Advanced computational statistics, lecture 5

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LINKÖPING UNIVERSITY

Course schedule

- Topic 1: **Gradient based optimisation**
- Topic 2: **Stochastic gradient based optimisation**
- Topic 3: **Gradient free optimisation**
- Topic 4: **Optimisation with constraints**
- Topic 5: **EM algorithm and bootstrap**
- Topic 6: **Simulation of random variables**
- Topic 7: **Importance sampling**

Course homepage:
http://www.adoptdesign.de/frankmillereu/adcompstat2023.html

Includes schedule, reading material, lecture notes, assignments

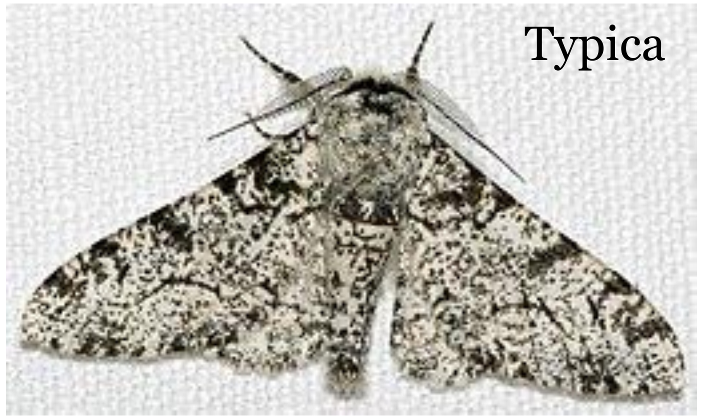
EM algorithm

EM algorithm

- EM = “Expectation-Maximization”
- Main application of this algorithm is in situations where not all data is observed
- E: Expectation will be taken over all (unobserved) data which lead to the observed data
- Algorithm is iterative:
  each iteration has an E step, followed by an M step

EM algorithm: Example 1

- Classical example: Genotype–phenotype
- Peppered moths (see Ex.4.2 in GH, “björkmätare”)



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- Alleles: C, I, T; genotypes: CC,CI,CT; II,IT; TT
- Observed only phenotype: *carbonaria; insularia; typica*
  Frequency observed: n_C; n_I; n_T
- Aim: estimate allele frequencies p_C, p_I, p_T based on observed phenotype frequencies

EM algorithm: Example 1

- Observed data: $\boldsymbol{X} = (N_C, N_I, N_T)$
- Complete data: $\boldsymbol{Y} = (N_{CC}, N_{CI}, N_{CT}, N_{II}, N_{IT}, N_{TT})$
- Aim: estimate $\boldsymbol{p} = (p_C, p_I, p_T)$
- We can specify
  - the expectations $E[\boldsymbol{Y}|\boldsymbol{X},\boldsymbol{p}]$ and
  - the complete data likelihood $f_{\boldsymbol{Y}}(\boldsymbol{y}|\boldsymbol{p})$

EM algorithm: Example 1

- According to biological theory:
  P(a random moth is CC) = $(p_C)^2$
  P(a random moth is CI) = $2p_C\, p_I$
  …
- The complete data likelihood $f_{\boldsymbol{Y}}(\boldsymbol{y}|\boldsymbol{p})$ is multinomial:

$$f_{\boldsymbol{Y}}(\boldsymbol{y}|\boldsymbol{p}) = (p_C^2)^{N_{CC}} * (2p_C p_I)^{N_{CI}} * \cdots * \binom{N}{N_{CC} \quad N_{CI} \quad \ldots}$$

- Complete data log likelihood:

$$\log f_{\boldsymbol{Y}}(\boldsymbol{y}|\boldsymbol{p}) = N_{CC} * \log(p_C^2) + N_{CI} * \log(2p_C p_I) + \cdots$$

- Expectations $E[\boldsymbol{Y}|\boldsymbol{X},\boldsymbol{p}]$ are for example:

$$E[N_{CC}|N_C, N_I, N_T, p] = N_C \frac{p_C^2}{p_C^2 + 2p_C p_I + 2P_C p_T}$$

EM algorithm

- Let $\boldsymbol{X}$ be observed data, $\boldsymbol{Y}$ complete data, $\boldsymbol{\theta}$ unknown parameter-vector, *$L(\boldsymbol{\theta}|\boldsymbol{x})$ likelihood to maximize*
- Iteration *t (t=0,1,…)*: $\boldsymbol{\theta}^{(t)}$
- Let $Q\left(\boldsymbol{\theta}\middle|\boldsymbol{x};\boldsymbol{\theta}^{(t)}\right) = E\left\{\log L(\boldsymbol{\theta}|Y)|\boldsymbol{x};\boldsymbol{\theta}^{(t)}\right\}$ be expectation of joint log likelihood for complete data conditional on observed data $\boldsymbol{X}=\boldsymbol{x}$
- EM algorithm:
  1. Initialize parameter-vector with a guess $\boldsymbol{\theta}^{(0)}$
  2. **E step:** Compute $Q\left(\boldsymbol{\theta}\middle|\boldsymbol{x};\boldsymbol{\theta}^{(t)}\right)$
  3. **M step:** Maximize $Q\left(\boldsymbol{\theta}\middle|\boldsymbol{x};\boldsymbol{\theta}^{(t)}\right)$ with respect to $\boldsymbol{\theta}$ -> $\boldsymbol{\theta}^{(t+1)}$
  4. Back to E step if not stopping criterion met (e.g. if $\left(\boldsymbol{\theta}^{(t+1)} - \boldsymbol{\theta}^{(t)}\right)$ small)

EM algorithm: Example 2

- Effect of a drug to be measured and *n* patients (randomly chosen out of a population of patients) treated with the drug
- X_i, *i=1,…,n*, observed for each patient after drug-treatment
- Known that population consists of two groups:
  - One group responds well to the drug (i.e. larger X_i)
  - Another group responds only barely (smaller X_i)
- It is not known which patient belongs to which group

Observed: X_i,

Unobserved: $Z_i = \begin{cases} \mathbf{1}, \text{if patient } i \text{ belongs to responder group} \\ \mathbf{0}, \text{otherwise} \end{cases}$

Complete data: $Y_i = (X_i, Z_i)$

- We assume a mixture distribution for X_i and want to estimate the parameters based on the observed data

Mixture distributions

- Generally, a density f_M of a finite **mixture distribution** is the sum of c weighted densities f_i of distributions:

$$f_M(\boldsymbol{x}) = \sum_{i=1}^{c} p_i f_i(\boldsymbol{x};\ \boldsymbol{\theta}_i)$$

  where p_i is a weight or mixing coefficient for the ith term ($p_i > 0$; $p_1 + \ldots + p_c = 1$), and $f_i(\boldsymbol{x};\ \boldsymbol{\theta}_i)$ is a probability density with parameter-vector $\boldsymbol{\theta}_i$
- If all c distributions in the mixture are (univariate or multivariate) normal distributions, we have a **normal mixture**
- In Lecture 1, we had an example of a bivariate normal mixture

EM algorithm: Example 2

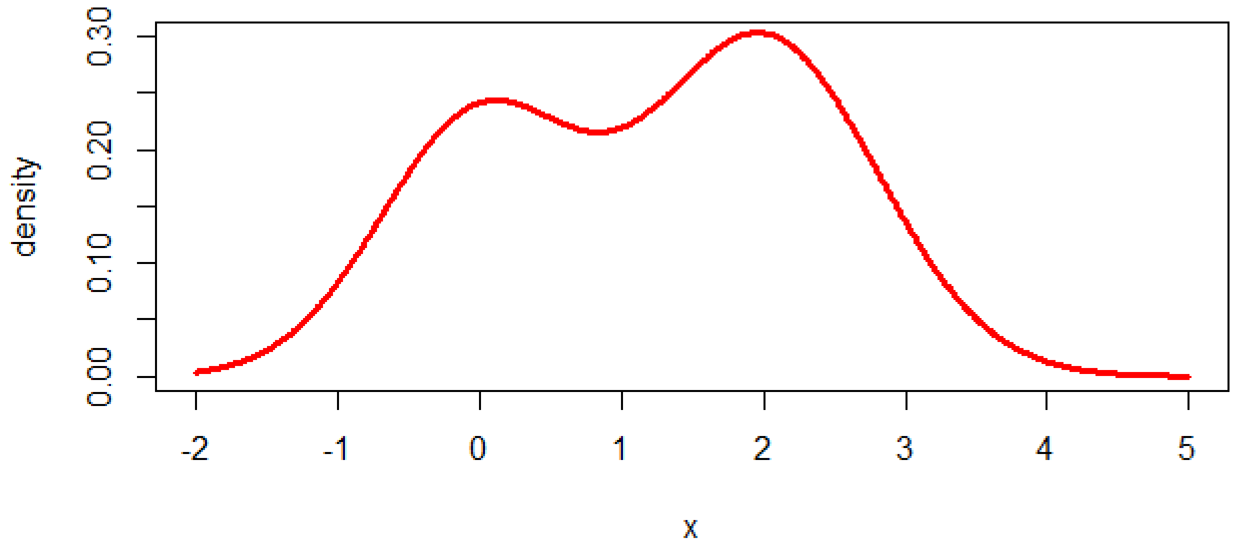
- In Example 2, assume that for both groups in the population (responders, non-responders), X_i follows normal distribution (unknown mean and variance)
- Appropriate mixture? How many parameters has it?

- Appropriate mixture: $f_M(x) = p\varphi(x;\ \mu_1; \sigma_1) + (1-p)\varphi(x; \mu_2; \sigma_2)$ with $\varphi(x; \mu; \sigma)$ being density of N(μ,σ) and p=mixing probability (probability to be a responder)

- 5 parameters: $p;\ \mu_1; \sigma_1; \mu_2; \sigma_2$

EM algorithm: Example 2

- $f_M(x) = p\varphi(x;\ \mu_1; \sigma_1) + (1-p)\varphi(x; \mu_2; \sigma_2)$
- parameters: $p;\ \mu_1; \sigma_1; \mu_2; \sigma_2$



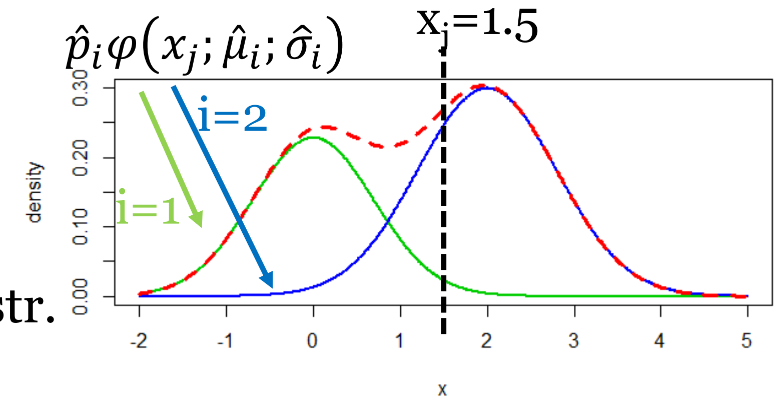
- Example here: $p = 0.4;\ \mu_1 = 0; \sigma_1 = 0.7; \mu_2 = 2; \sigma_2 = 0.8$

EM algorithm for normal mixtures

- The estimated probability that observation *j* belongs to group *i* is

$$\hat{\pi}_{ij} = \frac{\hat{p}_i \varphi(\boldsymbol{x}_j; \hat{\boldsymbol{\mu}}_i; \hat{\boldsymbol{\Sigma}}_i)}{\sum_{k=1}^{c} \hat{p}_k \varphi(\boldsymbol{x}_j; \hat{\boldsymbol{\mu}}_k; \hat{\boldsymbol{\Sigma}}_k)},$$

  where $\varphi(\cdot; \boldsymbol{\mu}; \boldsymbol{\Sigma})$ is density of (uni- or multivariate) normaldistr. with mean vector $\boldsymbol{\mu}$ and variance matrix $\boldsymbol{\Sigma}$ (in the univariate case, we use sd σ_i instead)



- Maximizers for Q of the model parameters are

$$\hat{p}_i = \frac{1}{n} \sum_{j=1}^{n} \hat{\pi}_{ij},$$

$$\hat{\boldsymbol{\mu}}_i = \frac{1}{\hat{p}_i n} \sum_{j=1}^{n} \hat{\pi}_{ij} \cdot \boldsymbol{x}_j,$$

$$\hat{\boldsymbol{\Sigma}}_i = \frac{1}{\hat{p}_i n} \sum_{j=1}^{n} \hat{\pi}_{ij} \cdot (\boldsymbol{x}_j - \hat{\boldsymbol{\mu}}_i)(\boldsymbol{x}_j - \hat{\boldsymbol{\mu}}_i)^T \longrightarrow$$

Unidimensional case for sd (instead of variance):

$$\hat{\sigma}_i = \sqrt{\frac{1}{\hat{p}_i n} \sum_{j=1}^{n} \hat{\pi}_{ij} \cdot (x_j - \hat{\mu}_i)^2}$$

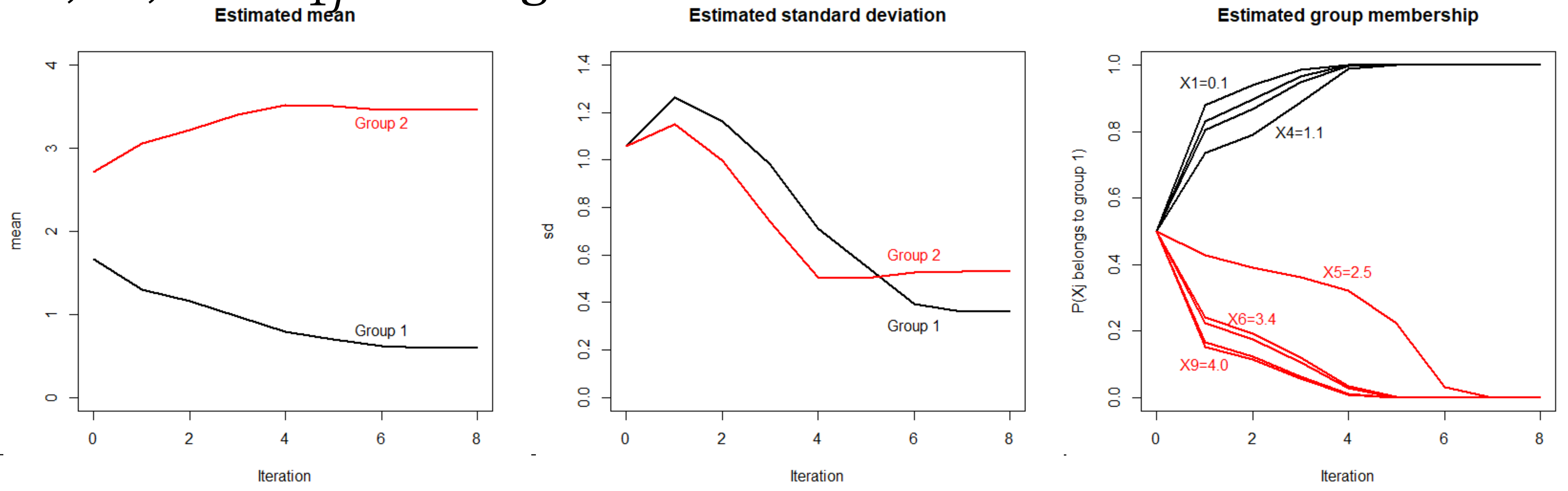
- $Q = \sum_{i=1}^{c} \sum_{j=1}^{n} \hat{\pi}_{ij} \{\log(\hat{p}_i) + \log \varphi(\boldsymbol{x}_j; \hat{\boldsymbol{\mu}}_i; \hat{\boldsymbol{\Sigma}}_i)\}$
- See Section 10.1 and 10.2 of Lindholm, Wahlström, Lindsten, Schön (2022)

EM algorithm for normal mixtures

- EM algorithm:
  1. Initialize parameter-vector with a guess
  $$\boldsymbol{\theta}^{(0)} = (p_1^{(0)}, \dots, p_c^{(0)}, \boldsymbol{\mu}_1^{(0)}, \dots, \boldsymbol{\mu}_c^{(0)}, \boldsymbol{\Sigma}_1^{(0)}, \dots, \boldsymbol{\Sigma}_c^{(0)})$$
  2. **E step:** Compute probabilities $\hat{\pi}_{ij}$ for individuals belonging to each group
  3. **M step:** Maximize model parameters with formulae given before. Result is:
  $$\boldsymbol{\theta}^{(t+1)} = (p_1^{(t+1)}, \dots, p_c^{(t+1)}, \boldsymbol{\mu}_1^{(t+1)}, \dots, \boldsymbol{\mu}_c^{(t+1)}, \boldsymbol{\Sigma}_1^{(t+1)}, \dots, \boldsymbol{\Sigma}_c^{(t+1)})$$
  4. Back to E step if not stopping criterion met

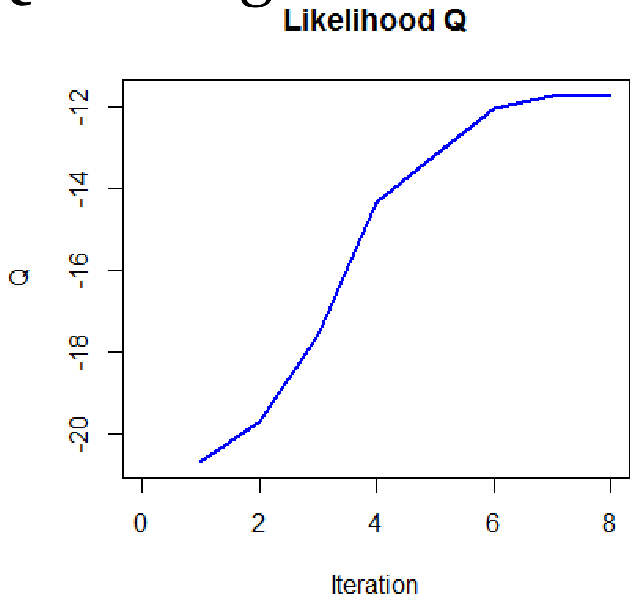
EM algorithm for normal mixtures

- Example for illustration: n=9 observations obtained. Ordered data: 0.1, 0.5, 0.7, 1.1, 2.5, 3.4, 3.5, 3.9, 4.0
- EM algorithm terminates after 8 iterations with: $(p_1^{(8)}, \mu_1^{(8)}, \mu_2^{(8)}, \sigma_1^{(8)}, \sigma_2^{(8)}) = (0.444, 0.600, 3.460, 0.361, 0.532)$
- Mean, sd, and $\hat{\pi}_{1j}$ converge as follows:



EM algorithm for normal mixtures

- Example for illustration: n=9 observations obtained. Ordered data: 0.1, 0.5, 0.7, 1.1, 2.5, 3.4, 3.5, 3.9, 4.0
- EM algorithm terminates after 8 iterations with: $(p_1^{(8)}, \mu_1^{(8)}, \mu_2^{(8)}, \sigma_1^{(8)}, \sigma_2^{(8)}) = (0.444, 0.600, 3.460, 0.361, 0.532)$
- Over the iterations, Q converges as follows:

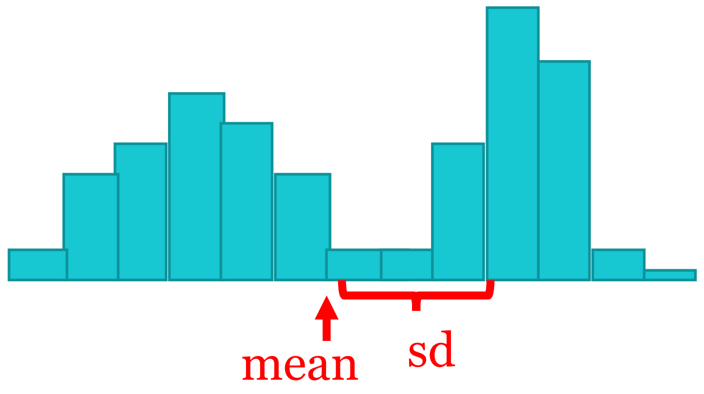


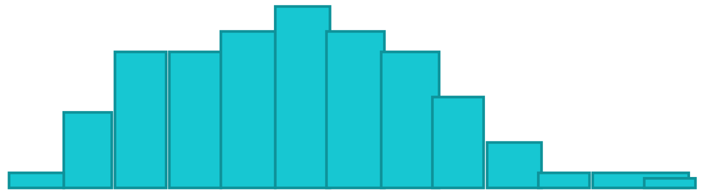
```
       Q
-20.69286
-19.68185
-17.56861
-14.35840
-13.19032
-12.03445
-11.71313
-11.71272
```

```
emalg <- function(dat, eps=0.000001){
  n      <- length(dat)
  pi     <- rep(NA, n)   #initialize vector for prob. to belong to group 1
  p      <- 0.5          #Starting value for mixing parameter
  sigma1 <- sd(dat)*2/3  #Starting value for variances
  sigma2 <- sigma1
  mu1    <- mean(dat)-sigma1/2 #Starting values for means
  mu2    <- mean(dat)+sigma1/2
  pv     <- c(p, mu1, mu2, sigma1, sigma2)  #parameter vector
  cc     <- eps + 100    #initialize conv. crit. not to stop directly
  while (cc>eps){
    pv1  <- pv           #Save previous parameter vector
    ### E step ###
    for (j in 1:n){
      pi1   <- p*dnorm(dat[j], mean=mu1, sd=sigma1)
      pi2   <- (1-p)*dnorm(dat[j], mean=mu2, sd=sigma2)
      pi[j] <- pi1/(pi1+pi2)
    }
    ### M step ###
    p      <- mean(pi)
    mu1    <- sum(pi*dat)/(p*n)
    mu2    <- sum((1-pi)*dat)/((1-p)*n)
    sigma1 <- sqrt(sum(pi*(dat-mu1)*(dat-mu1)/(p*n)))
    sigma2 <- sqrt(sum((1-pi)*(dat-mu2)*(dat-mu2)/((1-p)*n)))
    ######
    pv     <- c(p, mu1, mu2, sigma1, sigma2)
    cc     <- t(pv-pv1)%*%(pv-pv1)
  }
  pv
}
data <- c(0.1, 0.5, 0.7, 1.1, 2.5, 3.4, 3.5, 3.9, 4.0)
emalg(data)
```

Choice of starting values in example before

- We want to create automatically starting values which are meaningful for the data
- My heuristic rule to choose them in the R-code before:
  - Take total data and compute overall mean and sd
  - Overall sd is usually larger than sd’s for groups
  - Therefore, I took 2/3* overall sd for the sd in both groups
  - For group means, starting values with 1 sd difference chosen



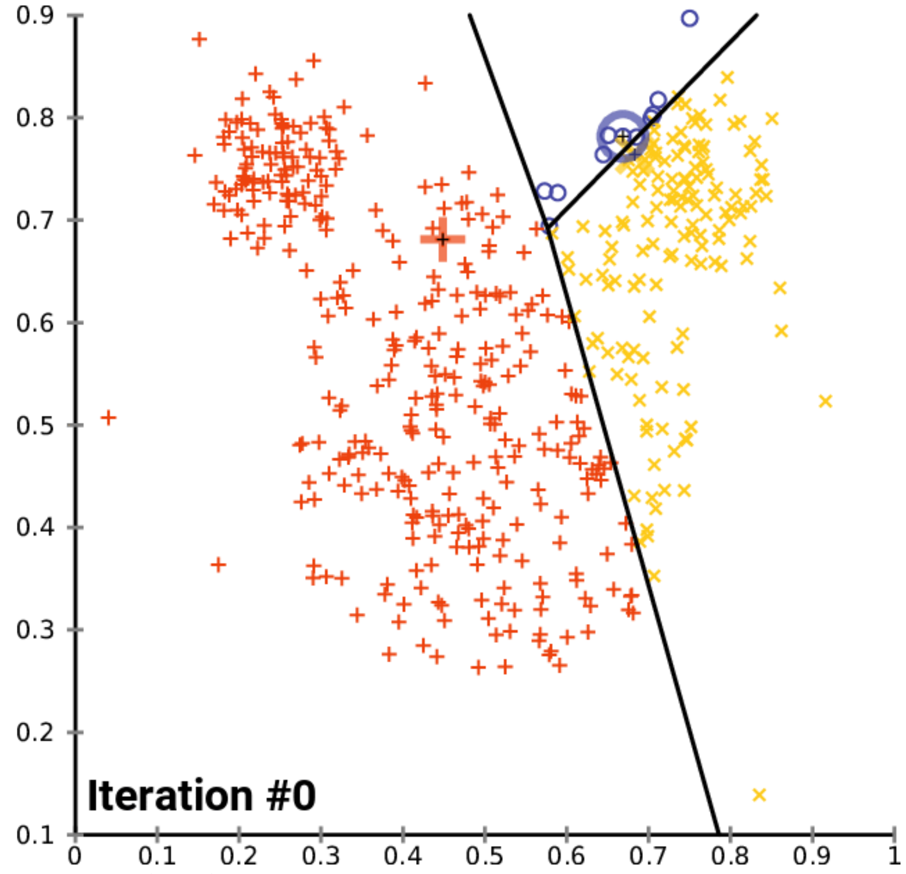


EM algorithm: Example 3

- We consider now an *unsupervised learning* situation with multivariate data coming from *c* groups, but it is unknown from which group each observation comes from (i.e., we have unlabeled data)
- Task: estimate to which group the observations belong to (i.e., classification)

Excursus: *K*-means clustering algorithm

- Initialize with *k* means
  $$\boldsymbol{\mu}_1^{(0)}, \cdots, \boldsymbol{\mu}_k^{(0)}$$
- <u>Assignment step:</u>
  Each observation is assigned to the nearest mean $\boldsymbol{\mu}_i^{(t)}$
- <u>Update step:</u>
  For each group *i* calculate the new mean $\boldsymbol{\mu}_i^{(t)}$
- Iterate until groups do no longer change



Annimation by: Chire
https://commons.wikimedia.org/wiki/File:K-means_convergence.gif

Excursus: *K*-means clustering algorithm

- The *k*-means algorithm creates clusters of similar size
- Sometimes more flexibility about cluster size desired

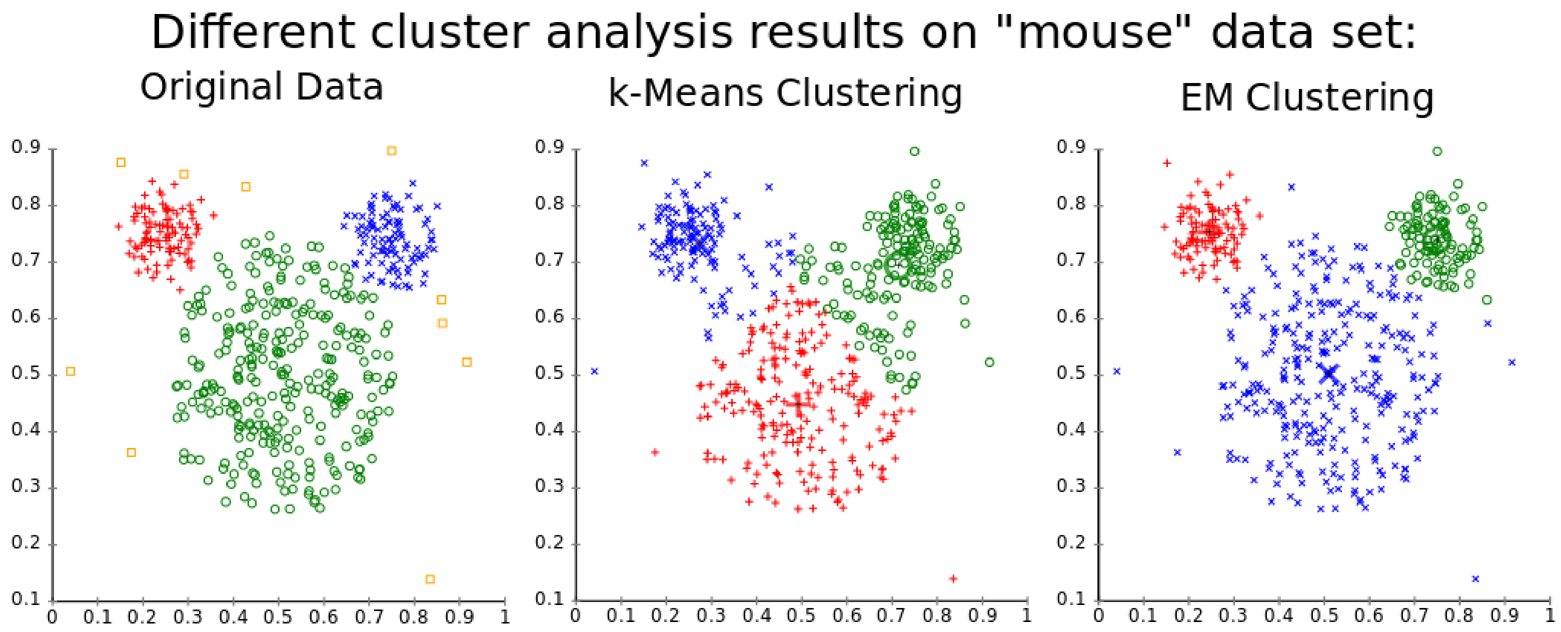


Figure by: Chire
https://upload.wikimedia.org/wikipedia/commons/0/09/ClusterAnalysis_Mouse.svg

- Assuming a multivariate normal mixture enables using the EM algorithm

Ways to choose starting values for the EM algorithm for normal mixtures

- We can look at the data and guess the components in the mixture, their mean and variance
- We can use a heuristic rule to determine starting values (like in Example 2)
- We can try a grid of starting parameter values
- We can first run a classification algorithm and use its result as starting values for the EM algorithm

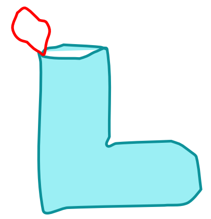
Stopping criteria for optimisation algorithms

- Stopping criterion e.g. $\left(\boldsymbol{\theta}^{(t+1)}-\boldsymbol{\theta}^{(t)}\right)^T\left(\boldsymbol{\theta}^{(t+1)}-\boldsymbol{\theta}^{(t)}\right)<\epsilon$
- Other stopping criteria:
  - Absolut stopping criterion, $\left\|\boldsymbol{\theta}^{(t+1)}-\boldsymbol{\theta}^{(t)}\right\|<\epsilon$,
  - Relative stopping criterion, $\left\|\boldsymbol{\theta}^{(t+1)}-\boldsymbol{\theta}^{(t)}\right\|/\left\|\boldsymbol{\theta}^{(t+1)}\right\|<\epsilon$,
  - Modified rel. stopping crit., $\frac{\left\|\boldsymbol{\theta}^{(t+1)}-\boldsymbol{\theta}^{(t)}\right\|}{\left\|\boldsymbol{\theta}^{(t+1)}\right\|+\varepsilon}<\varepsilon$
  - Different norms $\|\cdot\|$ can be used
  - EM: instead of parameter vector, can look at log-likelihood and compare it between iterations $\left|Q\left(\boldsymbol{\theta}\middle|\boldsymbol{x};\boldsymbol{\theta}^{(t+1)}\right)-Q\left(\boldsymbol{\theta}\middle|\boldsymbol{x};\boldsymbol{\theta}^{(t)}\right)\right|<\varepsilon$

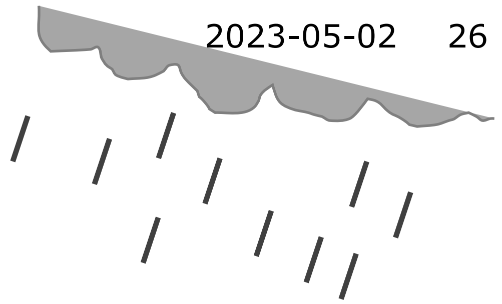
Bootstrap

Why bootstrap?

- Assume you have independent samples of some population
- In statistics, we have methods to construct confidence intervals (CIs) for a parameter θ of interest (e.g., mean) based on distributional assumptions; e.g., explicit formulas exist in case of normal distribution
- Sometimes not reasonable to make distributional assumptions
- With methods we will discuss here, we can **obtain CIs without these distributional assumption**
- The available sample is our best information about the population – we take the **available sample as assumption for distribution of population**
- We pull ourselves up by our own capabilities – like “pulling us up from the mud by our own **bootstraps**”



Example: precipitation data

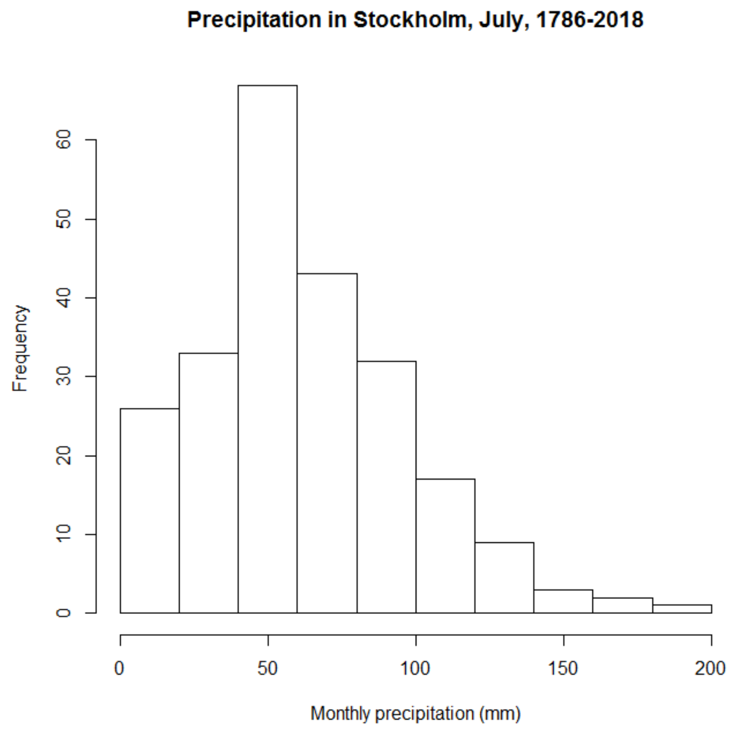


- Rainfall data from July in 233 years in Stockholm
- What is the mean and a 95%-CI for the mean?
- With standard formulae, we can calculate CI:

$$\bar{x} = 62.6mm, s = 35.0, n = 233,$$
$$s_{\bar{x}} = s/\sqrt{n} = 2.29,$$
$$t_{0.025,233} = 1.970$$

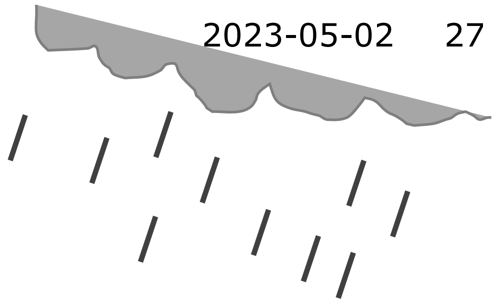
- 95%-CI-bounds: $\bar{x} \pm s_{\bar{x}} \cdot t_{0.025,233}$
- 95%-CI is here: $(58.1, 67.1)$

- But: normal distribution assumed

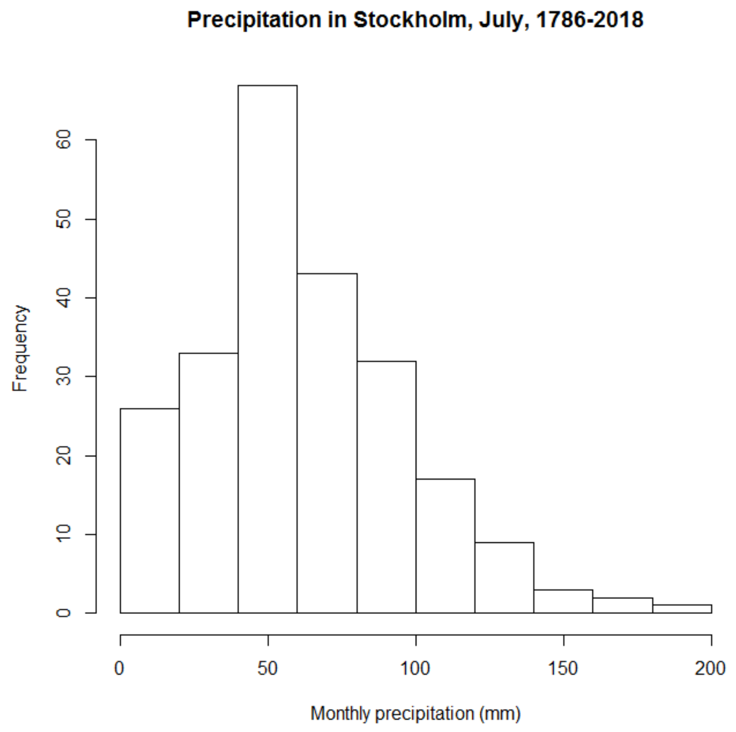


Data source: SMHI

Example: precipitation data



- This data is not normally distributed
- We want to make a more realistic assumption: Actual sample distribution is best information about distribution
- Idea: Given the 233 observations, **sample from them with replacement** until you have 233; calculate mean;
  repeat this B=1000 times;
  we have now 1000 means: the ”middle 950” give a 95%-CI



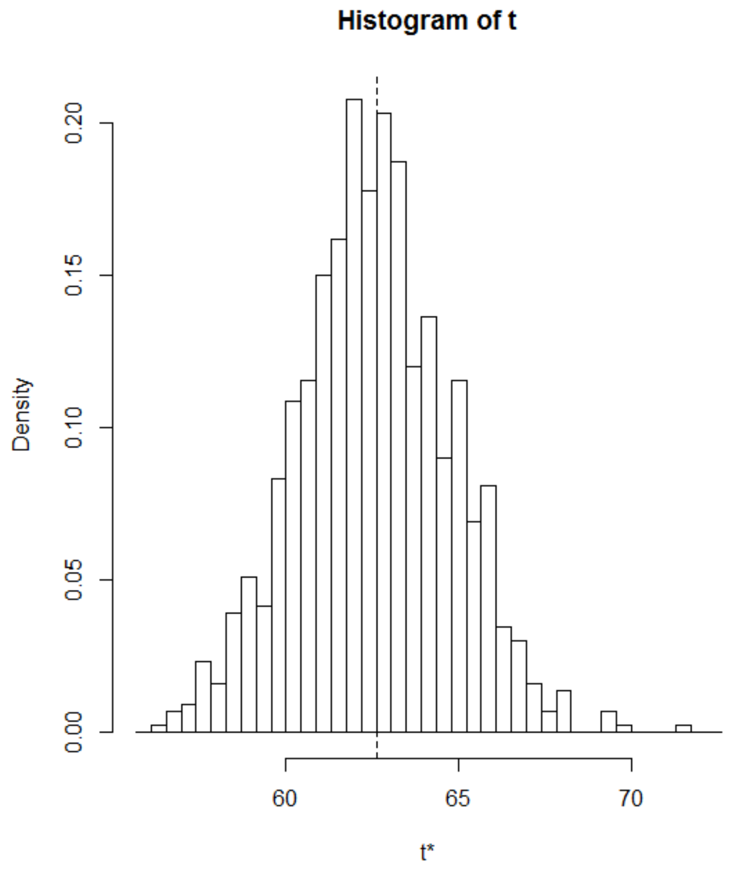
Example: precipitation data

- We illustrate the bootstrap using only the last 6 years: `42.3, 44.1, 91.9, 47.6, 14.6,  5.9`
- First resample: ` 5.9, 42.3,  5.9, 47.6, 91.9, 91.9`
- Second resample: `42.3, 44.1, 42.3, 91.9, 42.3, 14.6`
- Third resample: `47.6, 44.1, 42.3, 14.6, 91.9, 14.6`
- …
- 1000th resample: `47.6, 42.3, 91.9, 91.9,  5.9, 42.3`

- The mean of each resample: 47.6, 46.3, 42.5, …, 53.7

Example: precipitation data

- From the complete data, we made 1000 resamples; the 1000 means of those are in the histogram
- The mean of the means: 62.6 mm
  (bootstrap estimate is here the same as the usual estimate of the mean $\bar{x}$)
- The middle 95% of the means are from 58.2 to 66.7 – this is our 95%-bootstrap-CI for the mean



Bootstrap idea

- Original data of size n is given, a certain property θ (e.g. mean, variance, …) should be estimated by $\hat{\theta}$; its uncertainty should be quantified (e.g. CI for θ)
- Draw B resamples of size n of the original data with replacement
  B=500 or 1000 has been used historically; B=10000 is nowadays often no problem
- Usually, there are repetitions in a resample
- Calculate the property of interest for each resample: $\hat{\theta}_i$, i=1, …, B;
  the distribution of these B values (”bootstrap distribution”) can be used e.g. to compute a CI for θ
- Advantage: no assumption for distribution of original data

- Which assumption is still made?

Bootstrap in R

- R code using a loop for bootstrap replicates:

```
bo <- 1000   # bootstrap replicates
bs <- c()    # to save the results for the means
for (l in 1:bo){
  x  <- sample(mrain, size=length(mrain), replace=TRUE)
  bs <- c(bs, mean(x))
}
hist(bs)
bss  <- sort(bs)
ci95 <- c(bss[round(bo*0.025)], bss[round(bo*0.975)])
ci95
```

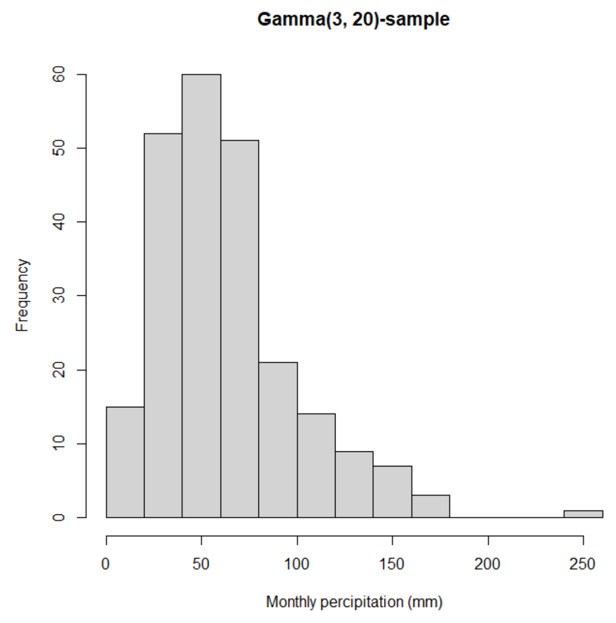
- A run of this code gave (58.2, 66.7) as 95% bootstrap confidence interval

Bootstrap in R with package `boot`

- As alternative, package `boot` with functions `boot` and `boot.ci` can be used
  ```
  library(boot)
  ```
- Define first function of interest, e.g. the mean:
  ```
  bootmean <- function(x, i) mean(x[i])
  ```
- Generate B bootstrap resamples with function `boot`:
  ```
  bss <- boot(mrain, bootmean, R=1000)
  ```
- You can plot a histogram of the bootstrap distribution:
  ```
  hist(bss$t)
  ```
- A 95%-CI is between 2.5%- and 97.5%-percentile of bootstrap distribution:
  ```
  boot.ci(bss, type=”perc”)
  ```
- The method used here for the CI-bounds is called “percentile method”

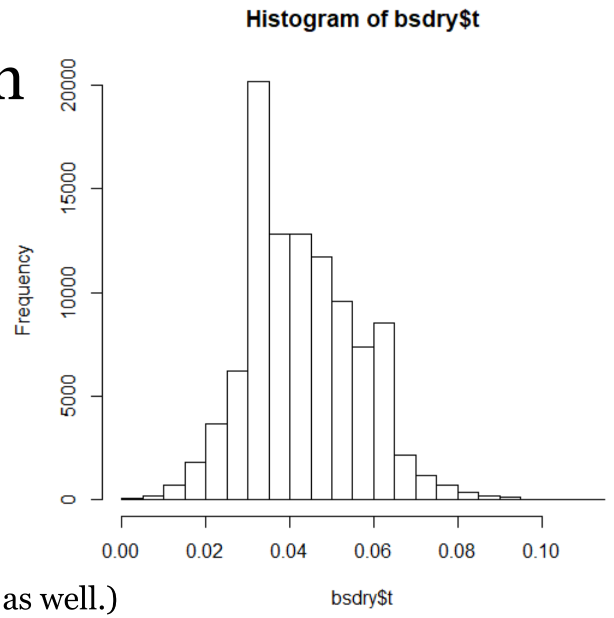
Parametric bootstrap

- When a parametric model for the data is known or believed to represent the reality well, we can do parametric bootstrap and sample according to the assumed model
- Example: We assume that monthly precipitation in July follows a Gamma(3, 20)-distribution
- We sample 233 datapoints from Gamma(3, 20) and calculate parameter of interest
- Do this B times and derive e.g. a confidence interval



Example: precipitation data

- What is an estimated probability for "less than 10mm rain in next July"? How good is our estimation? (➔ CI)
- Reasonable to calculate proportion of years with July-rain < 10mm. Here: in 10 of 233 years = 0.043
- To calculate a 95%-CI, we generate a bootstrap distribution
  (We resample B times and compute for each resample the proportion of years with July-rain < 10 mm)
- We use it's 2.5%- and 97.5%-percentile:
  `(0.0172, 0.0687)`
- Conclusion: The probability for < 10mm rain in July is between 1.7% and 6.9%; estimate is 4.3%
- (With normal assumption an estimate would be 6.6%. But a probability for < 0 mm rain would be 3.7%…
  To use bootstrap gives here much better estimates than with normal assumption! You get easily a confidence interval as well.)



Bootstrap in R with package `boot`

- Define function of interest, here proportion below 10mm:
  `bootdry <- function(x, i) mean((x[i]<10))`
- Generate B=100000 bootstrap resamples:
  `bsdry <- boot(mrain, bootdry, R=100000)`
- Plot a histogram of bootstrap distribution:
  `hist(bsdry$t)`
- Estimate proportion:
  `bootdry(mrain)`
- A 95%-CI is between the 2.5%- and 97.5%-percentile of the bootstrap distribution:
  `boot.ci(bsdry, type=”perc”)`

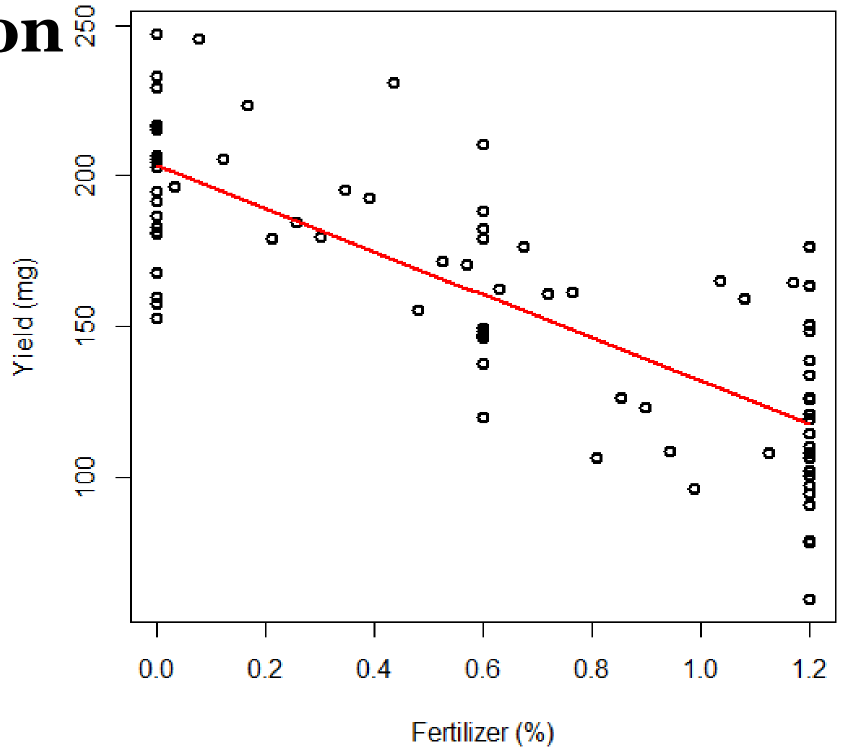
Bootstrap for regression models

- We can use the bootstrap method very flexibly, e.g. **in linear regression** if we want a **CI for the slope or the residual standarddeviation**
- Example: The (toxic) influence of a fertilizer on growth of garden cress was investigated in an experiment (yield vs. amount of fertilizer, n=81)
- Estimated linear regression:

$$yield = 203.3 - 71.3 \cdot fertilizer$$

with residual standarddeviation $\hat{\sigma} = 26.7$

- CI for slope? CI for $\hat{\sigma}$?

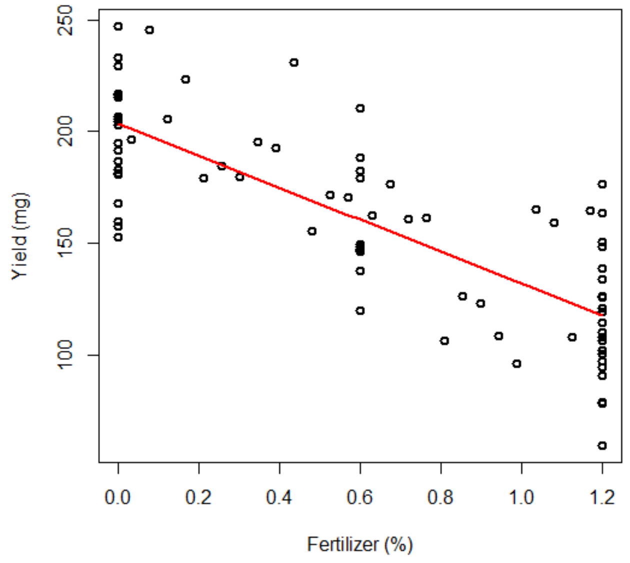


Bootstrap for regression models

- The dataset has n=81 pairs of fertilizer-yield-values
- The bootstrap resamples **n pairs** with replacement, computes regression-slope and $\hat{\sigma}$
- This is done B times; R-code:

```
cressdat <- data.frame(fertilizer,yield)
cmslope  <- function(dat, i)
{
  cm  <- lm(yield~fertilizer, subset=i, data=dat)
  coef(cm)[2]
}
cb <- boot(cressdat, cmslope, R=10000)
boot.ci(cb, type="perc")
```

- Result for CI-limits: -83.5, -58.7

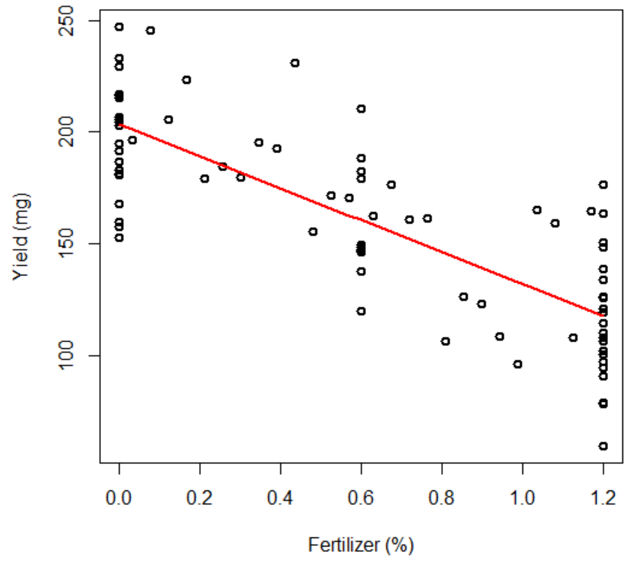


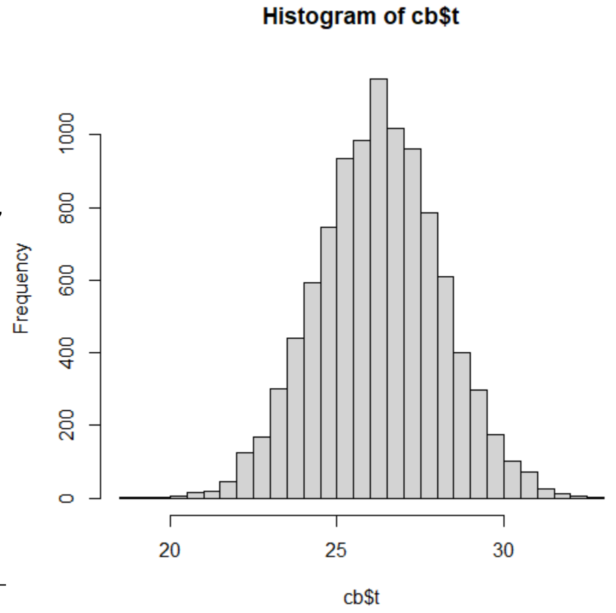
Bootstrap for regression models

- A function for analysis of the residual $\hat{\sigma}$ is:

```
cmressd <- function(dat, i)
{
  cm  <- lm(yield~fertilizer, subset=i, data=dat)
  summary(cm)$sigma
}
```

- Result for CI-limits: 22.62, 29.91 (percentile method)
- Median (50% percentile) of bootstrap distribution: 26.27
- Residual $\hat{\sigma}$ of data: 26.72
- Percentile CI is constructed around 26.27 while it should be constructed around 26.72 ➔ the CI is biased





Percentile method for CIs and alternatives

- The percentile method which we used so far can have drawbacks
- Bias: Estimate $\hat{\theta}$ might be very different from median of bootstrap distribution, median($\hat{\theta}_i$), but we would like a CI constructed around $\hat{\theta}$
- The bootstrap distribution might be heavily skewed implying that the se($\hat{\theta}$) changes with the true θ
- The BC_a method (bias correction – accelerated) improves the percentile method by
  - correcting for bias and
  - adjusting the boundary alpha-levels to handle dependence of se($\hat{\theta}$) on θ
- If bootstrap distribution has not these issues, BC_a = percentile
- For other methods (and BC_a) see Givens and Hoeting (2013), Chapter 9.3.

BC$_a$ method for bootstrap CIs

- Like percentile method, BC$_a$ uses quantiles from the bootstrap distribution, but instead of $\alpha/2$ and $1-\alpha/2$, it uses the two corrected quantiles $\Phi\left(z_0 + \frac{z_0 \pm z_{\alpha/2}}{1 - a\left(z_0 \pm z_{\alpha/2}\right)}\right)$
- Bias: Define $z_0 = \Phi^{-1}$(proportion of bootstrap values below estimate)
- Handling of skewness with acceleration factor a:

$$a = \frac{\sum_{i=1}^{n}\left(\hat{\theta}_{(\cdot)} - \hat{\theta}_{(i)}\right)^3}{6\left\{\sum_{i=1}^{n}\left(\hat{\theta}_{(\cdot)} - \hat{\theta}_{(i)}\right)^2\right\}^{3/2}}$$

  where $\hat{\theta}_{(i)}$ is estimated leaving out observation i and $\hat{\theta}_{(\cdot)}$ is mean of $\hat{\theta}_{(i)}$
- This is a *jackknife approach* for estimating the change of se$(\hat{\theta})$ when θ changes

Bagging (bootstrap aggregating)

- In the examples we discussed, we had an estimate $\hat{\theta}$ and got information about its uncertainty with the bootstrap approach, e.g. constructing a CI
- In bagging, bootstrap is used to improve the estimate $\hat{\theta}$ itself by $\frac{1}{B}\sum_{i=1}^{B}\hat{\theta}_i$
- For example, if $\hat{\theta}$ is based on model-fitting where very different models could be chosen only if some observations are changed, the bootstrap estimate is model averaging
- $\hat{\theta}$ might be based modelling with on neural networks or regression models with data-dependent feature selection
- See Section 7.1-7.2 of Lindholm, Wahlström, Lindsten, Schön (2022)