## Experiment planning: Factorial design, factor analysis

Most slides/figures taken from:
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## DOE (Design of Experiments)

- Introduction and motivation
- Comparing two alternative systems
- Linear and nonlinear regression
- Analysis of Variance (ANOVA)
- One-way ANOVA
- Two-way ANOVA
- Factorial designs
- $2^{k}$ factorial designs
- Fractional factorial designs
- Important background information (within above topics): Hypothesis testing


## Literature

- A. Law, D. Kelton: „Simulation Modeling \& Analysis", McGraw-Hill, 1991.
- G. Box, W. Hunter, J. Hunter: „Statistics for Experimenters", Wiley, 1978.
- D. Montgomery: „Design and Analysis of Experiments", Wiley, 1997.
- D. Goldberg: „Genetic Algorithms in Search, Optimization, and Machine Learning", AddisonWesley, 1989.


## Motivation

- Statistics chapter:
- Basic statistical concepts
- Hypothesis testing
- Analysis of a single simulation run
- But: Simulation not only used for single runs

We want to compare alternative designs!

- Approach for comparison
- Explorative approach ("Fiddle around with parameters" / "Hit or Miss" strategy) = inefficient or even dangerous
- $\rightarrow$ Methodic design of Experiments (DOE)


## Why compare system alternatives?

- Goals:
- Better understanding of system
- Better control of system
- Better performance of system
- Methods:
- Try out in different simulated environments
- Try out different workloads with different characteristics
- Try out different network topologies
- Try out with different system parameters


## Terminology

a factor: input variable (e.g., TCP window size), condition, structural assumption (e.g., TCP congestion control algorithm)

- level: one factor value that is used in our experiments
- response: system parameter of interest that depends on given set of factors (e.g., achieved TCP throughput)
a run: evaluation of response for a given set of factor values
- i.e., the analysed simulation result
- There will (should!) be multiple runs

Remember:

- In simulation experiments, responses vary for runs of the same factor values due to random effects
- Therefore: several runs have to be performed!


## Comparing two alternative systems

- Comparison of two systems:

Is there a difference in value for a given response variable?

- e.g., difference in achieved network throughput
- Test criterion:

1. Calculate difference between the two response variables
2. This difference is statistically significant if its confidence interval (CI) does not contain 0

- e.g.: Cl (throughput $_{T C P}$ Reno - throughput ${ }_{T C P}$ vegas ) $\neq 0$
$\rightarrow$ We can assume that the difference in throughput which the two congestion control algorithms TCP Reno and TCP Vegas achieve is statistically significant


## Is this enough?

- Good: Very simple
- Bad: Quite restricted applicability
- Only should be applied if the response has the same variance for the two levels - not often the case
- Better: Modified or Welch two-sample t confidence intervals
- Calculating the confidence interval for the response differences only can tell us if two levels of one factor make a difference
- What if we want to analyse more than two levels for a given factor?
- E.g., TCP Reno vs. TCP Vegas vs. TCP Cubic: 3 levels
- What if we have more than one factor?
- E.g., TCP congestion control algorithm, TCP window size, network delay, link bandwidth: 4 factors


## Linear model and regression

- Have $n$ samples $x_{1 \ldots n}$ and $y_{1 \ldots n}$ of two random variables $x$ and $y$
- $y$ is 'not really' a random variable:
it's also dependent on $x$
- Linear model: $y=a \cdot x+b+e$
- a: slope
- b: intercept
- e: error
a Idea: Chose $a$ and $b$ such that $e$ is minimised
- Calculate sum of squared errors:

$$
\text { SSE }=\sum_{i=1}^{n}\left(y_{i}-b-a x_{i}\right)^{2}
$$

- Minimise SSE


## Calculating $a$ and $b$

$$
\begin{aligned}
& a=\frac{\operatorname{Cov}(x, y)}{\operatorname{Var}(x)} \\
& b=\operatorname{mean}(y)-a \cdot \operatorname{mean}(x)
\end{aligned}
$$

- N.B.: different, but equivalent formulae in literature (you can omit dividing by n-1 in var and cov)
- Usually built into statistical programs
- Graphical interpretation:

Fit a straight line that goes through the points in the ( $x, y$ ) scatterplot

- b: intercept (Achsenabschnitt)
- a: slope (Steigung)


How good is our regression?

- Correlation coefficient r:

$$
r=\frac{\sum_{i=1}^{n}\left(\frac{x_{i}-\bar{x}}{s_{x}}\right)\left(\frac{y_{i}-\bar{y}}{s_{y}}\right)}{n-1}
$$

- Coefficient of determination: $r^{2}$
- i.e., simply square above result
- Can be better compared than non-squared $r$, because it is proportional to the correlation, e.g.: $r^{2}=0.4$ provides double the correlation than $r^{2}=0.2$
- Can be simply added up if multiple independent factors are combined
- Don't confuse these two with the covariance!


## Are we actually allowed to apply regression!?

- Warning:
- The residuals $e(a s$ in $y=a \cdot x+b+e)$ must be normally distributed!
- Exploit the central limit theorem: Calculate averages of multiple independent simulation runs with the same factor level
- Check that it looks normal: QQ plots or some normality test
- N.B.: This check has, of course, nothing to do with the "quality" of the regression expressed as $\mathrm{r}^{2}$
- Normality check: Are we allowed to look for linearity?
- $r^{2}$ : How much linearity is there?


## Regression and experiment planning

- In our nomenclature: $y=$ response, $x=$ factor level
- Regression can tell us how much the factor influences the response. Answers questions like:
- Does it make sense to explore further factor levels in a given direction?
- Does it make sense to check factor levels in between?
- Good:
- We now can have multiple factor levels
- Bad:
- We still have only one factor
- It must be linearly proportional
- The residuals must be normally distributed (but that constraint won't go away with ANOVA either)
- Often, the relationship between $x$ and $y$ is not linear
- Solution: Try to find a suitable transformation
- Let y be the simulation outcome (response)
- Then apply the model $y^{*}=a \cdot x+b+e$ where $y^{*}=f(y)$
- Transformation function f can be, for example:
- Logarithm
- Exponentiation
- Square root
- Square
- Some other polynomial (usually quadratic or cubic)
- Logistic function (logistic regression)
- Inverse (1/x)
- ...


## Nonlinear regression $2 / 2$

- Which transformation function is the right one?
- Careful consideration of the system: You have to think!
- Check if the $y^{*}$ are normally distributed - the $y$ are probably not normally distributed in this case
- QQ plots can help
- Admittedly, a matter of experience
- Warning:
- Overfitting, arbitrary curve fitting: "Just try around with some transformations and pick the one that matches best" - no, try to avoid that!
- A correlation can be coincidence
- Correlation does not imply causation
- Example: Decreasing number of pirates leads to increasing global temperatures (Church of the Flying Spaghetti Monster)
- Again: First think about the system, then postulate a meaningful transformation


## Multiple [linear] regression

- We want to look at multiple factors
- For historic reasons, we relabel our 'old' values a and $b$ from the regression formulae as
$\beta_{0} \ldots \beta_{\mathrm{m}}$ and the error as $\varepsilon$
- Linear model is now:

$$
y=\beta_{1} \cdot x_{1}+\beta_{2} \cdot x_{2}+\ldots+\beta_{m} \cdot x_{m}+\beta_{0}+\varepsilon
$$

- Warning about the indices: Now, $x_{1}$ means 'the first factor', not 'the first simulation run' (there may be many simulation runs for the same choice of the $\mathrm{x}_{\mathrm{i}}$ )
- Will not go into detail here


## ANOVA

- Short for 'analysis of variances'
- Historical term
- Explained in next slides
- Be careful: "variance analysis" is a more general term! Often, that term describes a slightly different analysis:
- Calculate variances of the responses for different levels of one (or several) factors
- Analyse statistically if the variances are the same
- Very similar to ANOVA, but slightly different!


## ANOVA nomenclature

- Factor has a levels ('treatments' for historical reasons: ANOVA was developed in pharmaceutical research)
- Each level is replicated/observed $n$ times
- Data:

| level | 1 | replication <br> L | $n$ |
| :---: | :---: | :---: | :---: |
| 1 | $y_{11}$ | L | $y_{1 n}$ |
| M | M |  | M |
| a | $y_{a 1}$ | L | $y_{a n}$ |

- Question we want to answer:
- Is there an effect of factor levels on system responses?
- If so: how much?


## The model for ANOVA

- Model for system responses with one factor

- i: factor level ('treatment')
a j: simulation run
- Please note: We're dealing with only one factor so far


## One-way ANOVA (1)

- Similar to linear regression:
- One factor, multiple levels
- $y_{i j}=\mu+\alpha_{i}+\varepsilon_{i}$
- $\mu$ : population mean (of the total population, i.e., across all different factor levels - in other words, across all simulation runs, regardless of their parameters!), also called grand average
- $\alpha_{i}$ : the influence of the different factor levels (how much do they contribute to a diversion from the mean?)
- $\varepsilon_{i}$ : errors, also called 'residuals' or 'noise'


## One-way ANOVA (2)

Important things to note about the model:

- Factor levels $\alpha_{i}$
- We do not require them to have a linear relationship on the response $y$
- They even can be categorical data, e.g.: \{male, female\} or \{child, student, employed, unemployed, retired, other\}
- Residuals $\varepsilon_{i}$
- Any deviation from the model that cannot be explained
- Usually, the index is dropped for the errors, as $\varepsilon$ is an independent random variable that must not (!) depend on the factor level
- If that is not the case, we do not have a truly random but a systematic error. That's bad - it violates our assumptions!


## One-way ANOVA (3)

- We suspect that the $\alpha_{\mathrm{i}}$ are different and influence the response variable y
- Formulate this as a statistical test


## Digression:

## Statistical tests, revisited

## Statistical tests

- So far, we've seen the $X^{2}$ distribution fitting test and the Kolmogorov-Smirnov test (KS)
- Both test if a given set of measurements is consistent with a theoretical distribution
- Note the wording: „Consistent with", but not „comes from"
- There are many, many other statistical tests for many, many other applications


## Statistical tests $=$ hypothesis tests

- We would like to „prove" some statement, based on statistical calculations


## Examples:

- Measurements $\mathrm{x}_{\mathrm{i}}$ are consistent with a normal distribution
- The mean of the measurements $x i$ is greater than 5
- Call this statement our 'work hypothesis' or 'alternative hypothesis' (Arbeitshypothese) $\mathrm{H}_{\mathrm{A}}$
- Formulate the contrary: null hypothesis $\mathrm{H}_{0}$
- $\mathrm{H}_{\mathrm{A}}$ and $\mathrm{H}_{0}$ need to be:
- Exclusive: Either $\mathrm{H}_{\mathrm{A}}$ is true or $\mathrm{H}_{0}$ is true
- Exhaustive: All possible results will satisfy one of the two


## Test statistic

- Hope to find statistical evidence that $\mathrm{H}_{0}$ is highly improbable
- Mathematically:
- Input data $=x_{i}$ (...rather arbitrary label)
- Calculate a so-called test statistic: TS $\left(\mathrm{x}_{\mathrm{i}}\right)$
- Usually: If test statistic is above some threshold, then refuse $\mathrm{H}_{0}$
- Test statistic depends on specific test
- Threshold depends on specific test and on desired accuracy


## Test accuracy: Error types

- As mentioned before: No test can give a $100 \%$ guarantee - we're talking about statistics here, and statistics always deals with the unknown
- Differentiate between two types of errors:

|  | Test rejects $\mathrm{H}_{0}$ | Test accepts $\mathrm{H}_{0}$ |
| :--- | :--- | :--- |
| In reality, $\mathrm{H}_{0}$ is false | Correct decision | Type II error, <br> $\beta$ error, <br> false negative |
| In reality, $\mathrm{H}_{0}$ is true | Type I error, <br> $\alpha$ error, <br> false positive | Correct decision <br> (albeit not the one that <br> we wanted in most <br> cases...) |

## Error types explained by example (1/2)

- Suppose you have developed a medical drug. Development has cost an enormous amount of money. Now you want to test if the drug is harmful to your patients
- Type I error ( $\alpha$ error)
- Probability that people get harmed
- Can cost lives: Invest a lot of effort to avoid it.
- Type II error ( $\beta$ error)
- Probability that you reject a drug that is actually perfectly safe
- Can waste money: Unpleasant, but more acceptable.


## Error types explained by example (2/2)

- Suppose you have developed a new network protocol. By applying a statistical test to the output of some network simulations, you hope to show that the protocol increases network performance $\left(=\mathrm{H}_{\mathrm{A}}\right)$.
- Type I error ( $\alpha$ error)
- Probability that you claim that the protocol is great, whereas it is actually rubbish
- If you don't specify your $\alpha$ error, or if it is too large (i.e., your confidence level is too low), then nobody will believe your results!
- Type II error ( $\beta$ error)
- Probability that you wrongly assume that your great protocol does not help anything
- Presumably interesting to you, but the reader of your paper does not care about the risk that you might have failed detecting the performance increase: Obviously, you did not fail, since otherwise the paper would not have been written...


## Balancing error types

- Problem:
- Reducing one error increases the other and vice versa. Damn.
- Only solution to reduce both: Increase the sample size. Usually a superlinear factor (e.g., to reduce one error by $1 / 2$ while keeping the other constant, we must increase sample size by 4)
- In the majority of the cases, keeping the $\alpha$ error low is more important
- $\alpha=5 \%$ has been accepted for years (although there has been some criticism), $1 \%$ is better, $0.1 \%$ is extremely good
- $\beta=10 \%$ or $20 \%$ is usually acceptable; but usually, it's not calculated
- Don't choose $\alpha$ too small if there are only few samples: Small sample size and small $\alpha$ both will increase $\beta$ to unacceptable values - then you would almost always accept the null hypothesis and thus (wrongly) reject your work hypothesis


## Power of a test

- 'Power' of a test := $(1-\beta)$
- Obviously the higher, the better
- Can be used to compare tests:
- Fix an $\alpha$ and a number of measurements
- The better test will feature a higher power for this input
- Rules of thumb:
- Parametric tests (make assumptions about input distribution) are stronger than nonparametric tests (work with any distribution)
- One-sided tests are stronger than two-sided tests (later slide).
- The more general the test, the weaker it is.


## Error types: summary

- Usually, Type-1 errors ( $\alpha$ errors) are the more serious ones
- In order to minimise one type of error (e.g., Type 1 error), you only have the choice between...:
- Increasing the Type 2 error
- Increasing the sample size
- Picking a different statistical test that has better error properties


## An „alternative": significance tests

P-value (R. A. Fisher): How likely is the result to happen?

- Test statistic is a dependent random variable that follows a specific distribution (test distribution, e.g., Student's t distribution or $X^{2}$ distribution) if the null hypothesis holds
- Using the theoretical distribution, calculate the probability that our measurements attain our given values or even more extreme values if the null hypothesis holds:
- This is defined as the $p$ value
- Note that the $p$ value itself is uniformly distributed in $[0 . . .1]$ if the null hypothesis holds, and it is near 0 if it does not hold.
- Refuse $H_{0}$ if this seems unlikely: i.e., refuse if $p \leq \alpha$
- In other words: Our threshold for the test statistic is the point where its distribution „has no meat", i.e., the p value gets too low


## We have two types of tests?

- In theory, distinguish:
- Hypothesis test that we just explained:

Fix an $\alpha$, calculate the test statistic and accept or reject the null hypothesis

- Fisher's probability test:

For the given data, calculate the $p$ value for the null hypothesis, and decide how likely the null hypothesis is

- In practice, combine both!
- $p$ value is more expressive
- Fixed $\alpha$ is more commonly known/accepted; often allows better comparisons to other studies


## How to combine both types of a test?

- With modern statistical programs, this is possible - in most cases, it's even done automatically!
- Good practice:
- Tell the reader your $p$ value (especially if null hypothesis sounds quite likely!)
- Traditionally, the $p$ value is judged with star symbols within braces:
- [***] means: $P \leq 0.1 \%$
- [**] means: $0.1 \%<\mathrm{P} \leq 1 \%$
- [*] means: $1 \%<\mathrm{P} \leq 5 \%$
- If possible, calculate the $p$ value and derive statements about $\alpha$
- e.g.: „The null hypothesis could be refused at a confidence level of $\alpha=0.5$, but not at a confidence level of $\alpha=0.1^{\prime \prime}$

One-sided tests, two-sided tests

- One-sided test:
$H_{A}: \mu<\mu_{0} \quad\left(\right.$ or $\left.\mu>\mu_{0}\right)$
- Example: „With the new routing protocol, network latency is significantly reduced from the old value"
- Two-sided test:
$H_{A}: \mu \neq \mu_{0}$
- Example: „With the new routing protocol, network throughput has significantly changed from the old value (either better or worse)"
- Which one to choose?
- One-sided tests are stronger than two-sided tests
- Two-sided tests are more expressive


## Back to one-way ANOVA! (4)

- Recall our model: $y_{i j}=\mu+\alpha_{i}+\varepsilon_{i}$
- We suspect that the $\alpha_{i}$ are different and influence the response variable y
- Formulate this as a statistical test:
- Hypothesis: At least one of the $\alpha_{i}$ influences $y$
- Null hypothesis: $\alpha_{1}=\alpha_{2}=\ldots=0$
- Equivalent formulation of null hypothesis:

The means of the factor levels are equal

## One-way ANOVA (5)

- Analysis of variance: Analyse total sum of squares
- Introduce these variables (SS = sum of squares):
- SS $_{\text {Total }}$
- The total variation across all samples
- I.e.: the total sum of squared deviations from the general mean $\mu$
- How much variability is in the general population?
- $\mathrm{SS}_{\text {Between }}$
- The variation between the different sample groups (i.e., one group for each different factor level)
- How much variability can be attributed to the different factor levels?
- $\mathrm{SS}_{\text {Within }}$
- The variation between the samples of one factor group (i.e., all samples that hold for the same factor)
- As we can see, we need to do multiple simulation runs for one factor level
- How much variability can be attributed to the errors (,noise')?


## One-way ANOVA (6)

- Important observation: $S_{\text {Total }}=S_{\text {Between }}+S_{\text {Within }}$
- Coarse idea:
- If $\mathrm{SS}_{\text {Between }}$ (the treatment variability) is much larger than $\mathrm{SS}_{\text {within }}$ (the error variability), then the overall variability is likely to be caused by the factor
- Otherwise, the overall variability is likely to be caused by ,random' noise
- Take care: The errors also can be unexplained effects
- More precisely: If $\mathrm{H}_{0}$ holds, then $\mathrm{SS}_{\text {Between }}$ and $\mathrm{SS}_{\text {Within }}$ have the same value
- Check this by applying the F test


## The F test

- Developed by R. A. Fisher
- Input: two samples from two different populations
- Populations have to be normally distributed (!)
a F test tells if the populations have a large difference in variance
- Test statistic: the F value

$$
F=\frac{\operatorname{Var}\left(X_{1}\right)}{\operatorname{Var}\left(X_{2}\right)}
$$

- If the null hypothesis holds, then the $F$ value is F distributed
- F distribution: a test distribution
- As usual: degrees of freedom = \#samples - 1


## One-way ANOVA (8)

- Further mathematical details...?
- Usually, the F test is built into statistical software
- Usually, ANOVA is built into statistical software
- We want to apply statistics, not learn any proofs of theorems $\rightarrow$ For more details, refer to literature


## ANOVA: Caveats

Prerequisites similar to linear regression:

- The measurements have to be normally distributed
- Easy if the response can be expected to be normally distributed (but that's generally not the case)
- Easy if means are sampled from several (i.e., enough!) simulation runs: central limit theorem
- The residuals have to be normally distributed
- Residuals: $e_{i j}=y_{i j}-\bar{y}_{i} \quad$ (i.e., the deviation from the group mean)
- Warning: You must ensure that this is really the case!
- If not, the result is meaningless!
- The variances of the $\alpha_{i}$ need to be equal
- F test
- How to check for normality?
- QQ-plots
- or some statistical test for normality


## Two-way ANOVA (1)

- Two factor response analysis

Factor $A$ and $B$ at levels $a$ and $b, n$ replications

- Change in quality of the results compared to oneway ANOVA?
Yes!
Both factor effects and effects from interacting factors
- main effect of each factor
- interaction of the two factors! $\begin{gathered}\text { grand } \\ \text { average }\end{gathered}$ error
- System model: $y_{i \mathrm{ijk}}=\widehat{\mu+\alpha_{i}+\beta_{j}+\gamma_{i j}+\varepsilon_{i j k}, ~}$



## Two-way ANOVA (2)

- Data

Factor A

|  | 1 | L | $b$ |  |
| :---: | :---: | :---: | :---: | :---: |
| Factor B | M | $y_{111} \mathrm{~L} y_{11 n}$ | L | $y_{1 b 1} \mathrm{~L} y_{1 b n}$ |
|  | M |  | M |  |
|  | $a$ | $y_{a 11} \mathrm{~L} y_{a 1 n}$ | L | $y_{a b 1} \mathrm{~L} y_{a b n}$ |

## Two-way ANOVA (3)

- Three null hypotheses:
- $\alpha_{i}=0$
- $\beta_{\mathrm{j}}=0$
- $\gamma_{i j}=0$
- Sums and averages similar to one-way ANOVA:
- $\mathrm{SS}_{\text {Total }}=\mathrm{SS}_{\mathrm{A}}+\mathrm{SS}_{\mathrm{B}}+\mathrm{SS}_{\mathrm{AB}}+\mathrm{SS}_{\text {Within }}$
- Usually built into statistical software packages


## Two-way ANOVA (5)

## - Two-way ANOVA table

| Source <br> of <br> Variation | Sum <br> of <br> Squares | Degrees <br> of <br> Freedom | Mean <br> Square | $F_{0}$ |
| :---: | :---: | :---: | :---: | :---: |
| A treatments | $S S_{A}$ | $a-1$ | $M S_{A}=\frac{S S_{A}}{a-1}$ | $\frac{M S_{A}}{M S_{E}}$ |
| B treatments | $S S_{B}$ | $b-1$ | $M S_{B}=\frac{S S_{B}}{b-1}$ | $\frac{M S_{B}}{M S_{E}}$ |
| Interaction | $S S_{A B}$ | $(a-1)(b-1)$ | $M S_{A B}=\frac{S S_{A B}}{(a-1)(b-1)}$ | $\frac{M S_{A B}}{M S_{E}}$ |
| Error | $S S_{E}$ | $a b(n-1)$ | $M S_{E}=\frac{S S_{E}}{a b(n-1)}$ |  |
| Total | $S S_{T}$ | $a b n-1$ |  |  |

## Two-way ANOVA (6)

- Interpretation of the results:

Check the p -values corresponding to the individual tests;
if they are small, there are significant effects.

- Note: statistical significance does not tell anything about practical relevance! Decide yourself!
- Check model adequacy by analysis of residuals:
- They should be consistent with a normal distribution
- They should be free of structure (e.g., check that a higher response value does not usually imply higher error values)


## Summary: ANOVA

- Generalisation: n-way ANOVA
- Usually performed using a statistical program
- Usually only two levels per factor. Examples:
- Small window size, large window size
- TCP Reno, TCP Cubic
- Tests if one or several factors have or have no influence on some response variable
- E.g.: Does TCP window size affect TCP throughput?
- Can tell how much influence the individual factors have
- Can tell how much influence the interactions of the factors have
- E.g.: Window size and congestion control algorithm taken together have significant influence


## ANOVA and experiment planning

- Usually many factors
- Example: TCP window size, TCP congestion control algorithm, network bandwidth, network delay, packet loss rate
- Which factor combinations should we try out? ANOVA can give answers to these questions:
- Which factors are interesting factors (i.e., have much influence), so we should try out more levels for them?
- Which factors have interesting interactions, so we should try out more factor level combinations for them?
- Which factors, which interactions can be left out?
- Structuring the experiments like this is called factorial design
- Of course, not limited to simulation experiments
- Problem with general factorial designs: explosion of number of runs for multi-factor multi-level designs
- Solution:

Two levels are often enough for detecting general trends and to screen out important factors

- k factors, each one with 2 levels: $2^{k}$ design points
- Underlying assumption: effects depend linearly on factors
- Example: 2 factors, i.e., a $2^{2}$ design
- 4 design points:

- Design matrix:

| Run | Factor A | Factor B | Response |
| :---: | :---: | :---: | :---: |
| 1 | - | - | $r_{1}$ |
| 2 | + | - | $r_{2}$ |
| 3 | - | + | $r_{3}$ |
| 4 | + | + | $r_{4}$ |

- Construction of the " $+/-$ " area of the design matrix:
- Each row is the binary coding of the run number minus 1
- with the least significant bit on the left side
- where ' - ' represents 0 and ' + ' represents 1
- Computation of the effects:
- Main effect of factor $A$ : how does the response change if $A$ is changed while $B$ is left constant?
- effect $_{\mathrm{A}}=1 / 2\left(\left(r_{2}-r_{1}\right)+\left(r_{4}-r_{3}\right)\right)$
- Main effect of factor $B$ : how does the response change if $B$ is changed while $A$ is left constant?
- effect $_{B}=1 / 2\left(\left(r_{3}-r_{1}\right)+\left(r_{4}-r_{2}\right)\right)$
- Main effect equations for other designs: Similar (Use factor column as signs for responses and sum up, then divide sum by $2^{k-1}$ )
- Usually, the ANOVA module of a statistical program will help
- Interaction of factors A and B : Is there a difference in the changes of the response if $A$ is changed while $B$ is kept either on level ' + ' or '-'?
- no interaction, i.e. no (or small) difference in changes:

- interaction, difference in changes:

- How to find the interaction equations for other designs?
- In theory: Multiply columns of factors of interest element by element and use the resulting column as signs for responses and sum up. Then divide sum by $2^{k-1}$.
- In practice: Built into statistical software...
- In addition to main effects and interactions, the average response is usually computed
- Example: main effects and interactions of the $2^{3}$ design

| average | A | B | C | AB | AC | BC | ABC |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| + | - | - | - | + | + | + | - |
| + | + | - | - | - | - | + | + |
| + | - | + | - | - | + | - | + |
| + | + | + | - | + | - | - | - |
| + | - | - | + | + | - | - | + |
| + | + | - | + | - | + | - | - |
| + | - | + | + | - | - | + | - |
| + | + | + | + | + | + | + | + |

## Fractional factorial designs (1)

- Full factorial design can be costly for larger number of factors
- In most cases, we are only interested in main effects and two-way interactions
- Example: Full $2^{7}$ design requires 128 times replications runs! (And each needs to be run multiple times.) Effects obtained:

| Avg. | Main effects | 2-way | 3-way | 4-way | 5 -way | 6 -way | 7 -way |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| 1 | 7 | 21 | 35 | 35 | 21 | 7 | 1 |

- More than $75 \%$ of the effects are 3-way interactions and higher
- Obtain the main effects and two-way interactions with less runs? Yes, by using fractional factorial designs!


## Fractional factorial designs (2)

- Example: Full $2^{3}$ design requires 8 runs

| Average | Main effects | 2-way inter. | 3-way inter. |
| :---: | :---: | :---: | :---: |
| 1 | 3 | 3 | 1 |

- Only interested in main effects - let's do only 4 runs and ignore the interactions
- $2^{3-1}$ design requires 4 runs, but:
how to accommodate 3 factors with a 2 factor design?



## Fractional factorial designs (3)

- Did we get information for free?

Half the runs to obtain the same result?

- NO! There are confounded (or aliased) effects!
- Main effects and two-way interactions are confounded, i.e.:
- Influence of $C$ indistinguishable from influence of interaction $A B$
- Influence of $B$ indistinguishable from influence of interaction $A C$
- Influence of A indistinguishable from influence of interaction BC
- What does this mean?
- Main effect of factor $C$ is only useful if interaction of $A$ and $B$ is small, i.e., $2^{3-1}$ design is a bad choice if two-way interactions are significant.
- N.B. There also is a graphical explanation for this ( $\rightarrow$ later slides)


## Fractional factorial designs (4)

- Resolution of a fractional design (denoted in Roman numbers)
- III: only main effects are not confounded
- IV: main effects/two-way interactions not confounded
- V: main effects/two-way interactions and two-way/two-way interactions not confounded
- Higher order effects are confounded!
- Practical advice:
- Use resolution III designs only in complete desperation!
- Interactions of more than 3 factors are rarely relevant
- Notation: $2_{\text {resolution }}^{k-p}$, e.g., $2_{i V}^{4-1}$
- Examples:
- III: $2_{I I I}^{3-1}, 2_{I I I}^{5-2}, 2_{I I I}^{6-3}, \mathrm{~K}$
- IV: $2_{V V}^{4-1}, 2_{V V}^{6-2}, 2_{i V}^{7-3}, \mathrm{~K}$
- $V: 2_{V}^{5-1}, 2_{V}^{8-2}, 2_{V}^{10.3}, \mathrm{~K}$


## Fractional factorial designs (5)

- Construction of the design matrix
- Basis is always full factorial design for $k$ —p factors, e.g., a $2^{3}$ matrix for a fractional $2_{I I \prime}^{5-2}$ design
- Missing columns are computed from existing ones by rules from DOE text books. These rules guarantee fractional designs of maximum resolution.
Example: for $2_{I I I}^{5-2}$ design, columns $D$ and $E$ missing

$$
\text { rules: } D=A B \text { or }-A B, E=A C \text { or }-A C
$$

( $A B$ : multiply signs of columns $A$ and $B$ )

- Resolution and construction of design matrix for fractional designs from DOE text books
- Often already built in run controllers of simulation tools or statistical programs


## Fractional factorial design, graphically explained

Motivation for the graphical approach:

- Successful application of graphical methods in other areas of statistics, in particular, for data analysis and data mining
- Application of the creative potential of the right brain half
- Intuitive understanding of "good" characteristics of DOE
- Approach was used for the development of DOE methods, but no longer in the application phase
- Straightforward approach, often even without use of computers

From the design matrix to the design graph

- Approach: Transform the design matrix into an appropriate and equivalent graphical representation
- 2 factors: | Run | Factor A | Factor B |
| :---: | :---: | :---: | :---: |
| 1 | - | - |
| 2 | + | - |
| 3 | - | + |



- 3 factors:



## Graphical representation of designs

- 4 factors: (hypercube)
(Problem:
 Humans don't have 4-D vision)


We're talking about an optimisation problem

- Goal: Minimize information loss of a fractional factorial design reduced by $p$ factors
- Graphically: Projections of the design graph where $p$ dimensions disappear (graph collapses)
- Example: 1 factor of a $2^{3}$ design disappears



## Optimum location of the design points

- Important graphical optimisation criteria for maximizing the information content in fractional designs:
- Each projection must be a complete design graph
- No multiple design points at the corners of the graph
- Example: Reduction of a $2^{3}$ design to a $2^{3-1}$ design, i.e., from 8 to 4 design points $\rightarrow$ optimum location?



## Optimum location of the design points



- Optimum $2^{3-1}$ design as as basic building block ("DOE lego")

- Projections as complete as possible, but with single design points at the corners
- Maximising the minimum distance of the design points (even distribution of points)


## Alternatives for a $2^{5-2}$ design



## D. Design graphs for presenting results



Purity

## 4. Design graphs for presenting results



