Experimental Design

Unit 1

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A letter from Günter Pilz (1/3)

Dear near-ring friends,

this time I want to tell you what near-rings have done for me. Since more than 50 years, I suffer from unusual tiredness in the late afternoon / early evening hours. Since the early 90's, this lead to total paralizations for 2-3 hours each, in which I could hear and see everything, but I could not move my eyes or any other part of my body. I was a Zombie.

After „using up" more than 120 doctors, a hospital in Marburg (near Frankfurt), specializing on rare diseases, found out that the paralyzations must be caused by a genetic defect in one of the (many) ion channels leading into the cells. But they told me that the investigation will be complicated and might take up to about 6 years. I found these 6 years too long, since some time before, a group of doctors had told me „If you are lucky, you have one more year to live. If you are unlucky, it might be 5 years". I asked what they meant, and they said that they expect my life to become so dreadful that I would like to die, the sooner the better. So I listed all substances which go into and out of cells, wrote down, what I had eaten (so I knew how much calcium, sodium, etc. were in my last meal), took a

A letter from Günter Pilz (2/3)

bathroom scale right after the meal, and pressed it with both hands. One hour after the meal, I did the same. The differences got up to + 12 kilos!

So I could use statistical regression (which is basically pure algebra) to find out that most chemicals are irrelevant, only a few remained „suspicious“. Since most procedures in the body do not rely on a single substance, I also used the best tool to study (positive and negative) synergies of these suspicious substances: balanced incomplete block (BIB) designs! Of course, I took them from planar near-rings, constructed by the Clay-Ferrero method. After only 6 weeks (due to my frequent meals), I had the result with 99.99% reliability: potassium is bad for me, and sodium is good. Nothing else counts. That also makes medical sense, since potassium and sodium are antagonists. I even can easily tell now, what kind of food will make me stronger by so many kg in the scale pressing. For instance, 100 g carrots will weaken me by 2.5 kg, while a hamburger will strengthen me by 7.2 kg. Mathematics and Statistics can really be super-cool !!

With these information, only a few weeks later the doctors in Germany could identify the ion channel and even the locus of the defect gene in it! This channel brings too much potassium ions into the cells; this destroyed the electric field inside the cells,

A letter from Günter Pilz (3/3)

my „batteries are empty“, and I cannot move for a while, until the cells are re-charged. Of course, there is neither a name nor a cure for this rare defect (just 1 case world-wide), but I can at least avoid total paralyzations by the intake of healthy food: very few vegetables and fruits, but much salt, sausages, and the like. Many diets are much worse than this one... That keeps me relatively OK, but I do not dare to travel non-trivial distances any more.

So I can really say: „ALGEBRA , STATISTICS, AND IN PARTICULAR PLANAR NEAR-RINGS, HAVE SAVED MY LIFE!“ That was REALLY Applied Algebra, at least for me! And the story became even more bizarre: the doctors in Marburg wanted to write a paper on my case, and due to my collaboration, they "forced"me to be a coauthor. This paper was written and sent to a journal. So I am now both coauthor and object of a study! Very strange. All good wishes and kindest regards!

Günter Pilz

Reference:

Pilz G., Weber F., Müller W., Schäfer J.: Statistical Methods to Support Difficult Diagnoses, in Diagnostics, Vol. 11, Nr. 7, Seite(n) 1300, 2021

Types of data acquisition

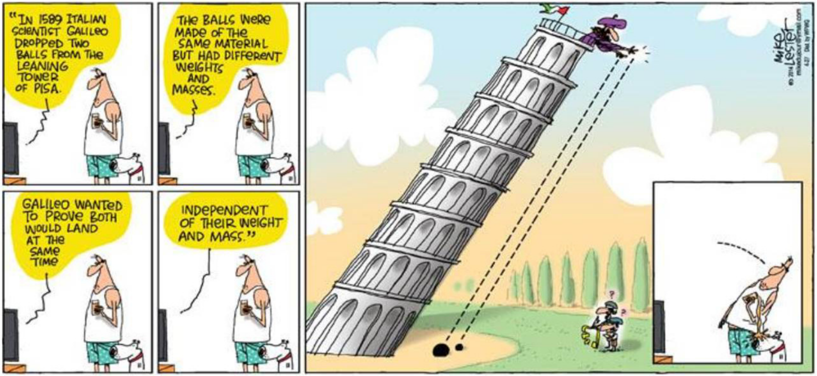
Observational:

- ideally randomly sampled
- also covariates are stochastic
- often unstructured: big data!

Experimental:

- conditions can be (partially) controlled
- covariates are deterministic
- allows for identifying causality

What is an experiment?



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An experiment is a procedure carried out to support, refute, or validate a hypothesis. Experiments provide insight into cause-and-effect by demonstrating what outcome occurs when a particular factor is manipulated. Experiments rely on repeatable procedure and logical analysis of the results.

WIKIPEDIA

Baking a cake

Controllable input factors:

sugar flour eggs temperature duration

experience of the cook type of oven

Uncontrollable input factors:

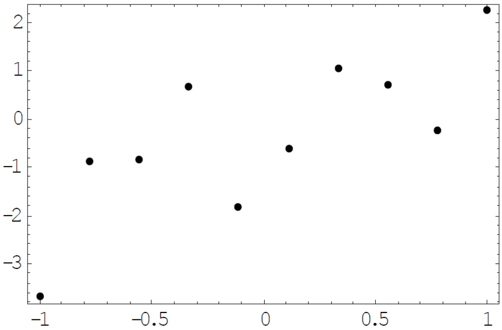
Components of experimental design

factors (variables inputs)	levels (settings)		responses (outcomes characteristics)
temperature →	160°C 180°C 150°C	→ conduct experiment and sample data →	
sugar →	150g 1 cup	→	taste
flour →	200g 2 cups	→	color
eggs →	3 eggs 4 eggs	→	consistency

Hierarchy of goals in experiments

- **Screening:** which factors/ingredients are influential?
- **Model-building:** what is a good recipe?
- **Learning:** which process leads to a (good) cake.
- **Prediction:** how will the cake taste under other baking conditions?
- **Optimization:** bake the best cake!

Motivating example: the estimation of the slope of a regression line



The assumed model is

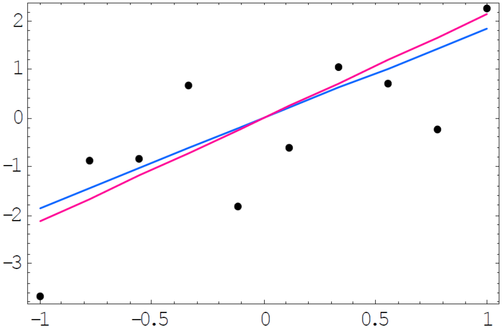
$$y_i = \beta x_i + \varepsilon_i$$

The experimenter may choose the design points, i.e. the x-values where he measures the output y in the experimental region $[-1; 1]$.

The experimenter may further choose the estimation method for β:

- The least squares estimator: $\hat{\beta} = \frac{\sum x_i y_i}{\sum x_i^2}$
- a plausible alternative: $\tilde{\beta} = \frac{1}{n} \sum \frac{y_i}{x_i}$

Motivating example: two possible estimators



The variances of the two estimators

$$\mathsf{Var}(\hat{\beta}) = \frac{\sigma_\varepsilon^2}{\sum x_i^2}$$

$$\mathsf{Var}(\tilde{\beta}) = \frac{\sigma_\varepsilon^2}{n^2} \sum \frac{1}{x_i^2}$$

depend both on the chosen design points x_i.

Compare two different designs:

- The **uniform design**: the design points are uniformly scattered on the experimental domain: $\{x_1, \ldots, x_n\} = \{\pm\frac{1}{n-1}, \pm\frac{3}{n-1}, \pm\frac{5}{n-1}, \ldots, \pm 1\}$
- The **optimal design** for this example: the design points are on the boundaries of the experimental domain, half of them on $x_i = -1$, half of them on $x_i = 1$

Motivating example: two possible designs

The variances of the uniform design are

$$\mathsf{Var}(\hat{\beta})_{unif} = \frac{(n-1)^2\sigma_\varepsilon^2}{2\sum_{i=1}^{n/2}(2i-1)^2} = \frac{3(n-1)\sigma_\varepsilon^2}{n(n+1)}$$

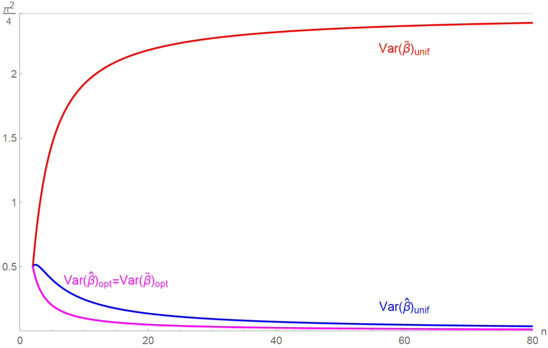
$$\mathsf{Var}(\tilde{\beta})_{unif} = \frac{2\sigma_\varepsilon^2}{n^2}\sum_{i=1}^{n/2}\frac{(n-1)^2}{(2i-1)^2} = \sigma_\varepsilon^2\left(\frac{n-1}{n}\right)^2\left(\frac{\pi^2}{4} - \frac{1}{2}\psi'\left(\frac{n+1}{2}\right)\right)$$

where $\psi'(z)$ is the first derivative of the digamma function $\psi(z) = \frac{\Gamma'(z)}{\Gamma(z)}$

The variances of the optimal design on the other hand are

$$\mathsf{Var}(\hat{\beta})_{opt} = \mathsf{Var}(\tilde{\beta})_{opt} = \frac{\sigma_\varepsilon^2}{n}$$

Motivating example: two possible designs



for big n we have

$$\lim_{n\to\infty} \mathsf{Var}(\hat{\beta})_{unif} = 0$$

$$\lim_{n\to\infty} \mathsf{Var}(\tilde{\beta})_{unif} = \frac{\sigma_\varepsilon^2\,\pi^2}{4}$$

$$\lim_{n\to\infty} \mathsf{Var}(\hat{\beta})_{opt} = \lim_{n\to\infty} \mathsf{Var}(\tilde{\beta})_{opt} = 0$$

So here the choice of an optimal design is more important than the choice of an optimal estimator!

Classic applications

- Agriculture
- Industrial production - quality- and process-control
- Clinical trials
- Computer Simulations
- Network tomography (study of a network's internal characteristics using information derived from end point data)
- Genetics - microarray analysis (method that uses microchips containing anchored arrays of short DNA elements (known as probes) for the large-scale interrogation of gene expression)

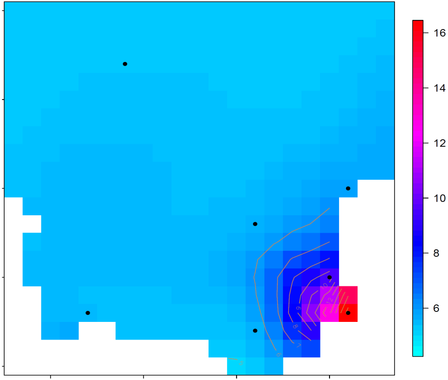
Discrete choice experiments in marketing

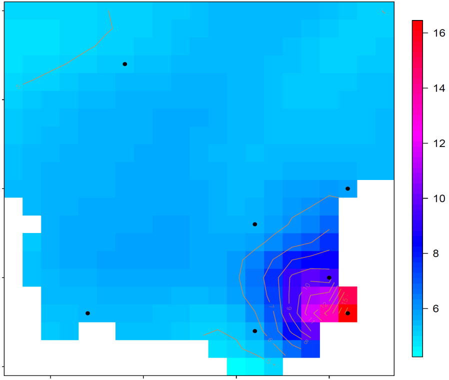
Focus Raven²	GIANT Dirt-E+ 0 Pro	Haibike SDURO FullLife LT 7.0	Riese & Müller Delite Mountain	BH Atom-X Lynx 6 Pro

Akku	**Akku**	**Akku**	**Akku**	**Akku**
250 Wh	500 Wh	500 Wh	1.000 Wh	500 Wh
Schaltung	**Schaltung**	**Schaltung**	**Schaltung**	**Schaltung**
Shimano Deore XT	Shimano Deore XT	Sram NX	Rohloff Speedhub	Shimano XT
11-Gang	11-Gang	11-Gang	14-Gang	11-Gang
Bremsen	**Bremsen**	**Bremsen**	**Bremsen**	**Bremsen**
Shimano Deore	Shimano Deore XT	Magura MT5	Shimano Deore XT	Shimano SLX
Gewicht	**Gewicht**	**Gewicht**	**Gewicht**	**Gewicht**
15,5 kg	22 kg	24,9 kg	25 kg	24,2 kg
zul. Gesamtgewicht	**zul. Gesamtgewicht**	**zul. Gesamtgewicht**	**zul. Gesamtgewicht**	**zul. Gesamtgewicht**
120 kg	150 kg	120 kg	140 kg	165 kg
Preis	**Preis**	**Preis**	**Preis**	**Preis**
ab 4.999 €	ab 3.999 €	ab 4.299 €	ab 6.799 €	5.499 €

Choice modelling attempts to model the decision process of an individual via preferences made in a particular context. Typically, it attempts to use discrete choices in order to infer positions of the items on some relevant latent scale - typically „utility“ in economics.

Environmental science: monitoring network design





In the left panel we see the measurements of ammonium concentrations in a part of the North Sea. The right panel shows the predicted values based on the measurements of only 7 design points.

Objectives

Students know the principles of effective data collection and corresponding software. They should be able to design a hands-on experiment and analysis in a simple situation.

Subject

- randomization, blocking, replication
- simple factorial designs, fractional factorials
- screening designs
- response surface designs
- optimal design of experiments
- design algorithms

Pre-requisites

none . . .

but you should remember the subjects of

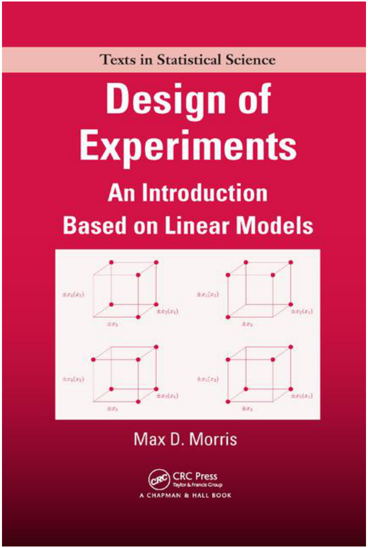
- Lineare Modelle
- Verallgemeinerte lineare Modelle
- Programmieren mit Statistischer Software (R !!!)

of our Bachelor programme Statistics and Data Science

General

- Email: `werner.mueller@jku.at`
- Study material
  Slides, exercises
  available on the Moodle-page of the lecture
- on the KUSSS pages you will just find the dates ...
- Address the secretariate `office-ifas@jku.at` for administrative issues!

Textbook for the course:



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Some Experimental Design Software

CRAN Task View: Design of Experiments (DoE) & Analysis of Experimental Data
Maintainer: Ulrike Groemping
Contact: groemping at bht-berlin.de
Version: 2018-05-26
URL: https://CRAN.R-project.org/view=ExperimentalDesign

DESIGN-EXPERT®
version 11

by Stat-Ease
free academic licenses
https://www.statease.com/software/dx-academic.html

Course

- Lecture
  - Compulsory attendance
  - Dates: Wednesday 13:45-15:15
  - Room S2 Z74
  - 10-14 dates, with a performed experiment and a pitch day
  - 4 ECTS $\approx$ 100 to 120 hrs workload ($\approx$ 7.7 to 9.25 hrs per date)
- Criteria for evaluation
  - Homework exercises (checkmarks and assignments submitted via moodle)
  - occasional presentation of homework exercises
  - design setup and report of your own experiment

Evaluation

- Short report on a performed experiment (weight: 2/3)
  - 10 - 15 pages
  - topics need to be pitched in the course of the semester
- Homework (weight: 1/3)
  - 42 exercises
  - students have to set checkmarks to indicate which exercises they have prepared for presentation – exercises for which checkmarks have been set have to be submitted (Moodle)
  - students may be called to present the prepared exercises (solutions have to be explained and justified), the presentations are graded, insufficient presentations result in the cancellation of all checkmarks of the date.
  - at least 50% checkmarks required

Consequences of absence

- Missing a date
  - without confirmation of a good reason (e.g. illness): no checkmarks for the corresponding date
  - with confirmation (e.g. doctor's certificate): unit will be neglected in calculation of percentage checked