Experiment Design for Computer Sciences (0AL0400)

Topic 01 - What is an experiment?

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Lecture Outline

In today's class, I want to cover some key concepts for the course:

1. What is an experiment;
2. What is the role of experiments in science;
3. Why experiments have to be designed;

In future lectures we will cover techniques related to the design and analysis of experiments, but the lecture today will be more conceptual. We will discuss WHY we want to do all these things.

Knowing the **WHY** is important to motivate the **WHAT**.

Part I: First, What is Science?

What is Science?

At the end of your 2-year course, you will receive a diploma that says:

Master in Computer Science

What do these words mean?

Let's have some discussion about this (and let me learn about you too!)

What is Science?

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Some answers from students in past years

- Science is a method to learn about the world;
- Science is a method to reach the truth;
- Science is useful when it contributes to society;
- Science is how we develop new technologies;

Thinking about science

(Not answering the question...)

- "Science" can mean different things, for different people, depending on context... not very satisfying.
- But maybe there are some common threads in the discussion ("science", the word, meaning knowledge):
  - The act of discovering knew knowledge about the world;
  - An activity that requires precision, detail, curiosity and honesty;
  - An activity that requires inspiration and creativity;
  - Trying to improve society, trying to improve technology (are these the same? are other entities that ask for improvement?)
- There are also some threads that are not often discussed:
  - Science as a **community**
  - Science as a **continuous process**
  - The relationship between **science and society** (is this relationship two way?)

What is Science

I know it when I see it

One way to understand science is to think about people, institutions, and events that we think of as "scientific", and reflect about them.

I also think it is important for us to have many role models we can get inspiration from. It is good to have heroes!

Let's talk a little about some famous scientists and scientific events.

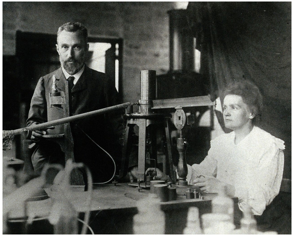
Marie Curie

Fact Sheet

- Marie Curie was Chemist from Poland. She discovered serveral radioactive materials and their properties.
- Won two nobel prizes: Physics and Chemistry
  (only person to receive two nobels in different scientific fields)

Marie Curie

Scientific Background



- Why did some materials emit radiation?
  - Was it a result of interaction between elements? Or a property of the element itself?
  - One of Curie's early significant discoveries was that the quantity of radiation depends only on the amount of the material.
- What is radiation useful for?
  - Until then, radiation was a pretty curiosity.
  - Curie developed several medical uses for radiation.

Marie Curie

Medical applications of radiation

- Observed that cancer tumour cells died more quickly to radiation than healthy cells;
- Designed mobile X-ray equipment that could be used for surgery in World War I ("little curies");
- Designed Radon gas syringes for sterilizing tissue and wounds;

Marie Curie

Open Science

- Refused to patent Radium or the technologies to extract and develop the material;
- Result: a Radium boom spread across the world, increasing its usage and study;
- She believed that by sharing scientific discoveries, this would allow science (and society) to progress faster.

"Physicists should always publish their researches completely. If our discovery has a commercial future that is a circumstance from which we should not profit. If radium is to be used in the treatment of disease, it is impossible for us to take advantage of that."

About the patenting of radium

Marie Curie

Personal Background

- Studied in an "underground university" (Flying University), and had to work as a tutor to support herself;
- Difficulty to get funding, sourcecrowded some of her research materials;
- Difficulties related to gender relations in Europe;
- The dangers of radioactivity were not well understood at the time:
  - Died early from radiation related diseases (like many chemists at the time);
  - Her research notebooks are still radioactive today!

Marie Curie
Legacy

What can we learn from the stories of famous scientists?

What are the scientists and stories that you know, that inspire you?

What is Science?

Scientific Discoveries

To define "science", it is also helpful to think about events that you consider as "scientific".

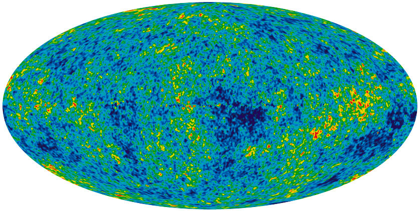
How are discoveries made?

Let's talk about two interesting discoveries.

Example 1: The Origins of the Universe

Discovery of the Cosmic Background Radiation and confirmation of the Big Bang Theory

- The origins of the universe is a key topics in physics research. However, it is "not very easy" to find data about this ancient event;
- The Cosmic Background Radiation, a faint noise that can be detected everywhere, supports the theory that the universe was originally hot and dense, and expanded quickly;
- It was discovered in 1965 by chance, when two astronomers found a noise in their telescope that they could not remove in any way, no matter how;

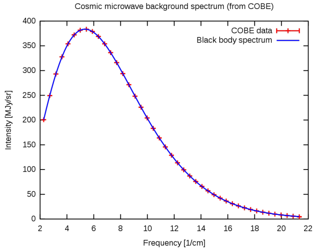


Example 1: The Origins of the Universe

Behind "chance" discoveries, there is a lot of preparation

Behind the "chance" discovery of CMB, there was a lot of preparation in reality.

- Scientists had investigated microwave radiation from the stars since 1890;
- A theoretical model for CMB had been predicted in 1948 by a different group;
- A third group was actively searching for the same data, and helped the chance findings;



Luck smile on those who are prepared (including humanity as a whole!)

Example 2: Proving that Citrus Fruit prevents Scurvy

Hail Britannia!

In the 18th century, the British Empire needed a large navy to control and plunder its dominion around the world.

However, sailors who spent too much time at sea would suffer a terrible **Rotting Disease**, which caused weakness, fatigue, bleeding, and eventually death from infection. This disease made constant stops at shore necessary.

Today we know that this disease, called **scurvy** is caused by the lack of vitamin C. But the way that the British Navy dealt with the problem is an interesting case of experimentation.

Example 2: Citrus fruits prevents scurvy

James Lind's experiment

James Lind (1747):

- Observation: scurvy in sailors;
- Conjecture: Caused by the body rottenning;
- Idea: attempt to avoid/reverse effects with acidic substances;

Separation of a group of 12 affected sailors in six groups with identical diets, except for the addition of a supplement:

Group 1	Group 2	Group 3
Cider.	Vitriol.	Vinegar.

Group 4	Group 5	Group 6
Sea water.	Oranges and lemons.	Tea.

Example 2: Proving that Citrus Fruit prevents Scurvy

Aftermatch

Of course, before Lind's experiment, there was already folk knowledge and recommendation about the relationship of Scurvy and Citrus. This includes memoirs by Spanish, French and Portuguese explorers.

Nevertheless, Lind's experiment is interesting to consider as an example of a general idea being formally demonstrated through a controlled experiment!

In spite of this experiment, the British Navy only formally started adding Lemon Juice to its rations from 1790...

A Framework for Science

Thinking about scientists and scientific discoveries, we start to see science as "something" with a set of characteristics. But what is it?

Many of you might have learned the following description in high school or university:

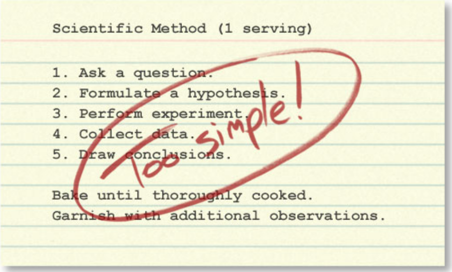
The Scientific Method

1. Observe a Phenomenom
2. Propose a Hypothesis
3. Perform an Experiment
4. Draw conclusions

Is this a good description of "What is Science?"

"The Scientific Method" – Too simple!

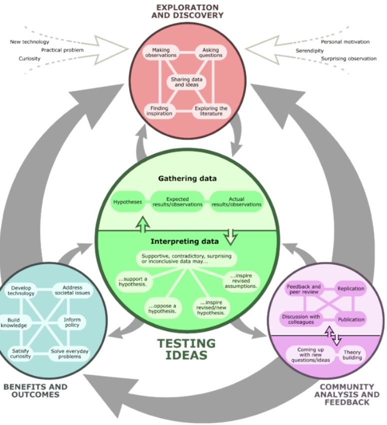
This description of the scientific method has a kernel of truth. But it has some limitations when compared to how science is actually done:



- It does not explain where questions or hypothesis come from.
- What happens when two scientists disagree about the data?
- It assumes that the scientific process ends after the data is collected.
  (How does this new knowledge reach society?)
  (How does this new knowledge influence science?)
- It assumes that old hypothesis or data never gets reviewed.
- etc...

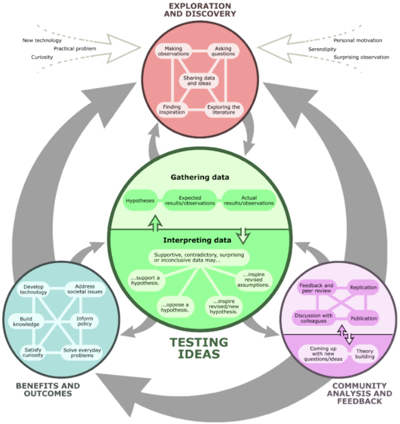
Science as an Interactive Process

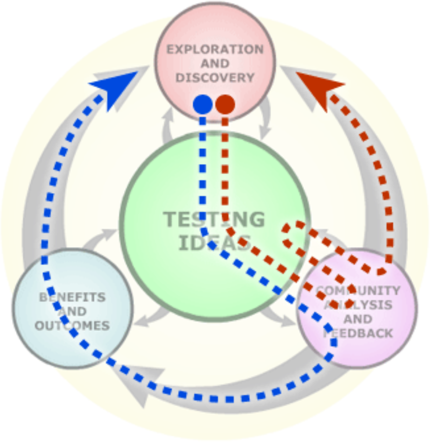
A more complete view of the process of science involves ideas, data, the scientific community, and society, in a continuous feedback circle.



Science as an Interactive Process

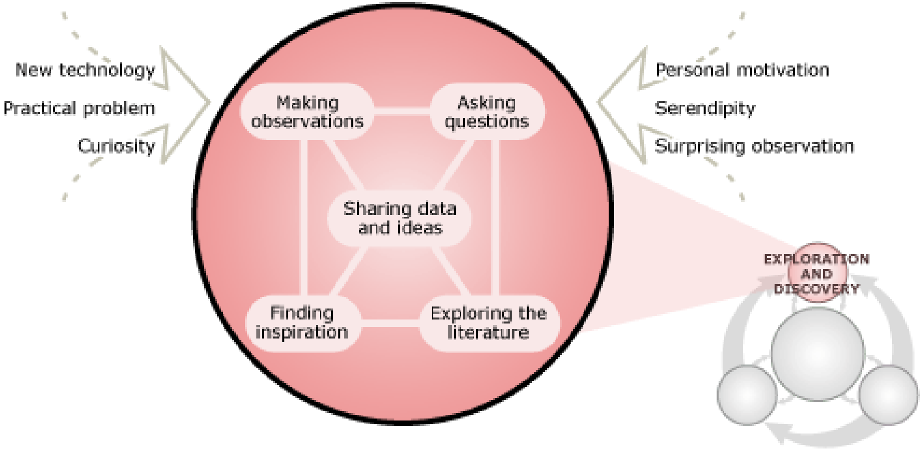
This understanding helps us see that there are many different paths to scientific discoveries. And these paths still have some common characteristics tying them together.





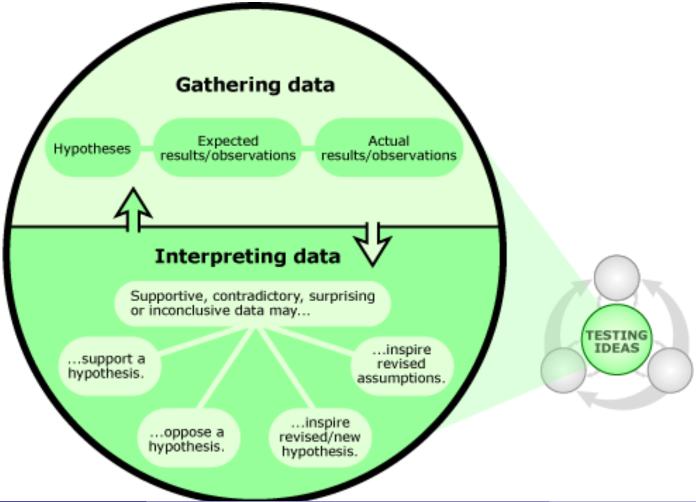
Science as an Interactive Process – Breakdown

Where do ideas come from?



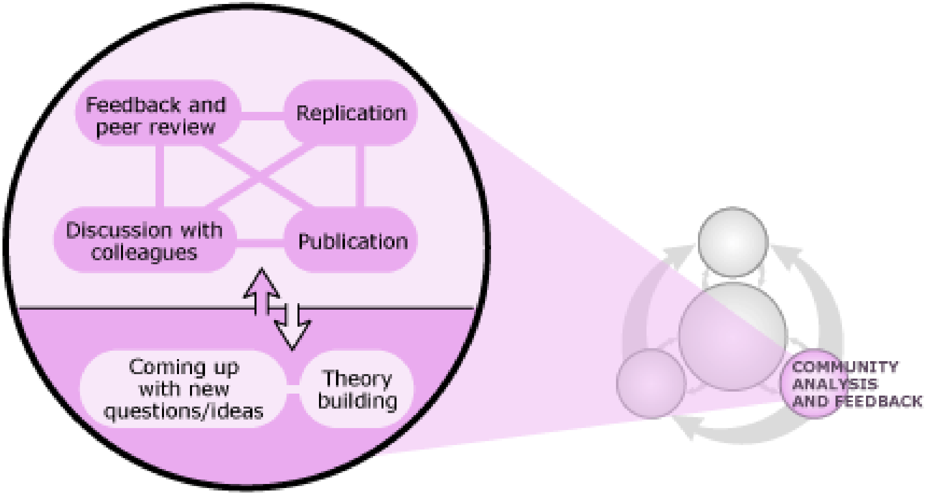
Science as an Interactive Process – Breakdown

Testing and Experimentation



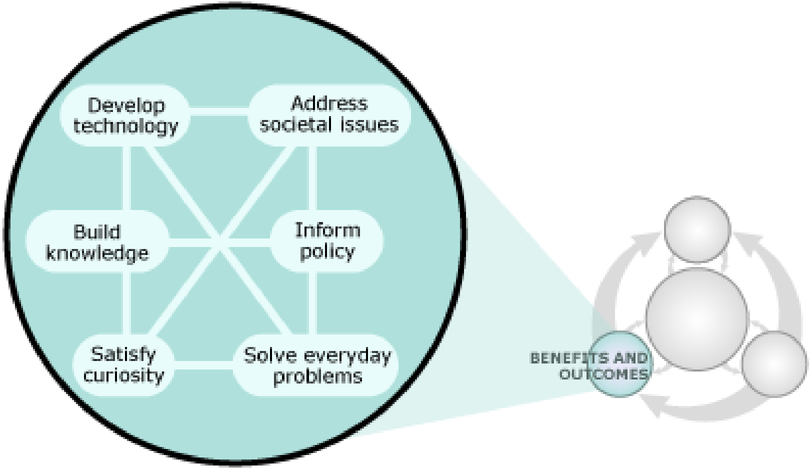
Science as an Interactive Process – Breakdown

The Scientific Community



Science as an Interactive Process – Breakdown

Science and Society



Wrap up – What is Science?

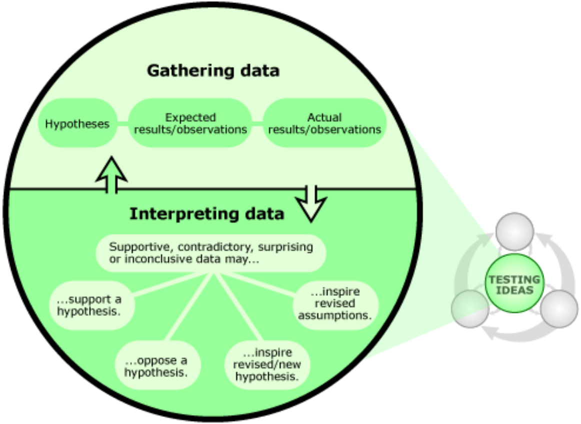
- Science is a method, a way of thinking, and also a community. A process of search and discovery that is continuously changing our society.
- I highly recommend that you read the "Understanding Science" webpage, for a much more in-depth discussion. See the manaba links.
- **What about Computer Sciences**? Popular discussion of science usually focus on physics, biology, social science, etc. How does Computer Science fit in this framework?

- In the next part of the lecture, we are going to focus on the role of experiments in science, which is also the focus for the rest of this class.

Part II: Experimentalism

The Role of Experiments in Science

Experiments occupy a central role in science. They are how we obtain information that help us answer our scientific questions.



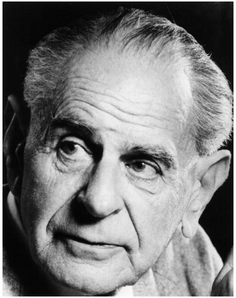
The Role of Experiments in Science

Philosophy and Experimentalism

- Philosophy of science: How can we know things?
  - Can we know things through logic? Can we trust our senses? Is knowledge immutable? etc.

- According to Popper, the only way to obtain knowledge about the world is through rigorous experimentation (Experimentalism);
  1. Formulate a question as a scientific hypothesis;
  2. Execute an experiment following the hypothesis;
  3. Support or reject the hypothesis;

- The definition of scientific hypothesis is important. In Experimentalism, a scientific hypothesis is one that produces falsifiable predictions.



Karl Popper (1902–1994)

Defining a "fair" experiment

Generally, we are interested in a "fair" experiment, that provides new evidence for the scientific question that we are trying to answer. A fair experiment has the following characteristics:

- It provides something to compare against;
- It controls the variables of interest;
- It avoids bias in the results;
- It is reproducible;
- It separates chance results from real differences;

"Provides Something to Compare Against"

Scientific Hypothesis

A scientific hypothesis is the question that we try to answer with an experiment. For an experiment to be useful, it is necessary that it has at least two possible results. Afterall, if you already know the result of your experiment, why do it?

Examples of scientific hypothesis:

- **Comparing different systems:**
  Chocolate cookies taste better than mint.
- **Comparing explanations to a phenomenom:**
  Bananas turn black in the refrigerator because of bacteria, not the temperature.
- **Test the characteristic of a system:**
  One apple tree is enough to feed our home for the entire year.

Scientific Hypothesis
Specific Hypothesis

One characteristic of good scientific hypothesis is that they are specific. The more detail you give to the question you want to answer, the easier it is to design a good experiment:

Example:

- "my Optimization method is the best!"
- "The optimization method proposed in this paper is better than existing methods!"
- "Using Polynomial mutation is better than gaussian mutation for optimization methods!"
- "Polynomial mutation increases the convergence rate of an optimization method, when compared to gaussian mutation!"

Scientific Hypothesis

Falsifiable Hypothesis

A good scientific hypothesis is falsifiable. A falsifiable hypothesis is one that **could be proven true or false** by the result of a experiment.

- Non Falsifiable Hypothesis: "This Neural Network can solve any problem if we find the right parameters".
  If the method does not solve the problem, it just means that the parameters are wrong, so we do another experiment... and another... and another...
- Falsifiable Hypothesis: "Using algorithm A and parameters θ, we achieve a speed-up of 1.5 on benchmark B."

An experiment control variables of interest

Types of Experiments

There are many variables that affect the result of an experiment. For example, if you want to test if chocolate ice cream tastes better than coffee, the result may be different if you ask children or PhD students.

If your scientific question is focused on the opinions of PhD students (WHY?), you can control the variables of the experiment, and not include children or professors in your survey.

Depending on how much freedom you have to control the variable in your experiments, we can classify experiments in three types:

- Observational Experiments;
- Retrospective Experiments;
- Controlled Experiments;

Types of Experiments

Observational Experiments

In an Observational Experiment, you obtain data by observing a phenomena without interacting with it directly.

Example: you count the number of people who use the train with and without masks every day.

- Requires care to observe representative situations;
- Allows the researcher to choose general conditions for observation;
- The situation of interest may be too rare to observe naturally;

Types of Experiments

Retrospective Experiments

In a Retrospective Experiment, the researcher obtains data from historical records (newspaper, reports, other scientific papers).

Example: you search from the relationship between announcements of celebrity marriages, and total number of registered marriages;

- Generally cheaper, and may be the only way to gather data over a very long period of time;
- Susceptible to missing records or bias in recording;

Types of Experiments

Controlled Experiments

In a Controlled Experiment, the researcher is able to define several variables in the experiment, and perform it in the conditions desired.

Example: You develop a new algorithm, and test it on some selected data sets, on a collection of different computational architectures;

- Gives a lot of control for the researcher;
- If not designed carefully, allows for the introduction of biases into the experiment;
- Can be the most expensive kind of experiment (although not always in CS);

3. A fair experiment control for biases

"With great power comes great responsibility"

When you control the variables of your experiment (**or when you don't!**). You can introduce biases to the result.

For example, if you compare the speed of two computer programs, it may be hard to see a difference, if you run your experiment in a very powerful computer. Or the difference may be exaggerated if you use a very slow one.

To have a fair experiment, it is important to be aware of these source of biases, and change your experiment to avoid those biases. This is one of the main tasks of Experimental Design.

Some Experiment Design Questions

- Which methods we compare in the experiment?
- Which data sets are used?
- How many times do we interview each participant?
- In what order do we perform the experiments?
- Which data is reported, and how is the data summarized?
- What criteria determines that the hypothesis was accepted or rejected?
- What hyper-parameters do we use?
- How many times is the experiment repeated? How are these repetitions sumarized?

Experiment Design

Example: Controlling for Variation

Let's say you are comparing two computer programs by measuring their running time (wallclock time).

You know that the running time of a program is affected by other programs that are running in the background of the operational system. For example, if a software update happens in the background, it could make a run much slower.

To control for this variation, you make sure to run your experiment in a system with a minimum number of running processes, and you also repeat the experiment many times and take the average running time;

Experiment Design

Example: Controlling for Independence

Imagine that you are comparing two website designs with the following experiment: You measure the time for a user to find some information on website A, then you measure the time for website B.

If you make this comparison always in the same order for all users, you discover that the users are a bit faster for website B, because they get used to the testing environment and are more relaxed.

To remove this influence, you make sure that the test order is always random, or you make sure that each user tests only one website.

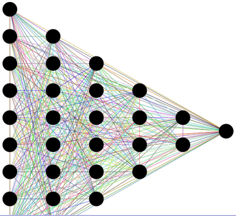
Experiment Design

Example: Controlling for Fairness

You propose a neural network architecture for a new vision problem, and you compare it against traditional architectures.

Because of the special characteristics of the problem, you fine-tune the hyper-parameters of your architecture to achieve the best performance.

To make sure that the comparison is fair, you use the same fine-tune techniques to the traditional architecture that you are comparing against, not using its old hyper-parameters from the literature.



Pre-registered Experiments

Pre-registration is the act of fully defining your research protocol **before you begin to collect or analyze data.**

By pre-registering your research, you avoid modifying your methods to fit your hypothesis (or modifying your hypothesis to fit your data)

Public pre-registration can prevent the loss of negative results. Private pre-registration can help you keep yourself in check.

Example: Center for Open Science
`https://cos.io/prereg/`

(Not a panacea: discuss partnership with Facebook in 2024 – can prereg work if you get to approve before sharing the data?)

Reproducible Experiments

Reproducibility is an important property of a good experiment:

- Others can confirm your results;
- Others can build on your results;
- Others can improve your results;
- Society can use your results;

Reproducible Experiments

How can we make experiments more reproducible?

Clear Experiment Design

Detailed steps taken to perform the experiment; Values of relevant parameters; How the results are processed and evaluated;

Open Data and Open Source

Data acquisition protocol is clearly defined; Raw data and pre-processing scripts are available; Data is well documented;

For CS, open source of proposed algorithms is essential;

Open Documentation

Code used for statistical analysis and data visualization;

Summary

Many scientific discoveries and scientific advancements (as well as your own master thesis!) depend on good experiments and data collection.

Unfortunately, good experiments are not as simple as simply going out on the streets and start collecting data.

Careful planning is necessary, not only to make sure that your experiment is not affected by biases, but also to make sure that your experiment is able to answer the question that you are asking.

Experiment Design is the proccess of carefully planning an experiment to make sure that it is fair and effective.

Part III: Outro

Summary of Lecture 01

- Experimentation is a key part of Science;
  - Experiments acquires data that can be used to validate or falsify scientific ideas, and to answer scientific questions;
- An experiment has to be performed carefully to guarantee its usefulness;
  - **Experimental design** defines the type of experiment, and how data is gathered;
  - Several factors can affect the **fairness and meaningfulness** of experiments;
  - **Reproducibility** is essential to guarantee the usefulness of an experiment;

Recommended Reading

Required Reading

- Understanding Science `https://undsci.berkeley.edu/article/intro_01`

Suggested Reading

- Videos: Crash Course Sociology and the Scientific Method, Sociology Research Methods; (link on manaba)
- Existential Comics `http://existentialcomics.com`;

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