Experiment Design for Computer Sciences (01CH740)

Topic 04 - Paired Comparison

Claus Aranha
caranha@cs.tsukuba.ac.jp

University of Tsukuba, Department of Computer Sciences

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Outline

In this lecture, we will continue studying the Null Hypothesis Statistical Testing.

We will learn about two specific cases that are quite common in algorithm studies:

- Hypothesis testing on the difference between two treatments. (**Comparison Testing**)
- Hypothesis testing when there is a strong correlation factor between the observations of the two treatments. (**Paired Testing**)

Treatments?

The word "treatment" is from the medicine literature, but here we use to indicate two different things that we want to compare. It could be two algorithms, or two parameter settings, or two experimental conditions, etc.

Part I – Two Sample Testing

Last Lecture Recap

In the last lecture we studied how we can use Statistical Inference to determine the answer to questions about experimental data. For example: **"are the observations produced by process B different from an expected value N?"**

We used the Null Hypothesis Statistical Testing method to answer this question: The process of interest is modeled as a Random Variable under a normal distribution. From the sample data, we calculate a **test statistic** that tells us "how surprising" that sample is under the null hypothesis.

Based on this information, we could answer that simple question. What about more complex situations?

Comparison of two processes

The comparison between two different approaches is a very common situation in scientific research:

- The efficacy of a new drug is compared against a control group;
- The precision of a new algorithm is compared against an old one;
- Two different website design proposals are compared regarding user preference;
- etc;

How can we adapt the Hypothesis testing procedure studied in the last lecture to these situations?

The analisys of these situations involves the calculation of statistics based on data from two different samples, so we will call it **two sample testing**.

Example: Comparing Methods for cutting steel rods

We will use the following situation to illustrate the hypothesis testing method:

A critical aspects of manufacturing steel rods is cutting the bars with a precise length.

Errors when cutting the bars will cause costs for reprocessing the rods.

An engineer is interested in comparing the current cutting process with a new method that could potentially improve the performance of the system by reducing the cutting error.

Comparing cutting methods

Quiz

We have two methods for cutting steel rods (old and new), and we want to find out which one has the smallest cutting error. Consider the following questions:

- How do we calculate / measure the cutting error of one of the methods?
- What is the observation / sample necessary to estimate this value?
- What is the variable that measures the cutting error difference between the two methods?
- What is a *statistical hypothesis* that represents the question of interest for this experiment?

Pause the video! Take some time to seriously answer these questions before you continue the material!

Modeling the cutting process

What is the cutting error?

Let's look at the first two questions:

- How do we calculate / measure the cutting error of one of the methods?
- What is the observation / sample necessary to estimate this value?

Let's consider a cutting error to be the difference between the length of a rod i and the target length l: $(|x_i - l|)$.

Assuming that the cutting error is a property of the method, we can estimate the mean cutting error using a sample X of n rods:

$$\hat{\mu}_e \text{ estimated by } e_X = \frac{\sum |x_i - l|}{n}$$

Modeling the cutting process

Cutting Error and Hypothesis

$$\hat{\mu}_e \text{ estimated by } e_X = \frac{\sum |x_i - l|}{n}$$

Using e_X as an estimate of the cutting error, it is possible to to perform statistical inference about one of the methods. For example:

- Is the error of method Y equal or under a required value r?
- $H_0 : e_Y \leq r$
- $H_1 : e_Y \geq r$

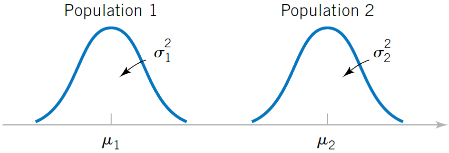
We can use the technique from the last lecture to solve this problem. But if we want to compare two methods: Y_1 and Y_2, what do we do?

Modeling the cutting process

Comparing Errors

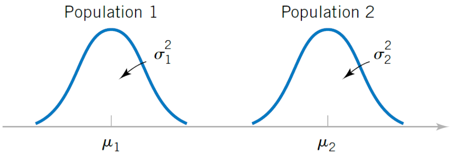
- What is the variable that measures the cutting error difference between the two methods?
- What is a *statistical hypothesis* that represents the question of interest for this experiment?

Let's consider these two questions. Remember that the error from each method is modeled as a random variable following a normal distribution.



Modeling the cutting process

Comparing Errors



The sum of two normal variables also follow a normal distribution. So, we can describe the difference between the cutting errors as the random variable $e_{\text{diff}} = (e_{\text{old}} - e_{\text{new}})$.

Because e_{diff} also follows a normal distribution, we can use the null hypothesis method to test the difference of the two methods:

- $H_0 : e_{\text{diff}} = 0$
- $H_1 : e_{\text{diff}} \neq 0$

A General Model for Comparing two Samples

Using the ideas from the previous example, let's describe a general statistical model to use when we want to test if two methods are quantitatively different.

Consider that we measure some observed value (y) taken from one of several methods ($i = 1, 2, \ldots$), we understand that the value comes from some distribution with mean μ_i, at it will also have an error (ϵ) away from that mean, which is different for each observation. So we describe the j-th observation taken from the i-th method as

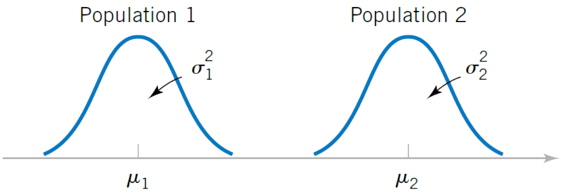
$$y_{ij} = \mu_i + \epsilon_{ij} \begin{cases} i = 1, 2 \\ j = 1, \ldots, n_i \end{cases}$$

Statistical Models

Two population Model

$$y_{ij} = \mu_i + \epsilon_{ij} \begin{cases} i = 1, 2 \\ j = 1, \ldots, n_i \end{cases}$$

Under this model for the observed variable (y_{ij}), we assume that the residuals ϵ_{ij} are independent and follow $\mathcal{N}\left(0, \sigma_i^2\right)$. Under these assumptions, the populations of the two samples look like this:



Comparison of two means

Null and Alternate Hypotheses

What should be the observed variable y? The goal of this experiment is to measure if the new method produces steel rods closer to the nominal value. In this case, a possible response variable would be the absolute error, e.g., $y = |\ell - \ell_{nominal}|$.

Keeping in mind our statistical model, we can build the hypothesis around the mean of the absolute error (μ_i). In that case, we can state the null and alternate hypotheses as:

$$\begin{cases} H_0 : \mu_1 - \mu_2 = 0 \\ H_1 : \mu_1 - \mu_2 < 0 \end{cases} \quad \textbf{or, equivalently,} \quad \begin{cases} H_0 : \mu_1 = \mu_2 \\ H_1 : \mu_1 < \mu_2 \end{cases}$$

Comparison of two means

Calculating the statistic

Lets assume (for the moment) that the variance of the process is unknown but similar for both systems. Since it is unknown, we have to estimate the variance from the sample data. As assume $\sigma_1^2 \approx \sigma_2^2$, we can use the pooled variance estimator:

$$s_p^2 = \frac{(n_1 - 1)\, s_1^2 + (n_2 - 1)\, s_2^2}{n_1 + n_2 - 2}$$

Based on this estimator and the stated assumptions, we calculate the T statistic:

$$T = \frac{(\bar{y}_1 - \bar{y}_2) - (\mu_1 - \mu_2)}{s_p \sqrt{\frac{1}{n_1} + \frac{1}{n_2}}} \sim t^{(n_1 + n_2 - 2)}$$

Back to the Steel Rods Example

Calculation of the Rejection threshold

If we recall our working hypotheses for the steel rod example:

$$\begin{cases} H_0 : \mu_1 - \mu_2 = 0 \\ H_1 : \mu_1 - \mu_2 < 0 \end{cases}$$

we have that, under H_0:

$$t_0 = \frac{(\bar{y}_1 - \bar{y}_2) - \cancelto{0}{(\mu_1 - \mu_2)}}{s_p\sqrt{\frac{1}{n_1} + \frac{1}{n_2}}} = \frac{(\bar{y}_1 - \bar{y}_2)}{s_p\sqrt{\frac{1}{n_1} + \frac{1}{n_2}}} \sim t^{(n_1+n_2-2)}$$

We'll reject H_0 at the $(1 - \alpha)$ confidence level if $t_0 \leq t_{\alpha/2}^{(n_1+n_2-2)}$

Back to the Steel Rods Example

Statistic Test Parameters

Remember that we need to decide three parameters that will specify the statistical test:

- **Significance level**: The probability of a **Type I error.** Let's assume that the desired significance level is $\alpha = 0.05$.
- **Power**: The probability of a **Type II Error.** Let's assume that the desired sensitivity is $1 - \beta = 0.8$.
- **Meaningful difference**: What is the minimum difference between the two methods that we are interested in detecting? Let's assume $15cm$.

The values for these variables depend on the needs of the specific experiment and/or application.

Calculating the Statistic

Computationally, we can perform the t-test for comparing the means of two independent populations by:

```
> y <- read.table("steelrods.csv", header = TRUE)
> t.test(y$Length.error ~ y$Process, alternative = "less",
+        mu          = 0, var.equal   = TRUE, conf.level  = 0.95)

data:  y$Length.error by y$Process
t = -14.312, df = 32, p-value = 9.244e-16
alternative hypothesis: true difference in means is less than 0
95 percent confidence interval:
      -Inf -7.156884
sample estimates:
mean in group new mean in group old
         7.782353         15.900000
```

Comparison of two means

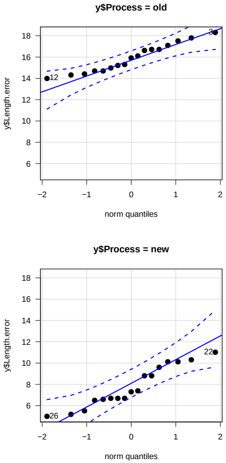
Testing the assumptions

The assumptions of the test must be verified. In this particular case:

- Normality;
- Equality of variances;
- Independence.

```
> qqPlot(y$Length.error, groups = y$Process,
         cex = 1.5, pch = 16,  las = 1,
         layout = c(2, 1))
> shapiro.test(y$Length.error[y$Process == "new"])
# W = 0.92269, p-value = 0.164
> shapiro.test(y$Length.error[y$Process == "old"])
# W = 0.94971, p-value = 0.4519
```

Reminder: the t-test is quite robust to mild to moderate violations of the normality of the residuals / groups.



Comparison of two means

Testing the assumptions

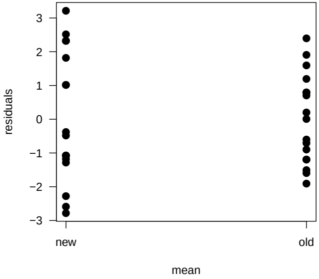
The assumptions of the test must be verified. In this particular case:

- Normality;
- Equality of variances;
- Independence;

```
> fligner.test(Length.error ~ Process, data = y)
# Fligner-Killeen:med chi-squared = 1.6837,
# df = 1, p-value = 0.1944

> resid <- tapply(X = y$Length.error,
         INDEX = y$Process,
         FUN   = function(x){x - mean(x)})

> stripchart(x          = resid,
             vertical = TRUE,
             pch      = 16,
             cex      = 1.5,
             las      = 1,
```



Comparison of two means

Testing the assumptions

The assumptions of the test must be verified. In this particular case:

- Normality;
- Equality of variances;
- Independence;

As mentioned in the last class, there is no general test for the independence assumption, and it has to be guaranteed in the design phase.

One can at most test for serial autocorrelation in the residuals using Durbin-Watson's test, but this test is absolutely dependent on the ordering of the observations - very useful to detect ordering-related trends in the residuals, but not much more than that.

Comparison of two means

Unequal variances

Suppose now a more general case, in which the variances of the two populations are unknown and cannot be assumed equal.

For this cases, a modification on the t-test called *Welch's t test* is usually employed. The Welch statistic can be calculated as:

$$t_0^* = \frac{\bar{y}_1 - \bar{y}_2}{\sqrt{\frac{s_1^2}{n_1} + \frac{s_2^2}{n_2}}}$$

Under the null hypothesis t_0^* is distributed approximately as a $t^{(\nu)}$ distribution, with:

$$\nu = \frac{\left(\frac{s_1^2}{n_1} + \frac{s_2^2}{n_2}\right)^2}{\frac{\left(s_1^2/n_1\right)^2}{n_1 - 1} + \frac{\left(s_2^2/n_2\right)^2}{n_2 - 1}}$$

Comparison of two means

Unequal variances

To illustrate this technique, let's use the data from the example[2]:

```
> with(y,
+      t.test(Length.error~Process,
+             alternative = "two.sided",
+             mu = 0,
+             var.equal = FALSE,             %% <- We only change this.
+             conf.level = 0.95))
Welch Two Sample t-test
data:  Length.error by Process
t = -14.312, df = 28.386, p-value = 1.645e-14
alternative hypothesis: true difference in means is not equal to 0
95 percent confidence interval:
-0.09278780 -0.06956515
sample estimates:
mean in group new mean in group old
      0.07782353        0.15900000
```

[2] Notice that this would not be necessary, since the data collected in the previous example did not violate the equality of variances assumption.

Comparison of two means

Summary

To compare an estimator from samples of two populations that (we assume) follow a normal distribution, we set our statistic and the corresponding hypotheses to be the difference of the target variables.

This technique for comparison testing is equally simple and extremely versatile.

Of course, there are cases where this approach does not apply. Next we will see a relatively common case where using the difference of the target variables would lead to a wrong inferential result.

Part II – Paired Testing

Comparison of two means

Dependent populations

Suppose the following situation: a young researcher develops an optimization algorithm (A) **for a given family of problems**, and wants to compare its convergence speed against a method that represents the state-of-the-art (B).

The researcher implements both methods and wants to determine whether the proposed one has a better average performance for problems of that particular family, which are represented by a given benchmark set.

The measurements are made under homogeneous conditions (same computer, same operational conditions, etc.) and the time is measured in a way that is not sensitive to other processes running in the system.

Comparison of two means

Dependent populations

This problem has some important questions worth considering:

- What is the actual question of interest?
- What is the *population* for which that question is relevant?
- What are the independent observations for that population?
- What are the relevant sample sizes for the experiment?

Consider carefully the difference between considering *individual runs* as a population against *individual problem instances* as a population. The important thing is to not mix both!

Paired Experimental Design

The variability of results due to the different test problems is a strong source of spurious variation (noise) that can and must be controlled;

An elegant solution to eliminate the influence of this nuisance parameter is the *pairing* of the measurements by problem:

- Observations are considered in pairs (A, B) for each problem;
- Hypothesis testing is done on the sample of *problem differences*;

Paired Design

Statistical Model

Let y_{Aj} and y_{Bj} denote paired observations of average time for methods A and B, for each problem instance j. The *paired difference* of an observation is simply $d_j = y_{Aj} - y_{Bj}$.

If we model our observations as an additive process:

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

where μ is the grand mean, τ_i is the effect of the i-th method on the mean, β_j is the effect of the j-th problem instance, and ε_{ij} is the model residual, then:

$$d_j = \mu + \tau_A + \beta_j + \varepsilon_{Aj} - (\mu + \tau_B + \beta_j + \varepsilon_{Bj})$$

$$\begin{aligned} d_j &= \cancelto{0}{(\mu + \beta_j - \mu - \beta_j)} + \tau_A - \tau_B + \varepsilon_{Aj} - \varepsilon_{Bj} \\ &= \mu_D + \varepsilon_j \end{aligned}$$

Paired Design

Hypotheses

The hypotheses of interest can now be defined in terms of μ_D, e.g.:

$$\begin{cases} H_0 : \mu_D = 0 \\ H_1 : \mu_D \neq 0 \end{cases}$$

which can now be treated as a test of hypotheses for a single sample: the population of interest is the differences in average times until convergence for the problems under investigation. The test statistic is given by:

$$T_0 = \frac{\bar{D}}{S_D/\sqrt{N}}$$

which is distributed under the null hypothesis as a Student-t variable with $N - 1$ degrees of freedom (where N is the number of test problem instances in the experiment);

Paired Design

Considerations

Some other important questions worth considering:

- In this example the minimally interesting effect size δ^* must be expressed in terms of *average time gains across problems* (not within individual instances);
- The most important sample size to consider in this situation refers to the *number of problem instances*, and not necessarily to the number of within-problems repeated measures;
- The number of repetitions within each problem will have an impact on the uncertainty associated to each observation (that is, to each value of mean time to convergence for each algorithm on each problem), which will propagate down to the residual variance.

Paired design

Considerations

Some other important questions worth considering:

- Pairing removes the effects of controllable nuisance factors from the analysis.
- Strongly indicated in cases with **strong correlations between samples** (e.g., heterogeneous experimental conditions).

Paired Comparison Example

Going back to our example, assume the following facts about the desired comparison:

- The benchmark set is composed of seven problem instances ($N = 7$);
- The researcher is interested in finding differences in mean time to convergence greater than ten seconds ($\delta^* = 10$) with a power of at least $(1 - \beta) = 0.8$, using a significance level $\alpha = 0.05$;
- The researcher performs $n = 30$ repeated runs[1] of each algorithm in each problem, from random initial conditions.

[1] Not that this number is necessarily good, but it is generally an easy alternative if you don't want to keep justifying your choices to less statistically-savvy reviewers.

Executing the Paired Analysis

Step 1: load and precondition the data

```
> # Read data
> data <- read.table("benchmark.csv",
+                     header=T)

# "Problem" is a categorical variable, not a continuous one
> data$Problem <- as.factor(data$Problem)

# Summarize within-problem observations by mean
> aggdata <- aggregate(Time ~ Problem:Algorithm,
+                      data = data,
+                      FUN  = mean)
> summary(aggdata)
 Problem Algorithm      Time
 1:2     A:7       Min.   : 37.63
 2:2     B:7       1st Qu.:109.45
 3:2               Median :178.73
 4:2               Mean   :175.48
 5:2               3rd Qu.:245.25
 6:2               Max.   :296.79
 7:2
```

Executing the Paired Analysis

Step 2: analysis

```
> # Perform paired t-test
> t.test(Time ~ Algorithm,
+        paired = TRUE,
+        data   = aggdata)

Paired t-test
data:  Time by Algorithm
t = -9.1585, df = 6, p-value = 9.54e-05
alternative hypothesis: true difference in means is not equal to 0
95 percent confidence interval:
 -21.85862 -12.64118
sample estimates:
mean of the differences
               -17.2499
```

Executing the Paired Analysis

Alternatively, we could have done:

```
> difTimes <- aggdata$Time[1:7] - aggdata$Time[8:14])
> t.test(difTimes)
```

```
One Sample t-test
data:  difTimes
t = -9.1585, df = 6, p-value = 9.54e-05
alternative hypothesis: true mean is not equal to 0
95 percent confidence interval:
 -21.85862 -12.64118
sample estimates:
mean of x
 -17.2499
```

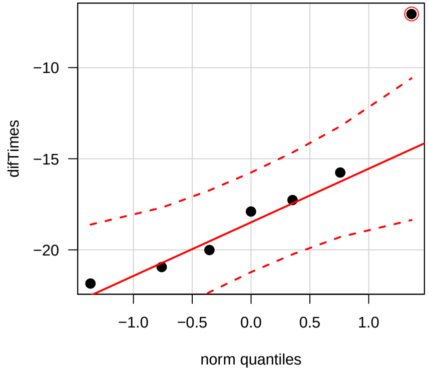
Check your understanding: Why is the paired test on two samples equivalent to the one sample test on the difference vector of the samples?

Verifying the Assumptions

```
> shapiro.test(difTimes)

Shapiro-Wilk normality test
data:  difTimes
W = 0.8387, p-value = 0.09655

# Redo test without outlier
> indx <- which(difTimes == max(difTimes))
> t.test(difTimes[-indx])$p.value
[1] 6.179743e-06
> t.test(difTimes[-indx])$conf.int
[1] -21.41856 -16.48037
```



Why is Pairing Important?

What happens if we fail to consider the problem effects?

```
> t.test(Time ~ Algorithm, data = aggdata)

Welch Two Sample t-test
data:  Time by Algorithm
t = -0.3609, df = 11.993, p-value = 0.7245
alternative hypothesis: true difference in means is not equal to 0
95 percent confidence interval:
 -121.40320   86.90341
sample estimates:
mean in group A mean in group B
       166.8527        184.1026
```

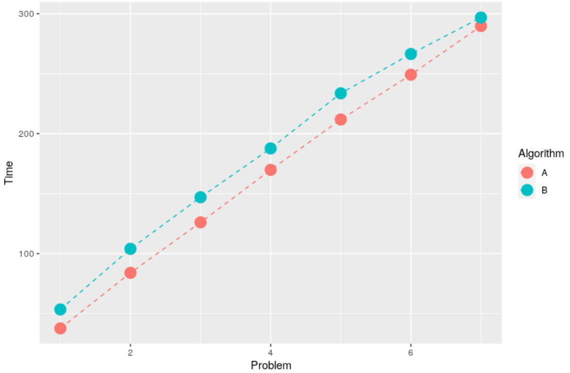
Failure to consider inter-unit variability can result in the masking of relevant effects by the nuisance factor.

Similarly, failure in recognizing the dependence structure of within-unit measurements yields tests with artificially inflated degrees of freedom, which results in the inflation of the effective value of α.

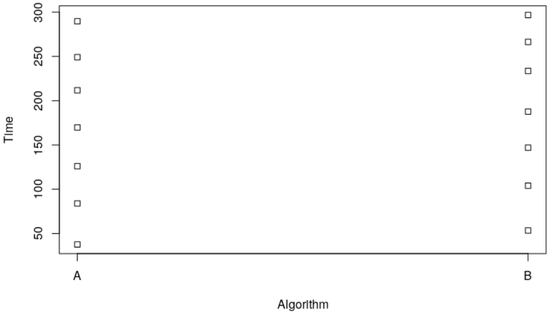
Why is Pairing Important?

A visual Comparison

Paired Samples



Unpaired Samples



- Estimating the mean of the differences vs the difference of the means;

Conclusion

Summary

- In the Last class, we described the Null Hypothesis testing method to perform **Statistical Inference** on a population parameter from a single sample;
- In this cless, we generalize this procedure to a common situation, where we want to compare two samples regarding a population parameter;
- The **Two Sample Hypothesis Testing** uses inference on a statistic based on the difference between sample estimators.
- When there is a high correlation between the observations of each sample, it is important to perform the pairing of the observations.

Report 2

Design, Execute and Analize a Scientific Experiment

In this report, you must choose a simple experiment to design, perform and analyze the results. Like in Report 1, your report must have:

- **Introduction**: Description of Scientific Question;
- **Experiment Design**: Plan of data collection and analysis
- **Data Collection:** Report on the data and results;
- **Analysis:** Conclusion based on hypotheses and statistic;

Important Notes

- Use techniques of Statistical Inference to analyze the results;
- In the Experiment Design section, describe the hypotheses used, and the variable of interest;
- In the Analysis section, do not forget to test the inferential assumptions (normality, variance, etc);
- Remember to follow practices of reproducible science!

A note about data re-use

Because this report is very similar to Report 01, a natural question is "Can I use the same data as in the first report, and just change the analysis?".

The short answer is **NO**.

The idea of experimental design is that the setup of the experiment, including the choice of variable, statistic, hypotheses, etc, should guide the data collection, not the other way around. Choosing the analysis **after** data collection is an easy way to bias the results.

How you can use your initial data:

You can, however, use your previous experiment data to guide the design of the new experiment. For example, you can use it to estimate variance, reasonable values for the hypotheses, etc.

Comments on Report 01

- I gave a quick look at the reports, but the full grading will take a bit of time, so please be patient;
- In general, everyone did great reports, I am very happy with the results;
- However, there were some common mistakes:
    - Many people did not include code for reproducibility; or the data used in the analysis; Non-reproducible reports will receive a lower grade.
    - A few students did not submit reports in PDF; The main file of the report MUST be a PDF
    - One student asked to use secret experimental data in the report; It is acceptable, but I recommend against it in the future;

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