Course "Empirical Evaluation in Informatics"

Data analysis techniques

Prof. Dr. Lutz Prechelt
Freie Universität Berlin, Institut für Informatik
http://www.inf.fu-berlin.de/inst/ag-se/

- Samples and populations
- The mean
- The variability
- Comparing samples
  - significance test, confidence interval
- Bootstrap
- Simple relationships of two variables
  - Plots, log-Scales
  - Correlation, linear models
  - local models (loess)
"Empirische Bewertung in der Informatik"

Techniken der Datenanalyse

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- Stichproben und Grundgesamtheiten
- Der Mittelwert
- Die Variabilität
- Vergleich von Stichproben
  - Signifikanztest, Vertrauensbereich
- Bootstrap
- Einfache Beziehungen zwischen zwei Variablen
  - Plots, log-Skalen
  - Korrelation, lineare Modelle
  - lokale Modelle (loess)
First note: samples and populations

- At the start of a statistical analysis, we usually have some subset ("sample", "Stichprobe") of all possible values of some kind ("population", "Grundgesamtheit")
  - e.g. data for a size 50 subset of all FUB Informatics students

- The goal of analysis is making valid statements about the population on the basis of
  - the sample alone (*frequentist approach*) or
  - the sample plus prior beliefs about the population (*Bayesian approach*)
Warning: sampling is difficult

- Both approaches will work well only if the sample is representative
  - that is, each member of the population had the same chance of being in the sample

- Obtaining a representative sample is very difficult
  - Often the boundaries of the population are unclear
    - Is a guest student a member?
    - Is a Nebenfach-student a member? etc.
  - It is unknown how to sample randomly with even chances
    - e.g. just catching people when passing the foyer is insufficient
  - Often the member we picked for our sample will refuse to cooperate

- So all conclusions must be considered with care
  - The conclusions are only "estimates"
Again: Possible tasks of data analysis

- Measure a variable
- Compare two (or more) variables
- Model a relationship
Measure a variable: 
what does the mean mean?

- Given: a set of measurements of the variable
- So we have a sample of a population. Which population?

**Case 1**: There is a single "true" value and we have a set of measurements with errors.
  - e.g. 10 measurements of the length of the same road
  - Case a): We are perhaps interested in the true value only, not in the population of measurements
    - The sample mean is an estimate of the true value
  - Case b): But maybe we try to understand the measurement method, not the road.
    - Think of research on review techniques

Then we are interested in the population, not the true value
  - The *error* in the measurements is what we want to characterize
What does the mean mean? (2)

- **Case 1**: There is a single "true" value and we have a set of measurements with errors. [...]

- **Case 2**: There is a stochastic variable (i.e. it has variability) and we have a sample of its values
  - e.g. each person's age within a group of people
  - We are interested in the "average" or "expected" case
    - The sample mean is an estimate of the mean age
  - There is a true value of the mean age of the population, though not a true value of the age of the population
    - The age of the population can be partially characterized by looking at the mean plus the variation of the age
What we need

- Estimates of the "expected" value of the variable
  - mean, median, mode, etc.
- Estimates of the variation ("variance") of the variable
  - standard deviation, median absolute deviation, quantile ranges, etc.
- Estimates of the error in the estimates
  - e.g. standard error of the mean, confidence limits

Note: There are different ways of defining "error", too
- They lead to different measures and methods
- They are appropriate in different situations
- But most of this is beyond the scope of this lecture
Estimators for expected value

- **Arithmetic mean**
  - Most common
  - Can be used only on a difference scale or ratio scale
- **Median (the 50/50 cut point)**
  - Required if all we have is an ordinal scale
  - Also useful if we want to be robust against few extreme values
    - Ignores distance; inefficient (i.e. much information remains unused)
- **Mode (the most frequent value)**
  - Required if we only have nominal data (unordered)
  - Sometimes useful for ordinal scales with few values
- **Trimmed mean (leave out a top/bottom fraction of the data points)**
  - Robust against outliers, without ignoring distance
- **M-estimators**
  - very advanced technique, robust and efficient
Expected value estimation example

- $x = (1:10)^2 = c(1, 4, 9, 16, 25, 36, 49, 64, 81, 100)$
- $\text{median}(x) = (25 + 36)/2 = 30.5$
- $\text{mean}(x, \text{tr}=0.1) = \text{mean}(c(4, 9, 16, 25, 36, 49, 64, 81)) = 35.5$
- $\text{mean}(x) = 38.5$

- Base plot: plot(x, rep(1, length(x)), type="h")
Expected value estimation example (2)

- From the TPC data:
  - median=6.1
  - 0.1-trimmed mean=8.5
  - mean=48
Estimators for variation

- **Standard deviation**
  - mean distance of a value from the mean
  - R: `sd(x)` or `sqrt(var(x))`

- **Median absolute deviation**
  - median distance of a value from the median
  - R: `mad(x, constant=1)` or `median(abs(median(x)-x))`
  - normal-consistent estimate is `mad(x)`
    - (i.e. equal to `sd(x)` for large samples from normal distributions)
    - less efficient estimator than std.dev., but robust to outliers

- **Interquartile range**
  - difference of the 0.75 and 0.25 quantiles
  - R: `IQR(x)` or `diff(quantiles(x, c(0.75,0.25)))`
  - normal-consistent estimate is `IQR(x)/1.349`
  - Note: interquartile range is related to the median, (not to the trimmed mean)
Variation estimation example

- $x = (1:10)^2 = c(1, 4, 9, 16, 25, 36, 49, 64, 81, 100)$
- $\sqrt{\text{var}(x)} = \text{sd}(x) = 34$
- $\text{mad}(x) = 36$
- $\text{IQR}(x) / 1.349 = 37$
- $\text{mad}(x, \text{const}=1) = 24$
- $\text{IQR}(x) = 49.5$
Variation estimation example (2)

- From the TPC data:
  \[ x = \text{dollarPerTpmC} \]
  - \( \text{sd}(x) = 214 \)
  - \( \text{mad}(x) = 4.1 \)
  - \( \frac{\text{IQR}(x)}{1.349} = 6.5 \)
The standard normal ("Gaussian") distribution

- 68%/95%/99.7% of all values fall within 1/2/3 standard deviations around the mean
  - R: `pnorm(1)-pnorm(-1)=0.683`
  - `pnorm(1:3)-pnorm(-1:-3) = 0.683 0.954 0.997`
Estimators for error: standard error

- Standard error (se, stderr) of the mean
  - is the standard deviation of the mean-estimates that are based on samples of size N from the same distribution
  - R: \( \text{se} = \frac{\text{sd}(x)}{\sqrt{\text{length}(x)}} = \sqrt{\frac{\text{var}(x)}{\text{length}(x)}} \)

- The best way of expressing estimated errors is by means of a confidence interval:
  - e.g. with 68% probability, the true mean will be in the range \( \text{mean-se} \ldots \text{mean+se} \)
    - so we have 68% confidence the mean will be in this range
    - \([\text{mean-se}, \text{mean+se}]\) is called a 68% confidence interval for the mean
  - \([\text{mean}-2\times\text{se}, \text{mean}+2\times\text{se}]\) is a 95% confidence interval for the mean, etc.

- TPC dollarPerTpmC: mean=48, std.err=19
Estimators for error: bootstrap

• Generally, estimating errors and confidence intervals is mathematically very challenging
  • std.err of the mean is one of the few simpler exceptions
• For the less mathematically inclined, the best replacement for strong theory is bootstrapping
  • More formally known as Bootstrap resampling
• Bootstrapping means simulating many trials by
  • treating the sample as if it was the population
  • computing many replicates of the statistic of interest
  • and observing the variation.
• However, for many kinds of statistics, further considerations are required
  • in particular, compensating for bias
  • again, this is beyond the scope of this lecture
Bootstrap example

- We bootstrap the median of dollarPerTpmC:
  - \( xx = \text{tpc}$dollarPerTpmC \)
  - \( \text{repl} = \text{replicate}(1000, \text{median}(\text{sample}(xx, \text{replace}=T))) \)
  - \( \text{mean}(xx)=48, \text{se}_{\text{mean}}=19, \text{median}(xx)=6.1, \text{se}_{\text{median}}=\text{sd}(\text{repl})=0.54 \)
  - bias = \( \text{mean}(\text{repl})-\text{median}(xx) = -0.02 \)

- R support:
  - library(boot)

![Density plot with boxplot](image-url)
Compare two or more samples

- We often want to compare two or more different samples of a variable (e.g. from 2 experiment groups)
- Essentially what we want is a confidence interval for the difference of the means
  - rather than the (much more common, but much less informative) p-value
  - The meaning of the p-value is this:
    - If there is in fact really no difference between the groups...
    - ...then the probability of obtaining a difference at least as large as the one you have seen is p.
  - If p is small, the difference is called "statistically significant"
    - (which basically tells you that the sample was large enough)
- If the samples are both from a normal distribution, the R procedure \textit{t.test} computes such an interval
  - iff you are sure that both distributions have the same variance, set var.equal=TRUE
Example: Comparing two pure normal distributions

- for each block of two pairs of samples (bottom to top):
  - $n=10, 50, 50$, $\mu_b=6, 6, 5.1$, $\mu_a=5, 5, 5$, $\sigma=1, 1, 0.2$
  - t-test, assuming unequal variance

$p$-value
80% confidence interval

$p=0.176$ 0.05...1.28
$p=0.036$ 0.44...1.70
Example:
Comparing tpmC per processor

- Now consider the tpmC performance per processor:
  - How large is the Windows/Unix difference and its 95% confidence interval?
Example, using normal distribution theory

- \( x = \frac{tpc[tpmC]}{tpc[cpus]}[tpc[ostype]=="Windows"] \)
- \( y = \frac{tpc[tpmC]}{tpc[cpus]}[tpc[ostype]=="Unix"] \)

- \( \text{t.test}(x,y): \) \( df = 43.62, \) \( p\text{-value} = 0.016 \)
  alternative hypothesis: true difference in means is not equal to 0
  95 percent confidence interval: 803 7258
  sample estimates: mean(x)=16544, mean(y)=12514

- or, assuming equal variances in the populations:
  - \( \text{t.test}(x,y, \text{var.equal=T}): df = 125, \) \( p\text{-value} = 0.0079 \)
  95 percent confidence interval: 1078 6983
Example, using bootstrap

- Bootstrapping is a general method for computing conf. interv.
  - making fewer assumptions (in particular: no normality needed)
- library(boot)
- dat = cbind(c(x,y), c(rep(1,length(x)),rep(0,length(y))))
- bb=boot(dat, function(d,i) mean(d[i,1][d[i,2]==1])-mean(d[i,1][d[i,2]==0]), R=1000)
- boot.ci(bb)
- Intervals:
  - Level      Normal              Basic
  - 95%   ( 953, 7195 )   (1094, 7446 )
  - Level     Percentile BCa
  - 95%   ( 615, 6967 )   ( 406, 6884 )
- For most cases, the BCa interval ("bias-corrected and accelerated") is to be preferred
Model a relationship

• Often we want to know whether there is a relationship between two or more variables
  • and what this relationship is
  • Its nature may be causal or purely correlational

• The basic case is two variables on a ratio scale

• The basic approach is the scatter plot
  • Example: tpmc vs. total clock speed
  • plot(cpus*freq, tpmC)
  • Is there a relationship? Probably yes, but the data cluster too much near the small values
  • Let us use a log scale instead
Log-log scale scatter plot, correlation

- plot(log(cpus*freq,2), log(tpmC,2))

- Yes, there is a quite obviously a strong linear relationship between these parameters

- The strength can be quantified by means of the correlation coefficient $r$
  - cor(log(cpus*freq,2), log(tpmC,2)) = 0.95
  - Watch out: Correlation is sensitive to the scale:
  - cor(cpus*freq, tpmC) = 0.88
  - Note: The computation assumes that the deviations from the relationship follow a normal distribution
    - So the non-log cor is not valid in this case
More on correlation

- \( \text{cor}(\log(\text{cpus*freq}, 2), \log(\text{tpmC}, 2)) = 0.95 \)
- \( \text{cor}(\text{cpus*freq}, \text{tpmC}) = 0.88 \)

- You can ignore scale entirely by using rank correlation:
  - \( \text{cor}(\text{rank}(\text{cpus*freq}), \text{rank}(\text{tpmC})) = 0.94 \)
    - uses rank numbers instead of actual data values (for data on less than a difference scale, this is the only allowed way)

- For less nice examples (with outliers), the results can be quite different
  - \( \text{cor}(\text{freq}, \text{tpmC}) = -0.195 \)
  - \( \text{cor}(\text{rank}(\text{freq}), \text{rank}(\text{tpmC})) = -0.28 \)
  - because the normality assumption is violated
Confidence interval for the correlation coefficient

- \( \text{cor}(\log(\text{cpus} \times \text{freq}, 2), \log(\text{tpmC}, 2)) = 0.95 \)
- \( \text{cor}(\text{cpus} \times \text{freq}, \text{tpmC}) = 0.88 \)

- Again we use the Bootstrap:
  - \( \text{xx} = \text{cbind}(\log(\text{cpus} \times \text{freq}, 2), \log(\text{tpmC}, 2)) \)
  - \( \text{bb} = \text{boot}(\text{xx}, \text{function}(\text{d}, \text{i}) \text{cor}(\text{d}[\text{i},1], \text{d}[\text{i},2]), \text{R}=1000) \)
  - \text{boot.ci}(.bb)
  - 95\% BCa interval: 0.929 0.964

- The other example:
  - \( \text{cor}(	ext{freq}, \text{tpmC}) = -0.195 \)
  - \( \text{xx} = \text{cbind}(	ext{freq}, \text{tpmC}) \)
  - \( \ldots \)
  - 95\% BCa interval: -0.285 -0.099
Note: Impressing laymen

• Some studies contain statements like this:
  • "The Pearson correlation coefficient is significant at level alpha = 0.05"
  • This talks about a hypothesis test against the null hypothesis that \( r = 0 \)

• This sounds impressive, but means nothing more than that there may be some correlation (however small)
  • precisely: it means that if there is no correlation at all in the population, it is unlikely (<5%) to obtain such samples
    • Hence if you had previous grounds to believe in correlation, the data does not suggest you need to drop that belief
  • In most cases this is of very little interest
• When you see such a statement, the best reaction is usually to be very heavily unimpressed
Correlation and causation

• Warning: **Remember that a correlation need not indicate causality**
  
  • \( \text{cor(freq, tpmC)} = -0.285...-0.099 \) (95% ci)
    
    means that increasing processor clock rate correlates with a *decreasing* rate of transactions per minute
    
    • This correlation can clearly not be causal: everything else the same, a faster clock would *increase* the transaction rate
  
  • So?
    
    • You need to know enough about your data:
  
  • The real reason is that the faster-clock (Windows) systems tend to have much fewer processors than the slower-clock (Unix) systems
    
    • The decreasing transaction rate is a property of the tpc data set, not of the clock frequency
freq and tpmC versus freq and cpus

- `xyplot(log(cpus,2)~freq, data=tpc, panel=panel.superpose, groups=ostype)`
Problems with summary statistics

- A further warning: The correlation, even in conjunction with other summary statistics, does not tell much about the nature of a relationship.

- The following plots all share the same correlation (0.82), means (x=9, y=7.5) and standard deviations (x=3.3, y=2)
  - data(anscombe)
    - 'stack' for repackaging
    - xyplot
Describing the relationship between x and y

- Since the correlation coefficient does not provide enough information, a scatter plot is usually advisable.

- Where appropriate(!), a linear regression line can be used to visualize a trend in the data:
  - use panel.lmline or type="r" with panel.xyplot
  - the function that computes the regression is `lm`
    - `lm="linear model"

- `lm` can also compute regressions for more than one predictor variable or results other than straight lines:
  - linear models are the most important technique of professional statisticians
  - Again, this is beyond the scope of this lecture
Attention with linear models!

• Assume we have a sample of pairs \((x, y)\) and we assume there is a systematic relationship (linear, for now)
  • Case 1: For any \(x\), there is a single "true" value of \(y\)
    • Case 1A: Our \(x\) are precise, but the \(y\) are measurements with errors (and those errors have normal distribution!)
    • Case 1B: The \(x\) have errors as well
  • Case 2: The relationship is stochastic. For any \(x\), there is a single expected value of \(y\), but actual values do vary
    • Case 2A: Our \(x\) are measured precisely, but the \(y\) may have errors
    • Case 2B: Our \(y\) are measured precisely, but the \(x\) have errors
    • Case 2C: Both \(x\) and \(y\) are measured with errors

• The standard linear regression formula makes assumptions that are met only by cases 1A and 2A
  • 1B and 2C require advanced theoretical knowledge!
  • So be careful what you do
Non-linear trends

• Often a straight regression line is not a suitable fit

• If we know a suitable fitting function \( f \), there are two approaches:
  • Transform the data, using the inverse of \( f \), so that the data fit with a straight line
  • or fit a curve rather than a straight line

• Transforming the data may also lead to a more uniform distribution of the data points
  • See the logarithmic transformations we have used
Local trends

- If no appropriate curve function can be found or we do not want to assume a specific kind, we can fit a local regression
  - *loess* = locally weighted regression
  - at each point of the line, we perform a linear regression, but far-away points a weighted less heavily
  - Parameter *span* controls weighting and ignoring of points
  - use e.g. *panel.loess* for plotting
Example: Loess curves

blue straight line: linear regression

green line: a loess curve
Things not covered

• In many cases, numerical linear models are insufficient to characterize the given data
  • Then advanced techniques such as nonlinear numerical models (e.g. neural networks) or partially qualitative models (e.g. classification trees) may help
• In particular, the data may have temporal aspects
  • Then topics such as time series analysis, random effects models, and survival analysis become relevant
• Or we are looking for a measure that can only be described by a yet unknown combination of our variables
  • Factor analysis, principal component analysis
• In many cases, the data to be analyzed is incomplete
  • "missing data": an important, often difficult, and subtle matter

• ...and many others
Final note: Statistics is difficult

- The techniques presented here only scratch the surface of statistical data analysis
  - In some cases, they are sufficient
  - If not, try to get help from a professional statistician

- Rules of thumb:
  - Stick to what you really understand
  - Beware of ignored assumptions
    - Violations may be OK, but you need to think about it
  - Back your numbers up by informative plots
    - Plots produce much higher credibility than bare numbers
    - And are not as likely to be grossly misinterpreted
Thank you!