Experimental design

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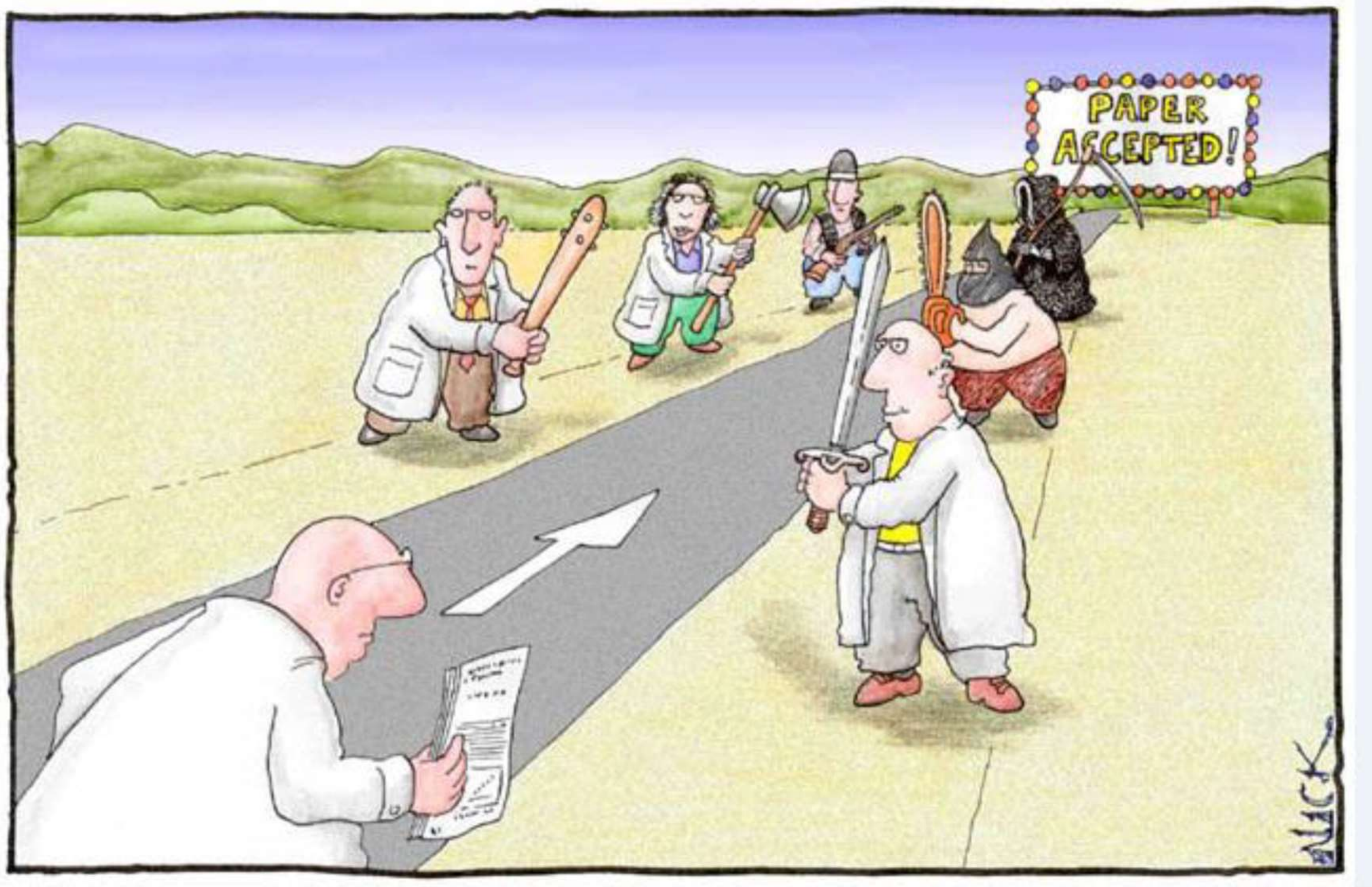
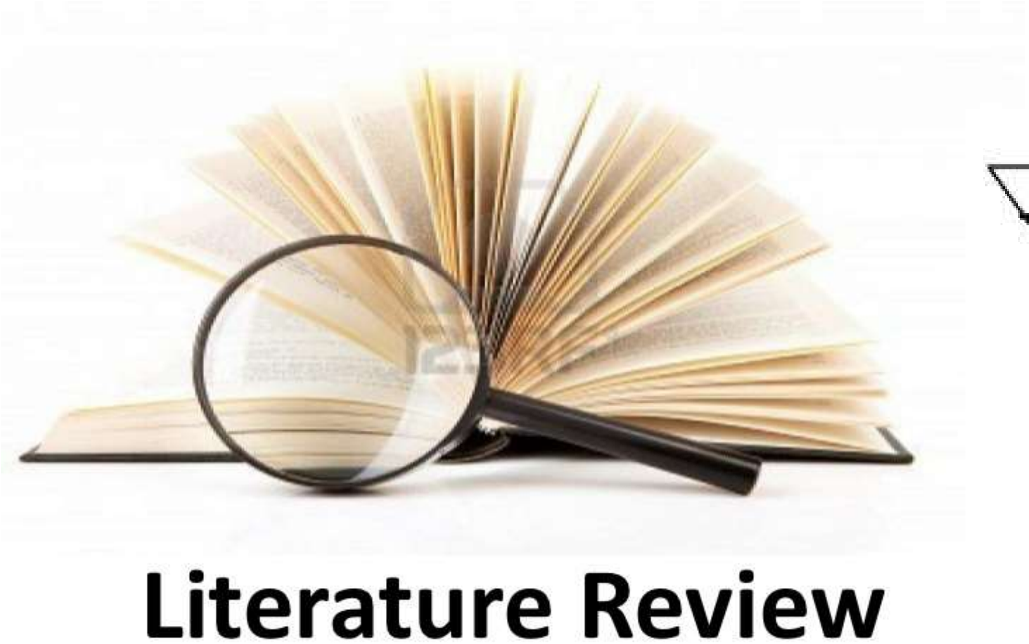
Ho Chi Minh, December 29th 2020

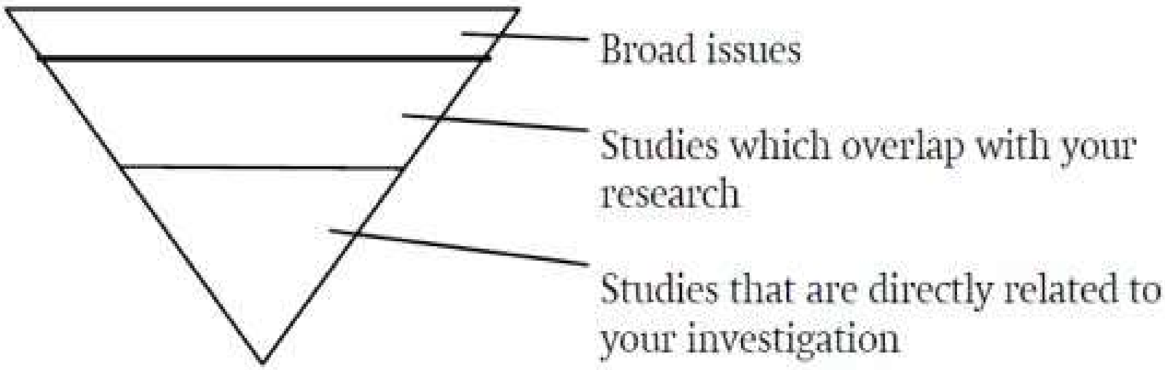
Experimetal design

What is goal?

Publishing is easy or not?




Literature Review


Broad issues
Studies which overlap with your research
Studies that are directly related to your investigation

Methodology of planning experiments

1. What is the goal?
   Why we do the experiment?
2. How we can answer the question?
   What kind of analysis can calculate we need?
3. What we have to measure?
   How many measurements and what combinations have to be performed?

Science vs Industry approach

There are different objectives for science and industry:

- Science: discover the statistical effect of particular factors on the feature of our interest.
  For example: how storage temperature is affecting fruit firmness?

- Industry: extract maximal unbiased (independent) information about factors affecting production from minimal observations.
  For example: what we can change in recipie to increase consumer acceptance?

* Hypothesis: a statement about the population

* Based on our collected data we conclude to the whole phenomenon (population)

* Whether our result (difference in samples) is greater than the difference caused **only by chance**.

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Experimetal design

Hypothesis, question

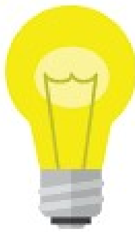
EXPERIMENT

Collected data

Type of question

STATISTICS

Conclusion



What is the goal?

The objective of the experiment determines what kind of methods will be available for analysis, as well as how many samples we need.

- Is it univariate relationship? $y = f(x)$
  Tipically no. Sorry, life is more complex.
- Is it multivariate relationship? $y = f(x_1, x_2, ...)$
  This is more realistic. The problem is to select the meaningful factors to save money and time.

What is the question?

The question determines the analysis type:

- Do you want to see the effect of change?
  Question: how long can fruit keep quality if I decrease storage temperature from 10 °C to 5 °C?
  Need comparison methods.
- Do you want to predict value without measurement?
  Question: how can I predict soluble solids content of fruit without destroying it?
  Need regression analysis.

How we can answer?

* Comparison methods

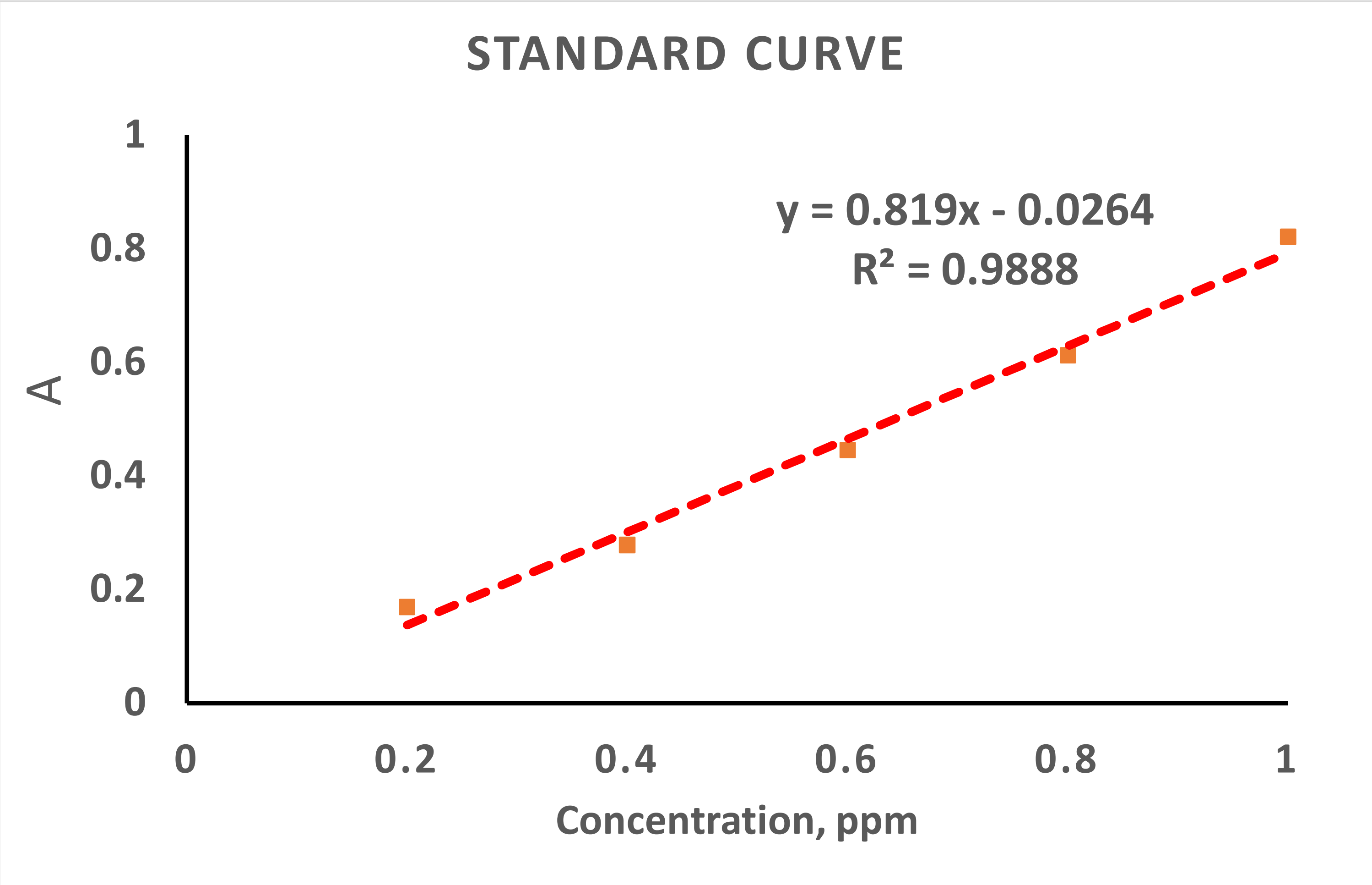
- **Two groups:**
  t-test (parametric test = requires normal distribution of data), Kolmogorov-Smirnov test (robust = for any distribution)
- **Many groups:**
  Analysis of Variances (ANOVA).
  Warning! **ANOVA** only can answer the question whether there is at least one group different from others! If you want to identify group differences, need to **run post-hoc test**: Tukey test, Duncan test, multiple range test, etc.

How we can answer?

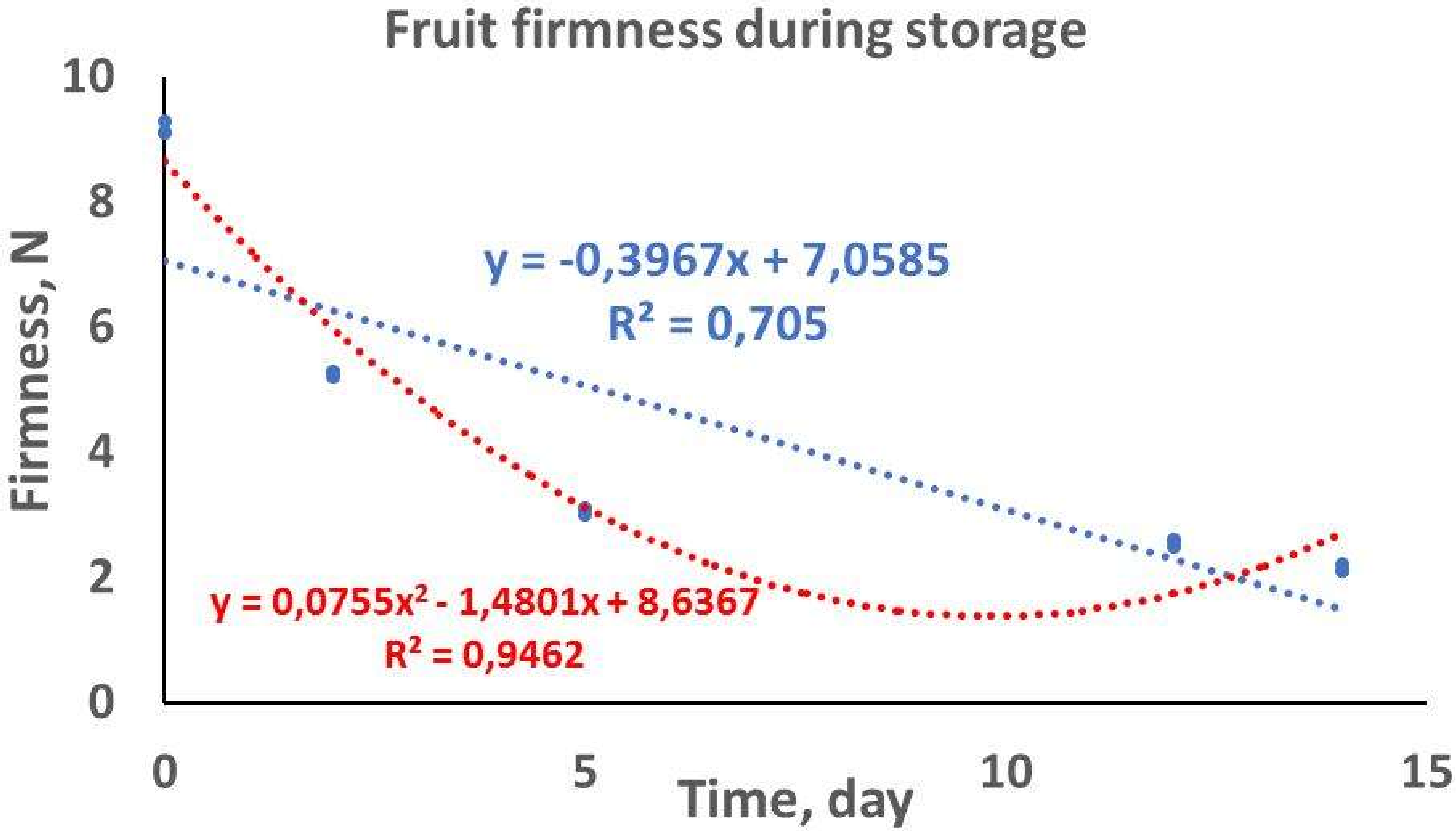
* Regression methods

- Is there **linear relationship** between them?
  Calculate Pearson correlation.
- Is there **non-linear relationship** between them?
  Calculate Kendall or Spearman (rank) correlation.
- How can I **predict feature or future value**?
  Fit curve on data:
  - Linear model for trend or calibration.
  - Model is usually given by chemistry (Arrhenius equation) or physics (Saturation model)

Example


STANDARD CURVE
y = 0.819x - 0.0264
R² = 0.9888
A
Concentration, ppm
0
0.2
0.4
0.6
0.8
1

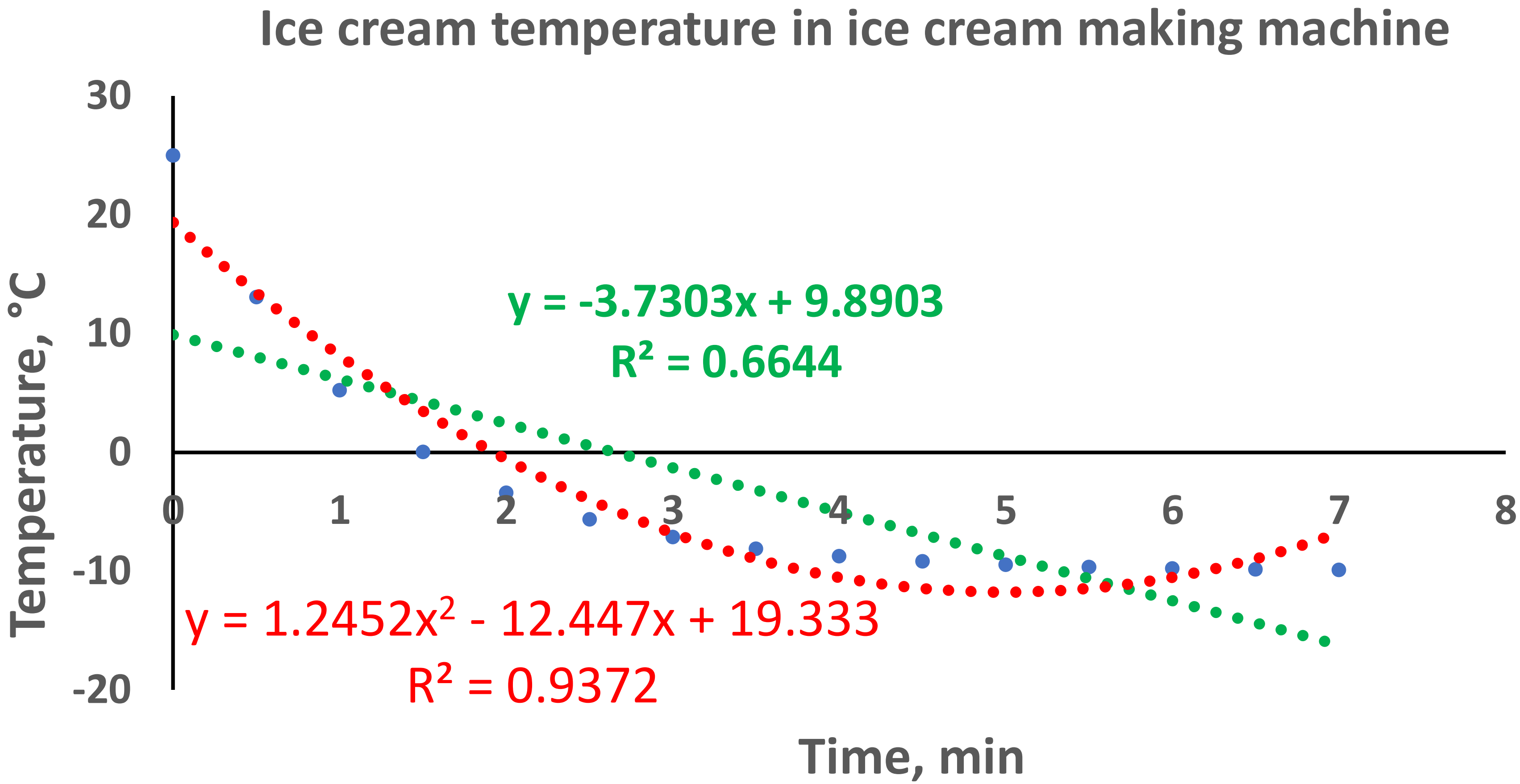
Example


Fruit firmness during storage
y = -0,3967x + 7,0585
R² = 0,705
y = 0,0755x² - 1,4801x + 8,6367
R² = 0,9462
Firmness, N
Time, day
10
8
6
4
2
0
0
5
10
15

Experimetal design

Example

What is the equation that can describe the presented phenomenon?



How we can answer?

* Regression methods

- What is the optimal combination?
  Response Surface Methodology (RSM).
  $$y = a + bx_1 + cx_2 + dx_1x_2 + ex_1^2 + fx_2^2 + \text{error}$$

- How can I predict soluble solids content (SSC)?
  Chemometry: use Near-Infrared (NIR) spectroscopy and make model with Partial Least Squares (PLS) regression.
  $SSC = f(\ LV_1(\text{spectra}),\ LV_2(\text{spectra}),\ \ldots\ )$

What combinations are measured?

Measurement groups:

	Cooking time		
	5 min	10 min	15 min
Temperature			
80 °C	______	______	______
100 °C	______	______	______
120 °C	______	______	______

This is called full factorial = all combinations are measured.

What combinations measure?

Statistical analysis uses level codes to balance differences between range of values:

Temperature	Cooking time: -1	0	+1
-1	______	______	______
0	______	______	______
+1	______	______	______

How we can answer?

What if we want to recognize quality class, infection, damage, etc?

Need classification methods. They are supervised methods. We teach the computer and it will calculate which group is closest to the new measurement?

- Discriminant Analysis (DA) is based on the variance of data.
- Support Vector Machine (SVM) is based on the high density locations of the data cloud.

Factorial design

Terminology in experimental design

Experiment

Treatment or factor

Level

Experimental unit

2^n factorial design

2^n

Number of factors = n

Level of factors = L

Total number of sample groups:

$$N_G = L^n$$

2^n factorial design

- What are **2^n factorial design**?

-design to determine effect of n factors, each with 2 levels

- Why consider **2^n factorial design**?

-easy to analyze

– factors that have significant impact → full factorial design

– factors have little impact → not of interest

- How to select 2 levels

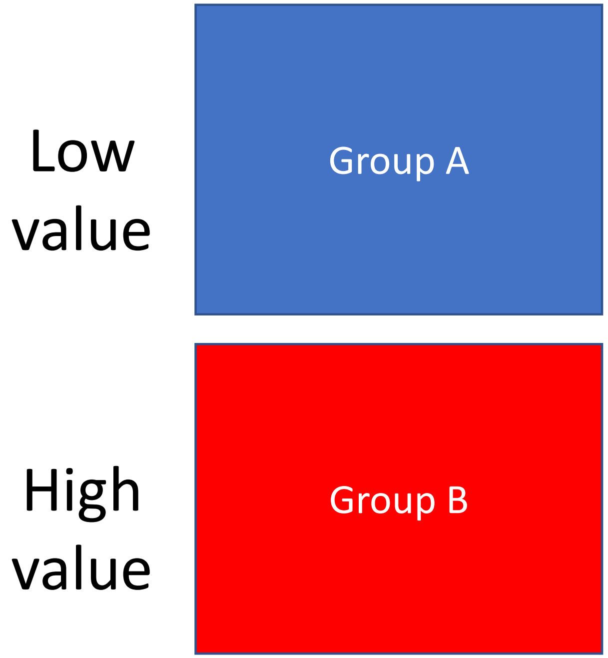
-if factor effect is expected to be unidirectional → select min, max

2^n factorial design

Number of factors = 1

Level of factors = 2

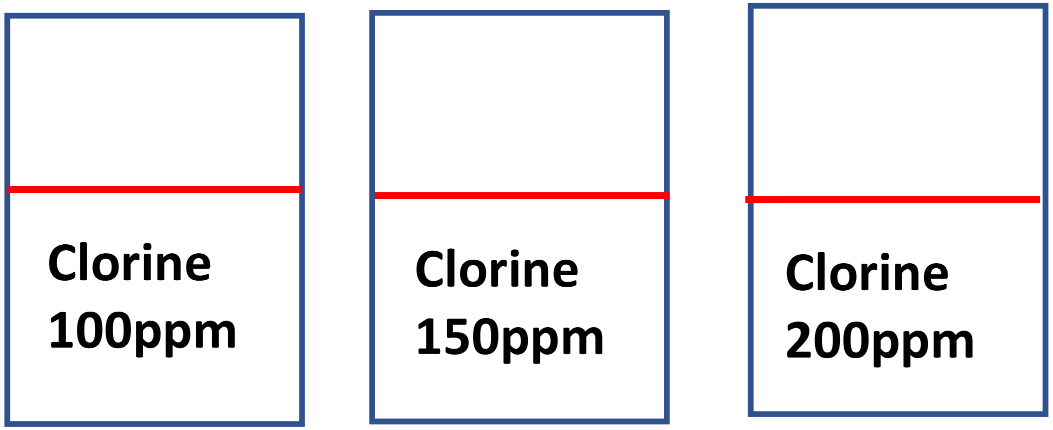
1 factor groups:



Experimetal design

Example

Evaluating the effect of clorine in washing fruit at different concentration: 100, 150, 200ppm.



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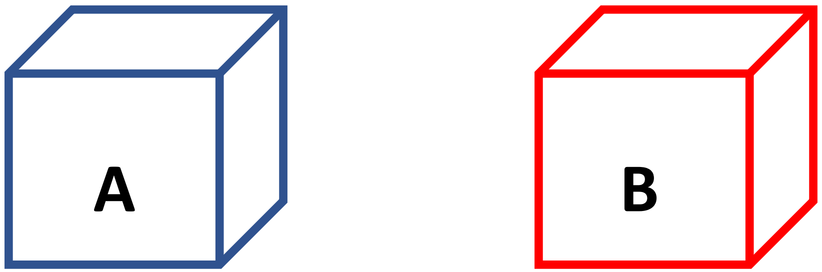
Experimetal design

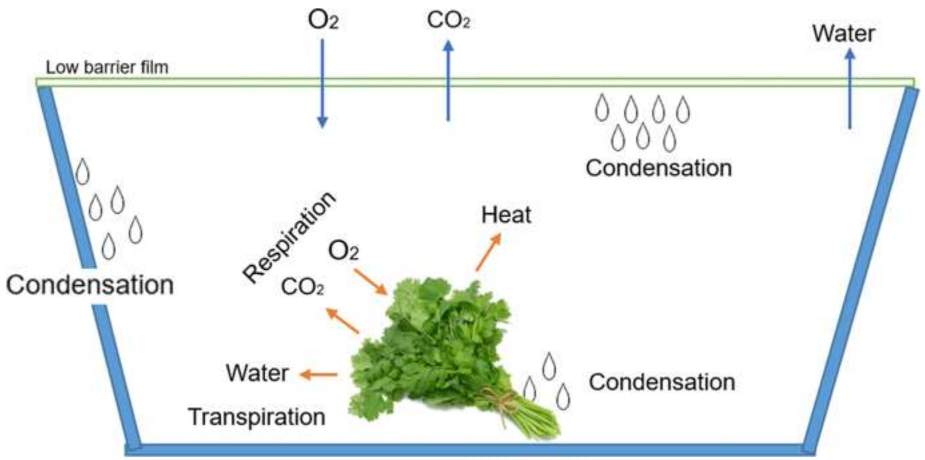
Example

- There are 2 types of packaging: A and B.
- Evaluating the effect of packaging on vegetable during storage for 10 days. How many groups?

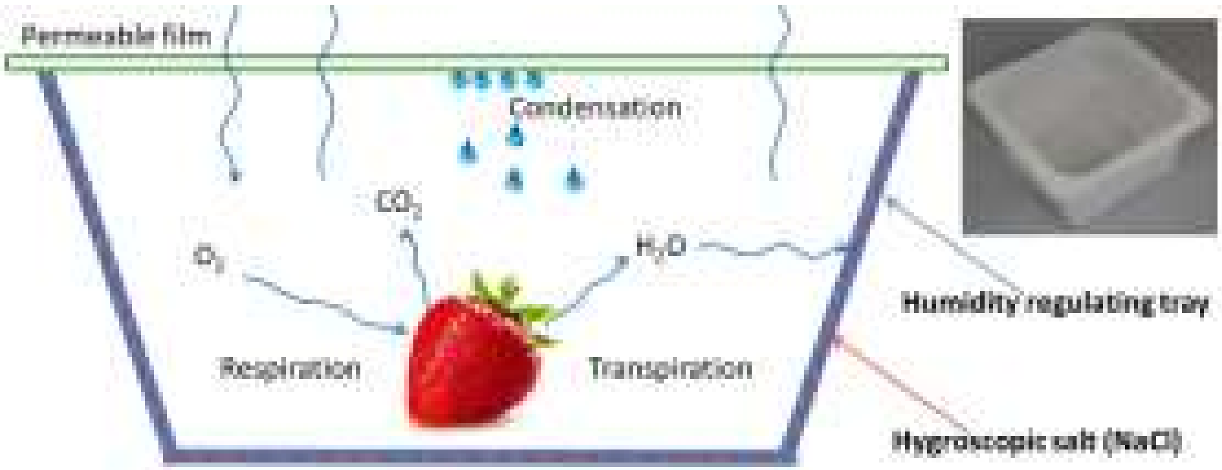


Experimetal design

Example

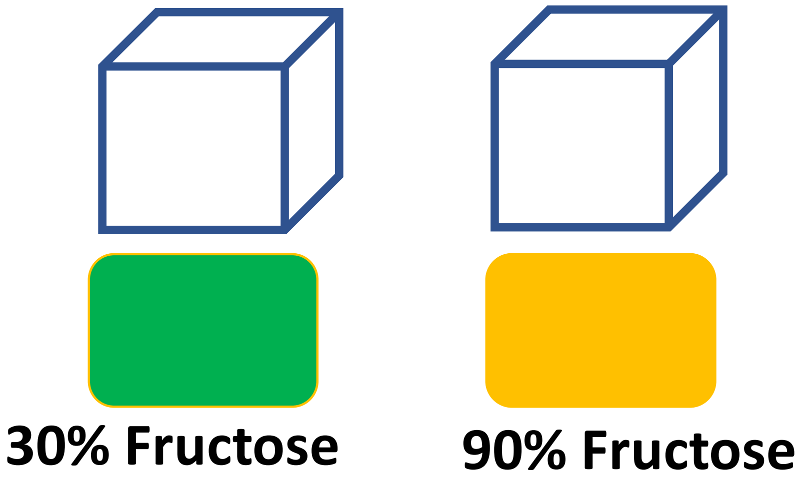


Moisture absorber pad



Example

-There are 2 types of moisture absorber: 30% fructose and 90% fructose. Evaluating the effect of moisture absorber on packaging vegetable during storage for 10 days. How many groups?



2^n factorial design

Number of factors = 2

Level of factors = 2

2 factor groups:

1 factor groups:

	Low value	High value
Low value	Group A	Group C
High value	Group B	Group D

Example

Measurement groups:

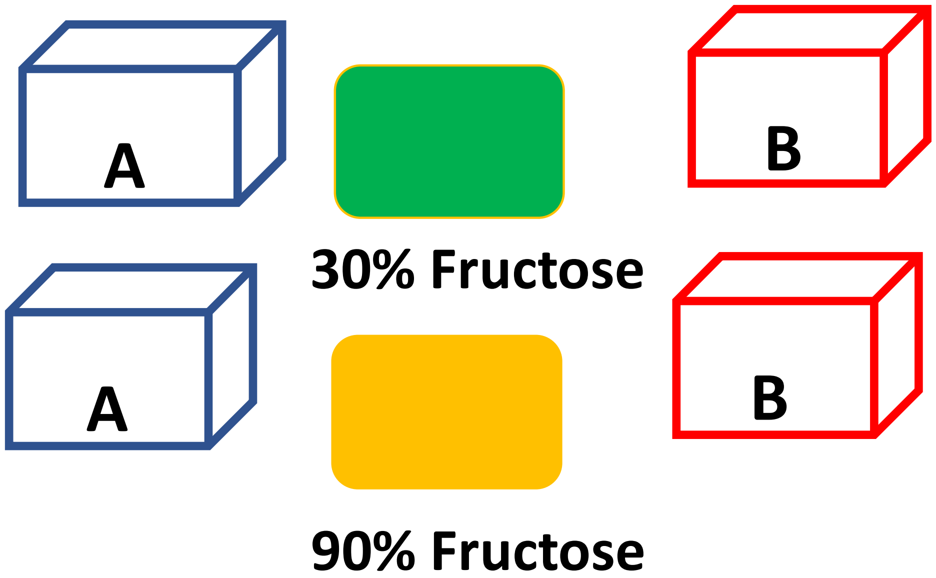
	Cooking time		
	5 min	10 min	15 min
Temperature			
80 °C	______	______	______
100 °C	______	______	______
120 °C	______	______	______

Full factorial = all combinations are measured.

Experimetal design

Experiment

-There are 2 types of packaging: A and B and 2 types of moisture absorber. Evaluating the effect of packaging and absorber on vegetable during storage. How many groups?



Experimental design:

- 2^n factorial design: two levels, n factor full design
- 3^n factorial design: three levels, n factor full design
- Central composite design (RSM)
- Latin square design
- Taguchi robust design
- Mixture design
- Fractional factorial design

What combinations are measured?

Number of measurements (N):

$$N = L^n \times R$$

n = number of factors (2 = cooking time, temperature)

L = number of levels adjusted (3 = low, medium, high)

R = number of replicates (3)

$$N = 3^2 \times 3 = 27$$

Example

Measurement groups:

	Cooking time		
	5 min	10 min	15 min
Temperature			
80 °C	______	______	______
100 °C	______	______	______
120 °C	______	______	______

This is called full factorial design = all combinations are measured.

Example

Temperature (°C)	pH	Time (min)
50	4.0	10
60	5.0	20
70	6.0	30

Full factorial design = ? combinations

$$Y=a_o + a_1X_1 + a_2X_2 + a_3X_3 + a_4X_1^2 + a_5X_2^2 + a_6X_3^2 + a_7X_1X_2 + a_8X_1X_3 + a_9X_2X_3$$

$$Y= 45.82 – 1.39X_1 + 1.19X_2 – 2.65X_1^2 – 2.1X_2^2 – 1.13X_3^2 + 0.65X_1X_2 + 0.65X_1X_3 + 1.22X_2X_3$$

Factorial design

What is block?

Block is a homogeneous unit of samples:

- Crops harvested at the same time
- Feeding made by the same company
- Animals living in the same barn
- Solutions prepared by the same technician

Block is usually added as additional factor to avoid systematic error. It makes statistic more robust and stronger. This is called block design.

What is mixture design?

In mixture design, the summary of all factors are always the same.

Example:

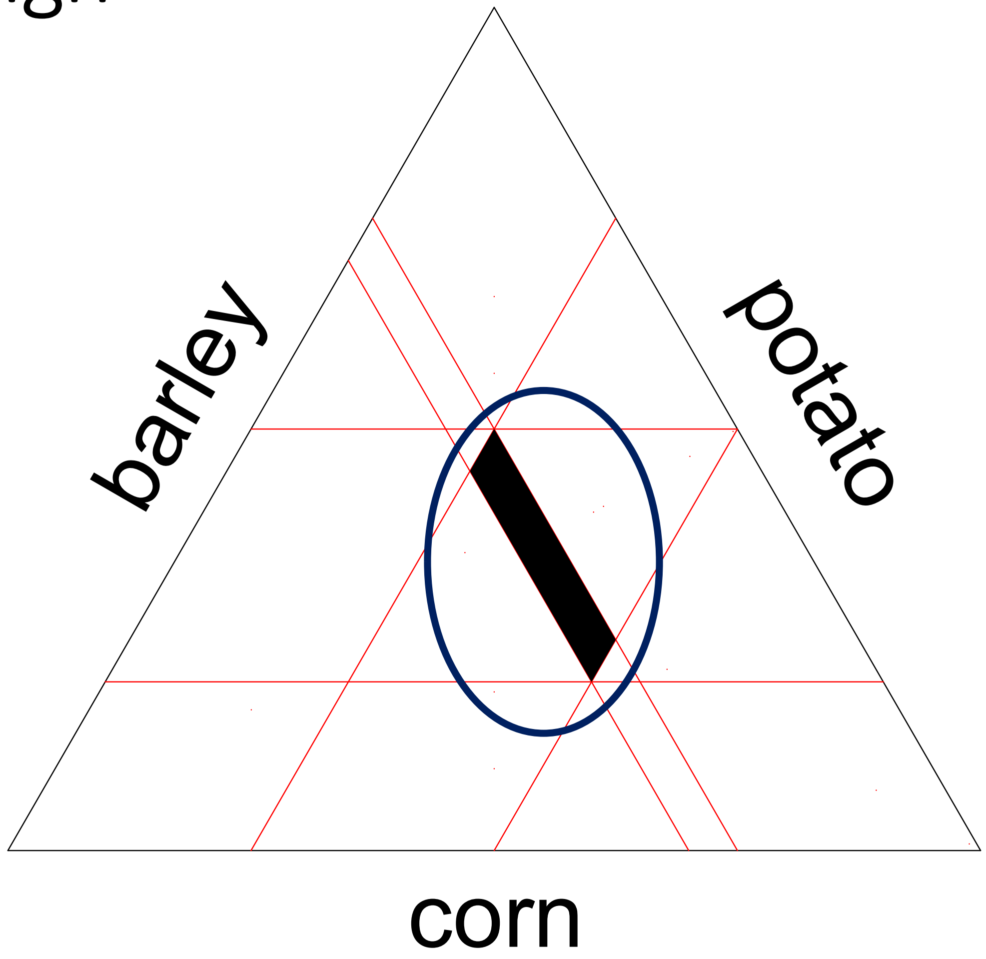
- Feeding #1: 20% corn, 50% barley, 30% potato
- Feeding #2: 50% corn, 25% barley, 25% potato

All feedings have the summary of 100%

Mixture design

Plotting mixture design

- Corn: 20 – 50%
- Barley: 25 – 50%
- Potato: 25 – 30%



Question

1. Which type of experimental design is suitable for this problem?
2. Please propose an experiment!

Problem: Our yoghurt product received 79% satisfaction on consumer survey. We want to improve by changing ingredients. The current contents of one portion:

- 110 g natural yoghurt
- 8 g cherry fruit pulp
- 7 g extruded cereal

One portion totally: 125 g

The cup size is given, filling must be 125 g.

Fractional factorial design

A full factorial design may require many experiments

- How can we get enough info with less: fractional factorial design

Temperature	Cooking time: 5 min	10 min	15 min
80 °C	x		x
100 °C		x	
120 °C	x		x

Full factorial design = all combinations are measured.

Example

Temperature (°C)	pH	Time (min)
50	4.0	10
60	5.0	20
70	6.0	30

$$Y = a_o + a_1X_1 + a_2X_2 + a_3X_3 + a_4X_1^2 + a_5X_2^2 + a_6X_3^2 + a_7X_1X_2 + a_8X_1X_3 + a_9X_2X_3$$

$$Y = 45.82 – 1.39X_1 + 1.19X_2 – 2.65X_1^2 – 2.1X_2^2 – 1.13X_3^2 + 0.65X_1X_2 + 0.65X_1X_3 + 1.22X_2X_3$$

Why experimental design?

- Obtain maximum information from fewest experiments

-minimize time spent gathering data

- Quantify effects from different factors using analysis

- Determine if a factor’s effect is significant

-differences might be random variations caused by
  - measurement errors
  - parameters not controlled

Basic principles

1. Thinking about the question in advance
2. Comparison/control
3. Replication
4. Randomization
5. Factorial experiments

Example

Question

Does chemical treatment/packaging affect the quality of the food?

Does the temperature/pH affect the …?

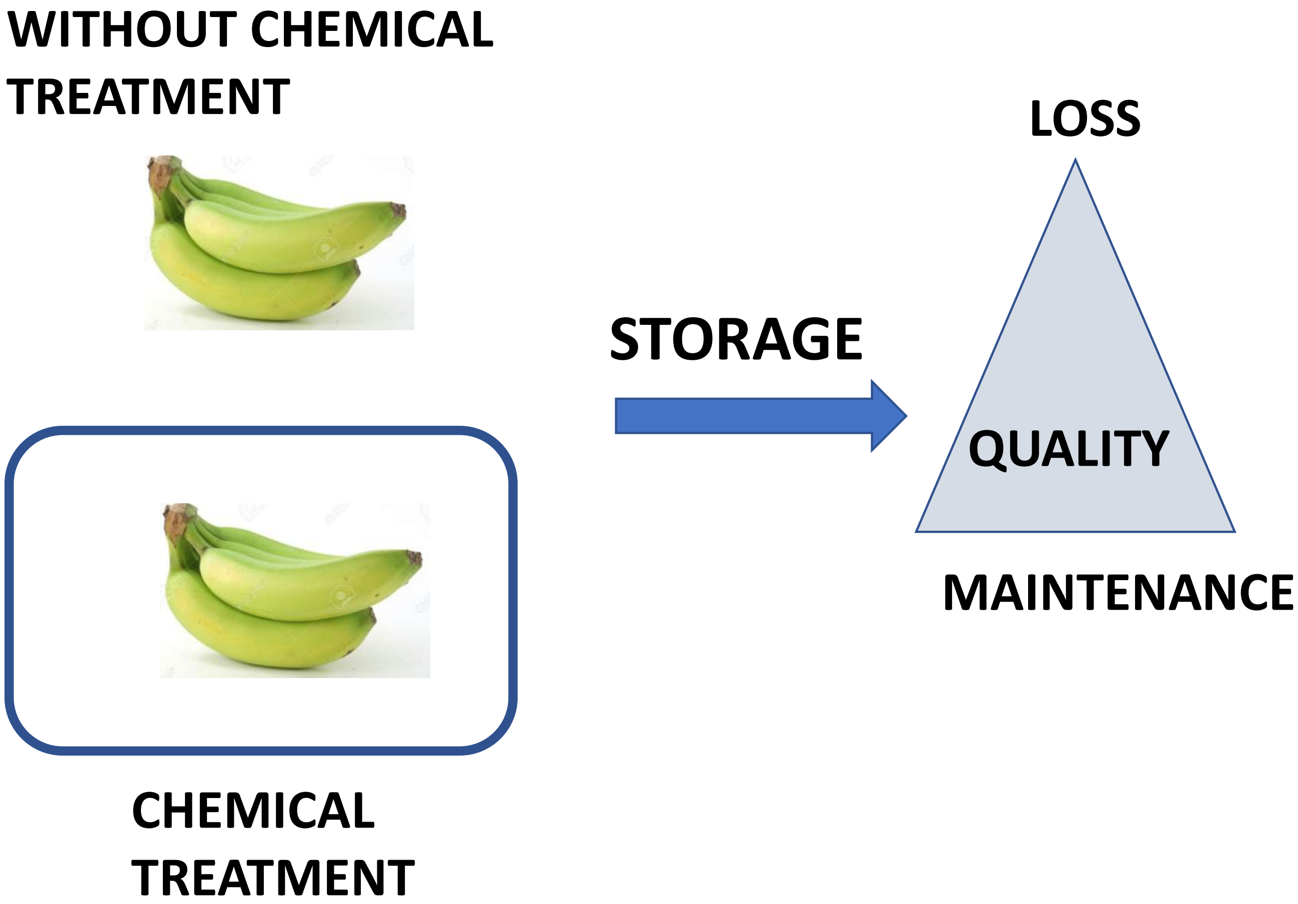
Does the solvent/time/… affect the…?

Experiment:

1. Treat the fruit with chemical
2. Wait 7 days
3. Measure the quality

Experimetal design

Example: How the chemical effect the quality of the fruit during storage?



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Experimetal design

Experiment

Initial

CONTROL

WITHOUT TREATMENT

TREATMENT

Comparison/control

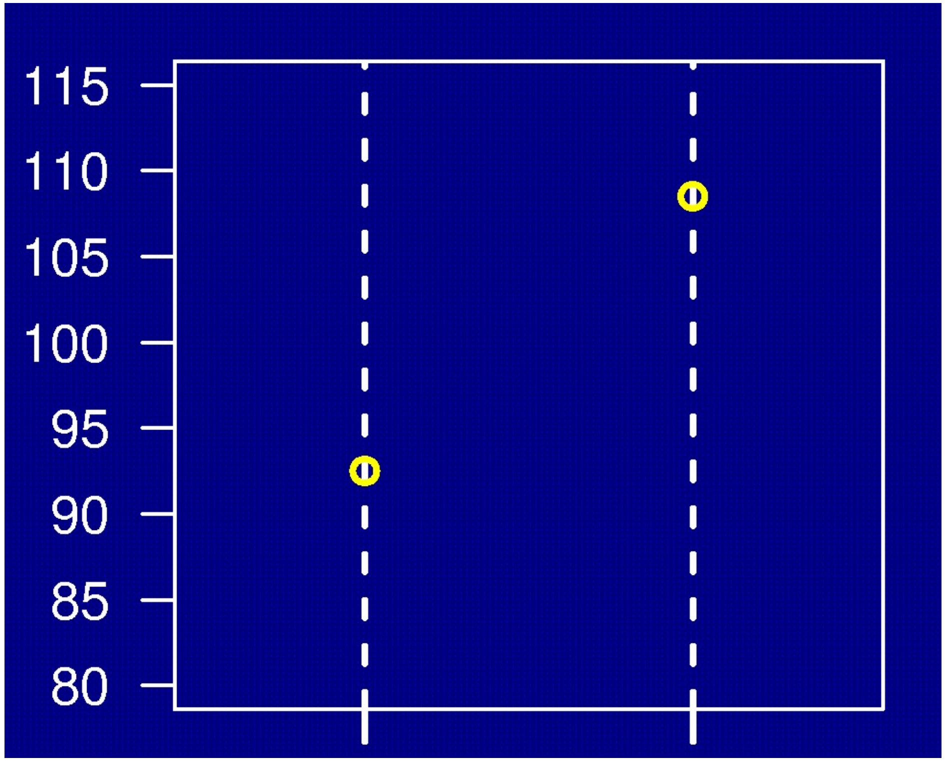
In the experimental design, group is compared to concurrent control (rather than to initial control).

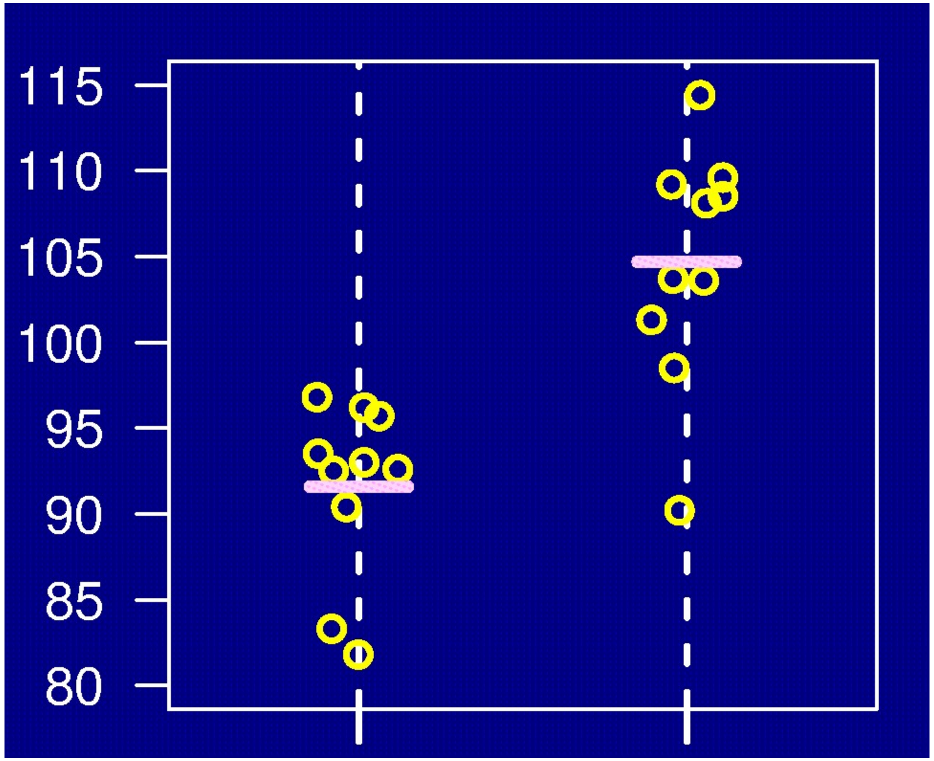
Example: chitosan treatment: 1%, 1.5%, 2%

– **don't make decision about factor's effect without comparison!**

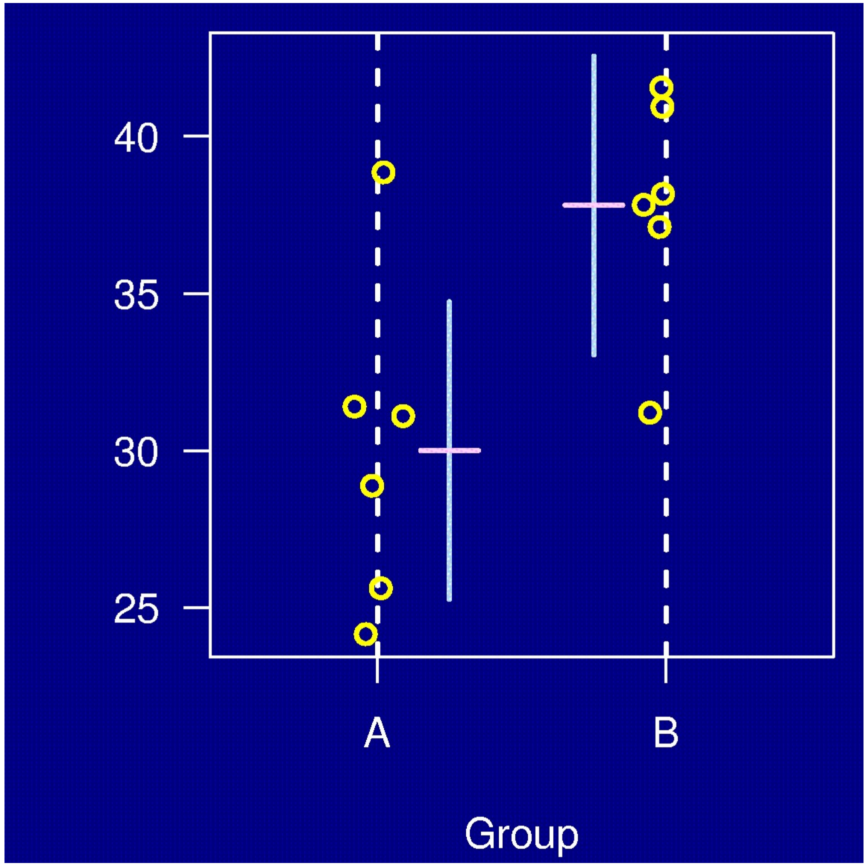
Replication

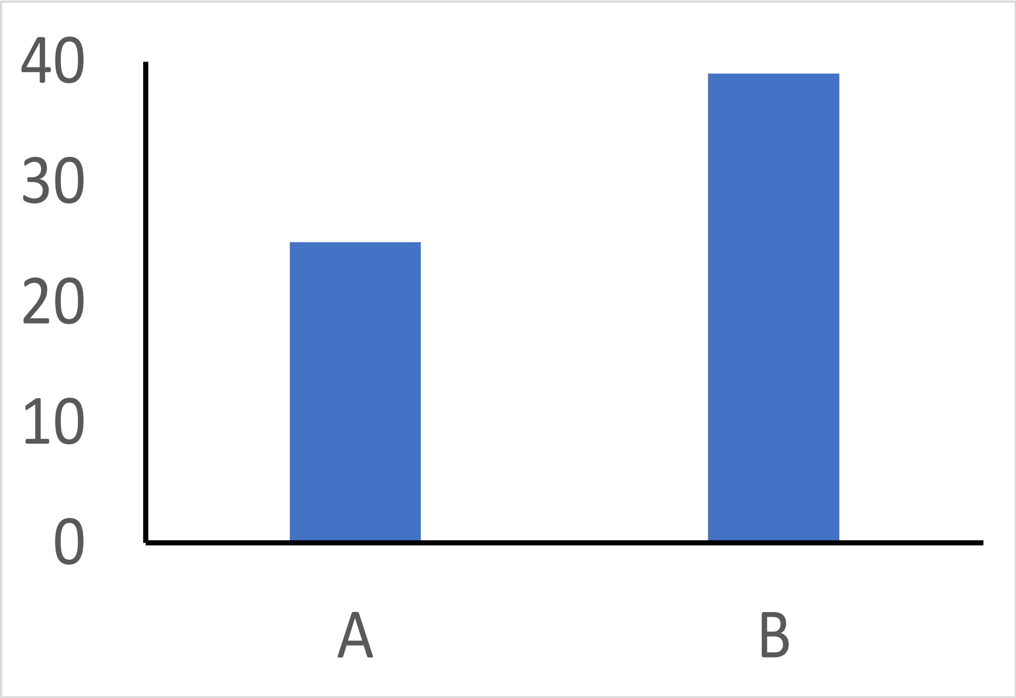
Example: Firmness (N) of apple (control & treated sample)





Why replicate?





Replication

Group	Mean	(SEM)
A	10.2	(0.6)
B	12.4	(0.8)
C	14.7	(0.6)

Group	Mean	(SEM)
A	10.2965	(0.63)
B	12.49	(0.7913)
C	14.787	(0.6108)

Why replicate?

- Reduce the effect of uncontrolled variation

Randomization

Experimental subjects (samples) should be assigned to treatment groups at random.

Using

- A computer, or
- Coins, dice or cards.

Why randomize?

Why randomize?

- Are the subjects you are studying really representative of the population you want to study?
- Ideally, your study material is a random sample from the population of interest.

Why randomize?

Randomized design for measurements:

in order to minimize systematic error

Randomized order / sequence:

Group D	Group B	Group A	Group C
1st measurement	2nd measurement	3rd measurement	4th measurement

Experimetal design

A Good measurement design or not?

Day 1	Day 2	Day 3	Day 4
G1	G1	G1	G1
G2	G2	G2	G2
G3	G3	G3	G3
G4	G4	G4	G4

G= group

Factorial experiments

We are interested in the effect of both salt water and a high-fat diet on blood pressure.

Good exp. design: look at all 4 treatments in one experiment.

Plain water	Normal diet
Salt water	High-fat diet

Why?

- We can learn more.
- More efficient than doing all single-factor experiments.

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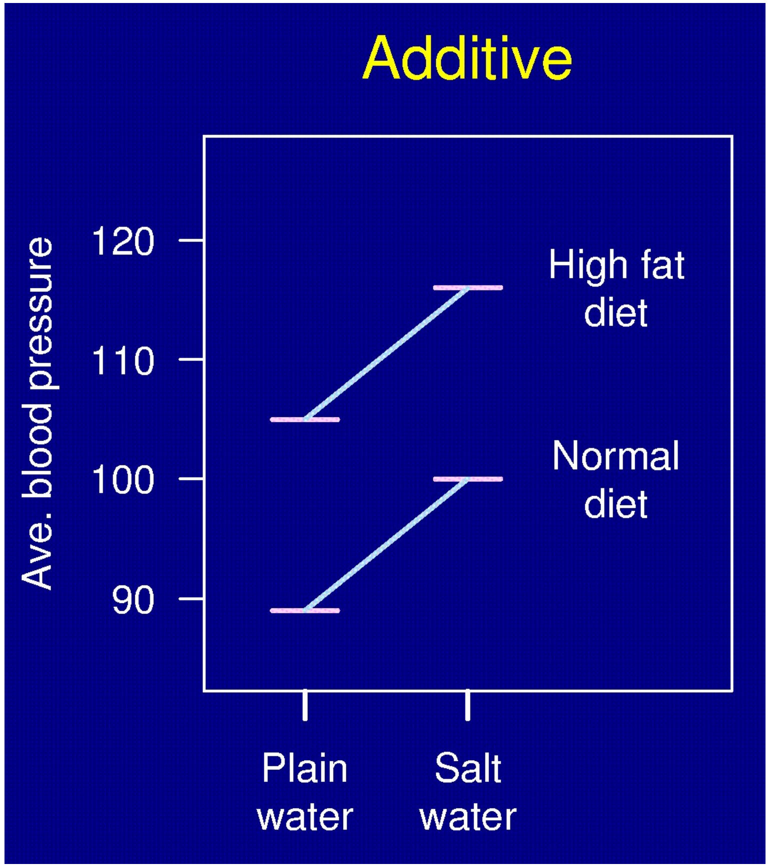
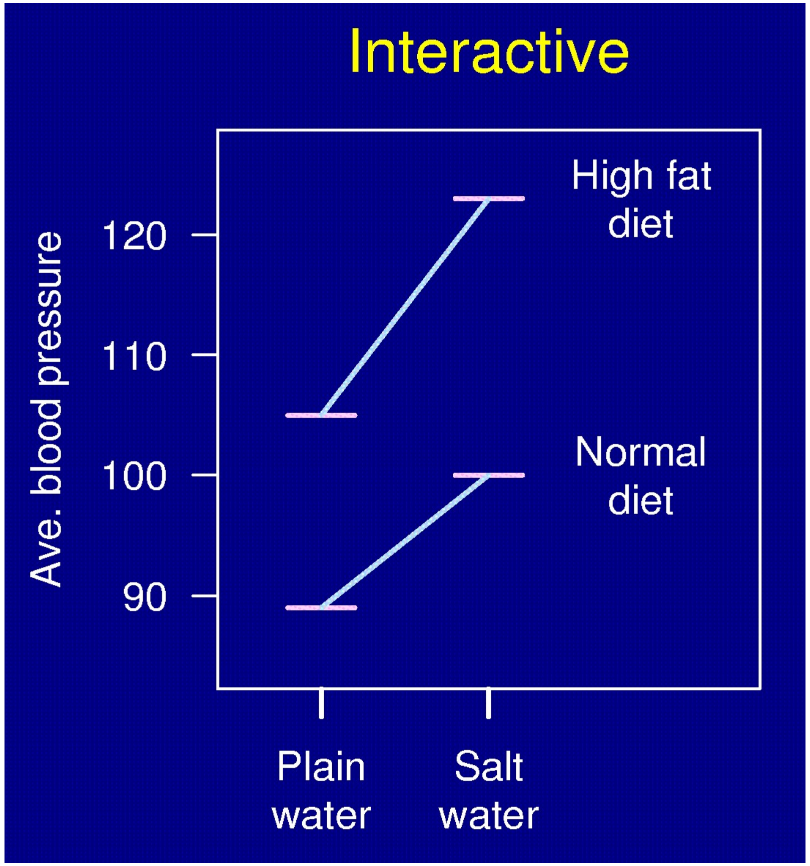
Experimetal design

Factorial experiments

Interaction: if level of A changes effect of level change of B



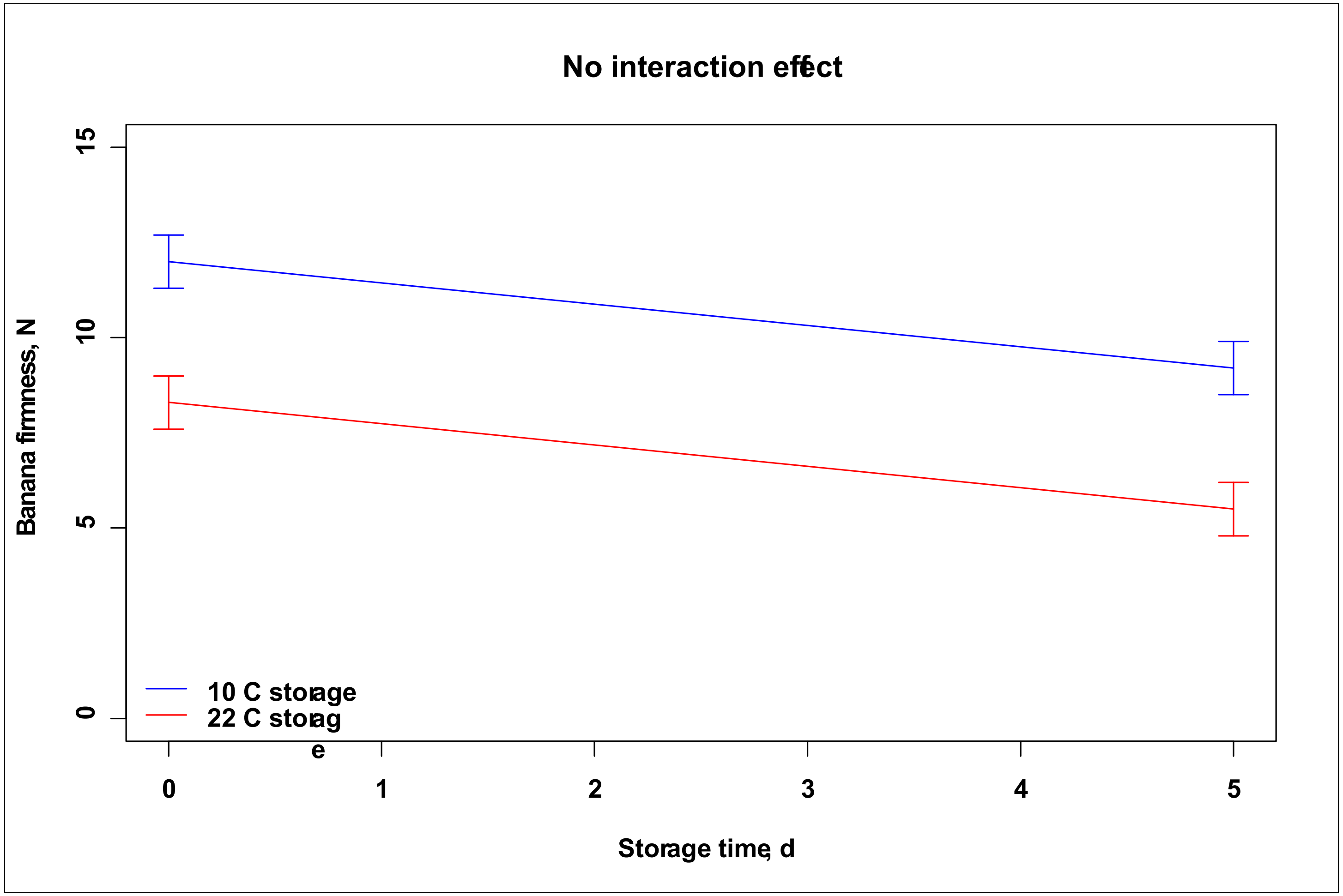


Experimetal design

Banana firmness

5 days storage
2 groups:
- 10 °C
- 22 °C

Cold stored pieces were harder.

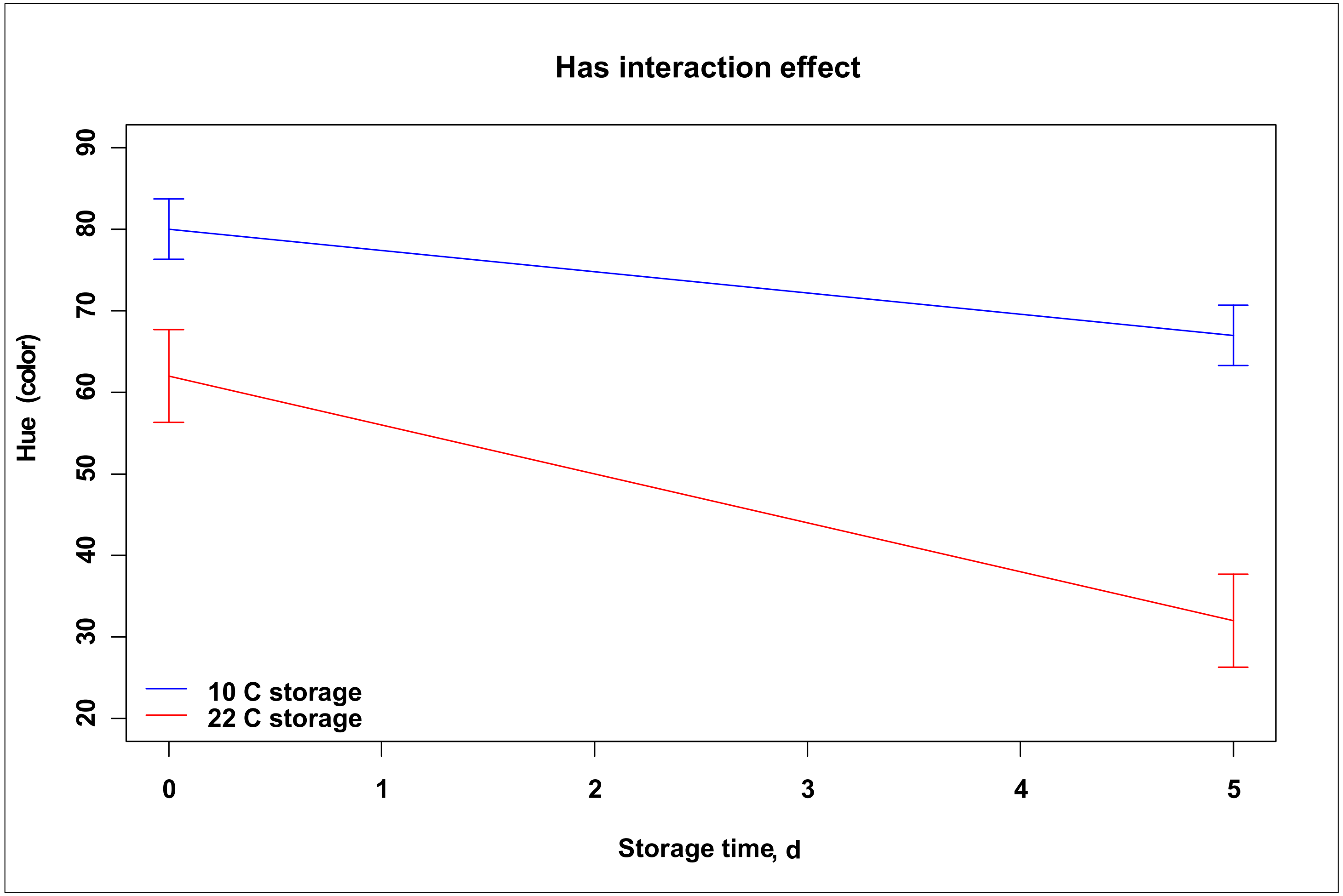


Experimetal design

Banana color

5 days storage
2 groups:
- 10 °C
- 22 °C

Cold stored pieces were more green, while warm pieces became brown.

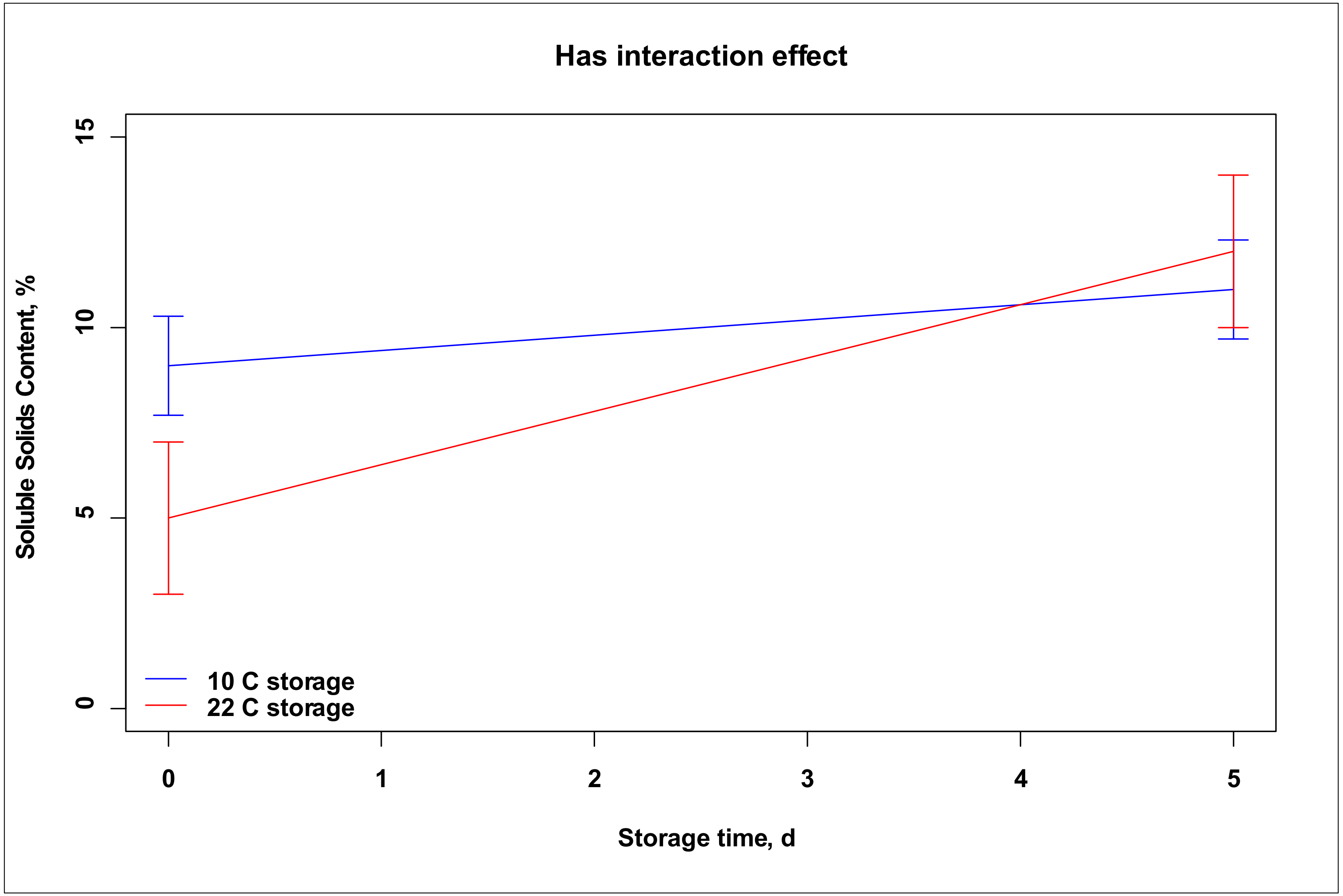


Experimetal design

Banana SSC

5 days storage
2 groups:
- 10 °C
- 22 °C

All pieces had similar SSC after 5 days, but warm pieces changed more.



Summary

Characteristics of good experiments:

- Unbiased
    - Randomization
    - Blinding
- High precision
    - Uniform material
    - Replication
    - Blocking
- Simple
    - Helps against mistakes

Common problems

Common mistakes

Vary one factor at a time to see how performance changes

Disadvantage

— if factors interact, may give wrong conclusions

	Cooking time		
	5 min	10 min	15 min
Temperature			
80 °C	x		
100 °C	x	x	x
120 °C	x		

This is called full factorial design = all combinations are measured.

Common mistakes

Example

Fix 2 factors, change 1 factor at a time?!

Temperature (°C)	**pH**	**Time (min)**
50	4.0	10
60	5.0	20
70	6.0	30

Full factorial design = 3^3 combinations

Common mistakes

• Use simple one-factor-at-a-time designs
-leads to many experiments, provides too little information per experiment

• Ignore interactions between factors
-cannot estimate interactions with one-factor-at-a-time experiments

• Conduct too many experiments
- The number of experiments needed depends upon # factors, # factor levels

↓

Be of simplicity, don’t attempt to do too much
write out the objectives, listed in order of priority

Common mistakes

Fail to isolate effects of different factors

-if varying several factors are being varied simultaneously

↓

Design experiments so that effects of factors can be separated

Cooking time

Temperature	5 min	10 min	15 min
80 °C	x		
100 °C		x	
120 °C			x

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Experimetal design

Explores every possible combination at all levels of factors

- Advantages

-detailed data

-can find effect of every factor, secondary factors, and interactions

- Disadvantages

-too many experiments, especially with repetitions

Solutions

—reduce number of levels per factor (2 is very popular)

—reduce number of factors:

– initially only examine a few levels of each factor

– delete unimportant factors, then try more factors per level

—use fractional factorial designs

What combinations are measured?

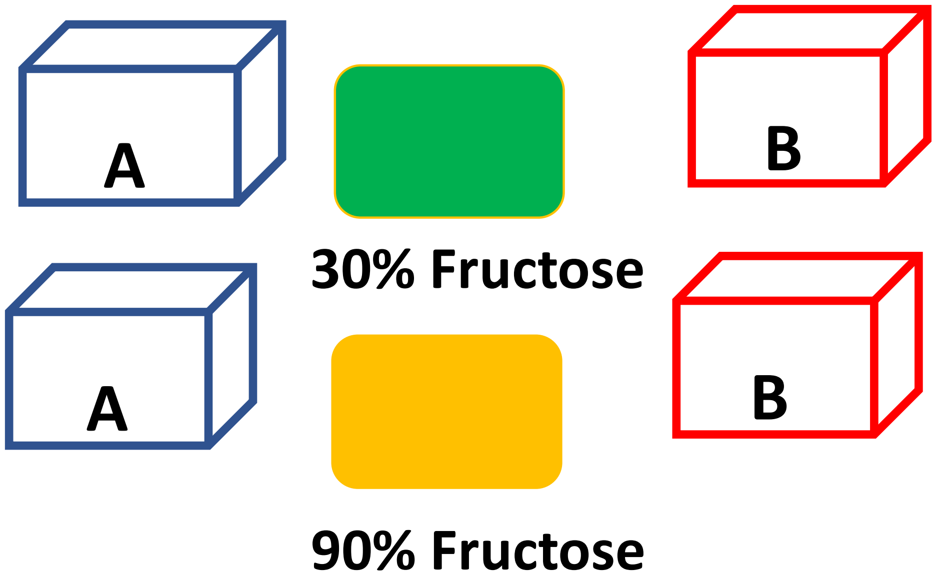
Measurement groups:

	Cooking time		
	5 min	10 min	15 min
Temperature			
80 °C	______	______	______
100 °C	______	______	______
120 °C	______	______	______

Full factorial design = all combinations are measured.

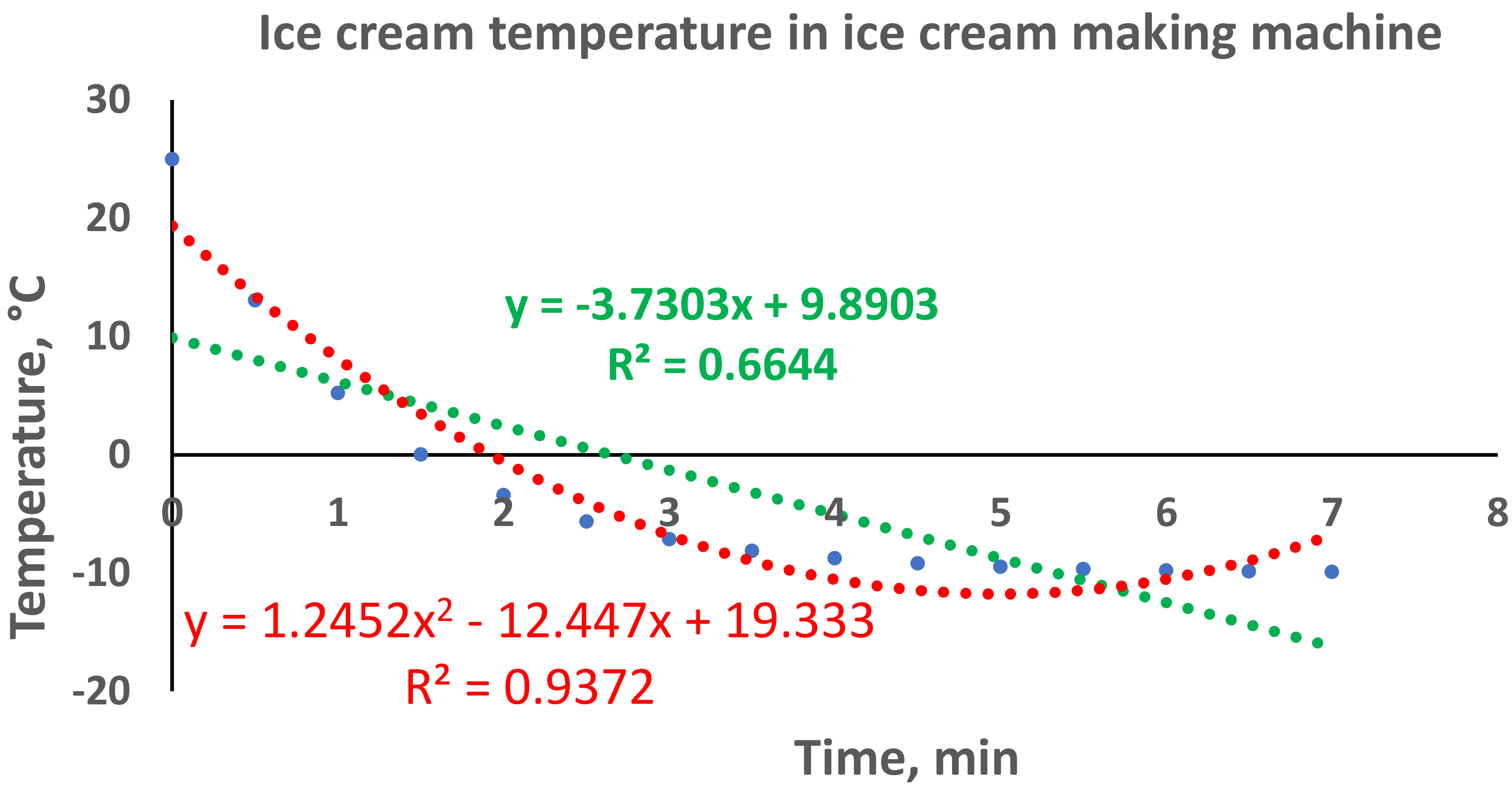
HOMEWORK

-There are 2 types of packaging: A and B and 2 types of moisture absorber. Evaluating the effect of packaging and absorber on vegetable during storage. How many groups?



HOMEWORK

What is the equation that can describe the presented phenomenon?



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THANK YOU FOR LISTENING!