Experimental Design
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Contents

Chapter 1

Introduction

1.1 Notation and Nomenclature

EXAMPLE 1.1.1: Experiment 1 — List View vs. Tile View

Suppose that Nike, the athletic apparel company, is experimenting with their mobile shopping interface, and they are interested in determining whether changing the user interface from *list view* to *tile view* will increase the proportion of customers that proceed to checkout.

EXAMPLE 1.1.2: Experiment 2 — Ad Themes

Suppose that Nixon, the watch and accessories brand, is experimenting with four different video ads that are to be shown on Instagram. The first has a surfing theme, the second has a rock climbing theme, the third has a camping theme, and the fourth has an urban professional theme. Interest lies in determining which of the four themes, on average, is watched the longest.

DEFINITION 1.1.3: Metric of interest

The **metric of interest** (MOI) is the statistic we wish the experiment investigates.

REMARK 1.1.4

Typically, we want to optimize for the metric of interest; that is, we would like to either maximize or minimize it.

EXAMPLE 1.1.5: Metric of Interest

- Key performance indicators (KPIs): a statistic that quantifies something about a business.
    - Click-through rates (CTRs).
    - Bounce rate.
    - Average time on page.
    - 95th percentile page load time.
- *Nike Example*: checkout rate (COR).
- *Nixon Example*: average viewing duration (AVD).

DEFINITION 1.1.6: Response variable

The **response variable**, denoted y, is the variable of primary interest.

REMARK 1.1.7

The response variable is what needs to be measured in order for the MOI to be calculated.

EXAMPLE 1.1.8: Response Variable

- *Nike Example*: binary indicator indicating whether a customer checked out.
- *Nixon Example*: the continuous measurement of viewing duration for each user.

DEFINITION 1.1.9: Factor

The **factor**, denoted x, is the variable(s) of secondary interest.

Also known as: **covariates**, **explanatory variates**, **predictors**, **features**, **independent variables**.

REMARK 1.1.10

We usually think the factors influence the response (dependent) variable.

EXAMPLE 1.1.11: Factor

- *Nike Example*: the factor is the *visual layout*.
- *Nixon Example*: the factor is the *ad theme*.

DEFINITION 1.1.12: Experimental conditions

The **experimental conditions** are the unique combinations of levels of one or more factors.

Also known as: **treatments**, **variants**, **buckets**.

DEFINITION 1.1.13: Levels

The **levels** are the values that a factor takes on in an experiment.

EXAMPLE 1.1.14: Levels

- *Nike Example*: {tile view, list view}.
- *Nixon Example*: {surfing, rock climbing, camping, business}.

DEFINITION 1.1.15: Experimental units

The **experimental units** are what is assigned to the experimental conditions, and on which we measure the response variable.

EXAMPLE 1.1.16: Experimental Units

- *Nike Example*: Nike mobile customers.
- *Nixon Example*: Instagram users.

REMARK 1.1.17

Often, in online experiments, the unit is a user/customer (i.e., person), but it does not have to be.

EXAMPLE 1.1.18

Uber matching algorithm experiment.

1.2 Experiments versus Observational Studies

DEFINITION 1.2.1: Experiment

An **experiment** is a collection of conditions defined by *purposeful changes* to one or more factors. Here, we intervene in the data collection.

- The goal is to identify and quantify the differences in response variable values across conditions.

- In determining whether a factor significantly influences a response, like whether a video ad's theme significantly influences its AVD, it is necessary to understand how experimental units' response when exposed to each of the corresponding conditions.

- However, it would be nice if we could observe how the *same* units behave in each of the experimental conditions, but we can't. We only observe their response in a single condition.

- **Counterfactual**: the hypothetical and unobservable value of a unit's response in a condition to which they were not assigned. We may think of this as an "alternate reality."

    EXAMPLE 1.2.2

    Nixon Example: the "camping" response variable for units assigned to the "surfing" condition.

- Because counterfactual outcomes cannot be observed, we require a **proxy**. Instead, we randomly assign *different units* to *different experimental conditions*, and we compare their responses.

- Ideally, the only difference between the units in each condition is the fact that they are in different conditions.

    - We want the units to be as homogenous as possible, this will help facilitate **causal inference** (establishing causal connections between variables).

    - This is typically guaranteed by *randomization*.

- The key here is that we purposefully control the factors to observe the resulting effect on the response. This facilitates causal conclusions.

- In an **observational study**, on the other hand, there is no measure of control in the data collection process. Instead, we collect the data passively and the relationship between the response and factor(s) is observed organically.

- This hinders our ability to establish causal connections between the factor(s) and the response variables. However, sometimes we have no choice.

    EXAMPLE 1.2.3: Unethical Experiments

    - *Unethical Experiment 1*: In evaluating whether smoking lung cancer, it would be unethical to have a '*smoking*' condition in which we force the subjects to smoke.
    - *Unethical Experiment 2*: In dynamic pricing experiments, it would be unethical to show different users different prices for the same products. For example, surge pricing in Uber/Lyft.

– *Unethical Experiment 3*: In social contagion experiments, it would be unethical to show some network users consistently negative content and others consistently positive content. But Facebook did this anyway.
– *Unethical Experiment 4*: Mozilla conducted an investigation in which the company was interested in determining whether Firefox users that installed an ad blocker were more engaged with the browser. However, it would have been unethical to force users to install an ad blocker, and so they were forced to perform an observational study with *propensity score matching* instead.

	Advantages	*Disadvantages*
Experiment	Causal inference is clean.	Experiments might be unethical, risky, or costly.
Observational Study	No additional cost, risk, or ethical concerns.	Causal inference is muddy.

1.3 QPDAC: A Strategy for Answering Questions with Data
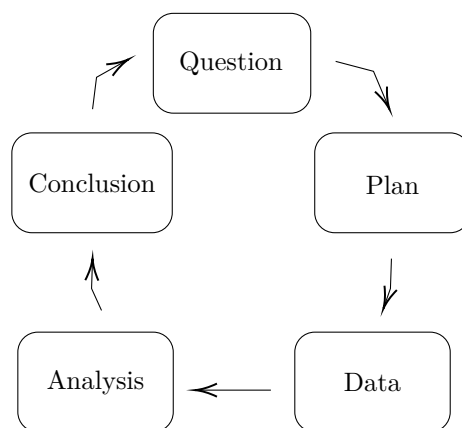
Figure 1.1: QPDAC Cycle

Question: Develop a clear statement of the question that needs to be answered.

- It is important that this is clear and concise and widely communicated, so all stakeholders are on the same page.
- The question should be quantifiable/measurable and typically stated in terms of the metric of interest.

EXAMPLE 1.3.1

- *Nike Example*: "which visual layout, tile view or list view, corresponds to the highest check-out rate?"
- *Nixon Example*: "which ad theme, camping, surfing, rock climbing, business, corresponds to the highest average viewing duration?"

Plan: In this stage, we design the experiment, and all pre-experimental questions should be answered.

- Choose the response variable. This should be dictated by the **Question** and the metric of interest.

- Choose the factor(s): brainstorm all factors that might influence the response and make decisions about whether and how they will be controlled in the experiment.

  i **Design factors**: factors that we will manipulate in the experiment. The factors we've discussed in the Nike and Nixon examples are design factors.

  ii **Nuisance factors**: factors that we expect to influence the response, but whose effect we do not care to quantify. Instead, we try to eliminate their effects with *blocking*.

  iii **Allowed-to-vary factors**: factors that we *cannot* control and factors that we are unaware of in an experiment.

     – *Nixon Example*: users' age, gender, nationality.

- Choose the experimental units. These are what we measure the response variable on.

- Choose the sample size and sampling mechanism.

  – Sample size: how many units per experimental condition?

  – Sampling mechanism: how are they selected?

Data: In this stage, we collect the data according to the **Plan**. It is extremely important that we do this step correctly; the suitability and effectiveness of the analysis relies on the correctness of the data. Computer scientists often use the phrase "garbage in, garbage out" to describe the phenomenon whereby poor quality input will always provide faulty output.

- A/A Test: we assign units to one of two *identical* conditions.

  – We do this to ensure the assignment of units to conditions is truly random.

  – Two groups should be indistinguishable in terms of response distribution and other demographics.

  – If things aren't indistinguishable, there is a problem.

  – *Sample Ratio Mismatch Test*: If the ratio of users (or any randomization unit) between the variants is not close to the designed ratio, the experiment suffers from a Sample Ratio Mismatch (SRM).

     * Hypothesis test can be used to determine whether the proportion of units in each condition match what would have been expected under random assignment.

Analysis: In this stage, we statistically analyze **Data** to provide an objective answer to the **Question**.

- This is typically achieved by way of estimating parameters, fitting models, and carrying out statistical hypothesis tests. This is where we spend most of our time in the course.

- If the experiment was well-designed, and we collected the data correctly, this step should be straight-forward.

Conclusion: In this stage, we consider the results of the **Analysis**, and one must draw conclusions about what has been learned.

- We clearly communicate these conclusions to all parties involved in — or impacted by — the experiment.

> • Communicating "wins" and "loses" will help to foster the culture of experimentation.

1.4 Fundamental Principles of Experimental Design

DEFINITION 1.4.1: Randomization

Randomization refers both to the manner in which we select experimental units for *inclusion* in the experiment and the manner in which we *assign* them to *experimental conditions*.

REMARK 1.4.2

Typically, we don't include the entire target/study population.

Thus, we have two levels of randomization:

- The first level of randomization exists to ensure the sample of units included in the experiment is *representative of those that were not.*
    - Allows us to generalize conclusions beyond just the experimental units to units in the population not in the experiment.
- The second level of randomization exists to *balance* the effects of *extraneous variables* not under study (i.e., the allowed-to-vary factors).
    - Balancing the effects of allowed-to-vary factors makes our conditions homogenous and thus best mimics the counterfactual, thereby making causal inference easy.

DEFINITION 1.4.3: Replication

Replication refers to the existence of multiple response observations within each experimental condition and thus corresponds to the situation in which we assign more than one unit to each condition.

- Assigning multiple units to each condition provides *assurance* that the observed results are genuine, and *not just due to chance.*
- For instance, consider the *Nike experiment* introduced previously. Suppose the CORs in the *list view* and *tile view* conditions were 0.5 and 1 respectively. This conclusion would be a lot more convincing if each condition had $n = 1000$ units as opposed to $n = 2$, where n is the sample size in *each* condition.
- How much replication do we need?
    - How big a sample size do we need?
    - Power analysis + sample size calculations will help answer this.

DEFINITION 1.4.4: Blocking

Blocking is the mechanism that we control the nuisance factors.

- To *eliminate* the influence of nuisance factors, we hold them fixed during the experiment.
- Thus, we run the experiment *at fixed levels of the nuisance factors*, i.e., within **blocks**.

  EXAMPLE 1.4.5: GAP — Email Promotion

  Consider an experiment in which the primary goal is to test different variations of the *message in the subject* line with the goal of maximizing '*open rate*.' However, suppose we know that the

'open rate' is also influenced by the "send time" (time of the day and the day of the week) of an email.

We send all the emails at the same time of day and on the same day of week to control/eliminate the effect of time/day nuisance factor. By *blocking*, in this way, the nuisance factor can't confound our conclusions.

Chapter 2

Experiments with Two Conditions

<div align="center">WEEK 2</div>

Anatomy of an A/B Test

- One design factor at two levels.

- We now consider the design and analysis of an experiment consisting of two experimental conditions — or what many data scientists broadly refer to as "A/B Testing" which is synonymous with "experimentation" in data science.

  - Canonical A/B test:

Figure 2.1: Canonical Button Colour Test.

  Here, the metric of interest might be click-through-rate, which we're interested in maximizing.

- Other, more tangible examples:

  - Amazon

    * Checkout reassurances

    * List view vs. tile view

  - Airbnb

    * Host landing page redesign

    * Next available date

- Typically, the goal of such an experiment is to decide which condition is optimal with respect to some metric of interest θ. This could be a

  - mean (e.g., average time on page, average purchase size, average revenue per customer)

  - proportion (e.g., CTR, bounce rate, retention rate)

  - variance

- quantile (e.g., median, 95th percentile of page load time)

- technically any statistic that can be from sample data

- Consider the button-colour example: imagine the observed click-through-rates (CTR) of the two conditions are: $\hat{\theta}_1 = 0.12$ (red) and $\hat{\theta}_2 = 0.03$ (blue).

  - Obviously, $\hat{\theta}_1 > \hat{\theta}_2$, but does that mean that $\theta_1 > \theta_2$?

- Formally, we phrase such a question as a statistical hypothesis that we test using the data collected from the experiment.

  - **H$_0$**: $\theta_1 = \theta_2$ versus **H$_\text{A}$**: $\theta_1 \neq \theta_2$ (two-sided).

  - **H$_0$**: $\theta_1 \leq \theta_2$ versus **H$_\text{A}$**: $\theta_1 > \theta_2$ (one-sided).

  - **H$_0$**: $\theta_1 \geq \theta_2$ versus **H$_\text{A}$**: $\theta_1 < \theta_2$ (one-sided).

- "Absence of evidence $\neq$ evidence of absence."

- No matter which hypothesis is appropriate, the goal is always the same: based on the observed data, we will decide to *reject* **H$_0$** or *not reject* **H$_0$**.

- In order to draw such a conclusion, we will define a **test statistic**.

> DEFINITION 2.0.1: Test statistic
>
> The **test statistic**, denoted T, is a random variable that satisfies three properties:
>   (i) It must be a function of the observed data.
>   (ii) It must be a function of the parameters θ_1 and θ_2.
>   (iii) Its distribution must not depend on θ_1 or θ_2.

- Assuming the null hypothesis is true, the test statistic T follows a particular distribution which we call the **null distribution**. For example, $\mathcal{N}(0,1)$, $t(\texttt{df})$, $F(\texttt{df1}, \texttt{df2})$, $\chi^2(\texttt{df})$.

- We then calculate t, the observed value of the test statistic, and evaluate its extremity relative to the null distribution.

  - If t is very extreme, this suggests that perhaps the null hypothesis is not true.

  - If t appears as though it could have come from the null distribution, then there is no reason to disbelieve the null hypothesis.

- We formalize the extremity of t using the **p-value** of the test.

> DEFINITION 2.0.2: **p**-value
>
> The probability of observing a value of the test statistic *at least as extreme* as the value we observed, if the null hypothesis is true.

  - Thus, the p-value formally quantifies how "extreme" the observed test statistic is.

  - The more extreme the value of t, the smaller the p-value, and the more evidence we have against it.

- How "extreme" t must be, and hence how small the p-value must be to reject **H$_0$**, is determined by the **significance level** of the test, denoted α.

  - If p-value $\leq \alpha$, we reject **H$_0$**.

  - If p-value $> \alpha$, we do not reject **H$_0$**.

> REMARK 2.0.3
>
> Common choices of α are 0.05 and 0.01.

- In order to choose α, one must understand the two types of errors that can be made when drawing conclusions in the context of a hypothesis test.

- Recall that by design, either $\mathbf{H}_0$ or $\mathbf{H}_A$ is true. This means that there are four possible outcomes when using data to decide which statement is true:

  (1) No Error: $\mathbf{H}_0$ is true, and we correctly do not reject it.

  (2) Type I Error: $\mathbf{H}_0$ is true, and we incorrectly reject it.

  (3) Type II Error: $\mathbf{H}_0$ is false, and we incorrectly do not reject it.

  (4) No Error: $\mathbf{H}_0$ is false, and we correctly reject it.

- We would like to reduce the likelihood of making either type of error.

  - But there are different consequences of each type of error.

  - So we may wish to treat them differently.

> EXAMPLE 2.0.4: Pregnancy Test
>
> $$\mathbf{H}_0\text{: person is not pregnant versus } \mathbf{H}_A\text{: person is pregnant.}$$
> - Type I Error: a non-pregnant person is pregnant (false positive).
> - Type II Error: a pregnant person is not pregnant (false negative).

> EXAMPLE 2.0.5: Courtroom
>
> Consider a courtroom analogy where we assume the defendant is innocent until proven guilty. Formally,
> $$\mathbf{H}_0\text{: the defendant is innocent versus } \mathbf{H}_A\text{: the defendant is guilty.}$$
> - Type I Error: sentencing an innocent person to jail.
> - Type II Error: letting a guilty person go free.

> DEFINITION 2.0.6: Significance level
>
> The **significance level** of a test is $\alpha = \mathbb{P}(\text{Type I Error})$.

> DEFINITION 2.0.7: Power
>
> The **power** of a test is $1 - \beta$ where $\beta = \mathbb{P}(\text{Type II Error})$.

- Fortunately, it is possible to control the frequency in which these types of errors occur.

- It is desirable to have a test with a small significance level, and a large power.

2.1 Comparing Means in Two Conditions

- Here, we restrict attention to the situation in which we measure the response variable of interest on a continuous scale.

- We assume that the response observations collected in the two conditions follow normal distributions, and in particular

$$Y_{i1} \sim \mathcal{N}(\mu_1, \sigma^2) \text{ and } Y_{i2} \sim \mathcal{N}(\mu_2, \sigma^2), \quad i = 1, 2, \dots, n_j \text{ for } j = 1, 2.$$

  - Y_{ij} = response observation for unit i in condition j.

- Using the observed data, we test hypotheses of the form:

  - **H$_0$**: $\mu_1 = \mu_2$ versus **H$_A$**: $\mu_1 \neq \mu_2$.
  - **H$_0$**: $\mu_1 \leq \mu_2$ versus **H$_A$**: $\mu_1 > \mu_2$.
  - **H$_0$**: $\mu_1 \geq \mu_2$ versus **H$_A$**: $\mu_1 < \mu_2$.

2.1.1 The Two-Sample t-Test

STATISTICAL TEST 2.1.1: Student's $\boldsymbol{t}$-test

- *Purpose*: Compare μ_1 versus μ_2 (assuming $\sigma_1 = \sigma_2$ are unknown).
- *Test Statistic*:

$$T = \frac{(\bar{Y}_1 - \bar{Y}_2) - \overbrace{(\mu_1 - \mu_2)}^{0}}{\hat{\sigma}\sqrt{\dfrac{1}{n_1} + \dfrac{1}{n_2}}} \sim t(n_1 + n_2 - 2)$$

  - $\hat{\sigma}$ is our estimator.
  - $t(n_1 + n_2 - 2)$ is our null distribution.
- *Observed Version*:

$$t = \frac{(\bar{y}_1 - \bar{y}_2) - 0}{\hat{\sigma}\sqrt{\dfrac{1}{n_1} + \dfrac{1}{n_2}}} = \frac{\hat{\mu}_1 - \hat{\mu}_2}{\hat{\sigma}\sqrt{\dfrac{1}{n_1} + \dfrac{1}{n_2}}}$$

  - $\bar{y}_j = \dfrac{1}{n_j} \sum\limits_{i=1}^{n_j} y_{ij} = \hat{\mu}_j$.
  - $\hat{\sigma}^2 = \dfrac{(n_1 - 1)\hat{\sigma}_1^2 + (n_2 - 1)\hat{\sigma}_2^2}{n_1 + n_2 - 2}$.
  - $\hat{\sigma}_j^2 = \dfrac{1}{n_j - 1} \sum\limits_{i=1}^{n_j} (y_{ij} - \bar{y}_j)^2$.
- *p-value Calculation*:
  - For **H$_0$**: $\mu_1 = \mu_2$ versus **H$_A$**: $\mu_1 \neq \mu_2$, we compute p-value $= \mathbb{P}(T \geq |t|) + \mathbb{P}(T \leq -|t|)$.
  - For **H$_0$**: $\mu_1 \leq \mu_2$ versus **H$_A$**: $\mu_1 > \mu_2$, we compute p-value $= \mathbb{P}(T \geq t)$.
  - For **H$_0$**: $\mu_1 \geq \mu_2$ versus **H$_A$**: $\mu_1 < \mu_2$, we compute p-value $= \mathbb{P}(T \leq t)$.

  REMARK 2.1.2

  In all cases above, $T \sim t(n_1 + n_2 - 2)$.

2.1.2 When Assumptions are Invalid

STATISTICAL TEST 2.1.3: Welch's $\boldsymbol{t}$-test

- *Purpose*: Compare μ_1 versus μ_2 (assuming $\sigma_1 \neq \sigma_2$ are unknown).
- *Test Statistic*: "Approximately," we have

$$T = \frac{(\bar{Y}_1 - \bar{Y}_2) - \overbrace{(\mu_1 - \mu_2)}^{0}}{\sqrt{\dfrac{\hat{\sigma}_1^2}{n_1} + \dfrac{\hat{\sigma}_2^2}{n_2}}} \,\dot{\sim}\, t(\nu)$$

where

$$\nu = \frac{\left(\frac{\hat{\sigma}_1^2}{n_1} + \frac{\hat{\sigma}_2^2}{n_2}\right)^2}{\frac{(\hat{\sigma}_1^2/n_1)^2}{n_1 - 1} + \frac{(\hat{\sigma}_2^2/n_2)^2}{n_2}} \approx \min(n_1, n_2) - 1$$

- *Observed Version*:

$$t = \frac{(\bar{y}_1 - \bar{y}_2) - 0}{\sqrt{\frac{\hat{\sigma}_1^2}{n_1} + \frac{\hat{\sigma}_2^2}{n_2}}} = \frac{\hat{\mu}_1 - \hat{\mu}_2}{\sqrt{\frac{\hat{\sigma}_1^2}{n_1} + \frac{\hat{\sigma}_2^2}{n_2}}}$$

- *p-value Calculation*: Same as Statistical Test 2.1.1, but where the null distribution is $T \sim t(\nu)$.

STATISTICAL TEST 2.1.4: **F**-test for Variances

- *Purpose*:
    - $\mathbf{H}_0$: $\sigma_1^2 = \sigma_2^2$ versus $\mathbf{H}_A$: $\sigma_1^2 \neq \sigma_2^2$.
    - $\mathbf{H}_0$: $\sigma_1^2/\sigma_2^2 = 1$ versus $\mathbf{H}_A$: $\sigma_1^2/\sigma_2^2 \neq 1$.
- *Test Statistic*:

$$T = \frac{\hat{\sigma}_1^2}{\hat{\sigma}_2^2} \sim F(n_1 - 1, n_2 - 1)$$

- *Observed Version*:

$$t = \frac{\hat{\sigma}_1^2}{\hat{\sigma}_2^2} \in \mathbf{R}$$

- *p-value Calculation*:
    - If $t \geq 1$, then p-value $= \mathbb{P}(T \geq t) + \mathbb{P}(T \leq 1/t)$.
    - If $t < 1$, then p-value $= \mathbb{P}(T \leq t) + \mathbb{P}(T \geq 1/t)$.

REMARK 2.1.5

In all cases above, $T \sim F(n_1 - 1, n_2 - 1)$.

2.1.3 Example: Instagram Ad Frequency

EXAMPLE 2.1.6: Instagram Ad frequency

- Suppose that you are a data scientist at Instagram, and you are interested in running an experiment to learn about the influence of ad frequency on user engagement.
- Currently, users see an ad every 8 posts in their social feed, but, in order to increase ad revenue, your manager is pressuring your team to show an ad every 5 posts.
    - Condition 1: 7:1 Ad Frequency
    - Condition 2: 4:1 Ad Frequency
- You are justifiably nervous about this change, and you worry that this will substantially decrease user engagement and hurt the overall user experience.
- The metric of interest you choose to optimize for is μ = average session time (where y = the length of time a user engages within the app, in minutes).
- The hypothesis here is:

$$\mathbf{H}_0: \mu_1 \leq \mu_2 \text{ versus } \mathbf{H}_A: \mu_1 > \mu_2$$

- The data summaries are:
    - $n_1 = 500$, $\hat{\mu}_1 = \bar{y}_1 = 4.92$, $\hat{\sigma}_1 = s_1 = 0.96$.
    - $n_2 = 500$, $\hat{\mu}_2 = \bar{y}_2 = 3.05$, $\hat{\sigma}_2 = s_2 = 0.99$.

F-test:
- $t = \hat{\sigma}_1^2 / \hat{\sigma}_2^2 = 0.96^2 / 0.99^2 = 0.938$.
- p-value $= \mathbb{P}(T \leq 0.938) + \mathbb{P}(T \geq 1/0.938) = 0.4720$ where $T \sim F(499, 499)$.
- This p-value is larger than any ordinary α, so we do not reject $\mathbf{H}_0$: $\sigma_1^2 = \sigma_2^2$, and so we continue with Student's t-test.

Student's t-test:
- $\hat{\sigma}^2 = \dfrac{499(0.96)^2 + 499(0.99)^2}{998} = 0.9793^2$.
- $t = \dfrac{4.92 - 3.05}{0.9793\sqrt{\frac{1}{500} + \frac{1}{500}}} = 30.1$.
- p-value $= \mathbb{P}(T \geq 30.1) = 1.84 \times 10^{-142} \approx 0$ where $T \sim t(998)$.
- This p-value is much smaller than any typical α, and so we reject $\mathbf{H}_0$: $\mu_1 \leq \mu_2$, and conclude that increasing ad frequency significantly reduces average session duration.

[R Code] `Comparing_two_means`

2.2 Comparing Proportions in Two Conditions

- Here, we restrict attention to the situation in which the response variable of interest is binary, indicating whether an experimental unit did, or did not, perform some action of interest. In cases like these, we let

$$Y_{ij} = \begin{cases} 1 & \text{if unit } i \text{ in condition } j \text{ performs an action of interest} \\ 0 & \text{if unit } i \text{ in condition } j \text{ does not perform an action of interest} \end{cases} \quad \begin{aligned} i &= 1, 2, \dots, n_j \\ j &= 1, 2 \end{aligned}$$

- Because the Y_{ij}'s are binary, it is common to assume that they follow a Bernoulli distribution; that is, $Y_{ij} \sim \text{Binomial}(1, \pi_j)$ where π_j represents the probability that $Y_{ij} = 1$. That is, the probability that unit i from condition j performs the "action of interest."

- Using the observed data, we test hypotheses of the form:

    - $\mathbf{H}_0$: $\pi_1 = \pi_2$ versus $\mathbf{H}_A$: $\pi_1 \neq \pi_2$.

    - $\mathbf{H}_0$: $\pi_1 \leq \pi_2$ versus $\mathbf{H}_A$: $\pi_1 > \pi_2$.

    - $\mathbf{H}_0$: $\pi_1 \geq \pi_2$ versus $\mathbf{H}_A$: $\pi_1 < \pi_2$.

2.2.1 *Z*-tests for Proportions

STATISTICAL TEST 2.2.1: **Z**-test for Proportions

- *Purpose*: Compare π_1 versus π_2.
- *Test Statistic*: "Approximately," we have

$$T = \frac{(\bar{Y}_1 - \bar{Y}_2) - \overset{0}{\overbrace{(\pi_1 - \pi_2)}}}{\sqrt{\hat{\pi}(1 - \hat{\pi})\left(\dfrac{1}{n_1} + \dfrac{1}{n_2}\right)}} \ \dot{\sim}\ \mathcal{N}(0, 1)$$

where $\hat{\pi} = \dfrac{n\hat{\pi}_1 + n_2\hat{\pi}_2}{n_1 + n_2} = \dfrac{\#\text{ units who performed action}}{\text{total \# units in exp.}}$ and $\hat{\pi}_j = \bar{y}_j$.

- *Observed Version*:

$$t = \frac{(\bar{y}_1 - \bar{y}_2) - 0}{\sqrt{\hat{\pi}(1 - \hat{\pi})\left(\dfrac{1}{n_1} + \dfrac{1}{n_2}\right)}} = \frac{\hat{\pi}_1 - \hat{\pi}_2}{\sqrt{\hat{\pi}(1 - \hat{\pi})\left(\dfrac{1}{n_1} + \dfrac{1}{n_2}\right)}}$$

- *p-value Calculation*: The *p*-values are calculated in the same way as in the *t*-tests, except here that $T \sim \mathcal{N}(0, 1)$.

2.2.2 Example: Optimizing Optimizely

EXAMPLE 2.2.2: Optimizing Optimizely

- During a website redesign, Optimizely was interested in how new versions of certain pages influenced things like conversion and engagement relative to the old version.
- One outcome they were interested in was whether the redesigned homepage lead to a significant increase in the number of new accounts created.
  - Condition 1: original homepage.
  - Condition 2: redesigned homepage.
- The metric of interest here is $\pi = $ conversion rate (where $y = 1$ if a homepage visitor signed up and 0 otherwise).
- The hypothesis tested here is:
$$\mathbf{H}_0\text{: } \pi_1 \geq \pi_2 \text{ versus } \mathbf{H}_A\text{: } \pi_1 < \pi_2$$
- We summarize the data from this experiment in a 2×2 contingency table:

		Condition		
		1	2	
Conversion	Yes	280	399	679
	No	8592	8243	16835
		8872	8642	17514

- $\hat{\pi}_1 = 280/8872 = 0.0316$ and $\hat{\pi}_2 = 399/8642 = 0.0462$. Thus,

$$\hat{\pi} = \frac{8872(0.0316) + 8642(0.0462)}{17514}$$

$$t = \frac{0.0316 - 0.0462}{\sqrt{(0.0388)(1 - 0.0388)(1/8872 + 1/8642)}} = -5.002$$

- *p*-value $= \mathbb{P}(T \leq -5.002) = 2.84 \times 10^{-7} \approx 0$ where $T \sim \mathcal{N}(0, 1)$.
- We reject $\mathbf{H}_0$ and conclude that the redesigned homepage significantly increases conversion rate.
- [R Code] Comparing_two_proportions

2.3 Power Analysis and Sample Size Calculations

- Used to control Type II Error.

- Power analyses help determine required sample sizes.

- Suppose, for illustration, that we are interested in testing the hypothesis:
$$\mathbf{H}_0\text{: } \theta_1 = \theta_2 \text{ versus } \mathbf{H}_A\text{: } \theta_1 \neq \theta_2$$

- Suppose, also for illustration, that the test statistic associated with this test has the form:

$$T = \frac{(\bar{Y}_1 - \bar{Y}_2) - \overset{0}{\overline{(\theta_1 - \theta_2)}}}{\sqrt{\dfrac{\mathbb{V}(Y_1)}{n} + \dfrac{\mathbb{V}(Y_2)}{n}}} \sim \mathcal{N}(0, 1)$$

DEFINITION 2.3.1: Rejection region

The **rejection region**, denoted $\mathcal{R}$, is all the values of the observed test statistic t that would lead to the rejection of $\mathbf{H}_0$:

$$\mathcal{R} = \{t : \mathbf{H}_0 \text{ is rejected}\}$$

- If $t \in \mathcal{R}$, we reject $\mathbf{H}_0$.
- If $t \in \mathcal{R}^c$, we do not reject $\mathbf{H}_0$.

Figure 2.2: $\mathbf{H}_0$: $\theta_1 = \theta_2$ versus $\mathbf{H}_A$: $\theta_1 \neq \theta_2$
$\mathcal{R} = \{t : t \leq -z_{\alpha/2} \text{ or } t \geq z_{\alpha/2}\}$

Figure 2.3: $\mathbf{H}_0$: $\theta_1 \leq \theta_2$ versus $\mathbf{H}_A$: $\theta_1 > \theta_2$
$\mathcal{R} = \{t : t \geq z_\alpha\}$

- Defining Type I and Type II error rates in terms of a rejection region is also useful:
    - $\alpha = \mathbb{P}(\text{Type I Error}) = \mathbb{P}(\text{Reject } \mathbf{H}_0 \mid \mathbf{H}_0 \text{ is true}) = \mathbb{P}(T \in \mathcal{R} \mid \mathbf{H}_0 \text{ is true})$.
    - $\beta = \mathbb{P}(\text{Type II Error}) = \mathbb{P}(\text{Do Not Reject } \mathbf{H}_0 \mid \mathbf{H}_0 \text{ is false}) = \mathbb{P}(T \in \mathcal{R}^c \mid \mathbf{H}_0 \text{ is false})$.
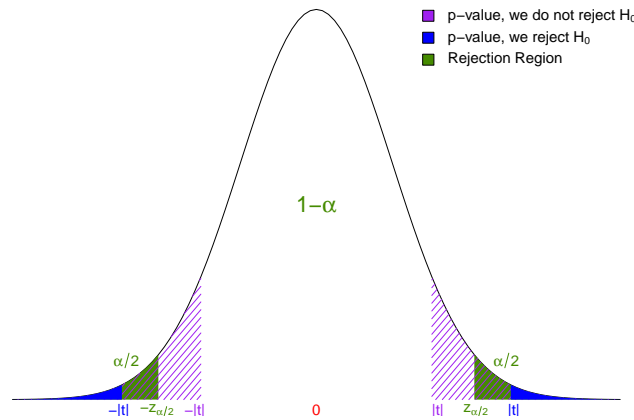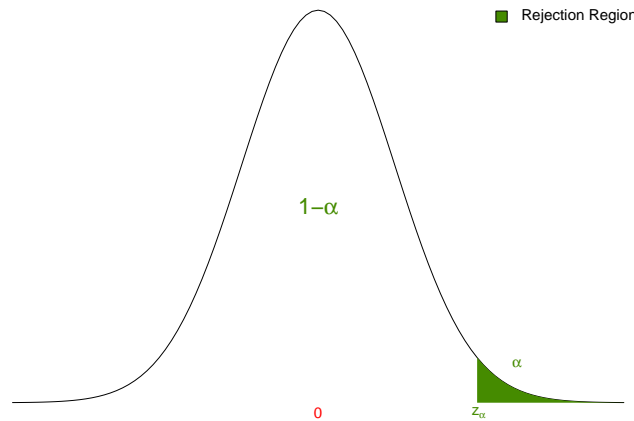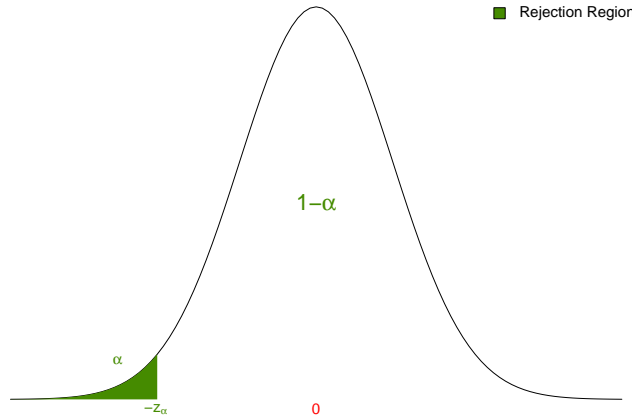
Figure 2.4: $\mathbf{H}_0$: $\theta_1 \geq \theta_2$ versus $\mathbf{H}_\mathrm{A}$: $\theta_1 < \theta_2$
$$\mathcal{R} = \{t : t \leq -z_\alpha\}$$

$$
\begin{aligned}
1 - \beta &= \text{Power} \\
&= 1 - \mathbb{P}(\text{Type II Error}) \\
&= 1 - \mathbb{P}(T \in \mathcal{R}^c \mid \mathbf{H}_0 \text{ is false}) \\
&= \mathbb{P}(T \in \mathcal{R} \mid \mathbf{H}_0 \text{ is false}) \\
&= \mathbb{P}\big(T \geq z_{\alpha/2} \cup T \leq -z_{\alpha/2} \,\big|\, \mathbf{H}_0 \text{ is false}\big) \\
&= \mathbb{P}\big(T \geq z_{\alpha/2} \,\big|\, \mathbf{H}_0 \text{ is false}\big) + \mathbb{P}\big(T \leq -z_{\alpha/2} \,\big|\, \mathbf{H}_0 \text{ is false}\big) \\
&= \mathbb{P}\left(\frac{\bar{Y}_1 - \bar{Y}_2}{\sqrt{\frac{\mathbb{V}(Y_1)+\mathbb{V}(Y_2)}{n}}} \geq z_{\alpha/2} \,\bigg|\, \mathbf{H}_0 \text{ is false} \right) + \mathbb{P}\left(\frac{\bar{Y}_1 - \bar{Y}_2}{\sqrt{\frac{\mathbb{V}(Y_1)+\mathbb{V}(Y_2)}{n}}} \leq -z_{\alpha/2} \,\bigg|\, \mathbf{H}_0 \text{ is false} \right)
\end{aligned}
$$

Assuming $\mathbf{H}_0$ is true, $\theta_1 - \theta_2 = 0$ and $\dfrac{\bar{Y}_1 - \bar{Y}_2}{\sqrt{\frac{\mathbb{V}(Y_1)+\mathbb{V}(Y_2)}{n}}} \sim \mathcal{N}(0,1)$. However, $\mathbf{H}_0$ is false, which means that $\theta_1 - \theta_2 = \delta$ for some $\delta \neq 0$. Thus,

$$\frac{(\bar{Y}_1 - \bar{Y}_2) - \delta}{\sqrt{\frac{\mathbb{V}(Y_1)+\mathbb{V}(Y_2)}{n}}} \sim \mathcal{N}(0,1)$$

Therefore, we need to account for this. Let $Z \sim \mathcal{N}(0,1)$, then

$$
\begin{aligned}
1 - \beta &= \mathbb{P}\left(\frac{(\bar{Y}_1 - \bar{Y}_2) - \delta}{\sqrt{\frac{\mathbb{V}(Y_1)+\mathbb{V}(Y_2)}{n}}} \geq z_{\alpha/2} - \frac{\delta}{\sqrt{\frac{\mathbb{V}(Y_1)+\mathbb{V}(Y_2)}{n}}} \right) + \mathbb{P}\left(\frac{(\bar{Y}_1 - \bar{Y}_2) - \delta}{\sqrt{\frac{\mathbb{V}(Y_1)+\mathbb{V}(Y_2)}{n}}} \leq -z_{\alpha/2} - \frac{\delta}{\sqrt{\frac{\mathbb{V}(Y_1)+\mathbb{V}(Y_2)}{n}}} \right) \\
&= \mathbb{P}\left(Z \geq z_{\alpha/2} - \frac{\delta}{\sqrt{\frac{\mathbb{V}(Y_1)+\mathbb{V}(Y_2)}{n}}} \right) + \mathbb{P}\left(Z \leq -z_{\alpha/2} - \frac{\delta}{\sqrt{\frac{\mathbb{V}(Y_1)+\mathbb{V}(Y_2)}{n}}} \right)
\end{aligned}
$$

Think about what happens to these terms when δ is positive versus negative. Without loss of generality, assume $\delta > 0$, in which case

$$1 - \beta = \mathbb{P}\left(Z \geq z_{\alpha/2} - \frac{\delta}{\sqrt{\frac{\mathbb{V}(Y_1)+\mathbb{V}(Y_2)}{n}}} \right)$$

We know that $\mathbb{P}\big(Z \geq z_{1-\beta}\big) = 1 - \beta$, therefore

$$z_{1-\beta} = z_{\alpha/2} - \frac{\delta}{\sqrt{\frac{\mathbb{V}(Y_1)+\mathbb{V}(Y_2)}{n}}}$$

Doing some algebra yields

$$n = \frac{(z_{\alpha/2} - z_{1-\beta})^2 [\mathbb{V}(Y_1) + \mathbb{V}(Y_2)]}{\delta^2}$$

- $\mathbb{V}(Y_1)$ and $\mathbb{V}(Y_2)$ are the variances of the response in the two conditions. This needs to be guessed or determined by historical information.

- $\delta = \theta_1 - \theta_2$ is called the **minimum detectable effect** (MDE).

> DEFINITION 2.3.2: Minimum detectable effect (MDE)
>
> The **minimum detectable effect**, denoted δ, is the smallest difference between conditions (i.e, between θ_1 and θ_2) that we find to be practically relevant and that we would like to detect as being statistically significant.

WEEK 3

2.4 Permutation and Randomization Tests

- All the previous tests have made some kind of distributional assumption for the response measurements, such as $Y_{ij} \sim \mathcal{N}(\mu_j, \sigma^2)$ or $Y_{ij} \sim \text{Binomial}(1, \pi_j)$.

- It would be preferable to have a test that does not rely on *any* assumptions.

- This is precisely the purpose of permutation and randomization tests.

  - These tests are *non-parametric* and rely on resampling.

  - The motivation is that if $\mathbf{H}_0$: $\theta_1 = \theta_2$ is true, any random rearrangement of the data is *equally likely to have been observed*. If $\mathbf{H}_0$ is true, then we have a single population/distribution from which our data has been drawn.

  - With n_1 and n_2 units in each condition, there are

  $$\text{Binomial}(n_1 + n_2)n_1 = \text{Binomial}(n_1 + n_2)n_2$$

  arrangements of the $n_1 + n_2$ observations into two groups of size n_1 and n_2 respectively.

  $$n_1 = n_2 = 50 \implies \text{Binomial}(n_1 + n_2)n_1 = \text{Binomial}(100)50 = 1.0089 \times 10^{29}$$

- A true **permutation test** considers *all possible rearrangements* of the original data.

  - The test statistic t is calculated on the original data and on every one of its rearrangements.

  - This collection of test statistic values generate the empirical null distribution.

- In a **randomization test**, we do not consider all possible rearrangements.

  - We just consider a large number N of them.

  - We use this in practice instead of a permutation test because the exact permutation tests have too many permutations to consider.

Randomization Test Algorithm

1. Collect response observations in each condition.

$$\{y_{11}, y_{21}, \ldots, y_{n_1 1}\} \rightarrow \hat{\theta}_1$$

$$\{y_{12}, y_{22}, \ldots, y_{n_2 2}\} \rightarrow \hat{\theta}_2$$

2. Calculate the test statistic t on the original data.

$$t = \hat{\theta}_1 - \hat{\theta}_2 \quad \text{or} \quad t = \frac{\hat{\theta}_1}{\hat{\theta}_2}$$

3. Pool all the observations together and randomly sample (without replacement) n_1 observations which will be assigned to "Condition 1" and the remaining n_2 observations that are assigned to "Condition 2." Repeat this N times.

$$\{y_{11}^\star, y_{21}^\star, \dots, y_{n_1 1}^\star\} \to \hat{\theta}_1^\star$$

$$\{y_{12}^\star, y_{22}^\star, \dots, y_{n_2 2}^\star\} \to \hat{\theta}_2^\star$$

4. Calculate the test statistic $t_k^\star$ on each of the "shuffled" datasets, $k = 1, 2, \dots, N$.

$$t_k^\star = \hat{\theta}_{1,k}^\star - \hat{\theta}_{2,k}^\star \quad \text{or} \quad t_k^\star = \frac{\hat{\theta}_{1,k}^\star}{\hat{\theta}_{2,k}^\star}$$

5. Compare to t to $\{t_1^\star, t_2^\star, \dots, t_N^\star\}$, the empirical null distribution, and calculate the p-value:

$$p\text{-value} = \frac{\# \text{ of } t^\star\text{'s that are at least as extreme as } t}{N} = \frac{1}{N} \sum_{k=1}^{N} \mathbb{I}\{t_k^\star \text{ at least as extreme as } t\}$$

- $\mathbf{H}_0$: $\theta_1 = \theta_2$ versus $\mathbf{H}_A$: $\theta_1 \neq \theta_2$. If $t = \hat{\theta}_1 - \hat{\theta}_2$, then the p-value is:

$$p\text{-value} = \frac{1}{N} \sum_{k=1}^{N} \mathbb{I}\{t_k^\star \geq |t| \cup t_k^\star \leq -|t|\}$$

- $\mathbf{H}_0$: $\theta_1 \geq \theta_2$ versus $\mathbf{H}_A$: $\theta_1 < \theta_2$. If $t = \hat{\theta}_1 - \hat{\theta}_2$, then the p-value is:

$$p\text{-value} = \frac{1}{N} \sum_{k=1}^{N} \mathbb{I}\{t_k^\star \leq t\}$$

- $\mathbf{H}_0$: $\theta_1 \leq \theta_2$ versus $\mathbf{H}_A$: $\theta_1 > \theta_2$. If $t = \hat{\theta}_1 - \hat{\theta}_2$, then the p-value is:

$$p\text{-value} = \frac{1}{N} \sum_{k=1}^{N} \mathbb{I}\{t_k^\star \geq t\}$$

EXAMPLE 2.4.1: Pokémon Go

- Suppose that Niantic Inc, is experimenting with two different promotions within Pokémon Go:
    - Condition 1: Give users nothing.
    - Condition 2: Give users 200 free Pokécoins.
    - Condition 3: Give users a 50% discount on Shop purchases.
- In a small pilot experiment, we randomize $n_1 = n_2 = n_3 = 100$ users to each condition.
- For each user, we record the amount of real money (in USD) they spend in the 30 days following the experiment.
- The data summaries are:

    – $\bar{y}_1 = \$10.74$, $Q_{y_1}(0.5) = \$9$.
    – $\bar{y}_2 = \$9.53$, $Q_{y_2}(0.5) = \$8$.
    – $\bar{y}_3 = \$13.41$, $Q_{y_3}(0.5) = \$10$.
Using R, we performed a randomization test with $N = 10\,000$ with respect to the mean we found that the control and free coin conditions did not significantly differ. But there was a significant increase in the amount of money spent in the discount condition relative to the other two.

The hypotheses that we tested to determine these conclusions were:
$$\mathbf{H}_0\text{: } \mu_1 = \mu_2 \text{ versus } \mathbf{H}_A\text{: } \mu_1 \neq \mu_2$$
$$\mathbf{H}_0\text{: } \mu_1 \geq \mu_2 \text{ versus } \mathbf{H}_A\text{: } \mu_1 < \mu_2$$
Interestingly, when you run these same tests, but on the basis of the median, we find no significant difference between any of the conditions.

- [R Code] `Randomization_test`

Chapter 3

Experiments with More than Two Conditions

Anatomy of an "A/B/m" Test

- One design factor at m levels.

- We will now consider a design and analysis of an experiment consisting of more than two experimental conditions — or what many data scientists broadly refer to as "A/B/m Testing."

  - Canonical A/B/m test:

Figure 3.1: Canonical Button Colour Test.

    What colour maximizes click-through rate?

- Other, more tangible, examples:

  - Netflix.

  - Etsy.

- Typically, the goal of such an experiment is to decide which condition is optimal with respect to some metric of interest θ. This could be a:

  - mean

  - proportion

  - variance

  - quantile

  - technically any statistic that can be calculated from sample data

- From a design standpoint, such an experiment is *very* similar to a two-condition experiment.

  1. Choose a metric of interest θ which addresses the question you are trying to answer.

  2. Determine the response variable y that must be measured on each unit to estimate $\hat{\theta}$.

3. Choose the design factor x and the m levels you will experiment with.

4. Choose $n_1, n_2, \ldots, n_m$ and assign units to conditions at random.

5. Collect the data and estimate the metric of interest in each condition:

$$\hat{\theta}_1, \hat{\theta}_2, \ldots, \hat{\theta}_m$$

- Determining which condition is optimal typically involves a series of pairwise comparisons: t-tests, z-tests, or randomization tests.

- But it is useful to begin such an investigation with a *gatekeeper* test (test of overall equality) which serves to determine whether there is *any* difference between the m experimental conditions. Formally, we phrase such a question as the following statistical hypothesis:
$$\mathbf{H}_0:\ \theta_1 = \theta_2 = \cdots = \theta_m \text{ versus } \mathbf{H}_A:\ \theta_j \neq \theta_k \text{ for some } j \neq k$$
In the case of means:
$$\mathbf{H}_0:\ \mu_1 = \mu_2 = \cdots = \mu_m \text{ versus } \mathbf{H}_A:\ \mu_j \neq \mu_k \text{ for some } j \neq k$$
In the case of proportions:
$$\mathbf{H}_0:\ \pi_1 = \pi_2 = \cdots = \pi_m \text{ versus } \mathbf{H}_A:\ \pi_j \neq \pi_k \text{ for some } j \neq k$$

3.1 Comparing Means in Multiple Conditions

- We assume that our response variable follows a normal distribution, and we assume that the mean of the distribution depends on the condition in which we take the measurements, and that the variance is the same across all conditions.

$$Y_{ij} \sim \mathcal{N}(\mu_j, \sigma^2) \quad \text{for } i = 1, 2, \ldots, n_j \text{ and } j = 1, 2, \ldots, m$$

- We use an F-test to test for means:
$$\mathbf{H}_0:\ \mu_1 = \mu_2 = \cdots = \mu_m \text{ versus } \mathbf{H}_A:\ \mu_j \neq \mu_k \text{ for some } j \neq k$$

3.1.1 The F-test for Overall Significance in a Linear Regression

- In particular, we use the F-test for overall significance in an *appropriately defined linear regression model*:

  - The *appropriately defined linear regression model* in this situation is one in which the response variable depends on $m - 1$ indicator variables:

  $$x_{ij} = \begin{cases} 1 & \text{if unit } i \text{ is in condition } j \\ 0 & \text{otherwise} \end{cases} \quad \text{for } j = 1, 2, \ldots, m - 1.$$

  - For a particular unit i, we adopt the model:

  $$Y_i = \beta_0 + \beta_1 x_{i1} + \beta_2 x_{i2} + \cdots + \beta_{m-1} x_{i,m-1} + \varepsilon_i$$

    * Y_i = response observation for unit $i = 1, 2, \ldots, N = \sum_{j=1}^{m} n_j$.

    * ε_i = random error term which we assume follows a $\mathcal{N}(0, \sigma^2)$ distribution independently for all $i = 1, 2, \ldots, N$.

    * Because we're about to do a regression analysis, the usual *residual diagnostics* are relevant.

  - In this model the β's are unknown parameters, and we interpret them in the context of the following expectations:

* Expected response in condition m:

$$\mathbb{E}[Y_i \mid x_{i1} = x_{i2} = \cdots = x_{i,m-1} = 0] = \beta_0 = \mu_m$$

* Expected response in condition j:

$$\mathbb{E}[Y_i \mid x_{ij} = 1] = \beta_0 + \beta_j = \mu_j \quad \text{for } j = 1, 2, \ldots, m-1$$

* β_0 is the expected response in condition m.

* β_j is the expected difference in response value in condition j versus condition m for $j = 1, 2, \ldots, m-1$.

$$\mu_1 = \beta_0 + \beta_1$$
$$\mu_2 = \beta_0 + \beta_2$$
$$\vdots$$
$$\mu_{m-1} = \beta_0 + \beta_{m-1}$$
$$\mu_m = \beta_0$$

- Based on these assumptions $\mathbf{H}_0$: $\theta_1 = \theta_2 = \cdots = \theta_m$ is true if and only if $\beta_1 = \beta_2 = \cdots = \beta_{m-1} = 0$, and hence is equivalent to testing:
$$\mathbf{H}_0: \beta_1 = \beta_2 = \cdots = \beta_{m-1} = 0 \text{ versus } \mathbf{H}_A: \beta_j \neq 0 \text{ for some } j$$

- This hypothesis corresponds, as noted, to the F-test for overall significance in the model.

• In regression parlance, the test statistic is the ratio of the regression mean squares (MSR) to the mean squared error (MSE) in a standard regression-based analysis of variance (ANOVA):

$$t = \frac{\text{MSR}}{\text{MSE}}$$

• In our setting we can more intuitively think of the test statistic as comparing the response variability between conditions to the response variability within conditions:

- Average response in condition j: $\bar{y}_{\bullet j} = \dfrac{1}{n_j} \displaystyle\sum_{i=1}^{n_j} y_{ij}$.

- Overall average response: $\bar{y}_{\bullet\bullet} = \dfrac{1}{N} \displaystyle\sum_{j=1}^{m} \sum_{i=1}^{n_j} y_{ij} = \dfrac{1}{N} \sum_{j=1}^{m} n_j \bar{y}_{\bullet j}$.

- Quantifies variability *between* conditions: $\text{SS}_{\text{C}} = \displaystyle\sum_{j=1}^{m} \sum_{i=1}^{n_j} (\bar{y}_{\bullet j} - \bar{y}_{\bullet\bullet})^2$.

- Quantifies variability *within* conditions: $\text{SS}_{\text{E}} = \displaystyle\sum_{j=1}^{m} \sum_{i=1}^{n_j} (y_{ij} - \bar{y}_{\bullet j})^2$.

- Quantifies *overall* variability: $\text{SS}_{\text{T}} = \displaystyle\sum_{j=1}^{m} \sum_{i=1}^{n_j} (y_{ij} - \bar{y}_{\bullet\bullet})^2 = \text{SS}_{\text{C}} + \text{SS}_{\text{E}}$.

• The null distribution for this test is $F(m-1, N-m)$.

• p-value $= \mathbb{P}(T \geq t)$ where $T \sim F(m-1, N-m)$.

• If $\mathbf{H}_0$: $\mu_1 = \cdots = \mu_m$ is true, then $\mathbb{E}[\text{MS}_{\text{C}}] = \sigma^2$ and $\mathbb{E}[\text{MS}_{\text{E}}] = \sigma^2$.

Table 3.1: ANOVA Table

Source	SS	d.f.	MS	Test Statistic
Condition	$\mathrm{SS_C}$	$m-1$	$\mathrm{MS_C} = \mathrm{SS_C}/(m-1)$	$t = \mathrm{MS_C}/\mathrm{MS_E}$
Error	$\mathrm{SS_E}$	$N-m$	$\mathrm{MS_E} = \mathrm{SS_E}/(N-m)$	
Total	$\mathrm{SS_T}$	$N-1$		

3.1.2 Example: Candy Crush Boosters

EXAMPLE 3.1.1: Candy Crush Boosters

- Candy Crush is experimenting with three different versions of in-game "boosters": the lollipop hammer, the jelly fish, and the colour bomb.
- We randomize each user to one of these three conditions ($n_1 = 121$, $n_2 = 135$, $n_3 = 117$) and they receive (for free) 5 boosters corresponding to their condition. Interest lies in evaluating the effect of these different boosters on the length of time a user plays the game.
- Let μ_j represent the average length of game play (in minutes) associated with booster condition $j = 1, 2, 3$. While interest lies in finding the condition associated with the longest average length of game play, here we first rule out the possibility that booster type does not influence the length of game play (i.e., $\mu_1 = \mu_2 = \mu_3$).
- In order to do this we fit the linear regression model:

$$Y = \beta_0 + \beta_1 x_1 + \beta_2 x_2 + \varepsilon$$

  where x_1 and x_2 are indicator variables indicating whether we observe a particular value of the response in the jelly fish or colour bomb conditions, respectively. The lollipop hammer is therefore the reference condition.
- In R, we found that the test statistic for testing:
  $$\mathbf{H}_0\colon \mu_1 = \mu_2 = \mu_3 \text{ versus } \mathbf{H}_A\colon \mu_j \neq \mu_k \text{ for some } j \neq k$$
  was $t = 851.8947$ and the null distribution was $T \sim F(2, 370)$. The corresponding p-value was:

  $$p\text{-value} = \mathbb{P}(T \geq 851.8947) = 3.28 \times 10^{-139}$$

- Therefore, we have very strong evidence against $\mathbf{H}_0$ and conclude that the average length of game play is not the same in the three booster conditions.
- [R Code] `Comparing_multiple_means`

3.2 Comparing Proportions in Multiple Conditions

- As is always the case when comparing proportions is of interest, we assume that our response variable is binary:

$$Y_{ij} = \begin{cases} 1 & \text{if unit } i \text{ in condition } j \text{ performs an action of interest} & i = 1, 2, \dots, n_j \\ 0 & \text{if unit } i \text{ in condition } j \text{ does not perform an action of interest} & j = 1, 2, \dots, m \end{cases}$$

- $Y_{ij} \sim \text{Binomial}(1, \pi_j)$ where π_j is the probability of a unit in condition j performing the action.

- We use a **chi-squared test of independence** (Pearson χ^2 test) to test for proportions:
  $$\mathbf{H}_0\colon \pi_1 = \pi_2 = \cdots = \pi_m \text{ versus } \mathbf{H}_A\colon \pi_j \neq \pi_k \text{ for some } j \neq k.$$

3.2.1 The Chi-squared Test of Independence

- We use the chi-squared test of independence as a test for 'no association' between two categorical variables that are summarized in a *contingency table.*

- We apply this methodology here to test the independence of the binary outcome (whether a unit performs the action of interest) and the particular condition they are in.

- To start, let's assume that $m = 2$, and let's use the Optimizely experiment as a reference.

  - If $\pi_1 = \pi_2 = \pi$, then we would expect the conversion rate in each condition to be the same.

  - An estimate of the pooled conversion rate in this case is $\hat{\pi} = 679/17514 = 0.0388$.

  - Let X = number of conversions in a condition with n units, therefore $X \sim \text{Binomial}(n, \pi)$ where $\mathbb{E}[X] = n\pi$.

  - Therefore, we would expect $n_1\hat{\pi} = 8872(0.0388) = 343.96$ conversions in condition 1, and $n_2\hat{\pi} = 8642(0.0388) = 335.04$ conversions in condition 2.

  - The chi-squared test formally evaluates if the difference between what was observed and what is expected under the null hypothesis is large enough to be considered *significantly* different.

  - The *general* 2×2 contingency table for a scenario like this is shown in Table 3.2.

Table 3.2: A General 2×2 Contingency Table

		Condition		
		1	2	
Conversion	Yes	$O_{1,1}$	$O_{1,2}$	O_1
	No	$O_{0,1}$	$O_{0,2}$	O_0
		n_1	n_2	$n_1 + n_2$

  * $O_{\ell,j}$: observed number of conversions ($\ell = 1$), and the observed number of non-conversions ($\ell = 0$) in condition $j = 1, 2$.

  * O_ℓ: overall number of conversions ($\ell = 1$) or non-conversions ($\ell = 0$)

  - So,

$$\hat{\pi} = \frac{O_1}{n_1 + n_2} \quad \text{and} \quad 1 - \hat{\pi} = \frac{O_0}{n_1 + n_2}$$

represent the overall proportions of units that did or did not convert, and they are estimates of overall conversion and non-conversion rates.

  - Let $E_{1,j}$ and $E_{0,j}$ represent the expected number of conversions and non-conversions in condition $j = 1, 2$,

$$E_{1,j} = n_j\hat{\pi} \quad \text{and} \quad E_{0,j} = n_j(1 - \hat{\pi})$$

  * This is what we expect if $\mathbf{H}_0$: $\pi_1 = \pi_2$ is true.

  - The χ^2 test statistic compares the observed count in each cell to the corresponding expected count, and is defined as

$$T = \sum_{\ell=0}^{1} \sum_{j=1}^{2} \frac{(O_{\ell_j} - E_{\ell,j})^2}{E_{\ell,j}} \sim \chi^2(1)$$

  - p-value = $\mathbb{P}(T \geq t)$ where $T \sim \chi^2(1)$.

  - Returning to the Optimizely example, the *expected* table is Table 3.3.

Table 3.3: 2×2 Contingency Table for Optimizely's Homepage Experiment

		Condition		
		1	2	
Conversion	Yes	343.96	335.04	679
	No	8528.04	8306.96	16835
		8872	8642	17514

- And the resultant test statistic and p-value are:

$$t = \frac{(280 - 343.96)^2}{343.96} + \frac{(399 - 335.04)^2}{335.04} + \frac{(8592 - 8528.04)^2}{8528.04} + \frac{(8243 - 8306.96)^2}{8306.96} = 25.075$$

$$p\text{-value} = \mathbb{P}(T \geq 25.075) = 5.52 \times 10^{-7} \quad \text{where } T \sim \chi^2(1)$$

- Let's now extend this for $m > 2$.

  - We've used the chi-squared test is a test of 'no association' between the binary outcome (whether a unit performs the action of interest) and the particular condition they are in.

    * But there is no requirement that there be only two conditions.

    * Here we generalize the test to any number of experimental conditions.

  - The information associated with this test can be summarized in a $2 \times m$ contingency table as seen in Table 3.4.

Table 3.4: A General $2 \times m$ Contingency Table

		Condition				
		1	2	$\cdots$	m	
Conversion	Yes	$O_{1,1}$	$O_{1,2}$	$\cdots$	$O_{1,m}$	O_1
	No	$O_{0,1}$	$O_{0,2}$	$\cdots$	$O_{0,m}$	O_0
		n_1	n_2	$\cdots$	n_m	$N = \sum_{j=1}^{m} n_j$

    * # of conversions ($\ell = 1$) or non-conversions ($\ell = 0$) is condition $j = 1, 2$.

    * $\hat{\pi} = O_1 / N$.

    * $1 - \hat{\pi} = O_0 / N$.

  - We compare each of the observed frequencies $O_{1,j}$ with the corresponding expected frequency $E_{\ell,j}$.

$$E_{1,j} = n_j \hat{\pi} \quad \text{and} \quad E_{0,j} = n_j (1 - \hat{\pi})$$

    * Expected number of conversions/non-conversions in condition j assuming $\mathbf{H}_0$: $\pi_1 = \pi_2 = \cdots = \pi_m$ is true.

  - The χ^2 test statistic compares the observed count in each cell to the corresponding expected count, and is defined as:

$$T = \sum_{\ell=0}^{1} \sum_{j=1}^{m} \frac{(O_{\ell,j} - E_{\ell,j})^2}{E_{\ell_j}} \sim \chi^2(m-1)$$

  - p-value $= \mathbb{P}(T \geq t)$ where $T \sim \chi^2(m-1)$.

3.2.2 Example: Nike SB Ads

EXAMPLE 3.2.1: Nike SB Ads

- Suppose that Nike is running an ad campaign for Nike SB, their skateboarding division, and the campaign involves $m = 5$ different video ads that are being shown in Facebook newsfeeds.
- A video ad is 'viewed' if it is watched for longer than 3 seconds, and interest lies in determining which ad is most popular and hence most profitable by comparing the viewing rates of the five different videos.
- We show each of these 5 videos to $n_1 = 5014$, $n_2 = 4971$, $n_3 = 5030$, $n_4 = 5007$, and $n_5 = 4980$ users, and summarize the results in Table 3.5.

Table 3.5: A 2×5 Observed Contingency Table for the Nike Example

		Condition					
		1	2	3	4	5	
View	Yes	160	95	141	293	197	886
	No	4854	4876	4889	4714	4783	24116
		5014	4971	5030	5007	4980	25002

- The overall watch rate (and its complement) are:

$$\hat{\pi} = \frac{O_1}{N} = \frac{886}{25002} = 0.0354 \quad \text{and} \quad 1 - \hat{\pi} = \frac{24116}{25002} = 0.9649$$

- We multiply n_j by $\hat{\pi}$ and $(1-\hat{\pi})$ for $j = 1, 2, 3, 4, 5$ to get the expected cell frequencies in Table 3.6.

Table 3.6: A 2×5 Expected Contingency Table for the Nike Example

		Condition					
		1	2	3	4	5	
View	Yes	177.68	176.16	178.25	177.43	176.48	886
	No	4836.32	4794.84	4851.75	4829.57	4803.52	24116
		5014	4971	5030	5007	4980	25002

- The resultant test statistic and p-value (where $T \sim \chi^2(4)$) are:

$$t = \sum_{\ell=0}^{1} \sum_{j=1}^{m} \frac{(O_{\ell,j} - E_{\ell,j})^2}{E_{\ell,j}} = 129.1686$$

$$p\text{-value} = \mathbb{P}(T \geq 129.1686) = 5.86 \times 10^{-27}$$

- Therefore, we reject $\mathbf{H}_0$: $\pi_1 = \pi_2 = \cdots = \pi_5$ and conclude that the "watch-rate" is not the same for each of the video ads.
- [R Code] `Comparing_multiple_proportions`

WEEK 4

3.3 The Problem of Multiple Comparisons

- We have seen that "gatekeeper" tests of overall equality such as:
$$\mathbf{H}_0: \theta_1 = \theta_2 = \cdots = \theta_m \text{ versus } \mathbf{H}_A: \theta_j \neq \theta_k \text{ for some } j \neq k$$
are often rejected.

- We may follow this up with a series of pairwise comparisons to determine which condition(s) is (are) optimal.

  - We already know how to do this!

* ∗ Z-tests, t-tests, F-tests, χ^2-tests, randomization tests.
* HOWEVER, when doing multiple comparisons like this, we encounter the **multiple comparison** or **multiple testing problem**.
  - Type I Errors are more likely to occur in a family of tests than an individual test.
* To frame this discussion, let's define some notation:
  - M: the number of hypotheses tested.
  - M_0: the number of true null hypotheses.
  - M_A: the number of false null hypotheses.
  - R: the number of null hypotheses that we reject.
  - $M - R$: the number of null hypotheses that we don't reject.
  - V: the number of true null hypotheses that were incorrectly rejected; that is, the number of Type I Errors.
  - S: the number of false null hypotheses that were incorrectly rejected.
  - U: the number of true null hypotheses that were correctly accepted.
  - T: the number of false null hypotheses that were incorrectly accepted; that is, the number of Type II Errors.
  - $M = M_0 + M_A$.
* We summarize the outcomes of these M decisions in Table 3.7.

Table 3.7: Outcomes From M Simultaneous Hypothesis Tests

		Decision		
		Reject $\mathbf{H}_0$	Accept $\mathbf{H}_0$	
Truth	$\mathbf{H}_0$ is True	V	U	M_0
	$\mathbf{H}_0$ is False	S	T	M_A
		R	$M - R$	M

  - R and $M - R$ are observable.
  - M_0, M_A, V, U, S, T are random variables; that is, the random process of collecting data and testing the M hypotheses determines their values. Therefore, they are all unobservable.
* Ideally, we would like V and T to be small.
  - T is controlled via sample size as it is related to power.
  - We control functions of V with sophisticated and clever statistical methods.

3.3.1 Family-Wise Error Rate

DEFINITION 3.3.1: Family-wise error rate

The **family-wise error rate** is the probability of committing a Type I Error in *any* of the M hypothesis tests.
$$\text{FWER} = \mathbb{P}(V \geq 1)$$
That is, the probability of making at least one Type I Error in M tests.

* If we use a significance level of α for each of the M tests, the FWER will be much greater than α.

- Boole's Inequality, which is $\mathbb{P}(A \cup B) = \mathbb{P}(A) + \mathbb{P}(B) - \mathbb{P}(A \cap B) \le \mathbb{P}(A) + \mathbb{P}(B)$, provides an upper bound:

$$
\begin{aligned}
\text{FWER} &= \mathbb{P}(V \ge 1) \\
&= \mathbb{P}(\text{At least one Type I Error in } M \text{ tests}) \\
&= \mathbb{P}\left(\bigcup_{k=1}^{M} \text{Type I Error on test } k \right) \\
&\le \sum_{k=1}^{M} \mathbb{P}(\text{Type I Error on test } k) \qquad \text{Boole's Inequality} \\
&= \sum_{k=1}^{M} \alpha \\
&= M\alpha
\end{aligned}
$$

> **EXAMPLE 3.3.2: FWER**
>
> If $M = 10$ and $\alpha = 0.05$, then FWER ≤ 0.5.

- If we're willing to assume that the M tests are independent then:

$$
\begin{aligned}
\text{FWER} &= \mathbb{P}(V \ge 1) \\
&= \mathbb{P}(\text{At least one Type I Error in } M \text{ tests}) \\
&= 1 - \mathbb{P}(\text{No Type I Error in } M \text{ tests}) \\
&= 1 - \mathbb{P}\left(\bigcap_{k=1}^{M} \text{No Type I Error on test } k \right) \\
&= 1 - \prod_{k=1}^{M} \mathbb{P}(\text{No Type I Error on test } k) \qquad \text{by independence} \\
&= 1 - \prod_{k=1}^{M} (1 - \alpha) \\
&= 1 - (1 - \alpha)^{M}
\end{aligned}
$$

- This error rate, as a function of M can be seen in Figure 3.2. As M increases, FWER also increases. In fact, $\lim\limits_{M \to \infty} \text{FWER} = 1$.

- A common value of M is Binomial$(m)2$: the number of pairwise comparisons necessary to compare each condition to every other condition.

> **EXAMPLE 3.3.3**
>
> If $m = 5$ and $\alpha = 0.05$, then $M = \text{Binomial}(5)2 = 10$. Therefore, FWER $= 1 - (1 - 0.05)^{10} = 0.4013$.

- Available to us are a variety of different statistical techniques that may be used to ensure the FWER does not exceed some threshold.

$$
\text{FWER} \le \alpha^{\star} \in [0, 1]
$$

> **REMARK 3.3.4: General Notation**
>
> - Denote the M null hypotheses as: $\mathbf{H}_{0,1}, \mathbf{H}_{0,2}, \dots, \mathbf{H}_{0,M}$.
> - Denote their corresponding p-values as: $p_1, p_2, \dots, p_M$.
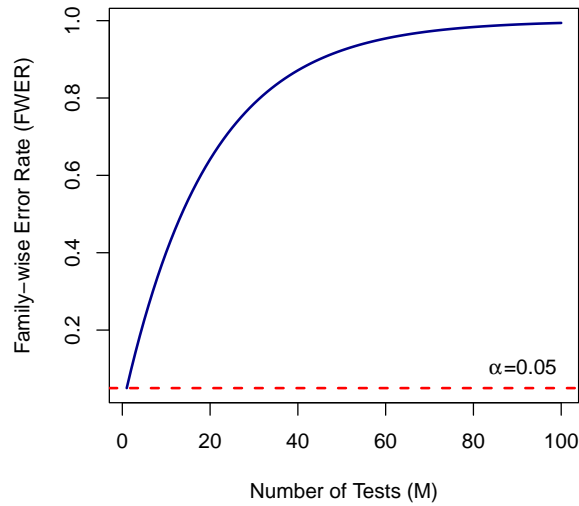
Figure 3.2: Family-Wise Error Rate Versus the Number of Hypothesis Tests, M.

EXAMPLE 3.3.5

Suppose we test $M = 4$ hypotheses, and the resulting p-values are $p_1 = 0.015$, $p_2 = 0.029$, $p_3 = 0.008$, and $p_4 = 0.026$.

The Bonferroni Correction

- This is the simplest method.

- Reject $\mathbf{H}_{0,k}$ if

$$p_k \leq \frac{\alpha^\star}{M} \quad \text{for } k = 1, 2, \ldots, M$$

So, we test all M hypotheses at a significance level of $\alpha^\star/M$.

- The procedure ensures FWER $\leq \alpha^\star$. From Boole's Inequality, we know that

$$\text{FWER} \leq M\left(\frac{\alpha^\star}{M}\right) = \alpha^\star$$

- If we assume independence, the Bonferroni-corrected FWER becomes

$$1 - \left(1 - \frac{\alpha^\star}{M}\right)^M$$

Taking the limit of $M \to \infty$ yields,

$$\lim_{M \to \infty} \left[1 - \left(1 - \frac{\alpha^\star}{M}\right)^M\right] = 1 - e^{-\alpha^\star}$$

which for typical values of $\alpha^\star$ in the range of $]0, 0.1]$ is approximately equal to $\alpha^\star$. For example, if $\alpha^\star = 0.1$, then the error is ≈ 0.005. The asymptotic error rate and line of equality can be seen in Figure 3.3.
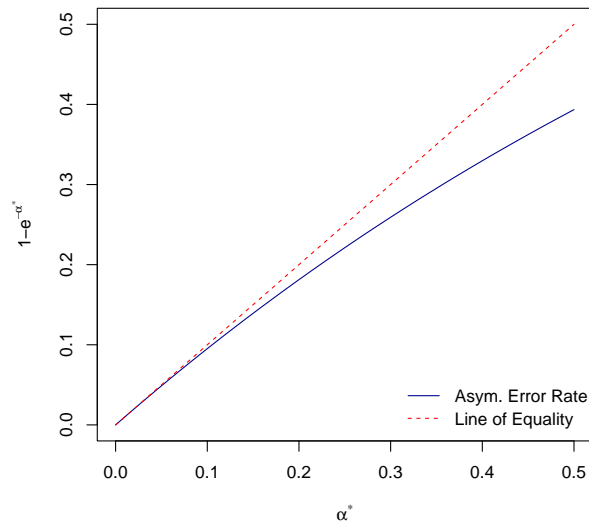
Figure 3.3: Illustration of the Bonferroni Correction for Asymptotically Large M.

> **EXAMPLE 3.3.6: Four-test Example — Bonferroni Correction**
>
> Let $p_1 = 0.015$, $p_2 = 0.029$, $p_3 = 0.008$, and $p_4 = 0.026$. Suppose that we wish to ensure FWER $\leq \alpha^\star = 0.05$.
>
> Under the Bonferroni Correction, we compare each p-value to $\alpha^\star/M = 0.05/4 = 0.0125$. Only $p_3 < 0.0125$, and hence only $\mathbf{H}_{0,3}$ is rejected.

The Šidák Correction

- This approach exploits the FWER formula derived when we assumed the M tests were independent.
- Reject $\mathbf{H}_{0,k}$ if

$$p_k \leq 1 - (1 - \alpha^\star)^{1/M} \quad \text{for } k = 1, 2, \ldots, M$$

> **REMARK 3.3.7**
>
> Where does the Šidák Correction come from?
>
> $$\begin{aligned} \alpha^\star = \text{FWER} = 1 - (1 - \alpha)^M &\iff 1 - \alpha^\star = (1 - \alpha)^M \\ &\iff (1 - \alpha^\star)^{1/M} = 1 - \alpha \\ &\iff \alpha = 1 - (1 - \alpha^\star)^{1/M} \end{aligned}$$

- This is actually not much different from the Bonferroni correction since

$$\frac{\alpha^\star}{M} \approx 1 - (1 - \alpha^\star)^{1/M}$$

> **EXAMPLE 3.3.8: Bonferroni versus Šidák Correction**
>
> Let $\alpha^\star = 0.05$ and $M = 10$. Then, $\alpha^\star/M = 0.005$, and $1 - (1 - \alpha^\star)^{1/M} = 0.005116$.

EXAMPLE 3.3.9: Four-test Example — Šidák Correction

Let $p_1 = 0.015$, $p_2 = 0.029$, $p_3 = 0.008$, and $p_4 = 0.026$. Suppose that we wish to ensure FWER $\leq \alpha^\star = 0.05$.

Under the Šidák Correction, we have

$$1 - (1 - \alpha^\star)^{1/M} = 1 - (0.95)^{0.25} = 0.012741$$

Therefore, we only reject $\mathbf{H}_{0,3}$ since only $p_3 < 0.012741$.

Holm's "Step-Up" Procedure

- The Bonferroni and Šidák corrections methods are very strict for large M.
    - In these cases *most* null hypotheses will not be rejected.
    - If we're too strict, we basically stop rejecting null hypotheses thereby eliminating Type I Errors, but we increase the Type II Errors.
- Ideally we would have an approach that is less strict but still controls the FWER at some $\alpha^\star$.
- This is exactly what Holm's Procedure gives us!

---

1. Order the M p-values from smallest to largest:

   $$p_{(1)}, p_{(2)}, \ldots, p_{(M)}$$

   where $p_{(k)}$ is the kth smallest p-value.

2. Starting from $k = 1$ and continuing incrementally, compare $p_{(k)}$ to $\alpha^\star/(M-k+1)$. Determine $k^\star$, the smallest value of k such that

   $$p_{(k)} > \frac{\alpha^\star}{M - k + 1}$$

3. Reject the null hypotheses $\mathbf{H}_{0,(1)}, \ldots, \mathbf{H}_{0,(k^\star-1)}$ and do not reject $\mathbf{H}_{0,(k^\star)}, \ldots, \mathbf{H}_{0,(M)}$.

- What's really happening?

$$p_{(1)} \text{ versus } \alpha^\star/M$$
$$p_{(2)} \text{ versus } \alpha^\star/(M-1)$$
$$p_{(3)} \text{ versus } \alpha^\star/(M-2)$$
$$\vdots$$
$$p_{(M)} \text{ versus } \alpha^\star$$

We compare each p-value to a Bonferroni-Corrected significance level based on the number of comparisons that remain to be made at a particular "step."

THEOREM 3.3.10

Holm's procedure controls the family-wise error rate.

Proof of Theorem 3.3.10 †

- We need to show that FWER $= \mathbb{P}(V \geq 1) \leq \alpha^\star \in [0, 1]$ when using the Holm's procedure.
- Let $p_{(1)}, p_{(2)}, \dots, p_{(M)}$ be the ordered p-values and let $\mathbf{H}_{0,(1)}, \mathbf{H}_{0,(2)}, \dots, \mathbf{H}_{0,(M)}$ be the corresponding null hypotheses.
- Define $K_0 \subset \{1, 2, \dots, M\}$ to be the subset of indices which correspond to true null hypotheses; that is, $\mathbf{H}_{0,k}$ is true for $k \in K_0$.
- We can visualize the sequential decisions made in Holm's Procedure as follows:

$$\overbrace{\underbrace{\mathbf{H}_{0,(1)} \cdots \mathbf{H}_{0,(h-1)}}_{\text{these are false } \mathbf{H}_0\text{'s}} \mathbf{H}_{0,(h)} \cdots \mathbf{H}_{0,(R)}}^{\text{these are rejected}} \mid \underbrace{\mathbf{H}_{0,(R+1)} \cdots \mathbf{H}_{0,(M)}}_{\text{these are not rejected}}$$

Let $\mathbf{H}_{0,(h)}$ be the first *true* $\mathbf{H}_0$ that was rejected. Since it was rejected by Holm's procedure, we know that

$$p_{(h)} \leq \frac{\alpha^\star}{M - h + 1}$$

Also, clearly we must have $h - 1 \leq M - M_0$ since $M - M_0$ is the total number of false $\mathbf{H}_0$'s and $h - 1$ is the number of false $\mathbf{H}_0$'s encountered by test h. And so,

$$M_0 \leq M - h + 1 \iff \frac{1}{M_0} \geq \frac{1}{M - h + 1} \iff \frac{\alpha^\star}{M_0} \geq \frac{\alpha^\star}{M - h + 1}$$

Thus, we must have $p_{(h)} \leq \alpha^\star/(M - h + 1) \leq \alpha^\star/M_0$. Therefore,

$$
\begin{aligned}
\text{FWER} &= \mathbb{P}(V \geq 1) \\
&= \mathbb{P}(\text{At least one Type I Error in } M \text{ tests}) \\
&= \mathbb{P}(\text{Reject at least one true } \mathbf{H}_0) \\
&= \mathbb{P}\left(\exists\, k \in K_0 \text{ such that } p_k \leq \frac{\alpha^\star}{M_0} \right) \\
&= \mathbb{P}\left(\bigcup_{k \in K_0} p_k \leq \frac{\alpha^\star}{M_0} \right) \\
&\leq \sum_{k \in K_0} \mathbb{P}\left(p_k \leq \frac{\alpha^\star}{M_0} \right) && \text{by Boole's Inequality} \\
&= \sum_{k \in K_0} \frac{\alpha^\star}{M_0} && \begin{array}{l}\text{since } p\text{-values for true null} \\ \text{hypotheses follow a Uniform}(0,1) \text{ distribution}\end{array} \\
&= M_0 \left(\frac{\alpha^\star}{M_0} \right) && \text{since the set } K_0 \text{ has cardinality } M_0 \\
&= \alpha^\star
\end{aligned}
$$

Therefore, FWER $\leq \alpha^\star$ as required.

EXAMPLE 3.3.11: Four-test Example ($M = 4$) — Holm's Procedure

Let $p_1 = 0.015$, $p_2 = 0.029$, $p_3 = 0.008$, and $p_4 = 0.026$. Suppose that we wish to ensure FWER $\leq$

$\alpha^\star = 0.05$.

$$p_{(1)} = p_3 = 0.008 \text{ versus } \alpha^\star/M = 0.05/4 = 0.0125$$
$$p_{(2)} = p_1 = 0.015 \text{ versus } \alpha^\star/(M-1) = 0.05/3 = 0.0167$$
$$p_{(3)} = p_4 = 0.026 \text{ versus } \alpha^\star/(M-2) = 0.05/2 = 0.025$$
$$p_{(4)} = p_2 = 0.029 \text{ versus } \alpha^\star/(M-3) = 0.05/1 = 0.05$$

We reject $\mathbf{H}_{0,(1)} = \mathbf{H}_{0,3}$ and $\mathbf{H}_{0,(2)} = \mathbf{H}_{0,1}$. We do not reject $\mathbf{H}_{0,(3)} = \mathbf{H}_{0,4}$ or $\mathbf{H}_{0,(4)} = \mathbf{H}_{0,2}$. Note that $k^\star = 3$.

- The decision process for all three of these methods can be visualized by plotting the ordered p-values $p_{(k)}$ versus their ranks $k = 1, 2, \ldots, M$ and overlay the significance thresholds which can be seen in Figure 3.4.
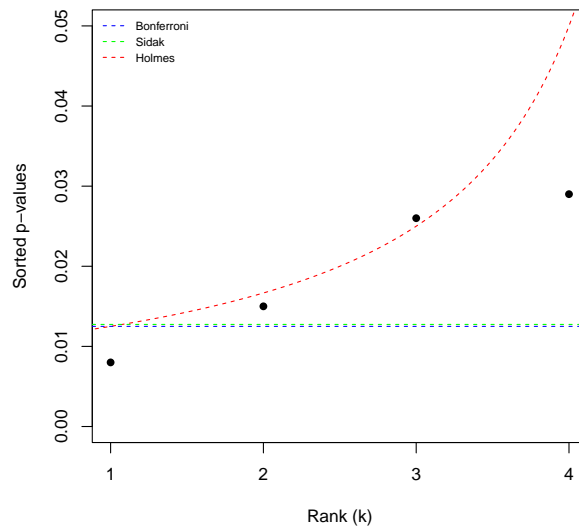
Figure 3.4: Significance Thresholds for Several Methods of Correction (1).

- The Bonferroni correction is most strict, followed by the Šidák correction, then by Holm's procedure.

Adjusted p-values

- So far we have framed each of the correction procedures above as an adjustment to the significance threshold against which each p-value is compared.

- Alternatively (and equivalently) we could invert this process and frame the decision in terms of a comparison of *adjusted p-values* to $\alpha^\star$.

- This is more familiar (compare our p-values to some constant threshold $\alpha^\star$).

  - We just need to adjust our p-values first.

- The decisions made with the following adjusted p-values are identical to that achieved by comparing unadjusted p-values to the methods' adjusted significance thresholds.

  - Bonferroni: Reject $\mathbf{H}_{0,k}$ if $p_k^\star \leq \alpha^\star$ where

$$p_k^\star = M p_k$$

> **EXAMPLE 3.3.12: Bonferroni's Adjusted *p*-values**
>
> In our four-test example, $p_1^\star = 0.06$, $p_2^\star = 0.116$, $p_3^\star = 0.032$, and $p_4^\star = 0.104$. Comparing to $\alpha^\star = 0.05$, we reject $\mathbf{H}_{0,3}$.

- Šidák: Reject $\mathbf{H}_{0,k}$ if $p_k^\star \leq \alpha^\star$ where

$$p_k^\star = 1 - (1 - p_k)^M$$

> **EXAMPLE 3.3.13: Šidák's Adjusted *p*-values**
>
> In our four-test example, $p_1^\star = 0.0587$, $p_2^\star = 0.1111$, $p_3^\star = 0.0316$, and $p_4^\star = 0.1$. Comparing to $\alpha^\star = 0.05$, we reject $\mathbf{H}_{0,3}$.

- Holm: Reject $\mathbf{H}_{0,k}$ if $p_{(k)}^\star \leq \alpha^\star$ where

$$p_{(k)}^\star = \max_{j \leq k}\left\{ p_{(j)}(M - j + 1) \right\}$$

> **EXAMPLE 3.3.14: Holm's Adjusted *p*-values**
>
> Let $p_1 = 0.015$, $p_2 = 0.029$, $p_3 = 0.008$, and $p_4 = 0.026$.
>
> | k | $p_{(k)}$ | $M - k + 1$ | $p_{(k)}(M - k + 1)$ | $p_{(k)}^\star = \max_{j \leq k}\left\{ p_{(j)}(M - j + 1) \right\}$ |
> |---|---|---|---|---|
> | 1 | 0.008 | 4 | 0.032 | $\max\{0.032\} = 0.032 = p_{(1)}^\star$ |
> | 2 | 0.015 | 3 | 0.045 | $\max\{0.032, 0.045\} = 0.045 = p_{(2)}^\star$ |
> | 3 | 0.026 | 2 | 0.052 | $\max\{0.032, 0.045, 0.052\} = 0.052 = p_{(3)}^\star$ |
> | 4 | 0.029 | 1 | 0.029 | $\max\{0.032, 0.045, 0.052, 0.029\} = 0.052 = p_{(4)}^\star$ |
>
> Thus, $p_1^\star = p_{(2)}^\star = 0.045$, $p_2^\star = p_{(4)}^\star = 0.052$, $p_3^\star = p_{(1)}^\star = 0.032$, and $p_4^\star = p_{(3)}^\star = 0.052$. Comparing to $\alpha^\star = 0.05$, we reject $\mathbf{H}_{0,1}$ and $\mathbf{H}_{0,3}$.

- Implemented in R with `p.adjust()`.

3.3.2 False Discovery Rate

- In the mid-1900s, Statisticians developed FWER methods with $M \approx 20$ comparisons in mind.

- In the era of Big Data, much larger values of M are typical.

- For larger values of M, traditional methods tend to be very conservative, and so FWER is perhaps not the best metric to control.

- More recently, emphasis has been placed on controlling the *rate* at which Type I Errors occur.

> **DEFINITION 3.3.15: False discovery proportion**
>
> The **false discovery proportion** (FDP) is
>
> $$Q = \frac{V}{R}$$
>
> Thus, Q is the proportion of all rejected null hypotheses that were rejected in error.

- In particular, interest lies in controlling the **false discovery rate** (FDR).

> **DEFINITION 3.3.16: False discovery rate**
>
> The **false discovery rate** is
> $$\mathbb{E}[Q] = \mathbb{E}\left[\frac{V}{R}\right]$$

- Unlike the FWER, the FDR is adaptive in the sense that the number of Type I Errors V has different implications depending on the size of M. That is,
    - Two Type I Errors in 10 tests might be unacceptable.
    - Two Type I Errors in 100 tests might be okay.
- Methods that control the FDR are less strict than methods that control FWER.
    - More Type I Errors will occur with such methods, but this is viewed as acceptable when M is very large.

Benjamini-Hochberg Procedure

- The Benjamini-Hochberg (BH) procedure for controlling FDR is a sequentially rejective procedure much like Holm's procedure for controlling FWER.

- We summarize the BH procedure, which aims to ensure FDR $\leq \alpha^\star$:

> 1. Order the M p-values from smallest to largest:
> $$p_{(1)}, p_{(2)}, \ldots, p_{(M)}$$
> where $p_{(k)}$ is the kth smallest p-value.
>
> 2. Starting from $k = 1$ and continuing incrementally, compare $p_{(k)}$ to $k\alpha^\star/M$. Determine $k^\star$ the largest value of k such that
> $$p_{(k)} \leq \frac{k\alpha^\star}{M}$$
>
> 3. Reject the null hypotheses $\mathbf{H}_{0,(1)}, \ldots, \mathbf{H}_{0,(k^\star)}$ and do not reject $\mathbf{H}_{0,(k^\star+1)}, \ldots, \mathbf{H}_{0,(M)}$.

- The decision process associated with this procedure is best visualized with a plot of the ordered p-values $p_{(k)}$ versus their ranks $k = 1, 2, \ldots, M$ with the significance threshold overlaid which can be seen in Figure 3.5.
    - The BH significance threshold is the line with intercept 0 and slope $\alpha^\star/M$.

> **EXAMPLE 3.3.17: Four-test Example — Benjamini-Hochberg Procedure**
>
> Let $p_1 = 0.015$, $p_2 = 0.029$, $p_3 = 0.008$, and $p_4 = 0.026$. Suppose that we wish to ensure FDR $\leq \alpha^\star = 0.05$. Since all p-values fall below the purple line in Figure 3.5, we reject all four null hypotheses.

- This threshold is much less strict than any of the FWER-control thresholds, but this is the appeal of the approach.

- The procedure that guarantees FDR $\leq \alpha^\star$ is beyond the scope of this course. However, the proof can be found in

- Like the FWER controlling methods we can define Benjamini-Hochberg-adjusted p-values and invert the decision framework by comparing the adjusted p-values to $\alpha^\star$.
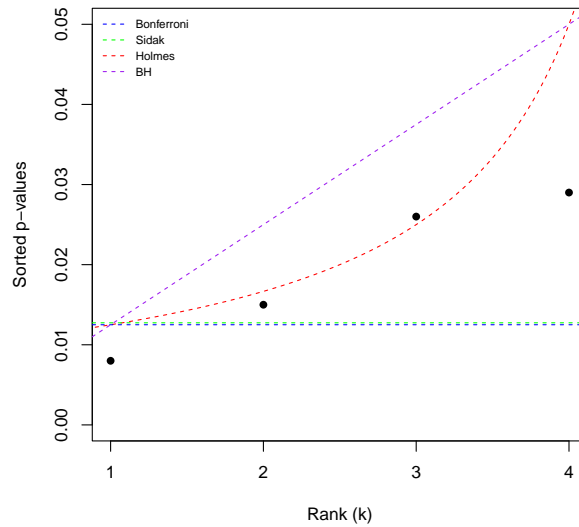
Figure 3.5: Significance Thresholds for Several Methods of Correction (2).

– Reject $\mathbf{H}_{0,(k)}$ if $p^{\star}_{(k)} \leq \alpha^{\star}$ where

$$p^{\star}_{(k)} = \min_{j \geq k}\left\{\frac{Mp_{(j)}}{j}\right\}$$

EXAMPLE 3.3.18: Benjamini-Hochberg Procedure's Adjusted p-values

Let $p_1 = 0.015$, $p_2 = 0.029$, $p_3 = 0.008$, and $p_4 = 0.026$.

k	$p_{(k)}$	$Mp_{(k)}/k$	$p^{\star}_{(k)} = \min_{j \geq k}\left\{Mp_{(j)}/j\right\}$
1	0.008	0.032	$\min\{0.032, 0.030, 0.035, 0.029\} = 0.029 = p^{\star}_{(1)}$
2	0.015	0.030	$\min\{0.030, 0.035, 0.029\} = 0.029 = p^{\star}_{(2)}$
3	0.026	0.035	$\min\{0.035, 0.029\} = 0.029 = p^{\star}_{(3)}$
4	0.029	0.029	$\min\{0.029\} = 0.029 = p^{\star}_{(4)}$

Thus, $p^{\star}_1 = p^{\star}_{(2)} = 0.029$, $p^{\star}_2 = p^{\star}_{(4)} = 0.029$, $p^{\star}_3 = p^{\star}_{(1)} = 0.029$, and $p^{\star}_4 = p^{\star}_{(3)} = 0.029$. Comparing to $\alpha^{\star} = 0.05$, we reject all $\mathbf{H}_0$'s.

[R Code] `Multiple_testing_example`

3.3.3 Sample Size Determination

- So what does all of this mean for power analyses and sample size calculations?

- There is a duality between significance level and power.

  – All else equal, reducing a test's significance level will increase the Type II Error rate and hence decrease power.

  – Play around with this interactive app to gain comfort with this notion.

    ∗ Assume $\mathcal{R} = \{t \mid t \geq z_{\alpha}\}$.

    ∗ Recall that:

· $\alpha = \mathbb{P}(\text{Type I Error}) = \mathbb{P}(T \in \mathcal{R} \mid \mathbf{H}_0 \text{ is true}) = \mathbb{P}(T \geq z_\alpha \mid \mathbf{H}_0 \text{ is true})$.

· $\beta = \mathbb{P}(\text{Type II Error}) = \mathbb{P}(T \notin \mathcal{R} \mid \mathbf{H}_A \text{ is true}) = \mathbb{P}(T < z_\alpha \mid \mathbf{H}_A \text{ is true})$.

- Thus, all the correction procedures discussed (which decrease the effective significance level) negatively impact power.

- In order to maintain power at some pre-specified level, we must compensate by increasing the sample size.

- Therefore, the more complicated your experiment (i.e., the more conditions it has), the larger your sample sizes will need to be.

    - Such modifications can be accounted for when selecting a sample size.

    - The significance level you use in your sample size calculations should be the adjusted one based on the correction method you use.

    - This is easier to do with *some* correction methods than others.

<div align="center">Week 5</div>

Primer on Logistic Regression

- Linear regression is an effective method of modelling the relationship between a single response variable (Y), and one or more explanatory variables ($x_1, x_2, \ldots, x_p$).

    - However, ordinary linear regression assumes that the response variable follows a normal distribution (i.e., $Y \sim \mathcal{N}(\mu, \sigma^2)$).

    - When the response variable is binary, this assumption is no longer valid.

- When we have a binary response, the Bernoulli distribution (i.e., $Y \sim \text{Binomial}(1, \pi)$) is a much more appropriate distributional assumption.

    - But ordinary linear regression is no longer appropriate.

    - Instead, we use **Logistic Regression**.

- In the context of a linear regression model, the expected response (given the values of the explanatory variables) is equated to the **linear predictor** $\beta_0 + \beta_1 x_1 + \cdots + \beta_p x_p$:

$$\mathbb{E}[Y \mid x_1, x_2, \ldots, x_p] = \mu = \beta_0 + \beta_1 x_1 + \cdots + \beta_p x_p$$

- In the context of Logistic Regression we also want to relate the expected response to the linear predictor.

    - But now, $\mathbb{E}[Y] = \pi \in [0, 1]$.

    - And equating π and $\beta_0 + \beta_1 x_1 + \cdots + \beta_p x_p$ does not make sense. In general, the linear predictor need not lie in $[0, 1]$.

$$\pi = \beta_0 + \beta_1 x_1 + \cdots + \beta_p x_p \quad \text{not a good thing to do}$$

- Instead, we relate the linear predictor to $\mathbb{E}[Y] = \pi$ through a monotonic differentiable **link function** that maps $[0, 1] \to \mathbf{R}$.

    - Logistic Regression arises when this link function is the **logit** function:

$$\text{logit}(\pi) = \log\left(\frac{\pi}{1 - \pi}\right) = \beta_0 + \beta_1 x_1 + \cdots + \beta_p x_p$$

– Inverting this yields the expected response (given the values of the explanatory variables):

$$\mathbb{E}[Y \mid \widehat{x_1, x_2}, ..., x_p] = \hat{\pi} = \frac{e^{\hat{\beta}_0 + \hat{\beta}_1 x_1 + \cdots + \hat{\beta}_p x_p}}{1 + e^{\hat{\beta}_0 + \hat{\beta}_1 x_1 + \cdots + \hat{\beta}_p x_p}} = \text{expit}(\beta_0 + \beta_1 x_1 + \cdots + \beta_p x_p)$$

- To interpret β_0, we set each explanatory variable to zero (i.e., $x_1 = x_2 = \cdots = x_p = 0$).

  – We see that β_0 is the **log-odds** that $Y = 1$ when $x_1 = x_2 = \cdots = x_p = 0$.

$$\log\left(\frac{\pi}{1 - \pi}\right) = \beta_0$$

  – Equivalently, e^{β_0} is the **odds** that the response would equal 1 when $x_1 = x_2 = \cdots = x_p = 0$. Exponentiating both sides yields

$$\frac{\pi}{1 - \pi} = e^{\beta_0}$$

DEFINITION 3.3.19: Odds

The **odds** of an event A is:

$$\frac{\mathbb{P}(A)}{\mathbb{P}(A^c)} = \frac{\mathbb{P}(A)}{1 - \mathbb{P}(A)}$$

- The interpretation of β_j, for $j = 1, 2, ..., p$, is uncovered by considering the Logistic Regression equation for different values of x_j.

  – Let π_x be the value of π when $x_j = x$ and let π_{x+1} be the value of π when $x_j = x + 1$.

$$\log\left(\frac{\pi_{x+1}}{1 - \pi_{x+1}}\right) - \log\left(\frac{\pi_x}{1 - \pi_x}\right) = (\beta_0 + \beta_1 x_1 + \cdots + \beta_j(x + 1) + \cdots + \beta_p x_p)$$
$$- (\beta_0 + \beta_1 x_1 + \cdots + \beta_j x + \cdots + \beta_p x_p)$$
$$= \beta_j$$

  – Thus:

$$\log\left(\frac{\pi_{x+1}}{1 - \pi_{x+1}} \middle/ \frac{\pi_x}{1 - \pi_x}\right) = \beta_j$$

  and so β_j is interpreted as a **log-odds ratio**, comparing the odds that $Y = 1$ when $x_j = x + 1$ versus $x_j = x$ (all else being equal).

  – Equivalently, e^{β_j} is interpreted as the **odds ratio**, comparing the odds that $Y = 1$ when $x_j = x+1$ versus $x_j = x$ (all else being equal). Exponentiating yields

$$\frac{\pi_{x+1}}{1 - \pi_{x+1}} \middle/ \frac{\pi_x}{1 - \pi_x} = e^{\beta_j}$$

- **Maximum likelihood estimation** is a method that is used to estimate parameters in Logistic Regression.

  – This means that the $\hat{\beta}$'s are maximum likelihood estimates, whose corresponding estimators have nice properties, such as:

$$\tilde{\beta} \sim \mathcal{N}\left(\beta, \frac{1}{J(\beta)}\right)$$

  where $J(\beta)$ is the Fisher Information.

– A consequence of this is that hypotheses of the form
$$\mathbf{H}_0\colon \beta_j = 0 \text{ versus } \mathbf{H}_{\mathrm{A}}\colon \beta_j \neq 0$$
are done with *Z-tests* with test statistics given by

$$t = \frac{\hat{\beta}_j - 0}{\mathrm{Se}\!\left(\hat{\beta}_j\right)} \,\dot{\sim}\, \mathcal{N}(0,1)$$

– In order to test hypotheses about several β's being simultaneously equal to zero, we use *likelihood ratio tests.*

Chapter 4

Blocking

- In the context of designed experiments we categorize factors as either:
  - *Design* factors: we manipulate these to quantify their impact on the response. They define the experimental conditions.
  - *Allowed-to-vary* factors: these are unknown, or known but uncontrollable factors that are <u>not</u> controlled in the experiment.
  - *Nuisance* factors: we control these to eliminate their effect on the response.
- But remember: in practice, context dictates whether a factor should be considered a design factor, a nuisance factor, or if it should be allowed to vary.

Figure 4.1: Four Levels of the *browser* Factor.

1. Usability testing involves studying the ease with which an individual uses a product or service for some intended purpose. Suppose investigators are performing a usability test to determine with which browser 70 to 80-year-old users find it easiest to look up the phone number of the nearest pharmacy. In this example, experimental units (70 to 80-year-olds) are randomly assigned to one of four browser conditions, and the investigators measure the time it takes to complete the task.

   - Browser is the design factor.

2. Suppose that Netflix is experimenting with server-side modifications to improve (reduce) the latency of Netflix.com. We hypothesize that the current infrastructure serves as a control condition and the modified infrastructure reduces median page load time. It is possible that a user's browser may also affect page load time, but this effect is not of interest to the investigators. To control for the potential impact of one's browser, Netflix initially experiments with only Firefox users.

   - Browser is the nuisance factor.

3. Suppose that Amazon.ca is experimenting with the width of their search bar. They hypothesize that a wider search bar will minimize the amount of mouse movement required to navigate to it, thereby

minimizing the average time-to-query. The experimenters do not care which browser a customer uses and so this factor is uncontrolled and hence is *allowed-to-vary* during their experiment.

- Browser is the allowed-to-vary factor.

- It's also important to understand the subtle distinction between nuisance factors and design factors in the context of a single experiment.

  – We control both factors in the experiment.

  – With a design factor we wish to quantify its influence on the response variable.

  – With a nuisance factor we do not care to quantify its effect, we wish only to *eliminate* it.

- We eliminate the effect of one or more nuisance factors with **blocking**.

  – To eliminate the effect of a nuisance factor, it cannot be allowed to vary on its own.

  – Blocking fixes the nuisance factor at one or more levels (**blocks**).

  – By holding a nuisance factor fixed, it cannot vary and hence cannot influence the response.

    * This is how Netflix handled the nuisance factor "browser" in Example 2.

4.1 Randomized Complete Block Designs

- The randomized complete block design (RCBD) is a simple experimental design that may be applied when we wish to investigate:

  – A single design factor; e.g., m levels, m conditions, while controlling for a single nuisance factor; e.g., b levels, b blocks.

- In a RCBD, we carry out each of the experimental conditions in every one of the blocks.

  – m conditions are happening inside each of the b blocks.

- The *observed* data in such an experiment is y_{ijk}.

  – Response observation for unit $i = 1, 2, \ldots, n_{jk}$ in condition $j = 1, 2, \ldots, m$ within block $k = 1, 2, \ldots, b$.

- We assume that there are n_{jk} units in (condition, block) $= (j, k)$ and thus an overall total of $N = \sum_{k=1}^{b} \sum_{j=1}^{m} n_{jk}$ units.

  – If $n_{jk} = n$ for all (j, k), we call the design "balanced."

- We tabulate the response data of this form below:

Table 4.1: Response Observations in a Randomized Complete Block Design

		Block			
		1	2	$\cdots$	b	
	1	$\{y_{i11}\}_{i=1}^{n_{11}}$	$\{y_{i12}\}_{i=1}^{n_{12}}$	$\cdots$	$\{y_{i1b}\}_{i=1}^{n_{1b}}$	$\bar{y}_{\bullet 1 \bullet}$
Condition	2	$\{y_{i21}\}_{i=1}^{n_{21}}$	$\{y_{i22}\}_{i=1}^{n_{22}}$	$\cdots$	$\{y_{i2b}\}_{i=1}^{n_{2b}}$	$\bar{y}_{\bullet 2 \bullet}$
	$\vdots$	$\vdots$	$\vdots$	$\ddots$	$\vdots$	$\vdots$
	m	$\{y_{im1}\}_{i=1}^{n_{m1}}$	$\{y_{im2}\}_{i=1}^{n_{m2}}$	$\cdots$	$\{y_{imb}\}_{i=1}^{n_{mb}}$	$\bar{y}_{\bullet m \bullet}$
		$\bar{y}_{\bullet \bullet 1}$	$\bar{y}_{\bullet \bullet 2}$	$\cdots$	$\bar{y}_{\bullet \bullet b}$	$\bar{y}_{\bullet \bullet \bullet}$

  – Block-specific average responses: $\bar{y}_{\bullet \bullet 1}, \bar{y}_{\bullet \bullet 2}, \ldots, \bar{y}_{\bullet \bullet b}$.

  – Overall average response: $\bar{y}_{\bullet \bullet \bullet}$.

- Condition-specific average responses: $\bar{y}_{\bullet 1 \bullet}, \bar{y}_{\bullet 2 \bullet}, \dots, \bar{y}_{\bullet m \bullet}$.

- We calculate the row, column, and overall means as follows:

$$\bar{y}_{\bullet j \bullet} = \frac{1}{n_{j+}} \sum_{k=1}^{b} n_{jk} \bar{y}_{\bullet jk} \quad \text{where } n_{j+} = \sum_{k=1}^{b} n_{jk}$$

$$\bar{y}_{\bullet \bullet k} = \frac{1}{n_{+k}} \sum_{j=1}^{m} n_{jk} \bar{y}_{\bullet jk} \quad \text{where } n_{+k} = \sum_{j=1}^{m} n_{jk}$$

$$\bar{y}_{\bullet \bullet \bullet} = \frac{1}{N} \sum_{k=1}^{b} \sum_{j=1}^{m} n_{jk} \bar{y}_{\bullet jk} = \frac{1}{N} \sum_{k=1}^{b} \sum_{j=1}^{m} \sum_{i=1}^{n_{jk}} y_{ijk}$$

where $\bar{y}_{\bullet jk}$ is the average response value in $(\text{condition}, \text{block}) = (j, k)$ cell, also

$$\bar{y}_{\bullet jk} = \frac{1}{n_{jk}} \sum_{i=1}^{n_{jk}} y_{ijk}$$

- Simple summaries such as these provide a crude assessment of whether the condition-to-condition and block-to-block variation is large.

  - If the condition-specific averages are very different, this suggests that the design factor influences the response.

  - If the block-specific averages are very different, this suggests that the nuisance factor influences the response, and that blocking was appropriate.

- The primary analysis goal in a RCBD is to determine whether the expected response differs significantly from one condition to another.

  - And if so, to identify the optimal condition, while controlling for the potential effect of the nuisance factor.

- We've previously done this with gatekeeper tests of the form:
  $$\mathbf{H}_0\colon \theta_1 = \theta_2 = \cdots = \theta_m \text{ versus } \mathbf{H}_A\colon \theta_j \neq \theta_k \text{ for some } j \neq k$$

- We do the same thing here, while accounting for the nuisance factor, with *appropriately defined* linear (continuous response) or logistic (binary response) regression models which contain:

  - An intercept.

  - $m - 1$ indicator variables for the design factor's levels.

  - $b - 1$ indicator variables for the nuisance factor's levels.

- We write the linear predictor as:

$$\alpha + \sum_{j=1}^{m-1} \beta_j x_{ij} + \sum_{k=1}^{b-1} \gamma_k z_{ij} \qquad (\star)$$

  - $x_{ij} = 1$ if unit i is in condition $j = 1, 2, \dots, m - 1$, and zero otherwise.

  - $z_{ik} = 1$ if unit i is in block $k = 1, 2, \dots, b - 1$, and zero otherwise.

  - The β's jointly quantify the effect of the design factor.

  - The γ's jointly quantify the effect of the nuisance factor.

- Two relevant hypotheses are:

  (1) $\mathbf{H}_0\colon \beta_1 = \beta_2 = \cdots = \beta_{m-1} = 0$ versus $\mathbf{H}_A\colon \beta_j \neq 0$ for some j.

- If we don't reject $\mathbf{H}_0$, this suggests the x's don't need to be in the model and hence the design factor doesn't significantly influence the response.

(2) $\mathbf{H}_0$: $\gamma_1 = \gamma_2 = \cdots = \gamma_{b-1} = 0$ versus $\mathbf{H}_A$: $\gamma_k \neq 0$ for some k.

- If we don't reject $\mathbf{H}_0$, this suggests the z's don't need to be in the model and hence the nuisance factor doesn't significantly influence the response. Therefore, blocking isn't necessary.

- We test these hypotheses by comparing a *full* model and *reduced* models where the *full* model is a model with a linear predictor given by $(\star)$, and a *reduced* model is a model with a linear predictor that arises when $\mathbf{H}_0$ is true.

  - We try to determine whether the full model fits the data significantly better than the reduced one.

4.1.1 RCBD to Compare Means

- Here, we're interested in testing the following hypothesis (while accounting for the influence of the nuisance factor):
$$\mathbf{H}_0: \mu_1 = \mu_2 = \cdots = \mu_m \text{ versus } \mathbf{H}_A: \mu_j \neq \mu_k \text{ for some } j \neq k$$
where μ_j is the expected response in condition $j = 1, 2, \dots, m$.

- We do this by testing:
$$\mathbf{H}_0: \beta_1 = \beta_2 = \cdots = \beta_{m-1} = 0 \text{ versus } \mathbf{H}_A: \beta_j \neq 0 \text{ for some } j$$
with an ANOVA in the context of the following linear regression model.

$$Y_i = \alpha + \sum_{j=1}^{m-1} \beta_j x_{ij} + \sum_{k=1}^{b-1} \gamma_k z_{ik} + \varepsilon_i$$

where Y_i is the response observation for unit $i = 1, 2, \dots, N = \sum_{k=1}^{b} \sum_{j=1}^{m} n_{jk}$ and $\varepsilon_i \overset{\text{iid}}{\sim} \mathcal{N}(0, \sigma^2)$ is a random error term.

- The relevant ANOVA table is Table 4.2.

Table 4.2: Two-Way ANOVA Table Associated With a Randomized Complete Block Design

Source	SS	d.f.	MS	Test Statistic
Condition	SS_C	$m-1$	$MS_C = SS_C/(m-1)$	$t_C = MS_C/MS_E$
Block	SS_B	$b-1$	$MS_B = SS_B/(b-1)$	$t_B = MS_B/MS_E$
Error	SS_E	$N-m-b+1$	$MS_E = SS_E/(N-m-b+1)$	
Total	SS_T	$N-1$		

- The sums of squares given in Table 4.2 are:
  - Total sum of squares (quantifies overall response variation):

$$SS_T = \sum_{k=1}^{b} \sum_{j=1}^{m} \sum_{i=1}^{n_{jk}} (y_{ijk} - \bar{y}_{\bullet\bullet\bullet})^2 = SS_C + SS_B + SS_E$$

  - Condition sum of squares (quantifies condition-to-condition response variation):

$$SS_C = \sum_{k=1}^{b} \sum_{j=1}^{m} \sum_{i=1}^{n_{jk}} (\bar{y}_{\bullet j \bullet} - \bar{y}_{\bullet\bullet\bullet})^2$$

– Block sum of squares (quantifies block-to-block response variation):

$$\text{SS}_\text{B} = \sum_{k=1}^{b} \sum_{j=1}^{m} \sum_{i=1}^{n_{jk}} (\bar{y}_{\bullet\bullet k} - \bar{y}_{\bullet\bullet\bullet})^2$$

– Error sum of squares (quantifies residual response variation not accounted for by conditions of blocks):

$$\text{SS}_\text{E} = \sum_{k=1}^{b} \sum_{j=1}^{m} \sum_{i=1}^{n_{jk}} (y_{ijk} - \bar{y}_{\bullet j\bullet} - \bar{y}_{\bullet\bullet k} + \bar{y}_{\bullet\bullet\bullet})^2$$

- So how do we use this table?

  – We test: $\mathbf{H}_0$: $\beta_1 = \beta_2 = \cdots = \beta_{m-1} = 0$ using $t_\text{C} = \text{MS}_\text{C}/\text{MS}_\text{E}$.

  * p-value $= \mathbb{P}(T \geq t_\text{C})$ where $T \sim F(m-1, N-m-b+1)$.

  – We test: $\mathbf{H}_0$: $\gamma_1 = \gamma_2 = \cdots = \gamma_{b-1} = 0$ using $t_\text{B} = \text{MS}_\text{B}/\text{MS}_\text{E}$.

  * p-value $= \mathbb{P}(T \geq t_\text{B})$ where $T \sim F(b-1, N-m-b+1)$.

4.1.2 Example: Promotions at The Gap

EXAMPLE 4.1.1: Promotions at The Gap

The Gap has three versions of an online weekday promotion that a customer sees when they go to gapcanada.ca:
- Version 1: 50% discount on one item.
- Version 2: 20% discount on your entire order.
- Version 3: Spend $50 and get a $10 gift card.

Interest lies in determining whether there is a difference in the average purchase total (i.e, the average dollar value of a customer's purchase) between promotion versions. However, the amount of money one spends may also be influenced by the nuisance factor, day of week. As such, we ran a randomized complete block design with $m = 3$ experimental conditions (corresponding to the three promotions) and $b = 5$ blocks (corresponding to the day of the week). Here $n_{jk} = 50$ for all (j, k), and so the design was "balanced." For each visitor to gapcanada.ca, their purchase total (in dollars) was recorded. The regression model fit to these response observations is:

$$Y_i = \alpha + \beta_2 x_{i2} + \beta_3 x_{i3} + \gamma_1 z_{i1} + \gamma_2 z_{i2} + \gamma_3 z_{i3} + \gamma_4 z_{i4} + \varepsilon_i$$

where x_{i2} and x_{i3} are condition indicators for promotions 2 and 3 (promotion 1 is the baseline) and $z_{i1}, \ldots, z_{i4}$ are block indicators for Monday-Thursday (Friday is the baseline). The ANOVA Table for this experiment is Table 4.3.

Table 4.3: The Gap RCBD ANOVA Table

Source	SS	d.f.	MS	Test Statistic
Condition	49618.34	2	24809.17	$t_\text{C} = 2165.39$
Block	19258.30	4	4814.58	$t_\text{B} = 420.22$
Error	8512.67	743	11.46	
Total	77389.32	749		

- $\mathbf{H}_0$: $\beta_2 = \beta_3 = 0$ tells us whether the design factor is significant.
  – p-value $= \mathbb{P}(T \geq t_\text{C}) = \mathbb{P}(T \geq 2165.39) = 1.101 \times 10^{-310}$ where $T \sim F(2, 743)$.
  – Therefore, we reject $\mathbf{H}_0$ and conclude that the expected response is not the same in all conditions.
- $\mathbf{H}_0$: $\gamma_1 = \gamma_2 = \gamma_3 = \gamma_4 = 0$ tells us whether the nuisance factor is significant.
  – p-value $= \mathbb{P}(T \geq t_\text{B}) = \mathbb{P}(T \geq 420.22) = 4.345 \times 10^{-189}$ where $T \sim F(4, 743)$.

– Therefore, we reject $\mathbf{H}_0$ and conclude that blocking was appropriate.

[R Code] `Comparing_means_within_blocks`

4.1.3 RCBD to Compare Proportions

- Here we're interested in testing the following hypothesis (while accounting for the influence of the nuisance factor):

$$\mathbf{H}_0\colon \pi_1 = \pi_2 = \cdots = \pi_m \text{ versus } \mathbf{H}_A\colon \pi_j \neq \pi_k \text{ for some } j \neq k$$

where π_j is the expected response in condition $j = 1, 2, \ldots, m$.

- We do this by testing:

$$\mathbf{H}_0\colon \beta_1 = \beta_2 = \cdots = \beta_{m-1} = 0 \text{ versus } \mathbf{H}_A\colon \beta_j \neq 0 \text{ for some } j$$

with a likelihood ratio test (LRT) in the context of the following logistic regression model:

$$\log\left(\frac{\pi_i}{1 - \pi_i}\right) = \alpha + \sum_{j=1}^{m-1} \beta_j x_{ij} + \sum_{k=1}^{b-1} \gamma_k z_{ik}$$

where Y_i is the response observation for unit $i = 1, 2, \ldots, N = \sum_{k=1}^{b} \sum_{j=1}^{m} n_{jk}$, and $\pi_i = \mathbb{E}[Y_i] = \mathbb{P}(Y_i = 1)$.

- The likelihood ratio test compares the full model to the one without the x's.

- Similarly, we test:

$$\mathbf{H}_0\colon \gamma_1 = \gamma_2 = \cdots = \gamma_{b-1} \text{ versus } \mathbf{H}_A\colon \gamma_k \neq 0 \text{ for some } k$$

with a LRT that compares the full model to the reduced one without the z's.

$$\mathbf{H}_0\colon \text{Reduced model fits as well versus } \mathbf{H}_A\colon \text{Full model fits better than reduced model.}$$

- The observed test statistic for both of these tests is:

$$
\begin{aligned}
t &= 2\log\left(\frac{\text{Likelihood}_{\text{Full Model}}}{\text{Likelihood}_{\text{Reduced Model}}}\right) \\
&= 2\Big[\text{Log-Likelihood}_{\text{Full Model}} - \text{Log-Likelihood}_{\text{Reduced Model}}\Big]
\end{aligned}
$$

which follows an approximate $\chi^2(\ell)$, if $\mathbf{H}_0$ is true, where

$$\ell = (\# \text{ parameters in full model}) - (\# \text{ parameters in reduced model})$$

- p-value $= \mathbb{P}(T \geq t)$ where $T \sim \chi^2(\ell)$.

4.1.4 Example: Enterprise Banner Ads

EXAMPLE 4.1.2: Enterprise Banner Ads

Enterprise is experimenting with $m = 3$ banner ads as a mechanism to drive traffic to their website. Since there are known regional differences in consumer preferences in the US, they wish to control for the nuisance factor "region" with $b = 4$ blocks corresponding to the four major US geographic regions: Northeast (NE), Northwest (NW), Southeast (SE), and Southwest (SW). We randomize a total of $n_{jk} = 5000$ for all (j, k) people to each ad condition in each region.

Interest lies in determining whether the different ads perform similarly with respect to click-through-rate (CTR) — and we wish to determine which one maximizes CTR — but we want to control for the effect of region. We do so with the following logistic regression model:

$$\log\left(\frac{\pi_i}{1 - \pi_i}\right) = \alpha + \beta_2 x_{i2} + \beta_3 x_{i3} + \gamma_1 z_{i1} + \gamma_2 z_{i2} + \gamma_3 z_{i3}$$

where x_{i2} and x_{i3} are condition indicators for ads 2 and 3 (ad 1 is the baseline), and z_{i1}, z_{i2}, z_{i3} are block indicators for NW, SE, SW regions (NE is the baseline).

- $\mathbf{H}_0$: $\beta_2 = \beta_3 = 0$.
  - p-value $= \mathbb{P}(T \geq t_{\mathrm{C}}) = \mathbb{P}(T \geq 249.924) = 5.367 \times 10^{-55}$ where $T \sim \chi^2(2)$.
  - Therefore, we reject $\mathbf{H}_0$ and conclude that the design factor is significant and the CTR is <u>not</u> the same in every condition.
- $\mathbf{H}_0$: $\gamma_1 = \gamma_2 = \gamma_3 = 0$.
  - p-value $= \mathbb{P}(T \geq t_{\mathrm{B}}) = \mathbb{P}(T \geq 139.824) = 4.126 \times 10^{-30}$ where $T \sim \chi^2(3)$.
  - Therefore, we reject $\mathbf{H}_0$ and conclude that the nuisance factor is significant and therefore blocking was a good thing to do.

[R Code] `Comparing_proportions_within_blocks`

WEEK 6

4.2 Balanced Incomplete Block Designs

- Randomized Complete Block Designs (RCBD) were a tool for the exploration of *one* design factor (m levels) while controlling for the effect of *one* nuisance factor (b blocks).

  - In a RCBD, we carry out *every* experimental condition inside *every* block.

  - But sometimes, due to practical constraints, this is not possible.

- The Gap is experimenting with $m = 3$ promotional offers:

  - Version 1: 50% discount on one item.

  - Version 2: 20% discount on your entire order.

  - Version 3: Spend \$50 and get a \$10 gift card.

- Experimenters would like to control for a possible day-of-week effect (block by day).

  - Naturally, one might consider a RCBD; that is, suppose we observe data in *every* block-condition combination as seen in Table 4.4.

Table 4.4: Complete Block Design

		Day					
		1	2	3	4	5	6
	1	✓	✓	✓	✓	✓	✓
Promotion	2	✓	✓	✓	✓	✓	✓
	3	✓	✓	✓	✓	✓	✓

- But The Gap may only offer two of the three promotions in a single day.

  - So we must consider an **incomplete** block design; that is, suppose we observe data in only *some* block-condition combinations.

- We refer to Table 4.5 as a **balanced incomplete block design** (BIBD).

REMARK 4.2.1: Notation

  - m: number of experimental conditions. In our previous example, $m = 3$.
  - b: number of blocks. In our previous example, $b = 6$.
  - $m^\star$: number of experimental conditions that can be run in each block. Also known as "block size." In our previous example, $m^\star = 2$.

Table 4.5: Incomplete Block Design

		Day					
		1	2	3	4	5	6
	1	✓	✓	×	✓	✓	×
Promotion	2	✓	×	✓	✓	×	✓
	3	×	✓	✓	×	✓	✓

> * RCBD: $m^\star = m$.
> * BIBD: $m^\star < m$.
> - r: number of blocks in which each condition appears. In our previous example, $r = 4$.
> - λ: number of blocks that *any* pair of conditions appear in together. In our previous example, $\lambda = 2$.

- The BIBD is "balanced" in the sense that:
  - The number of conditions in each block is the same for every block ($m^\star$).
  - The number of blocks each condition appears in is the same for every condition (r).
  - The number of blocks each pair of conditions appear in together is the same for every possible condition pairing (λ).

- This balance allows for the comparison of a metric of interest across m conditions while still accounting for a nuisance factor with b levels
  - But despite this balance, the "incompleteness" requires some sacrifice.

4.2.1 General Comments on the Design of a BIBD

- Not just any haphazard combination of $(m, b, m^\star, r, \lambda)$ values will yield a BIBD.

- Great care must go into planning a BIBD to ensure all forms of balance.

- A variety of restrictions must be met:
  - Consequences of "incompleteness:"
    * $m^\star < m$.
    * $r < b$.
    * $\lambda < r$.
  - Number of block-condition combinations for which we observe data:
    * $mr = bm^\star$
  - For condition X (doesn't matter which condition this is), $r(m^\star - 1) = \lambda(m - 1)$ is the total number of conditions that condition X appears within the same blocks.
    * Condition X appears in r blocks, and in each, it's grouped with $m^\star - 1$ *other* conditions.
    * We pair each of the other $m - 1$ conditions with condition X λ times.

- We use these restrictions as follows:
  1. Specify m, $m^\star$, and λ.
  2. Calculate $r = \lambda(m - 1)/(m^\star - 1)$, noting that it must be an integer.
  3. Calculate $b = mr/m^\star$, noting that it must be an integer.

EXAMPLE 4.2.2

Let $m = 3$, $m^\star = 2$, and $\lambda = 1$. We have $r = (1)(2)/(1) = 2$, and $b = (3)(2)/2 = 3$. See Table 4.6.

EXAMPLE 4.2.3: Pizza Table

Let $m = 3$, $m^\star = 2$, and $\lambda = 2$. We have $r = (2)(2)/(1) = 4$, and $b = (3)(4)/2 = 6$.

EXAMPLE 4.2.4

Let $m = 3$, $m^\star = 2$, and $\lambda = 3$. We have $r = (3)(2)/(1) = 6$, and $b = (3)(6)/2 = 9$. See Table 4.7.

- We select the design based on a trade-off between larger λ values and smaller b values.
    - Larger λ provides more information about pairwise comparisons.
    - Smaller b corresponds to fewer blocks and hence a smaller experiment.

Table 4.6: Incomplete Block Design

		Block		
		1	2	3
Condition	1	✓	✓	✗
	2	✓	✗	✓
	3	✗	✓	✓

Table 4.7: Incomplete Block Design

		Block								
		1	2	3	4	5	6	7	8	9
Condition	1	✓	✓	✓	✓	✓	✓	✗	✗	✗
	2	✓	✓	✓	✗	✗	✗	✓	✓	✓
	3	✗	✗	✗	✓	✓	✓	✓	✓	✓

4.2.2 General Comments on the Analysis of a BIBD

- Primary analysis goal:
    - Determine whether there exist significant differences among the expected response values from one experimental condition to another.

- In a RCBD, we do this by comparing the condition-specific means $\bar{y}_{\bullet j \bullet}$ to the overall mean $\bar{y}_{\bullet \bullet \bullet}$. This isn't fair in a BIBD because $\bar{y}_{\bullet \bullet \bullet}$ is calculated from data from blocks that condition j didn't appear in.

- In a BIBD, due to incompleteness, we compare $\bar{y}_{\bullet j \bullet}$ with the average response from the blocks that condition j appeared in:

$$\frac{\sum_{k \in \mathcal{B}_j} \sum_{i=1}^{n_{jk}} y_{ijk}}{\sum_{k \in \mathcal{B}_j} n_{jk}}$$

where $\mathcal{B}_j \subset \{1, 2, \ldots, B\}$ is the subset of indices indicating which blocks condition j appeared in.

- In general, the analysis of BIBDs involves an *adjustment* of this form when evaluating the effect of the design factor.

4.3 Latin Square Designs

- Until now, we have discussed experimental designs that employ blocking to control for *one* nuisance factor:

  - If we want to control for *two* nuisance factors, we should use a **Latin square design**.

  - If we want to control for *three* nuisance factors, we should use a **Graeco-Latin square design**.

  - If we want to control for *four* nuisance factors, we should use a **Hyper-Graeco-Latin square design**.

- A Latin square of order p is a $p \times p$ grid containing p unique symbols.

  - Each of these symbols occurs exactly once in each column.

  - Each of these symbols occurs exactly once in each row.

  - These "symbols" are typically denoted by Latin letters.

Table 4.8: 3×3, 4×4, and 5×5 Latin Square Examples

A	C	B
C	B	A
B	A	C

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

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

- A Sudoku puzzle is a special example of a 9×9 Latin square.

- We exploit this combinatorial structure to help us design experiments that facilitate blocking by two nuisance factors.

  - We arbitrarily associate the p rows with the levels of the first nuisance factor.

  - We arbitrarily associate the p columns with the levels of the second nuisance factor.

  - We arbitrarily associate the p Latin letters with the levels of the design factor.

- We present an example with $p = 4$ in Table 4.9.

Table 4.9: 4×4 Latin Square Design

		NF 2			
		1	2	3	4
NF 1	1	A	B	C	D
	2	D	A	B	C
	3	C	D	A	B
	4	B	C	D	A

  - **Limitation of LSD's**: we need to experiment with *all* of these factors at p levels.

  - $(3, 2)$ element represents the block where NF 1 is at level 3, NF 2 is at level 2, and DF is at level D.

- Each cell in this table represents a "block" in which we fix the nuisance factors' levels, and the Latin letter indicates the execution of an experimental condition.

- Rows, columns, and letters are all orthogonal, allowing us to separately estimate the effects of the design factor and each of the two nuisance factors.

- We may informally summarize these effects with the overall average and level-specific averages of the response variables.

  - Average response in a particular condition:

$$\bar{y}_{\bullet j \bullet \bullet} = \frac{1}{np} \sum_{(j,k,\ell) \in \mathcal{S}_j} \sum_{i=1}^{n} y_{ijk\ell}$$

  - Average response in a given row:

$$\bar{y}_{\bullet \bullet k \bullet} = \frac{1}{np} \sum_{(j,k,\ell) \in \mathcal{S}_k} \sum_{i=1}^{n} y_{ijk\ell}$$

  - Average response in a given column:

$$\bar{y}_{\bullet \bullet \bullet \ell} = \frac{1}{np} \sum_{(j,k,\ell) \in \mathcal{S}_\ell} \sum_{i=1}^{n} y_{ijk\ell}$$

  - Overall average:

$$\bar{y}_{\bullet \bullet \bullet \bullet} = \frac{1}{N} \sum_{(j,k,\ell) \in \mathcal{S}} \sum_{i=1}^{n} y_{ijk\ell}$$

    * $y_{ijk\ell}$ is the response observation for unit $i = 1, 2, \dots, n$ in block (k, ℓ) and hence condition j.
    * $j, k, \ell = 1, 2, \dots, p$.
    * n is the number of units in each block.
    * $N = np^2$.

- A comment about notation:

  - Each block contains just one condition, so each pair (k, ℓ) uniquely determines the value of j.
  - Consequently, there exist just p^2 tuples (j, k, ℓ).
  - Denote them by the set $\mathcal{S}$.
  - From Table 4.9, we have:

$(1,1,1)$	$(2,1,2)$	$(3,1,3)$	$(4,1,4)$
$(4,2,1)$	$(1,2,2)$	$(2,2,3)$	$(3,2,4)$
$(3,3,1)$	$(4,3,2)$	$(1,3,3)$	$(2,3,4)$
$(2,4,1)$	$(3,4,2)$	$(4,4,3)$	$(1,4,4)$

    * $\mathcal{S}_{j=1} = \{(1,1,1), (1,2,2), (1,3,3), (1,4,4)\}$.
    * We also define:
      · $\mathcal{S}_j \subset \mathcal{S}$: all tuples for which the design factor is level j.
      · $\mathcal{S}_k \subset \mathcal{S}$: all tuples for which the nuisance factor 1's is level k.
      · $\mathcal{S}_\ell \subset \mathcal{S}$: all tuples for which the nuisance factor 2's is level ℓ.

- The primary analysis goal in a Latin square design is to determine whether the expected response differs significantly from one condition to another.

- – If so, to identify the optimal condition while controlling for the potential effect of the nuisance factors.

- We've previously done this with gatekeeper tests of the form:
$$\mathbf{H}_0\text{: } \theta_1 = \theta_2 = \cdots = \theta_p \text{ versus } \mathbf{H}_A\text{: } \theta_j \neq \theta_{j'} \text{ for some } j \neq j'.$$

- We do the same thing here, while accounting for the nuisance factors, with *appropriately defined* linear or logistic regression models which contain:

    - – An intercept.
    - – $p-1$ indicator variables for the design factor's levels.
    - – $p-1$ indicator variables for nuisance factor 1's levels.
    - – $p-1$ indicator variables for nuisance factor 2's levels.

- We write the linear predictor as:

$$\alpha + \sum_{j=1}^{p-1} \beta_j x_{ij} + \sum_{k=1}^{p-1} \gamma_j z_{ik} + \sum_{\ell=1}^{p-1} \delta_\ell w_{i\ell}$$

    - – $x_{ij} = 1$ if unit i is in condition $j = 1, 2, \ldots, p-1$ (zero otherwise).
    - – $z_{ik} = 1$ if unit i is in a block for which nuisance factor 1 is at level $k = 1, 2, \ldots, p-1$ (zero otherwise).
    - – $w_{i\ell} = 1$ if unit i is in a block for which nuisance factor 2 is at level $\ell = 1, 2, \ldots, p-1$ (zero otherwise).
    - – The β's jointly quantify the effect of the design factor.
    - – The γ's jointly quantify the effect of nuisance factor 1.
    - – The δ's jointly quantify the effect of nuisance factor 2.

- Three relevant hypotheses are:
$$\mathbf{H}_0\text{: } \beta_1 = \beta_2 = \cdots = \beta_{p-1} = 0 \text{ versus } \mathbf{H}_A\text{: } \beta_j \neq 0 \text{ for some } j.$$
    - – Provides insight into whether DF is important.
$$\mathbf{H}_0\text{: } \gamma_1 = \beta_2 = \cdots = \gamma_{p-1} = 0 \text{ versus } \mathbf{H}_A\text{: } \gamma_k \neq 0 \text{ for some } k.$$
    - – Provides insight into whether NF 1 is important.
$$\mathbf{H}_0\text{: } \delta_1 = \delta_2 = \cdots = \delta_{p-1} = 0 \text{ versus } \mathbf{H}_A\text{: } \delta_\ell \neq 0 \text{ for some } \ell.$$
    - – Provides insight into whether NF 2 is important.

- We test these hypotheses by comparing a *full* (linear predictor) and *reduced* ($\mathbf{H}_0$ is true) model.

    - – We try to determine whether the full model fits the data significantly better than the reduced one.

4.3.1 Latin Squares to Compare Means

- Here we're interested in testing the following hypothesis (while accounting for the influence of the nuisance factors):
$$\mathbf{H}_0\text{: } \mu_1 = \mu_2 = \cdots = \mu_p \text{ versus } \mathbf{H}_A\text{: } \mu_j \neq \mu_{j'} \text{ for some } j \neq j'$$
where μ_j is the expected response in condition $j = 1, 2, \ldots, p$.

- We do this by testing:
$$\mathbf{H}_0\text{: } \beta_1 = \beta_2 = \cdots = \beta_{p-1} = 0 \text{ versus } \mathbf{H}_A\text{: } \beta_j \neq 0 \text{ for some } j$$
with an ANOVA in the context of the following linear regression model:

$$Y_i = \alpha + \sum_{j=1}^{p-1} \beta_j x_{ij} + \sum_{k=1}^{p-1} \gamma_k z_{ik} + \sum_{\ell=1}^{p-1} \delta_\ell w_{i\ell} + \varepsilon_i \quad \text{(Full Model)}$$

- Y_i is the response observation for unit $i = 1, 2, \ldots, N = np^2$.
- $\varepsilon_i \overset{\text{iid}}{\sim} \mathcal{N}(0, \sigma^2)$ is the random error term.

- The relevant sums of squares are:
  - The total sum of squares, which quantifies overall variation in response values:

  $$\text{SS}_{\text{T}} = \sum_{(j,k,\ell) \in \mathcal{S}} \sum_{i=1}^{n} (y_{ijk\ell} - \bar{y}_{\bullet\bullet\bullet\bullet})^2 = \text{SS}_{\text{C}} + \text{SS}_{\text{B}_1} + \text{SS}_{\text{B}_2} + \text{SS}_{\text{E}}$$

  - The condition sum of squares, which quantifies variability in the response from one condition to another:

  $$\text{SS}_{\text{C}} = \sum_{(j,k,\ell) \in \mathcal{S}} \sum_{i=1}^{n} (\bar{y}_{\bullet j\bullet\bullet} - \bar{y}_{\bullet\bullet\bullet\bullet})^2 = np \sum_{j=1}^{p} (\bar{y}_{\bullet j\bullet\bullet} - \bar{y}_{\bullet\bullet\bullet\bullet})^2$$

  - The first block sum of squares, which quantifies variability in the response from one level of nuisance factor 1 to another:

  $$\text{SS}_{\text{B}_1} = \sum_{(j,k,\ell) \in \mathcal{S}} \sum_{i=1}^{n} (\bar{y}_{\bullet\bullet k\bullet} - \bar{y}_{\bullet\bullet\bullet\bullet})^2 = np \sum_{k=1}^{p} (\bar{y}_{\bullet\bullet k\bullet} - \bar{y}_{\bullet\bullet\bullet\bullet})^2$$

  - The second block sum of squares, which quantifies variability in the response from one level of nuisance factor 2 to another:

  $$\text{SS}_{\text{B}_2} = \sum_{(j,k,\ell) \in \mathcal{S}} \sum_{i=1}^{n} (\bar{y}_{\bullet\bullet\bullet\ell} - \bar{y}_{\bullet\bullet\bullet\bullet})^2 = np \sum_{\ell=1}^{p} (\bar{y}_{\bullet\bullet\bullet\ell} - \bar{y}_{\bullet\bullet\bullet\bullet})^2$$

  - The error sum of squares, which quantifies variability in the response that was not explained by conditions or blocks (i.e., the design and nuisance factors):

  $$\text{SS}_{\text{E}} = \sum_{(j,k,\ell) \in \mathcal{S}} \sum_{i=1}^{n} (y_{ijk\ell} - \bar{y}_{\bullet j\bullet\bullet} - \bar{y}_{\bullet\bullet k\bullet} - \bar{y}_{\bullet\bullet\bullet\ell} - 2\bar{y}_{\bullet\bullet\bullet\bullet})^2$$

- We show the corresponding ANOVA table in Table 4.10.

Table 4.10: Three-Way ANOVA Table Associated with a Latin Square Design

Source	SS	d.f.	MS	Test Statistic
Design Factor	SS_{C}	$p-1$	$\text{MS}_{\text{C}} = \text{SS}_{\text{C}}/(p-1)$	$t_{\text{C}} = \text{MS}_{\text{C}}/\text{MS}_{\text{E}}$
Nuisance Factor 1	SS_{B_1}	$p-1$	$\text{MS}_{\text{B}_1} = \text{SS}_{\text{B}_1}/(p-1)$	$t_{\text{B}_1} = \text{MS}_{\text{B}_1}/\text{MS}_{\text{E}}$
Nuisance Factor 2	SS_{B_2}	$p-1$	$\text{MS}_{\text{B}_2} = \text{SS}_{\text{B}_2}/(p-1)$	$t_{\text{B}_2} = \text{MS}_{\text{B}_2}/\text{MS}_{\text{E}}$
Error	SS_{E}	$N - 3p + 2$	$\text{MS}_{\text{E}} = \text{SS}_{\text{E}}/(N - 3p + 2)$	
Total	SS_{T}	$N - 1$		

- So, how do we use this table?
  - We test $\mathbf{H}_0$: $\beta_1 = \beta_2 = \cdots = \beta_{p-1} = 0$ using $t_{\text{C}} = \text{MS}_{\text{C}}/\text{MS}_{\text{E}}$.
    * p-value: $\mathbb{P}(T \geq t_{\text{C}})$ where $T \sim F(p-1, N - 3p + 2)$.
  - We test: $\mathbf{H}_0$: $\gamma_1 = \gamma_2 = \cdots = \gamma_{p-1} = 0$ using $t_{\text{B}_1} = \text{MS}_{\text{B}_1}/\text{MS}_{\text{E}}$.
    * p-value: $\mathbb{P}\left(T \geq t_{\text{B}_1}\right)$ where $T \sim F(p-1, N - 3p + 2)$.

- We test: $\mathbf{H}_0$: $\delta_1 = \delta_2 = \cdots = \delta_{p-1} = 0$ using $t_{\mathrm{B}_2} = \mathrm{MS}_{\mathrm{B}_2}/\mathrm{MS}_{\mathrm{E}}$.
  * p-value: $\mathbb{P}\big(T \geq t_{\mathrm{B}_2}\big)$ where $T \sim F(p-1, N-3p+2)$.

4.3.2 Example: Netflix Latency

EXAMPLE 4.3.1: Netflix Latency

Consider the latency experiment described at the beginning of the chapter in which Netflix is experimenting with server-side modifications to improve (reduce) the latency of netflix.com. In particular, they have four different experimental conditions (A, B, C, D) that are intended to reduce average latency (in milliseconds). Two nuisance factors that may also influence latency are browser (Chrome, Microsoft Edge, Firefox, Safari), and time of day ([00:01,06:00], [06:01,12:00], [12:01,18:00], [18:01,00:00]). The design of the experiment is the 4×4 Latin square shown in Table 4.11. In order to determine whether the expected latency in each condition differs significantly, we randomize $n = 500$ users to each of the $p^2 = 16$ blocks.

Table 4.11: 4×4 Latin Square Design for the Netflix Experiment

| | | *Browser* | | | |
		Chrome	Edge	Firefox	Safari
	[00:01,06:00]	A	B	C	D
Time	[06:01,12:00]	D	A	B	C
	[12:01,18:00]	C	D	A	B
	[18:01,00:00]	B	C	D	A

We analyze the data with the following linear regression model:

$$Y_i = \alpha + \beta_2 x_{i2} + \beta_3 x_{i3} + \beta_4 x_{i4} + \gamma_1 z_{i1} + \gamma_2 z_{i2} + \gamma_3 z_{i3} + \delta_2 w_{i2} + \delta_3 w_{i3} + \delta_4 w_{i4} + \varepsilon_i$$

- x_{i2}, x_{i3}, x_{i4} are indicators for conditions B, C, D, where A is the baseline.
- z_{i1}, z_{i2}, z_{i3} are browser indicators for Microsoft Edge, Firefox, Safari, where Chrome is the baseline.
- w_{i2}, w_{i3}, w_{i4} are time indicators for time periods [06:01,12:00], [12:01,18:00], [18:01,00:00], where [00:01,06:00] is the baseline.

The ANOVA table associated with this model is Table 4.12.

Table 4.12: Netflix Latin Square ANOVA Table

Source	SS	d.f.	MS	Test Statistic
Condition	203903.38	3	67967.79	679.14
Browser	32.95	3	10.98	0.1097
Time	333242.01	3	111080.67	1109.92
Error	799636.18	7990	100.08	
Total	1336815	7999		

- $\mathbf{H}_0$: $\beta_2 = \beta_3 = \beta_4 = 0$.
  - p-value $= \mathbb{P}(T \geq t_{\mathrm{C}}) = \mathbb{P}(T \geq 679.14) \approx 0$ where $T \sim F(3, 7990)$.
  - Therefore, we reject $\mathbf{H}_0$ and conclude that the design factor significantly influences the response and hence the expected response is <u>not</u> the same in each condition.
- $\mathbf{H}_0$: $\gamma_1 = \gamma_2 = \gamma_3 = 0$.
  - p-value $= \mathbb{P}\big(T \geq t_{\mathrm{B}_1}\big) = \mathbb{P}(T \geq 0.1097) = 0.9545$ where $T \sim F(3, 7990)$.
  - Therefore, we do not reject $\mathbf{H}_0$ and conclude that "browser" does not significantly influence average latency, and so blocking by browser was probably not necessary.
- $\mathbf{H}_0$: $\delta_2 = \delta_3 = \delta_4 = 0$.
  - p-value $= \mathbb{P}\big(T \geq t_{\mathrm{B}_2}\big) = \mathbb{P}(T \geq 1109.92) \approx 0$ where $T \sim F(3, 7990)$.
  - Therefore, we reject $\mathbf{H}_0$ and conclude that the time of day significantly influences average latency and so blocking by it was sensible.

4.3.3 Latin Squares to Compare Proportions

- Here we're interested in testing the following hypothesis (while accounting for the influence of the nuisance factors):

  $$\mathbf{H}_0\text{: } \pi_1 = \pi_2 = \cdots = \pi_p \text{ versus } \mathbf{H}_A\text{: } \pi_j \neq \pi_{j'} \text{ for some } j \neq j'$$

  where π_j is the expected response in condition $j = 1, 2, \ldots, p$.

- We do this by testing:

  $$\mathbf{H}_0\text{: } \beta_1 = \beta_2 = \cdots = \beta_{p-1} = 0 \text{ versus } \mathbf{H}_A\text{: } \beta_j \neq 0 \text{ for some } j$$

  with a likelihood ratio test (LRT) in the context of the following logistic regression model:

  $$\log\left(\frac{\pi_i}{1 - \pi_i}\right) = \alpha + \sum_{j=1}^{p-1} \beta_j x_{ij} + \sum_{k=1}^{p-1} \gamma_k z_{ik} + \sum_{\ell=1}^{p-1} \delta_\ell w_{i\ell}$$

  - $Y_i = 1$ if unit i performs some action of interest, and $Y_i = 0$ otherwise.

  - $\pi_i = \mathbb{E}[Y_i] = $ expected response of unit i.

  - The likelihood ratio test compares the full model to the one without the x's.

- Similarly, we test:

  $$\mathbf{H}_0\text{: } \gamma_1 = \gamma_2 = \cdots = \gamma_{p-1} = 0 \text{ versus } \mathbf{H}_A\text{: } \gamma_k \neq 0 \text{ for some } k$$

  with a LRT that compares the full model to the reduced one without the z's.

- And we test:

  $$\mathbf{H}_0\text{: } \delta_1 = \delta_2 = \cdots = \delta_{p-1} = 0 \text{ versus } \mathbf{H}_A\text{: } \delta_\ell \neq 0 \text{ for some } \ell$$

  with a LRT that compares the full model to the reduced one without the w's.

- The observed test statistic for all of these tests is:

  $$t = 2 \log\left(\frac{\text{Likelihood}_{\text{Full Model}}}{\text{Likelihood}_{\text{Reduced Model}}}\right)$$

  $$= 2\Big[\text{Log-Likelihood}_{\text{Full Model}} - \text{Log-Likelihood}_{\text{Reduced Model}}\Big]$$

  which, if $\mathbf{H}_0$ is true, follows an approximate $\chi^2(p-1)$.

- p-value $= \mathbb{P}(T \geq t)$ where $T \sim \chi^2(p-1)$.

4.3.4 Example: Uber Weekend Promos

EXAMPLE 4.3.2: Uber Weekend Promos

Consider an experiment in which Uber is investigating the influence of three different promotional offers on ride-booking-rate (RBR).
- Promo A: None.
- Promo B: One free ride today.
- Promo C: Book a ride today and get 50% off your next 2 rides.

The experimenters would like to control for a possible day-of-week effect, and so they want to block by day. They would also like to control for possible city-to-city differences, and so they also want to block by city. To do so they run a 3×3 Latin square design as illustrated in Table 4.13. Interest lies in determining whether the different promotions perform similarly with respect to RBR — and they wish to determine which one maximizes RBR — while controlling for the effects of day and city. In order to do this they randomize $n = 1000$ users to each of the $p^2 = 9$ blocks.

Table 4.13: 3×3 Latin Square Design for the Uber Experiment

		City		
		Toronto	Vancouver	Montreal
Day	Friday	A	B	C
	Saturday	C	A	B
	Sunday	B	C	A

We analyze the data with the following logistic regression model:

$$\log\left(\frac{\pi_i}{1 - \pi_i}\right) = \alpha + \beta_2 x_{i2} + \beta_3 x_{i3} + \gamma_1 z_{i1} + \gamma_2 z_{i2} + \delta_1 w_{i1} + \delta_2 w_{i2}$$

- x_{i2}, x_{i3}, are condition indicators for promotions B, C, where A is the baseline.
- z_{i1}, z_{i2}, are day indicators for Saturday, Sunday, where Friday is the baseline.
- w_{i1}, w_{i2}, are city indicators for Toronto, Vancouver, where Montreal is the baseline.
- $\mathbf{H}_0$: $\beta_2 = \beta_3 = 0$.
  - p-value $= \mathbb{P}(T \geq t_C) = \mathbb{P}(T \geq 16.648) = 0.00024$ where $T \sim \chi^2(2)$.
  - Therefore, we reject $\mathbf{H}_0$ and conclude that the booking rate is <u>not</u> the same for each promotional offer.
- $\mathbf{H}_0$: $\gamma_1 = \gamma_2 = 0$.
  - p-value $= \mathbb{P}\left(T \geq t_{B_1}\right) = \mathbb{P}(T \geq 8.9107) = 0.01162$ where $T \sim \chi^2(2)$.
  - Therefore, we reject $\mathbf{H}_0$ and conclude that the day-of-week significantly influences booking, and so it is good that we blocked by this factor.
- $\mathbf{H}_0$: $\delta_1 = \delta_2 = 0$.
  - p-value $= \mathbb{P}\left(T \geq t_{B_2}\right) = \mathbb{P}(T \geq 2.1193) = 0.3466$ where $T \sim \chi^2(2)$.
  - Therefore, we do not reject $\mathbf{H}_0$ and conclude that "city" does not significantly influence booking rate, and so blocking by city may have not been necessary.

[R Code] `Latin_square_proportions`

Chapter 5

Experiments with Multiple Design Factors

- We now consider the design and analysis of experiments consisting of multiple conditions arising from multiple design factors.
    - This is often colloquially referred to as "multivariate testing" (MVT).
- Canonical MVT button test:

Many things influence click-through rate:
    - Colour.
    - Size.
    - Position.
    - Phrase.
- Some additional, more tangible, examples:
    - Etsy.
    - Netflix.
    - Airbnb.
- This week we describe how to design and analyze experiments that efficiently investigate multiple design factors.
- **Goals**:
    1. Determine which condition is optimal with respect to some metric of interest.

– But now a condition is defined by a specific combination of the levels of *multiple* design factors.

2. Determine *which* factors are influential and understand *how* the factors influence the response.

5.1 The Factorial Approach

- The key to multi-factor experiments is to *efficiently* investigate different combinations of the factor levels.

- **One-factor-at-a-time approach** (OFAT):

  – Sequence of experiments, each with just one factor being varied.

  – The winning level of this factor is retained.

  – Follow-up experiments manipulate some other factor, while the previous ones are held fixed at their optimal levels.

  > EXAMPLE 5.1.1: Button
  >
  > 1. Experiment with colour, and purple wins.
  > 2. Experiment with phrase, and "submit" wins.
  > 3. Experiment with size, and "large" wins.

EXAMPLE 5.1.2: Twitter ♡ versus ⋆

- In 2015 Twitter changed "favouriting" a tweet (expressed as stars) to "liking" a tweet (expressed as hearts) and the internet was pissed.
- In line with Twitter's "test everything" motto, this decision came about as a result of experimentation.
- A hypothetical experiment that could have lead to this decision might involve two factors at two levels.
  – DF1 = Shape → {Star, Heart}.
  – DF2 = Colour → {Yellow, Red}.
- A one-factor-at-a-time approach might look like this:
  – Experiment 1: ⋆ versus ♡.
  – Experiment 2: ⋆ versus ♡.
- Suppose they conclude that ♡ is the best, but what about ⋆? The problem with OFAT experiments is that we may never observe the truly optimal combination of factor levels.

EXAMPLE 5.1.3: Etsy Search Bar

- Check it out.

- **The Factorial approach**:

  – Experimental conditions are defined as every unique combination of the design factors' levels.

  – In the **Twitter** example, the factorial experiment would have looked like this: ⋆ ⋆ ♡♡.

  – In the **Etsy** example, the factorial experiment would have looked like this:
       Small Square Box, Small Rounded Box, Long Square Box, Long Rounded Box.

  – **Advantage**: it explores every possible condition.

    1. We don't miss the optimal condition.

    2. Our understanding of the relationship between the response and design factors is better with a factorial experiment than with an OFAT experiment.

- **Disadvantage**: it explores every possible condition.

  * With many design factors at many levels, the number of unique combinations might be unmanageably large.

  – As long as we choose our factors and their levels thoughtfully, the advantages outweigh the disadvantages.

- **Main effects**: The main effect of factor A, represents the change in the response variable produced by a change in that factor. In our **Twitter** example:

  – Main effect of shape: what happens to the response when we change the shape from ⋆ to ♡.

  – Main effect of colour: what happens to the response when we change the colour from yellow to red?

- **Interaction effects**: If the main effect of factor A depends on the level of some other factor B, we say that factors A and B interact. In our **Twitter** example:

  – Is there an interaction between shape and colour?

    ⟺ Does the effect of going from ⋆ to ♡ depend on colour?

    ⟺ Does the effect of going from yellow to red depend on shape?

- From a practical perspective it is critical to quantify both types of effects.

  – The only type of design that allows us to observe and estimate both main and interaction effects is the factorial design. The OFAT cannot do this.

5.2 Designing a Factorial Experiment

- Conceptually, the design of a factorial experiment is simple.

  1. Pick your metric of interest and define the corresponding response variable.

  2. Pick your design factors.

  3. Pick their levels.

  4. Define your experimental conditions (all possible combinations of our design factors' levels).

  5. Determine your sample sizes.

EXAMPLE 5.2.1: Button

Suppose you have $K = 3$ factors, *colour* (red, blue), *phrase* ("Continue", "Go"), and *size* (small, medium, large). These factors therefore have $m_1 = 2$, $m_2 = 2$, and $m_3 = 3$ levels respectively. Therefore, we have $m = m_1 m_2 m_3 = (2)(2)(3) = 12$ experimental conditions.

Go	Go	Go
Cont.	Continue	Continue
Go	Go	Go
Cont.	Continue	Continue

- In general, a factorial experiment with K factors requires $m = m_1 m_2 \cdots m_K$ conditions, where m_k is the number of levels of design factor k.

- As the number of factors and levels increase, the size of the experiment can get unmanageably large.

  – As such, we want to pick our factors and levels thoughtfully. Keep it simple.

1. Don't investigate factors that are highly correlated.

2. Don't choose levels that are very similar.

3. Don't choose factors that are hard to manipulate outside an experiment.

- Once the factors, levels, and hence experimental conditions have been established, experimental units must be randomized to each of the m conditions.

    - The number of experimental units assigned to each condition n_j, $j = 1, 2, \dots, m$, can be determined by sample size calculations associated with two-sample tests.

    - Make sure to account for the multiple comparison problem.

5.3   Analyzing a Factorial Experiment

- In order to determine which condition is optimal we use pairwise tests.

- In order to determine which factors are influential, and to quantify this influence we use regression.

- Whether it's a linear or logistic regression, we use a linear predictor which contains the following terms:

    - An intercept.

    - Main effect terms. We represent a factor with m_k levels using $m_k - 1$ variables.

    - Two-factor interaction terms, three-factor interaction terms, $\dots$, K-factor interaction terms.

    - In general, an h-factor interaction is represented by h-way products of the main effect indicators for the factors involved.

EXAMPLE 5.3.1: Button

With $K = 3$ factors with $m_1 = 2$, $m_2 = 2$, and $m_3 = 3$ levels, the required linear predictor will contain:
- Main effect terms, and
    - Let x_1 be an indicator for "colour."
    - Let x_2 be an indicator for "phrase."
    - Let x_3 and x_4 be indicators for "size."
- Two-factor interaction terms, and pairwise products of indicators for each pair of factors.
- Three-factor interaction terms. Three-way products of the indicators for all three factors.
- The linear predictor is given by:

$$\beta_0 + \underbrace{\beta_1 x_1 + \beta_2 x_2 + \beta_3 x_3 + \beta_4 x_4}_{\text{main effects}}$$
$$+ \underbrace{\beta_5 x_1 x_2 + \beta_6 x_1 x_3 + \beta_7 x_1 x_4 + \beta_8 x_2 x_3 + \beta_9 x_2 x_4}_{\text{two-factor interactions}}$$
$$+ \underbrace{\beta_{10} x_1 x_2 x_3 + \beta_{11} x_1 x_2 x_4}_{\text{three-factor interactions}}$$

- Hypotheses concerning the main effects will therefore involve $\beta_1, \beta_2, \beta_3, \beta_4$.
- Hypotheses concerning the two-factor interactions will involve $\beta_5, \beta_6, \beta_7, \beta_8, \beta_9$.
- Hypotheses concerning the three-factor interactions will involve β_{10}, β_{11}.

- In general, hypotheses of these sort will be performed by comparing full versus reduced models via partial F-tests (in the case of linear regression) and likelihood ratio tests (in the case of logistic regression).

5.3.1 Continuous Response — The Instagram Example

- We illustrate the topics discussed in this section in the context of an **Instagram Ad** example.

- Suppose that you are a data scientist at Instagram, and you are interested in running an experiment to learn about how ad frequency and ad type influences user engagement.

- Suppose that ad frequency has levels {9:1, 7:1, 4:1, 1:1} corresponding to ad frequencies of 1 in 10, 1 in 8, 1 in 5, and every other.

- Suppose also that ad type is a second design factor with levels {photo, video}.

- We will consider here the factorial experiment that considers every combination of these two factors' levels. Therefore, $m = m_1 m_2 = (4)(2) = 8$ conditions.

- Assume $n = 1000$ users are randomly assigned to each of these $m = 8$ conditions, and on each user we measure the length of time they engage with the app (in minutes).

- We use the resulting data to create the following **main effect plots** (i.e., the plots of MOI versus the levels of each factor) in Figure 5.1.
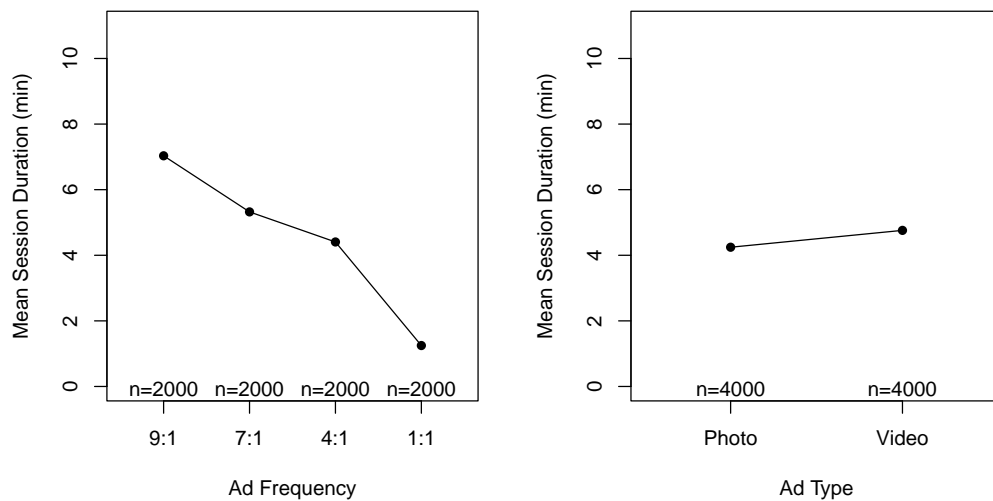

Figure 5.1: Left: Main Effect Plot for Ad Frequency; Right: Main Effect Plot for Ad Type

- As ad frequency increases, we see that average session duration increases.

- Average session duration increases with video ads relative to photo ads.

- Ad frequency appears to be more influential than ad type since the change in ASD produced by changes in frequency is large (in magnitude) than those produced by changes in ad type.

- **Important**:
  - Discussing main effects can be uninformative and potentially misleading if there is a significant interaction between the factors
  - In the presence of a significant interaction effect, it no longer makes sense to discuss the main effect of a factor in isolation, because doing so ignores the fact that this effect changes depending on the level of another factor.

- We can evaluate the presence of such interaction by studying **interaction effect plots** (i.e., plots of the MOI at each level of DF1 with different line types distinguishing the levels of DF2) in Figure 5.2.

- Non-parallel line segments on these plots would indicate the presence of an interaction since this would correspond to the main effect of one factor depending on the levels of the other factor.
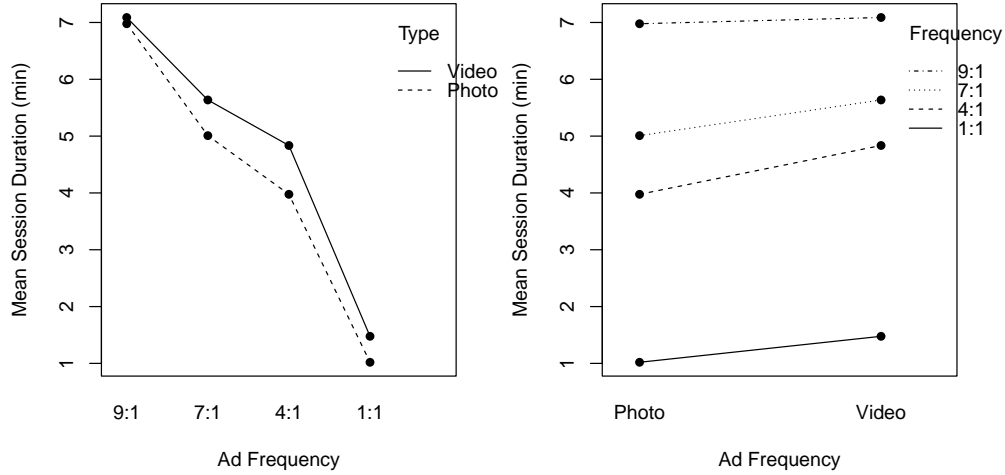
Figure 5.2: Interaction Plot for Ad Frequency and Ad Type.

- – The line segments in these plots are not perfectly parallel and so an interaction appears to exist.
  - – However, the departure from parallelism is not drastic, and so this interaction is perhaps not strong.
- To formally evaluate whether these main effects and interaction effects are significant we fit the following linear regression model:

$$Y_i = \beta_0 + \underbrace{\beta_1 x_{i1} + \beta_2 x_{i2} + \beta_3 x_{i3}}_{\text{main effects of frequency}} + \underbrace{\beta_4 x_{i4}}_{\text{main effects of type}} + \underbrace{\beta_5 x_{i1} x_{i4} + \beta_6 x_{i2} x_{i4} + \beta_7 x_{i3} x_{i4}}_{\text{two-factor interaction}} + \varepsilon_i$$

where the x's are indicator variables.

  - – $x_{i1} = 1$ if unit i is in a condition with the 7:1 ad frequency.
  - – $x_{i2} = 1$ if unit i is in a condition with the 4:1 ad frequency.
  - – $x_{i3} = 1$ if unit i is in a condition with the 1:1 ad frequency.
  - – $x_{i4} = 1$ if unit i is in a condition with video ads.
- The expected response in each condition, according to this model is Table 5.1.

		Ad Type	
		Photo	Video
Freq.	9:1	$\mathbb{E}[Y_i \mid x_{i1} = x_{i2} = x_{i3} = 0, x_{i4} = 0] = \beta_0$	$\mathbb{E}[Y_i \mid x_{i1} = x_{i2} = x_{i3} = 0, x_{i4} = 1] = \beta_0 + \beta_4$
	7:1	$\mathbb{E}[Y_i \mid x_{i1} = 1, x_{i4} = 0] = \beta_0 + \beta_1$	$\mathbb{E}[Y_i \mid x_{i1} = 1, x_{i4} = 1] = \beta_0 + \beta_1 + \beta_4 + \beta_5$
	4:1	$\mathbb{E}[Y_i \mid x_{i2} = 1, x_{i4} = 0] = \beta_0 + \beta_2$	$\mathbb{E}[Y_i \mid x_{i2} = 1, x_{i4} = 1] = \beta_0 + \beta_2 + \beta_4 + \beta_6$
	1:1	$\mathbb{E}[Y_i \mid x_{i3} = 1, x_{i4} = 0] = \beta_0 + \beta_3$	$\mathbb{E}[Y_i \mid x_{i3} = 1, x_{i4} = 1] = \beta_0 + \beta_3 + \beta_4 + \beta_7$

Table 5.1: Expected Response in Each Ad Frequency-Type Condition

- Clearly, a formal test of:

$$\mathbf{H}_0\text{: } \beta_5 = \beta_6 = \beta_7 = 0 \text{ versus } \mathbf{H}_A\text{: } \beta_j \neq 0$$

for $j = 5, 6, 7$ would evaluate the significance of the interaction effect.

  - – If we reject $\mathbf{H}_0$, any conclusions regarding the effect of one factor must be made in the context of the levels of the other factor.

– If we do not reject $\mathbf{H}_0$, the interaction terms can be removed from the model yielding the following simplified **main effects** model:

$$Y_i = \beta_0 + \beta_1 x_{i1} + \beta_2 x_{i2} + \beta_3 x_{i3} + \beta_4 x_{i4} + \varepsilon_i$$

which can be used to evaluate the significance of the main effect of each factor.

– The expected response in each condition, according to the main effects model is Table 5.2.

		Ad Type	
		Photo	Video
Freq.	9:1	$\mathbb{E}[Y_i \mid x_{i1} = x_{i2} = x_{i3} = 0, x_{i4} = 0] = \beta_0$	$\mathbb{E}[Y_i \mid x_{i1} = x_{i2} = x_{i3} = 0, x_{i4} = 1] = \beta_0 + \beta_4$
	7:1	$\mathbb{E}[Y_i \mid x_{i1} = 1, x_{i4} = 0] = \beta_0 + \beta_1$	$\mathbb{E}[Y_i \mid x_{i1} = 1, x_{i4} = 1] = \beta_0 + \beta_1 + \beta_4$
	4:1	$\mathbb{E}[Y_i \mid x_{i2} = 1, x_{i4} = 0] = \beta_0 + \beta_2$	$\mathbb{E}[Y_i \mid x_{i2} = 1, x_{i4} = 1] = \beta_0 + \beta_2 + \beta_4$
	1:1	$\mathbb{E}[Y_i \mid x_{i3} = 1, x_{i4} = 0] = \beta_0 + \beta_3$	$\mathbb{E}[Y_i \mid x_{i3} = 1, x_{i4} = 1] = \beta_0 + \beta_3 + \beta_4$

Table 5.2: Expected Response in Each Ad Frequency-Type Condition, Based on the Main Effects Model

– The hypothesis:

$$\mathbf{H}_0\text{: } \beta_1 = \beta_2 = \beta_3 = 0 \text{ versus } \mathbf{H}_A\text{: } \beta_j \neq 0$$

for $j = 1, 2, 3$ tests whether ad frequency is a significant factor.

– The hypothesis:

$$\mathbf{H}_0\text{: } \beta_4 = 0 \text{ versus } \mathbf{H}_A\text{: } \beta_4 \neq 0$$

tests whether ad type is a significant factor.

– **But remember**: these tests and the interpretation of main effects are only appropriate in the absence of interaction.

• Each of these null hypotheses generates a **reduced model** with fewer terms relative to a **full model** with all terms — we compare them using partial F-tests associated with an analysis of variance.

• Output from the relevant partial F-tests is shown in Figure 5.3.

• Conclusions:

– The p-value associated with $\mathbf{H}_0$: $\beta_5 = \beta_6 = \beta_7 = 0$ is very small, suggesting that the interaction between ad frequency and ad type is significant.

– The p-value associated with $\mathbf{H}_0$: $\beta_4 = 0$ is very small, suggesting that the main effect of ad type is significant.

– The p-value associated with $\mathbf{H}_0$: $\beta_1 = \beta_2 = \beta_3 = 0$ is very small, suggesting that the main effect of ad frequency is significant.

   * Strictly speaking, the last two conclusions are irrelevant because we know the interaction is significant. Although, I include this for instructional purposes.

• [R Code] `Factorial_example_means`

5.3.2   Binary Response — The TinyCo Example

• The informal and formal evaluation of main and interaction effects can be performed in the context of a binary response variable as well.

– Main effect and interaction effect plots are based on observed proportions.

– Logistic regression is used instead of ordinary linear regression.

• The structure of the linear predictor is identical to what we have discussed in general.

```
## Analysis of Variance Table
##
## Model 1: Time ~ Frequency + Type
## Model 2: Time ~ Frequency * Type
##   Res.Df    RSS Df Sum of Sq      F    Pr(>F)
## 1   7995 6522.2
## 2   7992 6372.9  3    149.27 62.398 < 2.2e-16 ***
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1

## Analysis of Variance Table
##
## Model 1: Time ~ Frequency
## Model 2: Time ~ Frequency + Type
##   Res.Df    RSS Df Sum of Sq      F    Pr(>F)
## 1   7996 7049.5
## 2   7995 6522.2  1    527.34 646.43 < 2.2e-16 ***
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1

## Analysis of Variance Table
##
## Model 1: Time ~ Type
## Model 2: Time ~ Frequency + Type
##   Res.Df    RSS Df Sum of Sq      F    Pr(>F)
## 1   7998 41875
## 2   7995  6522  3     35353 14445 < 2.2e-16 ***
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
```

Figure 5.3: ANOVA Output For Instagram Example

- For instance, if the Instagram experiment from the previous section had a binary response instead, the relevant logistic regression model would be

$$\log\left(\frac{\pi_i}{1-\pi_i}\right) = \beta_0 + \beta_1 x_{i1} + \beta_2 x_{i2} + \beta_3 x_{i3} + \beta_4 x_{i4} + \beta_5 x_{i1} x_{i4} + \beta_6 x_{i2} x_{i4} + \beta_7 x_{i3} x_{i4}$$

  where the x's are the indicator variables defined previously.

- Interest lies in determining whether subsets of the β's are equal to zero to evaluate the significance of various main and interaction effects.

  – We use **likelihood ratio tests** for the comparison of full and reduced logistic regression models.

  – The test statistic for the LRT is:

  $$t = 2\log\left(\frac{\text{Likelihood}_{\text{Full Model}}}{\text{Likelihood}_{\text{Reduced Model}}}\right)$$
  $$= 2\Big[\text{Log-Likelihood}_{\text{Full Model}} - \text{Log-Likelihood}_{\text{Reduced Model}}\Big]$$

  – If $\mathbf{H}_0$ is true, then t should look like it comes from a $\chi^2(\nu)$ distribution, where

  $$\nu = (\#\text{ coefficients in full model}) - (\#\text{ coefficients in reduced model})$$

  – p-value $= \mathbb{P}(T \geq t)$ where $T \sim \chi^2(\nu)$.

WEEK 8

Pit Stop: *Effects* vs. *Terms* in a Linear Predictor

Example: Suppose Factor A has $m_1 = 5$ levels, Factor B has $m_2 = 2$ levels, and Factor C has $m_3 = 3$ levels.

- The main effect for a given factor is represented by indicator variables corresponding to the levels of that factor.

  – **Factor A** will be represented in a regression model by $m_1 - 1 = 4$ indicator variables: x_1, x_2, x_3, x_4, and $m_1 - 1 = 4$ corresponding β's: $\beta_1 = \beta_2 = \beta_3 = \beta_4$.

  – Thus, the *main effect* of Factor A is composed of 4 *terms* in the model.

  – To determine the significance of the main effect of Factor A, we test:
  $$\mathbf{H}_0\colon \beta_1 = \beta_2 = \beta_3 = \beta_4 = 0.$$

  – **Factor B** will be represented in a regression model by $m_2 - 1 = 1$ indicator variable: x_5, and $m_2 - 1 = 1$ corresponding β: β_5.

  – Thus, the *main effect* of Factor B is composed of 1 *term* in the model.

  – To determine the significance of the main effect of Factor B, we test:
  $$\mathbf{H}_0\colon \beta_5 = 0.$$

  – **Factor C** will be represented in a regression model by $m_3 - 1 = 2$ indicator variables: x_6, x_7, and $m_3 - 1 = 2$ corresponding β's: β_6, β_7.

  – Thus, the *main effect* of Factor C is composed of 2 *terms* in the model.

  – To determine the significance of the main effect of Factor C, we test:
  $$\mathbf{H}_0\colon \beta_6 = \beta_7 = 0.$$

– **Note**: These three hypotheses are relevant only in the context of the *main effect* model which has linear predictor:

$$\beta_0 + \beta_1 x_1 + \beta_2 x_2 + \beta_3 x_3 + \beta_4 x_4 + \beta_5 x_5 + \beta_6 x_6 + \beta_7 x_7$$

- The interaction effect between *two* factors is represented by two-way products of the indicator variables corresponding to the main effects of the two factors.

  – The **A:B interaction** *effect* is composed of the $(m_1 - 1) \times (m_2 - 1) = 4 \times 1 = 4$ *terms* resulting from the two-way products between Factor A's and Factor B's indicator variables: $x_1 x_5, x_2 x_5, x_3 x_5, x_4 x_5$, with corresponding β's: $\beta_8, \beta_9, \beta_{10}, \beta_{11}$.

  – The significance of the A:B interaction effect is determined by testing:
  $$\mathbf{H}_0 \colon \beta_8 = \beta_9 = \beta_{10} = \beta_{11} = 0.$$

  – The **A:C interaction** *effect* is composed of the $(m_1 - 1) \times (m_3 - 1) = 4 \times 2 = 8$ *terms* resulting from the two-way products between Factor A's and Factor C's indicator variables:

  $$x_1 x_6, x_2 x_6, x_3 x_6, x_4 x_6, x_1 x_7, x_2 x_7, x_3 x_7, x_4 x_7,$$

  with corresponding β's: $\beta_{12}, \beta_{13}, \ldots, \beta_{19}$.

  – The significance of the A:C interaction effect is determined by testing:
  $$\mathbf{H}_0 \colon \beta_{12} = \beta_{13} = \beta_{14} = \beta_{15} = \beta_{16} = \beta_{17} = \beta_{18} = \beta_{19} = 0.$$

  – The **B:C interaction** *effect* is composed of the $(m_2 - 1) \times (m_3 - 1) = 1 \times 2 = 2$ *terms* resulting from the two-way products between Factor B's and Factor C's indicator variables: $x_5 x_6, x_5 x_7$, with corresponding β's: β_{20}, β_{21}.

  – The significance of the B:C interaction effect is determined by testing:
  $$\mathbf{H}_0 \colon \beta_{20} = \beta_{21} = 0.$$

- The interaction effect between *three* factors is represented by three-way products of the indicator variables corresponding to the main effects of the three factors.

  – The **A:B:C interaction** *effect* is composed of the $(m_1 - 1) \times (m_2 - 1) \times (m_3 - 1) = 4 \times 1 \times 2 = 8$ *terms* resulting from the three-way products between Factor A's, Factor B's, and Factor C's indicator variables:

  $$x_1 x_5 x_6, x_1 x_5 x_7, x_2 x_5 x_6, x_2 x_5 x_7, x_3 x_5 x_6, x_3 x_5 x_7, x_4 x_5 x_6, x_4 x_5 x_7,$$

  with corresponding β's: $\beta_{22}, \ldots, \beta_{29}$.

  – The significance of the A:B:C interaction effect is determined by testing:
  $$\mathbf{H}_0 \colon \beta_{22} = \beta_{23} = \beta_{24} = \beta_{25} = \beta_{26} = \beta_{27} = \beta_{28} = \beta_{29} = 0.$$

  – **Note**: The hypotheses concerning the significance of interaction effects are relevant only in the context of the *full model* which has linear predictor:

$$
\begin{aligned}
\text{Intercept} \to{}& \beta_0 + \\
\text{ME's} \to{}& \beta_1 x_1 + \beta_2 x_2 + \beta_3 x_3 + \beta_4 x_4 + \beta_5 x_5 + \beta_6 x_6 + \beta_7 x_7 + \\
\text{2FI's} \to{}& \left\{
\begin{array}{l}
\beta_8 x_1 x_5 + \beta_9 x_2 x_5 + \beta_{10} x_3 x_5 + \beta_{11} x_4 x_5 + \beta_{12} x_1 x_6 + \beta_{13} x_2 x_6 + \beta_{14} x_3 x_6 + \\
\beta_{15} x_4 x_6 + \beta_{16} x_1 x_7 + \beta_{17} x_2 x_7 + \beta_{18} x_3 x_7 + \beta_{19} x_4 x_7 + \beta_{20} x_5 x_6 + \beta_{21} x_5 x_7 +
\end{array}
\right. \\
\text{3FI's} \to{}& \left\{
\begin{array}{l}
\beta_{22} x_1 x_5 x_6 + \beta_{23} x_1 x_5 x_7 + \beta_{24} x_2 x_5 x_6 + \beta_{25} x_2 x_5 x_7 + \\
\beta_{26} x_3 x_5 x_6 + \beta_{27} x_3 x_5 x_7 + \beta_{28} x_4 x_5 x_6 + \beta_{29} x_4 x_5 x_7
\end{array}
\right.
\end{aligned}
$$

- **ALL** the tests discussed here are carried by either a **partial F-test** or a **likelihood ratio test**.

- Partial F-test: p-value $= \mathbb{P}(T \geq t)$ where $T \sim F(\nu, h)$.
- Likelihood ratio test: p-value $= \mathbb{P}(T \geq t)$ where $T \sim \chi^2(\nu)$.
- $\nu = (\# \ \beta$'s in "full" model$) - (\# \ \beta$'s in "reduced" model$)$.
- $h =$ error degrees of freedom in the "full" model $= N - \# \ \beta$'s in "full" model.

TinyCo is a mobile video game studio that develops the Tiny Zoo game. In this game users own zoos and collect animals to put in their zoos. An experiment is performed in which a new animal, the "bananimal," is released for purchase as a part of the Super Sweet Series. Interest lies in understanding the relationship between conversion (purchase rate) and two factors: the bananimal's colour (yellow or gold) and the bananimal's price ($10, $20, or $30 of in-game currency). A factorial experiment with 6 conditions was performed to investigate these relationships. A summary of the data resulting from this experiment is shown below.

Condition	Sample Size	Purchase Rate
$10 + Yellow	500	0.1720
$20 + Yellow	483	0.0973
$30 + Yellow	488	0.0492
$10 + Gold	500	0.2260
$20 + Gold	500	0.1840
$30 + Gold	487	0.1992

- What does the main effect plots tell us?
    - ME of colour: gold bananimals are purchased more frequently than yellow.
    - ME of price: we expect purchase rate to decrease as bananimal price increases.
    - However, we should not stop here because an interaction exists.
- What does the interaction effect plots tell us?
    - A price-colour interaction exists.
    - We see that increasing price from $20 to $30 for gold bananimals increases purchase rate, whereas the same increase for yellow bananimals decreases purchase rate.
- To formally analyze the data, we fit the *full* logistic regression model with linear predictor:

$$\beta_0 + \beta_1 x_{i1} + \beta_2 x_{i2} + \beta_3 x_{i3} + \beta_4 x_{i1} x_{i2} + \beta_5 x_{i1} x_{i3}$$

    - $x_{i1} = 1$ if unit i is in a gold bananimal condition.
    - $x_{i2} = 1$ if unit i is in a $20 bananimal condition.
    - $x_{i3} = 1$ if unit i is in a $30 bananimal condition.
- We test the significance of the interaction effects via the hypothesis:
$$\mathbf{H_0}: \ \beta_4 = \beta_5 = 0 \text{ vs. } \mathbf{H_A}: \ \beta_j \neq 0 \text{ for some } j = 4, 5.$$
- This involves a comparison between the full model and the reduced *main effects* model with linear predictor:
$$\beta_0 + \beta_1 x_{i1} + \beta_2 x_{i2} + \beta_3 x_{i3}$$
    - p-value $= \mathbb{P}(T \geq 19.918) = 4.731 \times 10^{-5}$ where $T \sim \chi^2(2)$.
    - Therefore, we reject $\mathbf{H_0}$ and conclude that the price-colour interaction is significant.
- We can also test the main effect of colour with $\mathbf{H_0}: \ \beta_1 = 0$ in the context of the main effects model:
    - $t = 53.757$.
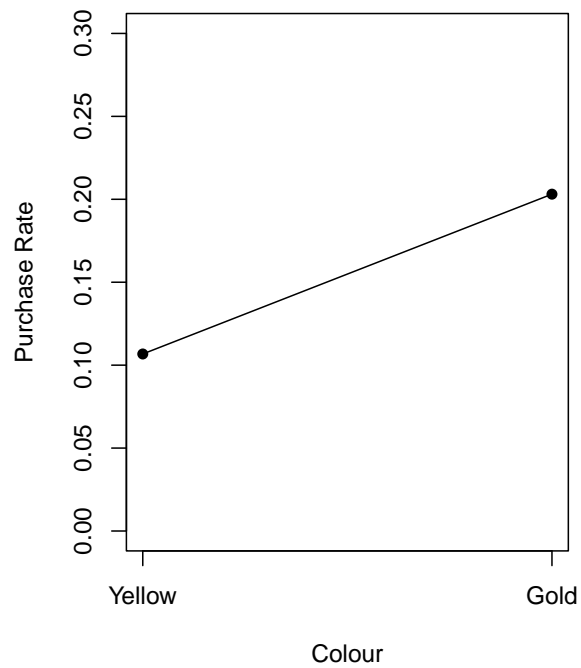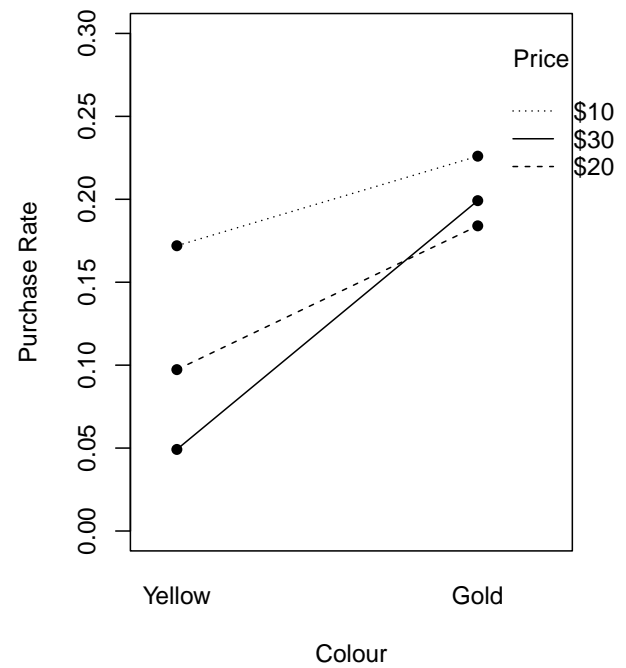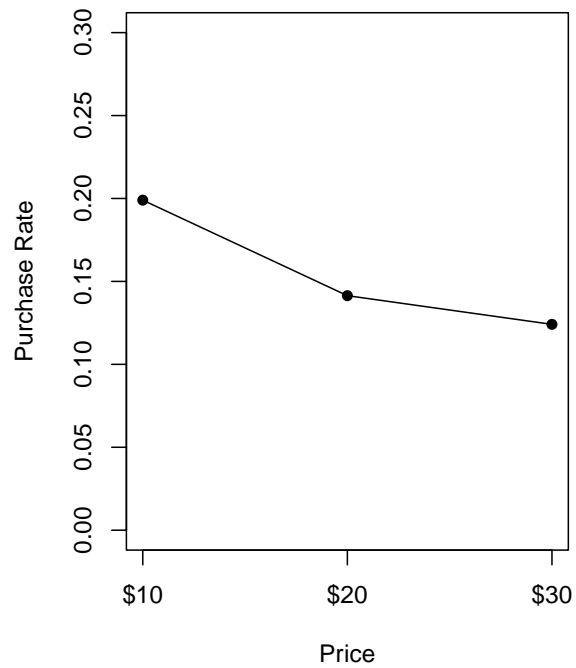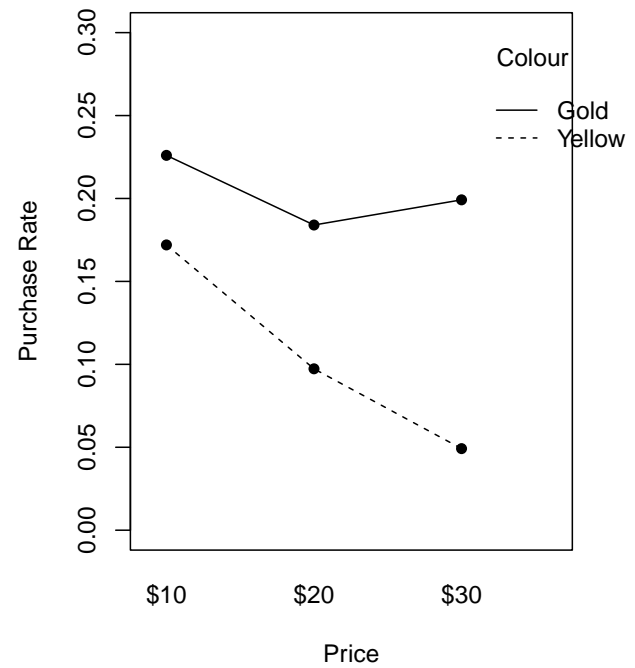
- p-value $= 2.269 \times 10^{-13}$.

    - Therefore, we reject $\mathbf{H}_0$ and conclude that colour <u>does</u> significantly influence purchase rate.

- We can also test the main effect of price with $\mathbf{H}_0$: $\beta_2 = \beta_3 = 0$ in the context of the main effects model:

    - $t = 23.324$.

    - p-value $= 8.614 \times 10^{-6}$.

    - Therefore, we reject $\mathbf{H}_0$ and conclude that price <u>does</u> significantly influence purchase rate.

- So what have we learned about the influence of these factors?

    - Colour and price both significantly influence purchase rate.

    - Gold bananimals tend to be purchased more often than yellow.

    - Increasing price from \$10 to \$20 decreases purchase rate (for both colours) and increasing price from \$20 to \$30 increase purchase rate for gold but not yellow bananimal.

- And which condition was optimal?

    - It turns out that the purchase rate is not statistically significantly different in the three gold bananimal conditions. So, \$30 gold bananimals seem like a good choice for TinyCo.

- [R Code] `Factorial_example_proportions`

5.4   Two-Level Factorial Experiments

- Factorial experiments are the most informative means of exploring several design factors.

- But this may require a larger number of experimental conditions than is practically feasible.

- As a compromise, we might consider **two-level factorial experiments**.

    - This is a factorial experiment where each factor is experimented at just two levels.

- Such an experiment is typically used for **factor screening**.

    - Among a larger number of factors, we want to determine which significantly influence the response.

- Factoring screening is predicated on the **Pareto Principle**.

    - Only a "vital few" factors will be important relative to the "trivial many."

- We will discuss two types of two-level factorial experiments:

    - $\mathbf{2^K}$ **factorial designs**: investigates K design factors in 2^K conditions (i.e., all possible combinations of the factors' levels).

    - $\mathbf{2^{K-p}}$ **factorial designs**: investigates K design factors in 2^{K-p} conditions (i.e., just a <u>fraction</u> of all possible combinations of the factors' levels).

Chapter 6

2^K Factorial Experiments

6.1 Designing 2^K Factorial Experiments

<div align="center">WEEK 9</div>

---

* 2^K factorial experiments involved K design factors, each at two levels.

- These experiments are typically used for factor screening.

    → **Primary Goal**: Determine which among the K factors significantly influence the response variable.

    → **Secondary Goal**: Determine which combination of levels is optimal.

        ↪ This is only relevant if the levels experimented with are the only ones of interest.

→ The design of the experiment involves:

1. Choose the MOI and response variables.

    ↪ Dictated by the question.

2. Choose the design factors.

    ↪ Choose K factors that may influence the response and that you want to learn about.

3. Choose the levels of the design factors.

    ↪ With the goal of factor screening we want to give influential factors as an opportunity as possible to show themselves as being influential.

    ↪ Pick levels that are quite different. For example, colour and discount amount.

4. Define experimental conditions.

    ↪ These are the 2^K unique combinations of the K factors' levels.

5. Assign n experimental units to each condition.

    ↪ Balance is not necessary, it's just notationally convenient.

    ↪ Overall sample size: $N = n2^K$.

- In two-level experiments we regard the two levels of a factor as *low* and *high* values of that factor.

    – If a factor is categorical, then "low" vs. "high" labelling is arbitrary.

- We represent each factor by a binary variable:

$$x = \begin{cases} -1 & \text{if the factor is at its "low" level} \\ 1 & \text{if the factor is at its "high" level} \end{cases}$$

  * We <u>could</u> alternatively code each x as an indicator variable, but the ± 1 coding gives rise to some convenient statistical properties.

→ With the factor levels coded in this way, each experimental condition can be identified by a unique combination of plus and minus ones.

- The experimental design can be completely summarized by the **design matrix**.

  − 2^K rows (for each condition) and K columns (for each factor) of plus and minus ones.

  → The ± 1 entries are organized such that each row corresponds to a unique condition and the columns correspond to each of the factors.

  → The design matrix provides a prescription for running the 2^K factorial experiment.

EXAMPLE 6.1.1: 2^1 Design Matrix

$$\begin{array}{c} C1 \to \\ C2 \to \end{array} \begin{bmatrix} -1 \\ +1 \end{bmatrix} = [\boldsymbol{x}_1]$$

EXAMPLE 6.1.2: 2^2 Design Matrix

$$\begin{array}{c} C1 \to \\ C2 \to \\ C3 \to \\ C4 \to \end{array} \begin{bmatrix} -1 & -1 \\ +1 & -1 \\ -1 & +1 \\ +1 & +1 \end{bmatrix} = [\boldsymbol{x}_1 \quad \boldsymbol{x}_2]$$

EXAMPLE 6.1.3: 2^3 Design Matrix

$$\begin{array}{c} C1 \to \\ C2 \to \\ C3 \to \\ C4 \to \\ C5 \to \\ C6 \to \\ C7 \to \\ C8 \to \end{array} \begin{bmatrix} -1 & -1 & -1 \\ +1 & -1 & -1 \\ -1 & +1 & -1 \\ +1 & +1 & -1 \\ -1 & -1 & +1 \\ +1 & -1 & +1 \\ -1 & +1 & +1 \\ +1 & -1 & +1 \end{bmatrix} = [\boldsymbol{x}_1 \quad \boldsymbol{x}_2 \quad \boldsymbol{x}_3]$$

→ 2^K experiments may also be visualized geometrically as K-dimensional hypercubes.

  − Vertices correspond to the unique configurations of the K factors' levels, and hence experimental conditions.

    <u>Design Space</u>: the space of all possible combinations of the design factors' values.

6.2 Analyzing 2^K Factorial Experiments

- Primary goal of a 2^K factorial experiment is factor screening.

  − Interest lies primarily in estimation of main and interaction effects.

* The **main effect** of a factor is defined as the expected change in response produced by changing that factor from its low to its high level.

* The **interaction effect** between two factors quantifies the difference between the main effect of one factor at the two levels of the other.

6.2.1 An Intuition-Based Analysis

EXAMPLE 6.2.1: Toy Example

Factors A and B are investigated in a 2^2 factorial experiment with $n = 3$.

Condition	Factor A	Factor B	Response (y)	Average Response ($\bar{y}$)
1	-1	-1	$\{1, 1, 2\}$	$4/3$
2	$+1$	-1	$\{3, 4, 5\}$	$12/3$
3	-1	$+1$	$\{2, 1, 3\}$	$6/3$
4	$+1$	$+1$	$\{1, 2, 5\}$	$8/3$

* Intuitive estimate of the main effect of A:

$$\widehat{\text{ME}}_A = \bar{y}_{A^+} - \bar{y}_{A^-} = \frac{\bar{y}_{A^+ \cap B^-} + \bar{y}_{A^+ \cap B^+}}{2} - \frac{\bar{y}_{A^- \cap B^-} + \bar{y}_{A^- \cap B^+}}{2}$$
$$= \frac{(12/3) + (8/3)}{2} - \frac{(4/3) + (6/3)}{2}$$
$$= -1/3$$

  Therefore, we expect the average response to go up by $10/6$ when A is moved from its low to high level.
* Intuitive estimate of the main effect of B:

$$\widehat{\text{ME}}_B = \bar{y}_{B^+} - \bar{y}_{B^-} = \frac{\bar{y}_{A^- \cap B^+} + \bar{y}_{A^+ \cap B^+}}{2} - \frac{\bar{y}_{A^- \cap B^-} + \bar{y}_{A^+ \cap B^-}}{2}$$
$$= \frac{(6/3) + (8/3)}{2} - \frac{(4/3) + (12/3)}{2}$$
$$= -1/3$$

  Therefore, we expect the average response to go down by $1/3$ when B is moved from its low to high level.
* To evaluate whether factors A and B interact, we should compare the main effect of A when B is at its high level to the main effect of A when B is at its low level.
    − Conditional ME of A when B is high:

$$\widehat{\text{ME}}_{A|B^+} = \bar{y}_{A^+ \cap B^+} - \bar{y}_{A^- \cap B^+} = \frac{8}{3} - \frac{6}{3} = \frac{2}{3}$$

    − Conditional ME of A when B is low:

$$\widehat{\text{ME}}_{A|B^-} = \bar{y}_{A^+ \cap B^-} - \bar{y}_{A^- \cap B^-} = \frac{12}{3} - \frac{4}{3} = \frac{8}{3}$$

    Therefore, because $\widehat{\text{ME}}_{A|B^+} \neq \widehat{\text{ME}}_{A|B^-}$ we know there exists an A:B interaction.
* The interaction effect is defined as the average difference between the conditional main effects:

$$\widehat{\text{IE}}_{AB} = \frac{\widehat{\text{ME}}_{A|B^+}}{2} - \frac{\widehat{\text{ME}}_{A|B^-}}{2}$$
$$= \frac{\widehat{\text{ME}}_{B|A^+}}{2} - \frac{\widehat{\text{ME}}_{B|A^-}}{2}$$
$$= \frac{\bar{y}_{A^+ \cap B^+} + \bar{y}_{A^- \cap B^-}}{2} - \frac{\bar{y}_{A^+ \cap B^-} + \bar{y}_{A^- \cap B^+}}{2}$$
$$= \frac{2}{6} - \frac{8}{6}$$
$$= -1$$

- If a third factor C were involved, we may define the three-way ABC interaction as:

$$
\begin{aligned}
\widehat{\text{IE}}_{\text{ABC}} &= \frac{\widehat{\text{IE}}_{\text{AB}|\text{C}^+}}{2} - \frac{\widehat{IE}_{\text{AB}|\text{C}^-}}{2} \\
&= \frac{\widehat{\text{IE}}_{\text{AC}|\text{B}^+}}{2} - \frac{\widehat{IE}_{\text{AC}|\text{B}^-}}{2} \\
&= \frac{\widehat{\text{IE}}_{\text{BC}|\text{A}^+}}{2} - \frac{\widehat{IE}_{\text{BC}|\text{A}^-}}{2}
\end{aligned}
$$

- So what actually happened here?
  - ME of A: average response in the rightmost corners, minus the average response in the leftmost corners.
  - ME of B: average response in the topmost corners, minus the average response in the bottommost corners.
  - IE of AB: difference of the average response in ellipses joining opposing corners.
- These intuitive comparisons are still relevant when the response variable is binary:

$$
\widehat{\text{ME}}_{\text{A}} = \sqrt{\frac{\bar{y}_{\text{A}^+ \cap \text{B}^-}}{1 - \bar{y}_{\text{A}^+ \cap \text{B}^-}} \times \frac{\bar{y}_{\text{A}^+ \cap \text{B}^+}}{1 - \bar{y}_{\text{A}^+ \cap \text{B}^+}}} \div \sqrt{\frac{\bar{y}_{\text{A}^- \cap \text{B}^-}}{1 - \bar{y}_{\text{A}^- \cap \text{B}^-}} \times \frac{\bar{y}_{\text{A}^- \cap \text{B}^+}}{1 - \bar{y}_{\text{A}^- \cap \text{B}^+}}}
$$

$$
\widehat{\text{ME}}_{\text{B}} = \sqrt{\frac{\bar{y}_{\text{A}^- \cap \text{B}^+}}{1 - \bar{y}_{\text{A}^- \cap \text{B}^+}} \times \frac{\bar{y}_{\text{A}^+ \cap \text{B}^+}}{1 - \bar{y}_{\text{A}^+ \cap \text{B}^+}}} \div \sqrt{\frac{\bar{y}_{\text{A}^+ \cap \text{B}^-}}{1 - \bar{y}_{\text{A}^+ \cap \text{B}^-}} \times \frac{\bar{y}_{\text{A}^- \cap \text{B}^-}}{1 - \bar{y}_{\text{A}^- \cap \text{B}^-}}}
$$

$$
\widehat{\text{IE}}_{\text{AB}} = \sqrt{\frac{\bar{y}_{\text{A}^+ \cap \text{B}^+}}{1 - \bar{y}_{\text{A}^+ \cap \text{B}^+}} \times \frac{\bar{y}_{\text{A}^- \cap \text{B}^-}}{1 - \bar{y}_{\text{A}^- \cap \text{B}^-}}} \div \sqrt{\frac{\bar{y}_{\text{A}^+ \cap \text{B}^-}}{1 - \bar{y}_{\text{A}^+ \cap \text{B}^-}} \times \frac{\bar{y}_{\text{A}^- \cap \text{B}^+}}{1 - \bar{y}_{\text{A}^- \cap \text{B}^+}}}
$$

  ↪ Where do these come from?
    * Calculate the odds that $Y = 1$ in each corner (condition).
    * Compare the corners in one red ellipse to the other.
    * This comparison is based on a ratio of geometric means (as opposed to a difference of arithmetic means like in the non-binary case).

6.2.2 A Regression-Based Analysis

The Model

- Fitted regression models provide an estimate of the **response surface**.
  ↪ **Response surface**: functional relationship between the response and design factors.
- Each of the K factors is represented by the binary variables.

$$
x_j = \begin{cases} -1 & \text{if the factor is at its "low" level} \\ 1 & \text{if the factor is at its "high" level} \end{cases} \quad \text{for } j = 1, 2, \dots, K
$$

- Since each factor is represented by a single term, the linear predictor contains:
  - An intercept: β_0.
  - K main effect terms corresponding to $x_1, x_2, \dots, x_K$.
  - $\binom{K}{2}$ two-factor interaction terms corresponding to $x_1 x_2, x_1 x_3, x_1 x_4, \dots$.

- $\binom{K}{3}$ three-factor interaction terms corresponding to $x_1 x_2 x_3, x_1 x_2 x_4, \dots$.

- $\vdots$

- $\binom{K}{K} = 1$ K-factor interaction term corresponding to $x_1 x_2 \cdots x_K$.

In total, there are $\sum_{j=0}^{K} \binom{k}{j} = 2^K$ terms.

EXAMPLE 6.2.2: 2^1 Example

$$\beta_0 + \beta_1 x_1$$

EXAMPLE 6.2.3: 2^2 Example

$$\beta_0 + \beta_1 x_1 + \beta_2 x_2 + \beta_{12} x_2$$

EXAMPLE 6.2.4: 2^3 Example

$$\beta_0 + \underbrace{\beta_1 x_1 + \beta_2 x_2 + \beta_3 x_3}_{\text{main effects}} + \underbrace{\beta_{12} x_1 x_2 + \beta_{13} x_1 x_3 + \beta_{23} x_2 x_3}_{\text{two-factor interactions}} + \underbrace{\beta_{123} x_1 x_2 x_3}_{\text{three-factor interaction}}$$

Estimation

- Estimation of the β's is carried out by:

  ↪ Ordinary least squares (in the case of linear regression).

  ↪ Maximum likelihood (in the case of logistic regression).

- In both cases there is a one-to-one connection between the main and interaction effects. Note that $\widehat{\text{Effect}}$ are calculated using the "intuitive" formulas described above.

  - Continuous response:
  $$\widehat{\text{Effect}} = 2\hat{\beta}$$

  - Binary response:
  $$\widehat{\text{Effect}} = e^{2\hat{\beta}}$$

  where β is the regression coefficient corresponding to the effect of interest.

- Recall the **Toy Example**:

  - The linear predictor for that experiment is:
  $$\beta_0 + \beta_1 x_1 + \beta_2 x_2 + \beta_{12} x_1 x_2$$

  where x_1 and x_2 correspond to factors A and B respectively.

  - The linear regression model is:
  $$Y_i = \beta_0 + \beta_1 x_{i1} + \beta_2 x_{i2} + \beta_{12} x_{i1} x_{i2} + \varepsilon_i \quad i = 1, 2, \dots, N = n2^K$$

  which can be written in matrix-vector notation as:
  $$\boldsymbol{Y} = \mathbf{X}\boldsymbol{\beta} + \boldsymbol{\varepsilon}$$

where

$$
\boldsymbol{Y} = \begin{bmatrix} 1 \\ 1 \\ 2 \\ 3 \\ 4 \\ 5 \\ 2 \\ 1 \\ 3 \\ 1 \\ 2 \\ 5 \end{bmatrix}, \quad
\mathbf{X} = \begin{bmatrix}
1 & -1 & -1 & 1 \\
1 & -1 & -1 & 1 \\
1 & -1 & -1 & 1 \\
1 & 1 & -1 & -1 \\
1 & 1 & -1 & -1 \\
1 & 1 & -1 & -1 \\
1 & -1 & 1 & -1 \\
1 & -1 & 1 & -1 \\
1 & -1 & 1 & -1 \\
1 & 1 & 1 & 1 \\
1 & 1 & 1 & 1 \\
1 & 1 & 1 & 1
\end{bmatrix} = \begin{bmatrix} \mathbf{1} & \boldsymbol{x}_1 & \boldsymbol{x}_2 & \boldsymbol{x}_{12} \end{bmatrix}, \quad
\boldsymbol{\beta} = \begin{bmatrix} \beta_0 \\ \beta_1 \\ \beta_2 \\ \beta_{12} \end{bmatrix}, \quad
\boldsymbol{\varepsilon} = \begin{bmatrix} \varepsilon_1 \\ \varepsilon_2 \\ \vdots \\ \varepsilon_{12} \end{bmatrix}
$$

⋆ The columns of X are orthogonal!

· This is why we code x's using ± 1's.

– The least squares estimate of $\boldsymbol{\beta}$ is:

$$\hat{\boldsymbol{\beta}} = (\mathbf{X}^\top \mathbf{X})^{-1} \mathbf{X}^\top \boldsymbol{Y}$$

Therefore,

$$
\mathbf{X}^\top \mathbf{X} = \begin{bmatrix}
12 & 0 & 0 & 0 \\
0 & 12 & 0 & 0 \\
0 & 0 & 12 & 0 \\
0 & 0 & 0 & 12
\end{bmatrix}_{4\times 4} \rightarrow (\mathbf{X}^\top \mathbf{X})^{-1} = \frac{1}{12} \mathbf{I}_4
$$

$$
\mathbf{X}^\top \boldsymbol{Y} = \begin{bmatrix} \mathbf{1}^\top \boldsymbol{Y} \\ \boldsymbol{x}_1^\top \boldsymbol{Y} \\ \boldsymbol{x}_2^\top \boldsymbol{Y} \\ \boldsymbol{x}_3^\top \boldsymbol{Y} \end{bmatrix} = \begin{bmatrix}
\displaystyle\sum_{i=1}^{N} Y_i \\
\displaystyle\sum_{i:A^+} Y_i - \sum_{i:A^-} Y_i \\
\displaystyle\sum_{i:B^+} Y_i - \sum_{i:B^-} Y_i \\
\displaystyle\sum_{i:A^+\cap B^+} Y_i + \sum_{i:A^-B^-} Y_i - \sum_{i:A^-B^+} Y_i - \sum_{i:A^+B^-} Y_i
\end{bmatrix}
$$

$$
\hat{\boldsymbol{\beta}} = (\mathbf{X}^\top \mathbf{X})^{-1} \mathbf{X}^\top \boldsymbol{Y} = \begin{bmatrix} 5/2 \\ 10/12 \\ -1/6 \\ -1/2 \end{bmatrix}
$$

– Notice that:

$$
\hat{\boldsymbol{\beta}} = \begin{bmatrix} 5 \\ 10/6 \\ -1/3 \\ -1 \end{bmatrix} = \begin{bmatrix} 2\bar{y} \\ \widehat{\text{ME}}_A \\ \widehat{\text{ME}}_B \\ \widehat{\text{IE}}_{AB} \end{bmatrix}
$$

This is the same as what we calculated using the "intuitive" formulas. This is <u>not</u> a coincidence!

• In general:

– $\boldsymbol{Y}$ is an $N \times 1$ vector of response observations.

– $\boldsymbol{\varepsilon}$ is an $N \times 1$ random vector of error terms.

– $\boldsymbol{\beta}$ is a $2^K \times 1$ vector of regression coefficients.

– $\mathbf{X}$ is the $N \times 2^K$ **model matrix** containing plus and minus ones.

* Each column represents a different effect (i.e., term in the linear predictor).

* Interaction columns are obtained from element-wise multiplication of the main effects columns involved in the interaction.

* ± 1's in the rows are defined in terms of the design matrix (i.e., which condition the response observation was observed in).

* The columns of the model matrix are <u>always</u> orthogonal $\to \mathbf{X}^\top \mathbf{X} = N\mathbf{I}_{2^K} \to (\mathbf{X}^\top \mathbf{X})^{-1} = \frac{1}{N}\mathbf{I}_{2^K}$.

– Due to the orthogonality of the model matrix, any effect (whether main or interaction) is estimated as:

$$\widehat{\text{Effect}} = 2\hat{\beta} = \frac{\mathbf{X}^\top \mathbf{Y}}{n2^{K-1}}$$

where $\boldsymbol{x}$ is the column of $\mathbf{X}$ corresponding to the effect of interest, and β is the corresponding regression coefficient.

* This should make sense: β's in ordinary regression are interpreted as the expected change in response resulting from a unit increase in x. Here, we care about two-unit increases (i.e., low $\to$ high, $-1 \to +1$).

Hypothesis Testing

* The significance of main and interaction effects is determined by testing hypotheses that set the relevant β's equal to 0.

* But now, because each effect is represented by just a single term, the hypotheses of interest involve just a single β.

* In the **Toy Example**, if we wanted to determine the significance of factor A, we simply test
$$\mathbf{H}_0\colon \beta_1 = 0$$
or if we want to determine whether the A:B interaction is significant, we test
$$\mathbf{H}_0\colon \beta_{12} = 0.$$

* Hypotheses like these are tested with ordinary significance tests for individual regression coefficients.

– t-tests in the case of linear regression.

– Z-tests in the case of logistic regression.

* <u>All</u> tests can be done in the <u>full model</u> (linear predictor with 2^K terms).

* But if for some reason we still want to test hypotheses about several β's simultaneously, we can compare full and reduced models with the usual:

– Partial F-tests in the case of linear regression.

– Likelihood ratio tests in the case of logistic regression.

6.2.3 The Credit Card Example

* To illustrate a complete analysis of a 2^K factorial experiment, we consider an example from Montgomery (2019) in which an experiment was performed to test new ideas to improve the conversion rate of credit card offers. For this example, the response is binary — indicating whether an individual signed up for a credit card as a result of the offer — and so an analysis based on logistic regression is performed.

* A 2^4 factorial experiment was carried out to investigate four factors and their influence on credit card sign-ups. The four factors and each of their levels are summarized in Table 6.1.

Table 6.1: Factors and levels for the credit card example.

Factor	Low ($-$)	High ($+$)
Annual Fee (x_1)	Current	Lower
Account-Opening Fee (x_2)	No	Yes
Initial Interest Rate (x_3)	Current	Lower
Long-term Interest Rate (x_4)	Low	High

- The $2^4 = 16$ unique combinations of these factor levels produced 16 experimental conditions, each of which was assigned $n = 7500$ units. Practically speaking, 16 credit card offers were devised (one corresponding to each condition) and each was mailed to 7500 customers. The design matrix and a summary of the conversion rates are provided in Table 6.2.

Table 6.2: Design matrix and response summary for the 2^4 factorial credit card experiment.

Condition	Factor 1	Factor 2	Factor 3	Factor 4	Sign-ups	Conversion Rate
1	-1	-1	-1	-1	184	2.45%
2	$+1$	-1	-1	-1	252	3.36%
3	-1	$+1$	-1	-1	162	2.16%
4	$+1$	$+1$	-1	-1	172	2.29%
5	-1	-1	$+1$	-1	187	2.49%
6	$+1$	-1	$+1$	-1	254	3.39%
7	-1	$+1$	$+1$	-1	174	2.32%
8	$+1$	$+1$	$+1$	-1	183	2.44%
9	-1	-1	-1	$+1$	138	1.84%
10	$+1$	-1	-1	$+1$	168	2.24%
11	-1	$+1$	-1	$+1$	127	1.69%
12	$+1$	$+1$	-1	$+1$	140	1.87%
13	-1	-1	$+1$	$+1$	172	2.29%
14	$+1$	-1	$+1$	$+1$	219	2.92%
15	-1	$+1$	$+1$	$+1$	153	2.04%
16	$+1$	$+1$	$+1$	$+1$	152	2.03%

- Using this data we fit a logistic regression model with the following linear predictor:

$$
\begin{aligned}
\text{Intercept} &\rightarrow \beta_0 + \\
\text{ME's} &\rightarrow \beta_{12}x_1x_2 + \beta_{13}x_1x_3 + \beta_{14}x_1x_4 + \beta_{23}x_2x_3 + \beta_{24}x_2x_4 + \beta_{34}x_3x_4 + \\
\text{2FI's} &\rightarrow \beta_8 x_1 x_5 + \beta_9 x_2 x_5 + \beta_{10} x_3 x_5 + \beta_{11} x_4 x_5 + \beta_{12} x_1 x_6 + \beta_{13} x_2 x_6 + \beta_{14} x_3 x_6 + \\
\text{3FI's} &\rightarrow \beta_{123}x_1x_2x_3 + \beta_{124}x_1x_2x_4 + \beta_{134}x_1x_3x_4 + \beta_{234}x_2x_3x_4 + \\
\text{4FI} &\rightarrow \beta_{1234}x_1x_2x_3x_4
\end{aligned}
$$

- The regression output associated with this model is in Figure 6.1.

  - The p-value for $\mathbf{H_0}$: $\beta_1 = 0$ is 2.92×10^{-5}.

  - The p-value for $\mathbf{H_0}$: $\beta_2 = 0$ is 3.99×10^{-8}.

  - The p-value for $\mathbf{H_0}$: $\beta_3 = 0$ is 0.00260.

  - The p-value for $\mathbf{H_0}$: $\beta_4 = 0$ is 2.29×10^{-8}.

  - The p-value for $\mathbf{H_0}$: $\beta_{12} = 0$ is 0.00434.

  - The p-value for $\mathbf{H_0}$: $\beta_{34} = 0$ is 0.04899.

Figure 6.1: `glm()` for Credit Card Example

```
Coefficients:
             Estimate Std. Error  z value Pr(>|z|)
(Intercept) -3.739697   0.019342 -193.347  < 2e-16 ***
x1           0.080845   0.019342    4.180 2.92e-05 ***
x2          -0.106211   0.019342   -5.491 3.99e-08 ***
x3           0.058248   0.019342    3.011  0.00260 **
x4          -0.108086   0.019342   -5.588 2.29e-08 ***
x1:x2       -0.055164   0.019342   -2.852  0.00434 **
x1:x3       -0.004794   0.019342   -0.248  0.80426
x2:x3       -0.006967   0.019342   -0.360  0.71868
x1:x4       -0.013178   0.019342   -0.681  0.49566
x2:x4        0.010625   0.019342    0.549  0.58280
x3:x4        0.038079   0.019342    1.969  0.04899 *
x1:x2:x3    -0.009646   0.019342   -0.499  0.61799
x1:x2:x4     0.010629   0.019342    0.550  0.58265
x1:x3:x4    -0.002543   0.019342   -0.131  0.89539
x2:x3:x4    -0.020946   0.019342   -1.083  0.27885
x1:x2:x3:x4 -0.009496   0.019342   -0.491  0.62347
---
Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0
```

- We now know which main and interaction effects are significant (i.e., all main effects x_1:x_2 and x_3:x_4).

  – Let's use main and interaction effect plots to help us interpret these effects.

    * In Figure 6.2, the conversion rate is maximized when the annual fee is low, no account opening fee, and when initial and long-term interest rates are low.

    * In Figure 6.3:

      · When an account opening fee exists, the effect of the annual fee is less than if there wasn't an account opening fee.

      · As long as long-term interest is low, the effect of initial interest rate is not large.

Figure 6.2: Main effect plots for the credit card example.
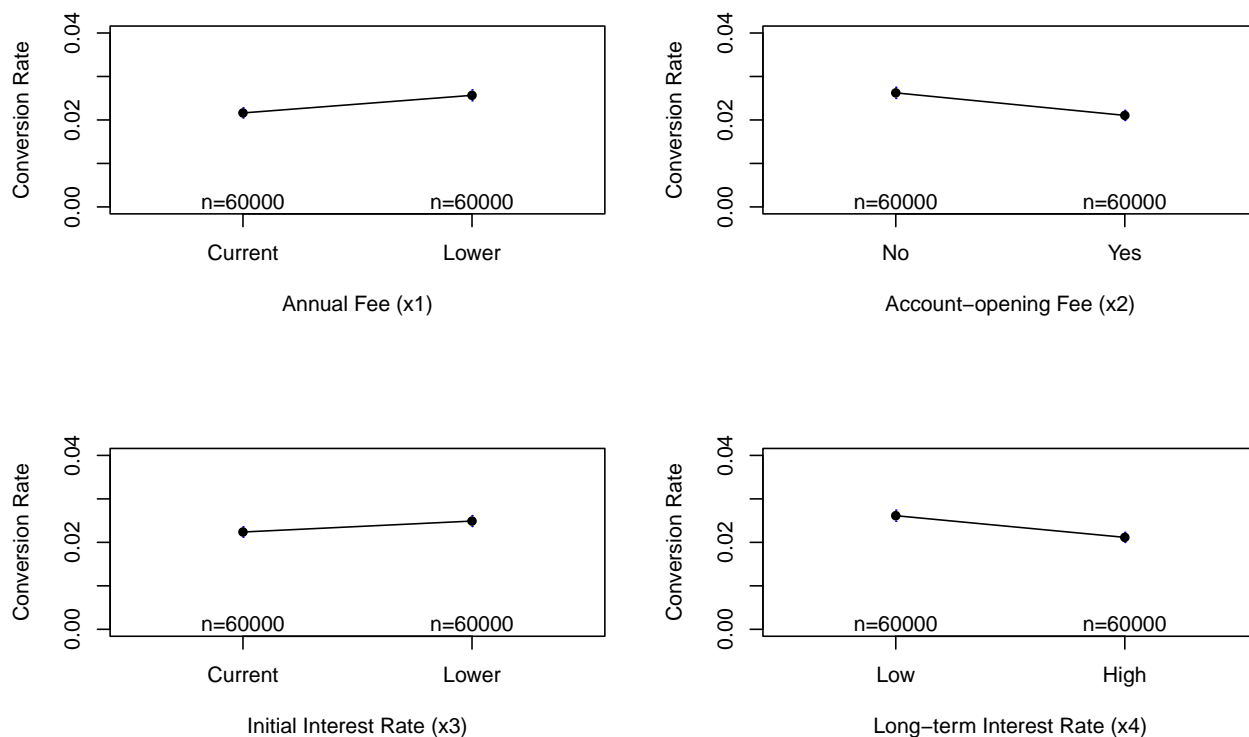
- [R Code] 2^4_Factorial_Example

Figure 6.3: Interaction effect plots for the credit card example