# Lecture #20: Experimental Design

CS 109A, STAT 121A, AC 209A: Data Science

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# Announcements

- **HW 8**: due tomorrow by 11:59pm.
- **Projects**:
  - Last Milestone due Monday, Nov 28
  - Look for an announcement in coming week about poster days.
- **Midterm**: to be released Sat at 9am and due Tues at 9am (you have get to choose your favorite 24 hour window).
- We will have a 'Grading Concerns Day' on Dec. 6.
- No class on Monday.
- No Quiz today. Last Quiz will be on Monday, Nov. 28.
- HW 7, Prob 2. Quantitatve vs. Legal vs. Moral Choices.

# Lecture Outline

**Causal Effects**

Experiments and *AB*-testing

t-tests, binomial z-test, fisher exact test, oh my!

Adaptive Experimental Design

# Association vs. Causation

In many of our methods (regression, for example) we often want to measure the association between two variables: the response, $Y$, and the predictor, $X$. For example, this association is modeled by a $\beta$ coefficient in regression, or amount of increase in $R^2$ in a classification tree associated with a predictor, etc...

If $\beta$ is *significantly different* from zero (or amount of $R^2$ is greater than by chance alone), then there is evidence that the response is associated with the predictor. But what can we say about a *causal association*? That is, can we manipulate $X$ in order to influence $Y$?

Not necessarily. Why not? There is potential for confounding factors to be the driving force for the observed association./

# Controlling for confounding

How can we fix this issue of confounding variables?

There are 2 main choices:

1. Model all possible confounders by including them into the model (multiple regression, for example).
2. An *experiment* can be performed where the scientist manipulates the levels of the predictor (now called the *treatment*) to see how this leads to changes in values of the response.

What are the advantages and disadvantages of each approach?

# Controlling for confounding

1. Modeling the confounders
   - Advantages: cheap
   - Diasadvantages: not all confounders may be measured.
2. Performing an experiment
   - Advantages: confounders will be balanced, on average, across treatment groups
   - Diasadvantages: expensive, can be an artificial environment

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# Experiments and *AB*-testing

There are many ways to design an experiment, depending on the number of types of treatments, number of treatment groups, how the treatment effect may vary across subgroups, etc...

The simplest type of experiment is called a *Completely Randomized Design*. If two treatments, call them treatment $A$ and treatment $B$, are to be compared across $n$ subjects, then $n/2$ subject are randomly assigned to each group. If $n = 100$, this is equivalent to putting all 100 names in a hat, and pulling 50 names out and assigning them to treatment $A$.

In the world of Data Science, this is called *AB-testing*.

*AB*-testing is often used in the tech industry to determine which form of website design (the treatment) leads to more ad clicks, purchases, etc... (the response).

# Assigning subject to treatments

In order to balance confounders, the subject must be properly randomly assigned to the treatment groups, and sufficient enough sample sizes need to be used.

For a CRD with 2 treatment arms, how can this randomization be performed via a computer?

You can just sample $n/2$ numbers from the values $1, 2, ..., n$ without replacement and assign those individuals (in a list) to treatment group $A$, and the rest to treatments group $B$. This is equivalent to sorting the list of numbers, with the first half going to treatment $A$ and the rest going to treatment $B$.

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# Analyzing the results

Just like in statistical/machine learning, the analysis of results for any experiment depends on the form of the response variable (categorical vs. quantitative), but also depends on the design of the experiment.

For $AB$-testing (classically called a 2-arm CRD), this ends up just being a 2-group comparison procedure, and depends on the form of the response variable (aka, if $Y$ is binary, categorical, or quantitative).

# Analyzing the results (cont.)

For those of you who have taken Stat 100/101/102/104/111/139: If the response is quantitative, what is the classical approach to determining if the means are different in 2 independent groups? - a 2-sample $t$-test for means

If the response is binary, what is the classical approach to determining if the proportions of successes are different in 2 independent groups? - a 2-sample $z$-test for proportions

# 2-sample $t$-test

Formally, the 2-sample $t$ test for the mean difference between 2 treatment groups is:

$$H_0 : \mu_A = \mu_B \quad \text{vs.} \quad H_A : \mu_A \neq \mu_B$$

$$t = \frac{\bar{Y}_A - \bar{Y}_B}{\sqrt{\frac{S_A^2}{n_A} + \frac{S_B^2}{n_B}}}$$

The $p$-value can then be calculated based on a $t_{\min(n_A, n_B)-1}$ distribution.

The assumptions for this test include (i) independent observations nad (ii) normally distributed responses within each group (or sufficiently large sample size).

# 2-sample $z$-test for proportions

Formally, the 2-sample $z$ test for the difference in proportions between 2 treatment groups is:

$$H_0 : p_A = p_B \quad \text{vs.} \quad H_A : p_A \neq p_B$$

$$z = \frac{\hat{p}_A - \hat{p}_B}{\sqrt{\hat{p}_p(1-\hat{p}_p)\left(\frac{1}{n_A} + \frac{1}{n_B}\right)}}$$

where $\hat{p}_p = \frac{n_A \cdot \hat{p}_A + n_B \cdot \hat{p}_B}{n_A + n_B}$ is the overall proportion of successes.

The $p$-value can then be calculated based on a standard normal distribution.

The use of the standard normal here is based on the fact that the binomial distribution can be approximated by a normal, which is reliable when $np \geq 10$ and $n(1-p) \geq 10$.

# Summary of analysis procedures for CRD Experiments

| Variable Type | # Trt's | Classic Approach | Alternative Approach |
|---|---|---|---|
| Quantitative | 2 | $t$-test | Randomization test |
| | 3+ | ANOVA | |
| Binary | 2 | $z$-test | Fisher's exact test |
| | 3+ | $\chi^2$ test | |
| Categorical (3+) | 2+ | $\chi^2$ test | Fisher's exact test |

The classical approaches are typically *parametric*, based on some underlying distributional assumptions of the individual data, and work well for large $n$ (or if those assumptions are actually true). The alternative approaches are *nonparameteric* in that there is no assumptions of an underlying distribution, but they have slightly less power is assumptions are true and may take more time & care to calculate.

# ANOVA procedure

The classic approach to compare 3+ means is through the Analysis of Variance procedure (aka, ANOVA).

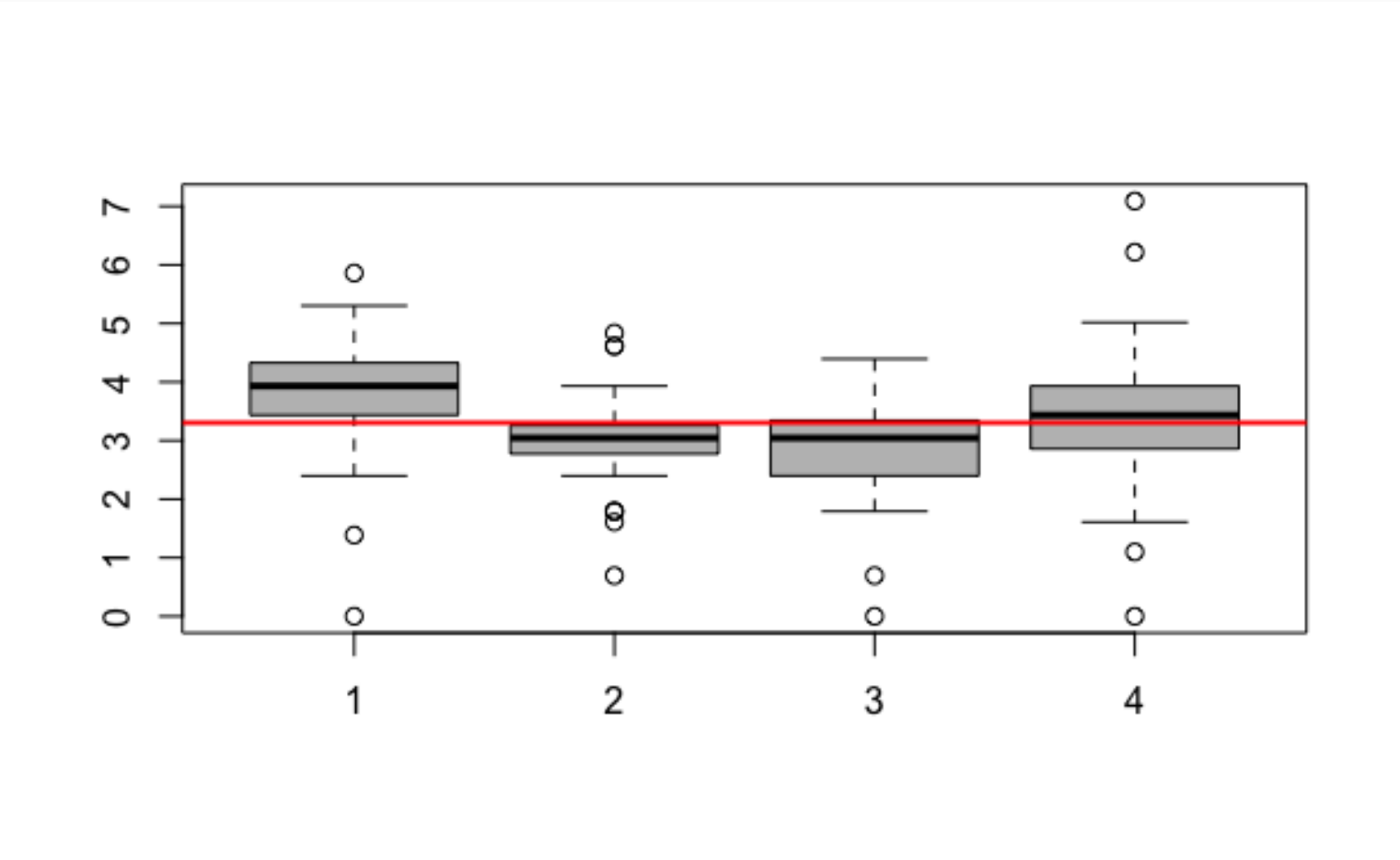
The ANOVA procedure's $F$-test is based on the decomposition of sums of squares in the response variable (which we have indirectly used before when calculating $R^2$).

$$SST = SSM + SSE$$

In this multi-group problem, it boils down to comparing how far the group means are from the overall grand mean (SSM) in comparison to how spread out the observations are from their respective group means (SSE).

A picture is worth a thousand words...

# Boxplot to illustrate ANOVA




Which line performs the best? How do you know?

# ANOVA $F$-test

Formally, the ANOVA $F$ test for differences in means among 3+ groups can be calculated as follows:

$H_0$: the mean response is equal in all $K$ treatment groups.

$H_A$: there is a difference in mean response somewhere among the treatment group.

$$F = \frac{\sum_{k=1}^{K} n_k(\bar{Y}_k - \bar{Y})^2/(K-1)}{\sum_{k=1}^{K}(n_k-1)S_k^2/(n-K)}$$

where $n_k$ is the sample size in treatment group $k$, $\bar{Y}_k$ is the mean response in treatment group $k$, $S_k^2$ is th variance of responses in treatment group $k$, $\bar{Y}$ is the overall mean response, and $n = \sum n_k$ is the total sample size.

The $p$-value can then be calculated based on a $F_{df_1=(K-1),df_2=(n-K)}$ distribution.

# $\chi^2$ test for independence

The classic approach to see if a categorical response variable is different between 2 or more groups is the $\chi^2$ test for independence. A *contingency* table (we called it a confusion matrix) illustrates the idea:

| Abortion Should be | Republican | Democrat | total |
|---|---|---|---|
| Legal | 166 | 430 | 596 |
| Illegal | 366 | 345 | 711 |
| Total | 532 | 775 | 1307 |

If the two variables were independent, then:
$P(Y = 1 \cap X = 1) = P(Y = 1)P(X = 1)$.

How far the inner cell counts are from what they are expected to be under this condition is the basis for the test.

# $\chi^2$ test for independence

Formally, the $\chi^2$ test for independence can be calculated as follows:

$H_0$: the 2 categorical variables are independent

$H_A$: the 2 categorical variables are not independent (response depends on the treatment).

$$\chi^2 = \sum_{allcells} \frac{(Obs - Exp)^2}{Exp}$$

where $Obs$ is the observed cell count and $Exp$ is the expected cell count: $Exp = \frac{(rowtotal) \times (columntotal)}{n}$

The $p$-value can then be calculated based on a $\chi^2_{df=(r-1)\times(c-1)}$ distribution ($r$ is the # categories for the row variable, $c$ is the # categories for the column variable).

# Randomization test

A randomization test is the non-parametric approach to analyzing quantitative data in an experiment. It is an example of a *resampling* approach (the bootstrap is another resampling approach).

The basic assumption of the randomization test is that if the treatments are truly the same, then the measured response variable for subject $i$ would not change if that subject was instead randomly assigned to a different treatment. This is sometimes called *exchangeability*.

# Randomization test (cont.)

So to analyze the results, we re-randomize the individuals to treatment through simulation (keeping the sample sizes the same). We then re-calculate the statistic of interest (difference in sample 2-means or sums of squares between 3+ groups) many-many times and build a histogram of the results. This histogram is then used as the reference distribution to determine how extreme are actual observed result is.

This approach is also called a permutation test, since we are re-permuting each of the subjects into the treatment groups (and then assume this has no bearing on the response).

# Fisher's exact test

R.A. Fisher also came up with what is known as Fisher's exact test.

This analysis approach is useful for a contingency table, and does not need to rely on large sample size.

It fixes the row and column totals, and then determines all the ways in which the inner cells can be calculated given those row and column totals.

The probability of any of these filled out tables, given the row and column totals is fixed, is then based on a hypergeometric distribution.

Then the possible filled out tables that are less likely to occur than what was actually observed contribute to the p-value (by adding up their probabilities).

# Fisher's exact test

| Abortion Should be | Republican | Democrat | total |
|---|---|---|---|
| Legal | 166 | 430 | 596 |
| Illegal | 366 | 345 | 711 |
| Total | 532 | 775 | 1307 |

$$P(X_1 = 166) = \frac{\binom{596}{166}\binom{711}{366}}{\binom{1307}{532}} \approx 1.33 \times 10^{-18}$$

Then a similar calculation is done for all possible values of $X_1$, and these probabilities are summed up for those cases of $X_1$ that are not more likely to occur.

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# Beyond CRD designs

The approaches we have seen to experiments all rely on the completely randomized design (CRD) approach.

There are many extensions to the CRD approach depending on the setting. For example:

- If there are more than two types of treatments (for example: (i) font type and (ii) old vs. new layout), then a *factorial* approach can be used to test both types of treatments at the same time.
- If the treatment effect is expected to be different across different subgroups (for example possibly different for men vs. women), then a stratified/cluster randomized design should be used.

# Beyond CRD designs (cont.)

These different experimental designs will need to have adjusted analysis approaches to analyze them appropriately (for example, a multi-way ANOVA for a factorial design with quantitive response variable and a stratified analysis, like the Mantel-Haenszel test, for the cluster randomized design with a categorical response variable).

But all of these procedures rely on the fact that there is a fixed sample size for the experiment. This has a glaring limitation: you have to wait to analyze until $n$ is recruited/reached.

If you peak at the results before $n$ is reached, then this is a form of *multiple comparisons* and thus overall Type I error rate is inflated.

# Bandit Designs

A *sequential* or *adaptive* procedure can be used if you would like to intermittently check the results as subject are recruited (or want to look at the results after each and every new subject is enrolled).

One example of a sequential test/procedure is a *bandit-armed* design. In this design, after a burn-in period based on a CRD, then the treatment that is performing better is chosen more often to be administered to the subjects.

For example, in the *play the winner* approach for a binary outcome, if treatment $A$ is successful for a subject, then you continue to administer this treatment to the next subject until it fails, and then you skip to treatment $B$, and vice versa.

The advantage to this approach is that if one treatment is truly better, then the number of subjects exposed to the worse treatment is lessened.

# Bayesian Bandit Designs

Our friend Bayes' theorem comes into play again if we would like to have a bandit design for a quantitative outcome.

The randomization to treatment for each subject is based on a biased coin, where the probability of being assigned to treatment $A$ is based on the poster probability that treatment $A$ is a better treatment.

This probability can be calculated based on the Bayes theorem as follows:

$$P(\mu_{Y|trtA} > \mu_{Y|trtB}|Data) \propto P(Data|\mu_{Y|trtA} > \mu_{Y|trtB})P(\mu_{Y|trtA} > \mu_{Y|trtB})$$

where $P(\mu_{Y|trtA} > \mu_{Y|trtB})$ is the prior belief (can be set to 0.5).

This can easily extend to more than just 2 treatment groups.