model and Geometry of BBD for Three Factors

- ◆ Design Points of Three Factor BBD

Comments

- ◆ BBD contains edge points of a cube and points at the center of cube.
- ◆ Edge points contains two factors at extreme levels, i.e., at lowest level (-1) and/or at the highest level ($+1$).
- ◆ Center point contains all factors at middle levels.

Lesson 251: Properties of BBD

BBD (Box-Behnken Design)

- ◆ BBD is a second order design can be used to estimate a second order model.
- ◆ BBDs are constructed for three or above number of factors.
- ◆ The design contains three equally spaced levels of each included factors.

Properties of BBD

- ◆ BBD offers sufficient degrees of freedom to test lack-of-fit and pure error, as design has extra unique trials and center runs replications.
- ◆ Design is exactly rotatable for **four** and **seven** factors and does not substantially deviates from rotatability for other number of factors.
- ◆ BBD is a spherical design
- ◆ All the design points lie in the middle of the edges of a cube/ hypercube and are at equal distance from the center.
- ◆ Design does not include any corner/ factorial points or axial points.
- ◆ Design has limited capability of orthogonal blocking as compared to some other response surface designs.

Lesson 252: Application of a BBD

- ◆ BBD is a second order design can be used to estimate a second order model.
- ◆ BBD are constructed for three or above number of factors.
- ◆ The design contains three equally spaced levels of each included factors.

Application

- ◆ BBD does not properly cover the cuboidal experimental region as design does allocation points on the corners.
- ◆ BBD should be chosen when experimenter does not want to predict response at extreme points.
- ◆ If experimenter needs three level design and coverage of corners is necessary, then face-centered CCD is a better choice.
- ◆ Center runs are necessary in BBD to avoid singularity.
- ◆ 3-5 center runs are recommended in a BBD.
- ◆ BBD can be a better choice for small number of factors as the design size is smaller or equal to the other compatible response surface designs.

Some Examples of Application

- ◆ Manohar, et al. (2013) used Box-Behnken design in the experiments for turning Inconel 718 alloy with an overall objective of optimizing the process to yield higher metal removal, better surface quality and lower cutting forces.
- ◆ Ye, et al. (2017) applied BBD for modeling the influence of some variables on the performance of coal flotation. They performed verification experiments at optimum conditions to determine the validity of the predicted models.

Lesson 253: Comparison of CCD and BBD

Nature of Factors

- ◆ Both designs preferably include continuous factors.
- ◆ Factors are independently varied at different levels.
- ◆ BBD includes three equally spaced levels of each factor whereas CCD may contain three equally spaced levels or five levels which may or may not be equally spaced.

Visual Comparison

Model Comparison

- ◆ Both designs can be used first order and second order polynomial model.
- ◆ CCD can be used to estimate third order and fourth order model if the design contains enough runs.

Response Prediction

- ◆ BBD is not capable of predicting response at points at extreme distance from the center, coverage of experimental region is poor in case of BBD.
- ◆ CCD can predict response at extreme corner points and anywhere at axis.

Rotatability

- ◆ Rotatable CCD can be constructed for any number of factors by choosing suitable axial distance.
- ◆ BBD is rotatable for four and seven factors and generally near rotatable for other number of factors.

Comparison of Size

No. of Factors	CCD	BBD
2	$8 + n_c$	-
3	$14 + n_c$	$12 + n_c$
4	$24 + n_c$	$24 + n_c$
5	$26 + n_c$	$40 + n_c$
6	$44 + n_c$	$48 + n_c$
7	$60 + n_c$	$56 + n_c$
8	$80 + n_c$	-
9	$82 + n_c$	$96 + n_c$
10	$148 + n_c$	$160 + n_c$

Lesson 254: Comparison of 3^3 Factorial Design and a Face-centered CCD

Nature of Factors

- ◆ Both designs preferably include continuous factors.
- ◆ All factors are independently varied.
- ◆ Each factor is applied at three equally spaced levels.

Design Structure of Two Factor 3-Level Designs.

- a) 3^2 factorial b) Face-centered CCD

X_1	X_2
-1	-1
1	-1
-1	1
1	1
-1	0
0	-1
0	1
0	0

(a) 3^3 Factorial = 27 runs

(b) Face-Centered CCD = $14 + n_c$

Figure 42.1: Three Factor 3-Level Designs

Three Factor 3-Level Designs

Comparison

- ◆ 3^3 and face-centered CCD both are second-order designs.
- ◆ 3^3 design contains 27 runs whereas face-centered CCD has $14 + n_c$ design points.
- ◆ 3^3 design includes 12 extra edge points, hence less economical than face-centered CCD.
- ◆ Both designs have 25 common points.
- ◆ **As second order model contains 10 parameters,**
 - ★ 3^3 design spares 17 degrees of freedom all for estimation of lack-of-fit. No degree of freedom for pure error.
 - ★ Face-centered CCD allocates 4 degrees of freedom for lack-of-fit and for pure error with replication of center runs.

Lecture 43

Small Composite Design

Lesson 255: Small Composite Design (SCD)

Definition 43.1

SCD is constructed on the basic structure of CCD but the fractional factorial portion is neither a k-factor full factorial nor a resolution V factorial.

SCD contains a special resolution III fraction with no four letter word in the defining relation, denoted by resolution III*.

Comparison of SCD and CCD

◆ 3-Factor SCD and CCD

$$SCD = \begin{bmatrix} -1 & -1 & -1 \\ 1 & 1 & -1 \\ 1 & -1 & 1 \\ -1 & 1 & 1 \\ -\alpha & 0 & 0 \\ \alpha & 0 & 0 \\ 0 & \alpha & 0 \\ 0 & -\alpha & 0 \\ 0 & 0 & -\alpha \\ 0 & 0 & -\alpha \\ 0 & 0 & 0 \end{bmatrix} \quad CCD = \begin{bmatrix} -1 & -1 & -1 \\ 1 & -1 & -1 \\ -1 & 1 & -1 \\ 1 & 1 & -1 \\ -1 & -1 & 1 \\ 1 & -1 & 1 \\ -1 & 1 & 1 \\ 1 & 1 & 1 \\ -\alpha & 0 & 0 \\ \alpha & 0 & 0 \\ 0 & -\alpha & 0 \\ 0 & \alpha & 0 \\ 0 & 0 & -\alpha \\ 0 & 0 & \alpha \\ 0 & 0 & 0 \end{bmatrix}$$

◆ Information Matrices

$$X'X_{SCD} = \begin{matrix} & \begin{matrix} 1 & x_1 & x_2 & x_3 & x_1^2 & x_2^2 & x_3^2 & x_1x_2 & x_1x_3 & x_2x_3 \end{matrix} \\ \begin{matrix} 1 \\ x_1 \\ x_2 \\ x_3 \\ x_1^2 \\ x_2^2 \\ x_3^2 \\ x_1x_2 \\ x_1x_3 \\ x_2x_3 \end{matrix} & \left[\begin{array}{ccccccccccc} 11 & 0 & 0 & 0 & 4+2\alpha^2 & 4+2\alpha^2 & 4+2\alpha^2 & 0 & 0 & 0 \\ & 4+2\alpha^2 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & -4 \\ & & 4+2\alpha^2 & 0 & 0 & 0 & 0 & 0 & -4 & 0 \\ & & & 4+2\alpha^2 & 0 & 0 & 0 & -4 & 0 & 0 \\ & & & & 4+2\alpha^4 & 4 & 4 & 0 & 0 & 0 \\ & & & & & 4+2\alpha^4 & 4 & 0 & 0 & 0 \\ & & & & & & 4+2\alpha^4 & 0 & 0 & 0 \\ & & & & & & & 4 & 0 & 0 \\ & & & & & & & & 4 & 0 \\ & & & & & & & & & 4 \end{array} \right] \end{matrix}$$

$$X'X_{CCD} = \begin{matrix} & \begin{matrix} 1 & x_1 & x_2 & x_3 & x_1^2 & x_2^2 & x_3^2 & x_1x_2 & x_1x_3 & x_2x_3 \end{matrix} \\ \begin{matrix} 1 \\ x_1 \\ x_2 \\ x_3 \\ x_1^2 \\ x_2^2 \\ x_3^2 \\ x_1x_2 \\ x_1x_3 \\ x_2x_3 \end{matrix} & \left[\begin{array}{ccccccccccc} 15 & 0 & 0 & 0 & 4+2\alpha^2 & 4+2\alpha^2 & 4+2\alpha^2 & 0 & 0 & 0 \\ & 8+2\alpha^2 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & -4 \\ & & 8+2\alpha^2 & 0 & 0 & 0 & 0 & 0 & -4 & 0 \\ & & & 8+2\alpha^2 & 0 & 0 & 0 & -4 & 0 & 0 \\ & & & & 8+2\alpha^4 & 8 & 8 & 0 & 0 & 0 \\ & & & & & 8+2\alpha^4 & 8 & 0 & 0 & 0 \\ & & & & & & 8+2\alpha^4 & 0 & 0 & 0 \\ & & & & & & & 8 & 0 & 0 \\ & & & & & & & & 8 & 0 \\ & & & & & & & & & 8 \end{array} \right] \end{matrix}$$

Discussion

- ◆ Second order polynomial model contains 10 terms, SCD contains just one run above saturation.
- ◆ One degree of freedom is available for lack-of-fit.
- ◆ Multiple center runs can provide degrees of freedom for pure error.
- ◆ Information matrix of SCD shows that linear terms are aliased with two factor interactions.
- ◆ Linear effects may benefit from axial points, therefore, all terms of second order model are estimable.
- ◆ SCD and CCD are nearly identical for estimation of quadratic terms.

Lesson 256: Use of Plackett-Burman Design in SCD

Why PBD in SCD?

- ◆ SCD usually contains a special resolution III fraction with no four letter word in the defining relation, denoted by resolution III*.
- ◆ There are some situations when resolution III* fraction can be usefully replaced by columns from Plackett-Burman design.
- ◆ Draper (1985) and Draper and Lin (1990) have shown that many SCDs exist that can be constructed using PBDs.
- ◆ In some cases SCDs produced by PBDs are smaller than SCDs produced by using resolution III*.
- ◆ Saturated SCDs can be avoided with the use of PBDs.

Example 1: SSD for $k = 5$

	+	−	+	−	−
	+	+	−	+	−
	−	+	+	−	+
	+	−	+	+	−
	+	+	−	+	+
	+	+	+	−	+
	−	+	+	+	−
	−	−	+	+	+
	−	−	−	+	+
	+	−	−	−	+
	−	+	−	−	−
	−	−	−	−	−
$\pm\alpha$	0	0	0		
0	$\pm\alpha$	0	0	0	
0	0	$\pm\alpha$	0	0	
0	0	0	$\pm\alpha$	0	
0	0	0	0	$\pm\alpha$	
0	0	0	0	0	

- ◆ This is 23-run SCD.
- ◆ Design contains 5 columns from 12-run PBD.
- ◆ Design contains 2 degrees of freedom for lack-of-fit.
- ◆ Pure error can be estimated by taking replication on center runs.

Further Comments

- ◆ For a three level SCD set $\alpha = 1$, a face-centered SCD.
- ◆ For a spherical SCD set $a = \sqrt{k}$.

Lesson 257: Application of a SCD

SCDs are economical, near saturated designs constructed on the basic structure of CCD. Factorial portion of SCD usually contains resolution III fraction in place of resolution V as in CCD.

Size of SCD

No. of Factors	Model Parameters	Design Points
2	6	6
3	10	10
4	15	16
5	21	26
6	28	28
7	36	46
8	45	48
9	55	82

Important About SCD

- ◆ Though all second order model terms are estimable through SCD, design considerably suffers in efficiency for estimation of linear and interaction terms.

- ◆ SCD cannot be an alternate to CCD unless run economy is the top most priority for the experimenter.
- ◆ Most attractive virtue of SCD is, probably, its use in sequential experimentation.
- ◆ RSM nearly always involves iterative decision making, a first-stage experiment with an SCD may suggest that current experimentation is near the optimum and there are no ridge conditions.

Lesson 258: Alphabetic Design Optimalities

Key Points

◆ The Model

$$y = X\beta + \varepsilon$$

$X_{n \times p}$ = Model matrix
 $\beta_{p \times 1}$ = Vector of regression coefficients
 $\varepsilon_{n \times 1}$ = Vector of errors
 $y_{n \times 1}$ = Vector of observed responses

◆ Model Estimates

$$\hat{\beta} = (X^T X)^{-1} X^T y$$

$$Var(\hat{\beta}) = \sigma^2 (X^T X)^{-1}$$

$$\hat{y} = X\hat{\beta}$$

$$Var(\hat{y}) = \sigma^2 x (X^T X)^{-1} x^T \quad x_{1 \times p} = \text{is a row in the model matrix}$$

Optimal Design

- ◆ The design problem consists of selecting row vectors $x_{1 \times p}$, from the design space such that the design defined by these n vectors is, in some desired sense, optimal.
- ◆ Experimenter may wish to have
 - ★ Efficient estimation of regression coefficients.
 - ★ Minimize the variances of regression coefficients.
 - ★ Minimize the prediction variances on different locations of design space.

Alphabetic Optimalities

- ◆ Design optimality criteria are commonly characterized by letters of alphabet, A, D, E, G , etc. Hence called alphabetic optimality criteria.
- ◆ Each alphabetic criterion focuses on a specific desired characteristic of the design.

Lesson 259: D-Optimality and D-Efficiency

Key Points

◆ The Model

$$y = X\beta + \varepsilon$$

$X_{n \times p}$ = Model matrix
 $\beta_{p \times 1}$ = Vector of regression coefficients
 $\varepsilon_{n \times 1}$ = Vector of errors
 $y_{n \times 1}$ = Vector of observed responses

◆ Moment Matrix

$$M = \frac{X^T X}{N}$$

★ Scaled Dispersion Matrix

$$M^{-1} = N(X^T X)^{-1}$$

★ Determinant of Moment Matrix

$$|M| = \frac{|X^T X|}{N^p}$$

◆ Under the assumption

- ★ Independent normal model errors and
- ★ Constant variance

$|M|$ is inversely proportional to the square of the volume of the confidence region on the regression coefficients, which reflects how well coefficient are estimated.

Definition 43.2

D-Optimality

Wald (1943) proposed D-optimality criterion which focuses on maximizing the determinant of moment matrix M over the design space $\mathfrak{R}$, i.e.,

$$D = \max_{\mathfrak{R}} |M(\mathfrak{R})|$$

A large $|X^T X|$ or small $|(X^T X)^{-1}|$ implies a good estimation of vector of coefficients, β .

Definition 43.3

D-Efficiency

D-efficiency of a design $\mathfrak{R}^*$ can be defined as

$$D_{eff} = \left(|M(\mathfrak{R}^*)| / \max_{\mathfrak{R}} |M(\mathfrak{R})| \right)^{\frac{1}{p}}$$

The power $1/p$ takes account of the number of model parameters being assessed.

Alphabetic Design Optimalities

Lesson 260: A-Optimality and A-Efficiency

Key Points

◆ The Model

$$y = X\beta + \varepsilon$$

$X_{n \times p}$ = Model matrix
 $\beta_{p \times 1}$ = Vector of regression coefficients
 $\varepsilon_{n \times 1}$ = Vector of errors
 $y_{n \times 1}$ = Vector of observed responses

◆ Moment Matrix

$$M = \frac{X^T X}{N}$$

★ Scaled Dispersion Matrix

$$M^{-1} = N(X^T X)^{-1}$$

★ Determinant of Moment Matrix

$$|M| = \frac{|X^T X|}{N^p}$$

Definition 43.4

A-Optimality

A-optimality deals with individual variances rather than considering the joint confidence ellipsoid in the form of $|M(\mathfrak{R})|$ as was in case of D-optimality.

Variances of regression coefficients appear on the diagonal of $(X^T X)^{-1}$.

Thus A-optimality:

$$A = \min_{\mathfrak{R}} \text{trace} |M(\mathfrak{R})|^{-1}$$

A-Efficiency

$$A_{eff} = 100 \times \left(\frac{p}{\text{trace}(N \times (X^T X)^{-1})} \right)$$

Lesson 261: E-Optimality and E-Efficiency

Let us define eigen values as E-optimality based on eigen values.

Definition 43.5

Eigen values

Eigenvalues are a special set of scalars associated with a linear system of equations (i.e., a matrix equation) that are sometimes also known as characteristic roots or characteristic values.

Each eigenvalue is paired with a corresponding (so-called) eigenvector

Let A be a linear transformation represented by a matrix A . If there is a vector Z such that

$$AZ = \lambda Z$$

for some scalar λ , then λ is called the eigenvalue of A with corresponding eigenvector Z .

Definition 43.6

E-Optimality

A design is E -optimal if it maximizes the smallest eigenvalue of

$$M = \frac{X'X}{N}$$

over the design space.

where $X_{n \times p}$ is the model matrix under the model $y = X\beta + \varepsilon$

Definition 43.7

E-Efficiency

A design is E -efficient if it chooses the design points over the whole design space which maximize the smallest eigenvalue when compared to other design over this space.

Lesson 262: G-Optimality and G-Efficiency

Key Points

◆ The Model

$$y = X\beta + \varepsilon$$

$X_{n \times p}$ = Model matrix

$\beta_{p \times 1}$ = Vector of regression coefficients

$\varepsilon_{n \times 1}$ = Vector of errors

$y_{n \times 1}$ = Vector of observed responses

◆ Scaled Prediction Variance

$$V(x) = N \cdot x^{(x)T} (X^T X)^{-1} x^{(m)}$$

$x^{(m)}$ is the location in the design space extended to through the model terms. For example, for the first order model

$$x^{(1)T} = \begin{bmatrix} 1 & x_1 & x_2 & \cdots & x_k \end{bmatrix}$$

Definition 43.8

G-Optimality

A design ξ is called G -optimal if it minimizes the maximum prediction variance over the whole experimental region $\mathfrak{R}$, i.e.,

$$G = \min_{\xi} [\max_{x \in \mathfrak{R}} V(x)]$$

Or equivalently

$$\min_{\xi} [\max_{x \in \mathfrak{R}} \{x^{(m)T} (M(\xi))^{-1} x^{(m)}\}]$$

Definition 43.9

G-Efficiency

For a design ξ , under the p -parameter model G -efficiency is computed as:

$$G_{eff} = \frac{p}{\max_{x \in \mathfrak{R}} V(x)}$$

Lesson 263: Variance Dispersion Graphs

◆ The Model

$$y = X\beta + \varepsilon$$

$X_{n \times p}$ = Model matrix

$\beta_{p \times 1}$ = Vector of regression coefficients

$\varepsilon_{n \times 1}$ = Vector of errors

$y_{n \times 1}$ = Vector of observed responses

◆ Scaled Prediction Variance

$$V(x) = N \cdot x^{(x)T} (X^T X)^{-1} x^{(m)}$$

$x^{(m)}$ is the location in the design space extended to through the model terms. For example, for the first order model

$$x^{(1)T} = \begin{bmatrix} 1 & x_1 & x_2 & \cdots & x_k \end{bmatrix}$$

Scaled Prediction Variance Graph

The curve represents

- ◆ Maximum
- ◆ Average and
- ◆ Minimum

Scaled prediction
variance for a design.

Fraction of Design Space (FDS) Plot

The FDS Plot shows the proportion of
the design space over which the relative
prediction variance lies below a given
value.

Other Graphs on Prediction Variance

Variance Dispersion Graph for esti-
mated difference of response

Fraction of design space plot for esti-
mated difference of response

Lecture 44

Orthoogonal Blocking in Second Order Design

Lesson 264: Tradeoff Between Different Optimality Criteria

Definition 44.1

Optimality Criteria

Selecting among several candidate designs. Practitioners are typically forced to make trade-off between their objectives when choosing the final design. Many competing criteria that could be considered in selecting the design are discussed by Anderson-Cook et al. (2009).

Traditionally a single-number summary, such as the precision with which the model parameters are estimated that can not be generalized easily.

A design which is optimal under one criterion may not necessarily be optimal under the other criterion. But these measures are often used in evaluating and comparing competing designs.

Other important considerations include the robustness of the design to model misspecification and potential problems arising from spurious or missing data.

Graphical methods, like VDG and FDS plot, are generally superior to the simplistic summaries of alphabetic optimality criteria.

Lesson 265: Orthogonal Blocking in Second Order Designs

◆ Blocking

- ★ In the statistical theory of the DOE, blocking is the arranging of experimental units in groups (blocks) that are identical to one another.
- ★ Typically, a blocking factor is a source of variability that is not of primary interest to the experimenter.

◆ Blocked Design

- ★ With a randomized block design, the experimenter divides experimental units into blocks, such that the variability within blocks is less than the variability between blocks.
- ★ Units within each block are randomly assigned to treatment conditions.

◆ Orthogonal Blocks

- ★ In RSM, the estimation of the polynomial effects is often influenced by the block effect.
- ★ A desired blocking strategy is to minimize the blocking effect on the model coefficients.
- ★ Orthogonal blocking provides the same estimate of the model coefficients as would have been obtained by ignoring the blocks.

Lesson 266: Conditions for Orthogonal Blocking in Second Order Designs

Second order model for k factors and b blocks

$$y_u = \beta_0^* + \sum_{i=1}^k \beta_i x_{ui} + \sum_{i=1}^k \beta_{ii} x_{ui}^2 + \sum_{i < j}^k \sum_{j=2}^k \beta_{ij} x_{ui} x_{uj} + \sum_{m=1}^b \delta_m (z_{um} - \bar{z}_m)$$

, $u = 1, 2, \dots, N$,

where, the indicator variable

$$z_{um} = \begin{cases} 1 & \text{if the } u\text{th observation is in the } m\text{th block} \\ 0 & \text{otherwise} \end{cases}$$

Orthogonal Blocking

Necessary conditions for block effects to be orthogonal to regression coefficients:

$$\begin{aligned} \sum_{u=1}^N x_{ui} (z_{um} - \bar{z}_m) &= 0, \quad i = 1, 2, \dots, k, \quad m = 1, 2, \dots, b \\ \sum_{u=1}^N x_{ui} x_{uj} (z_{um} - \bar{z}_m) &= 0, \quad i \neq j, \quad m = 1, 2, \dots, b \\ \sum_{u=1}^N x_{ui}^2 (z_{um} - \bar{z}_m) &= 0, \quad i = 1, 2, \dots, k, \quad m = 1, 2, \dots, b \end{aligned}$$

Condition-I in Orthogonal Blocking

From above we can find that for a specific block, m :

$$\sum_{block m} x_{ui} = \sum_{block m} x_{ui} x_{uj} = 0,$$

$i, j = 1, 2, \dots, k$

In each block first and second mixed moments should be zero.

Condition-II in Orthogonal Blocking

Again for block m we can find:

$$\sum_{u=1}^N x_{ui}^2 z_{um} = \bar{z}_m \sum_{u=1}^N x_{ui}^2,$$

for $i = 1, 2, \dots, k$

For each design variable the sum of squared contribution from each block is proportional to block size.

Lesson 267: Orthogonal Blocking: Two Blocks CCD

Rotatable CCD for $k = 2$

Consider

- ◆ A rotatable CCD for two factors,
- ◆ Constructed in two blocks,
- ◆ With two center runs in each block.

The Design

- ◆ Block I contains 2^2 full factorial runs and center runs.

Block-I	
x_1	x_2
-1	-1
-1	1
1	-1
1	1
0	0
0	0

- ◆ Block II contains four axial runs and center runs.

Block-II	
x_1	x_2
$\sqrt{2}$	0
$\sqrt{2}$	0
0	$-\sqrt{2}$
0	$\sqrt{2}$
0	0
0	0

Orthogonal Blocking

This CCD has orthogonal blocking because:

- ◆ **Condition I**
Each block contains first order orthogonal design, i.e. first moment and mixed second moment are both zero.
- ◆ **Condition II**
The sum of squares of each design variable is equal to 4 and both blocks are also of equal size.

Note that any even number of center runs assigned equally to both blocks would result in orthogonal blocking.

Derivation of α : For a CCD with n_f factorial runs and n_0 center runs, the design to be

orthogonally blocked we need:

$$\frac{\sum_{\text{axial block}} x_{iu}^2}{\sum_{\text{factblock}} x_{iu}^2} = \frac{2k + n_0}{n_f + n_0}, \quad i = 1, 2, \dots, k$$

$$\frac{2\alpha^2}{n_f} = \frac{2k + n_0}{n_f + n_0}$$

$$\alpha = \sqrt{\frac{n_f(2k + n_0)}{2(n_f + n_0)}}$$

Lesson 268: General Comments on Blocking of CCD

Spherical Region

We can easily see that orthogonal blocking in CCD can mostly be achieved when the:

- ◆ Experimental region is spherical, i.e. $\alpha = \sqrt{k}$ and
- ◆ Center runs are evenly distributed among blocks. In case of more than two blocks center runs may vary.

Three Blocks

- ◆ Factorial runs are evenly divided in two blocks.
- ◆ Axial runs are Put in the same block.
- ◆ We must use $\alpha = \sqrt{3}$.

Block I			Block II			Block III		
X_1	X_2	X_3	X_1	X_2	X_3	X_1	X_2	X_3
-1	-1	-1	1	-1	-1	$-\alpha$	0	0
1	1	-1	-1	1	-1	α	0	0
1	-1	1	-1	-1	1	0	$-\alpha$	0
-1	1	1	1	1	1	0	α	0
0	0	0	0	0	0	0	0	α
0	0	0	0	0	0	0	0	$-\alpha$
						0	0	0
						0	0	0
						0	0	0

Cuboidal Region

- ◆ Orthogonal blocking in case of cuboidal region is not so straight forward.
- ◆ The block size is usually quite disproportionate. Which may not be acceptable for the experimenter.

Cuboidal Region (Orthogonal Blocks)

Consider Face-Centered CCD for $k = 2$:

- ◆ Block I contains 8 runs with 4 center runs
- ◆ Block II contains 4 runs with no center run

Block I		Block II	
X_1	X_2	x_1	x_2
-1	-1	-1	0
-1	1	1	0
1	-1	0	-1
1	1	0	1
0	0		
0	0		
0	0		
0	0		

Lesson 269: Blocking in BBD

BBD: Three level response surface designs constructed on the basic structure of Balanced Incomplete Block Design (BIBD) in which not all treatments are applied in each block.

General Structure for three factors Treatment

	Treatment		
	A	B	C
Block I	*	*	
Block II	*		*
Block III		*	*

Two treatments are paired together in a 2^2 factorial.

Blocking BBD

A BBD with:

- ◆ Three factors cannot have blocks.
- ◆ Four factors can be done in three blocks.
- ◆ Five, six, seven, or ten factors can be done in two blocks.
- ◆ Nine factors can be done in five or ten blocks.

Orthogonal Blocking

- ◆ The capacity of BBD for orthogonal blocking is limited.
- ◆ Orthogonal blocking in BBD can be done for $k = 4$ and 5.
- ◆ Center runs should be equally assigned to each block.

Orthogonal Blocking in BBD for $k = 4$

Lesson 270: Analysis of a Second Order Blocked Experiment Under Blocked CCD

Example

A chemical is required to fit the response surface and find conditions on time (A) and temperature (B) to maximize the response, yield. Two batches of raw material must be used. The design in coded form in two blocks and the observed response are given below:

Block	A (Time)	B (Temp.)	Resp
1	-1	-1	80.5
1	1	-1	82
1	-1	1	81.5
1	1	1	83.5
1	0	0	83.9
1	0	0	84.3
1	0	0	84
2	-1.41421	0	75.6
2	1.41421	0	78.4
2	0	-1.41421	77
2	0	1.41421	78.5
2	0	0	78.5
2	0	0	79.5
2	0	0	79.7
2	0	0	79.8

Unblocked CCD

Blocked CCD

Contour Plot

Response Optimization

Lecture 45

Use of Statistical Software in DOE

Lesson 271: Use of Software

- ◆ Software advancements gave rise to solving complex factorial statistical equations.
- ◆ Statisticians began in earnest to design experiments with more than one factor (multifactor) being tested at a time.
- ◆ Computerized multifactor DOE began supplanting one-factor-at-a-time experiments.
- ◆ Computer software are available from various leading software companies in the 1980s and included packages such as JMP, Minitab, Matlab, R Language, and Design-Expert.

Benefits

- ◆ Identifying key factors for process or product improvements.
- ◆ Setting up and analyzing general factorial, two-level factorial, fractional factorial and Plackett–Burman designs.
- ◆ Performing numerical optimizations.
- ◆ Screening for critical factors and their interactions.
- ◆ Analyzing process factors or mixture components.
- ◆ Combining mixture and process variables in designs.
- ◆ Rotating 3D plots to visualize response surfaces.
- ◆ Exploring 2D contours with a computer mouse, setting flags along the way to identify coordinates and predict responses.
- ◆ Precisely locating where all specified requirements meet using numerical optimization functions within DOE software.
- ◆ Finding the most desirable factor settings for multiple responses simultaneously.

Lesson 272: Use of Statistical Software in DOE

272.1 One-Way ANOVA in Minitab

Consider the data

Control	F1	F2	F3
21.0	32.0	22.5	28.0
19.5	30.5	26.0	27.5
22.5	25.0	28.0	31.0
21.5	27.5	27.0	29.5
20.5	28.0	26.5	30.0
21.0	28.6	25.2	29.2

Residual plots to check model assumptions

Tukey’s Test (Post-hoc test)

Lesson 273: Two-Way ANOVA in Minitab

Consider data (data does not seems to be complete)

Interest in Politics	Gender	Education Level
38.0	Male	School
39.0	Male	School
35.0	Male	School
38.0	Male	School
47.0	Male	School
41.0	Male	School
40.0	Male	School
36.0	Male	School
37.0	Male	School
31.0	Male	School
41.5	Male	College
54.5	Male	College
41.5	Male	College
44.5	Male	College
44.5	Male	College
44.0	Male	College
46.5	Male	College

Lesson 274: Factorial ANOVA in Minitab

274.1 Response Surface Design

Stat > DOE > Response Surface > Create Response Surface Design

Analysis of Response Surface Design

Stat > DOE > Response Surface > Analyze Response Surface Design...

