

Biological Statistics III – Lecture 12

Computer based methods: randomization, bootstrap

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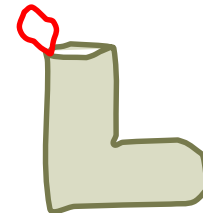
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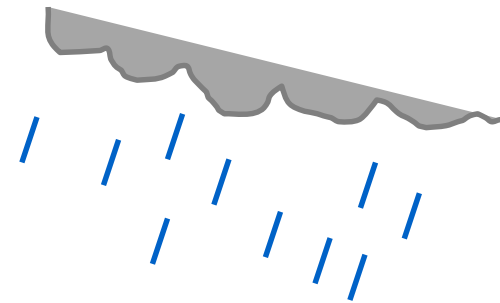
Outline

- Bootstrap
 - Idea, method and examples
 - Bootstrap in the context of regression models
- Permutation tests
 - Idea, method and examples
 - The Mantel test in ecology

Why bootstrap?

- You have tested hypotheses or constructed confidence intervals (CIs) for parameters of interest (e.g. mean) assuming normal distribution with help of formulae
- Sometimes not reasonable to assume normal distribution and inference based on it might then mislead
- We want to **obtain CIs without any distributional assumption**
- The available sample is our best information about the population – we take the **available sample as assumption for distribution of population**
- Like “pulling us up from the mud by our own **bootstraps**”

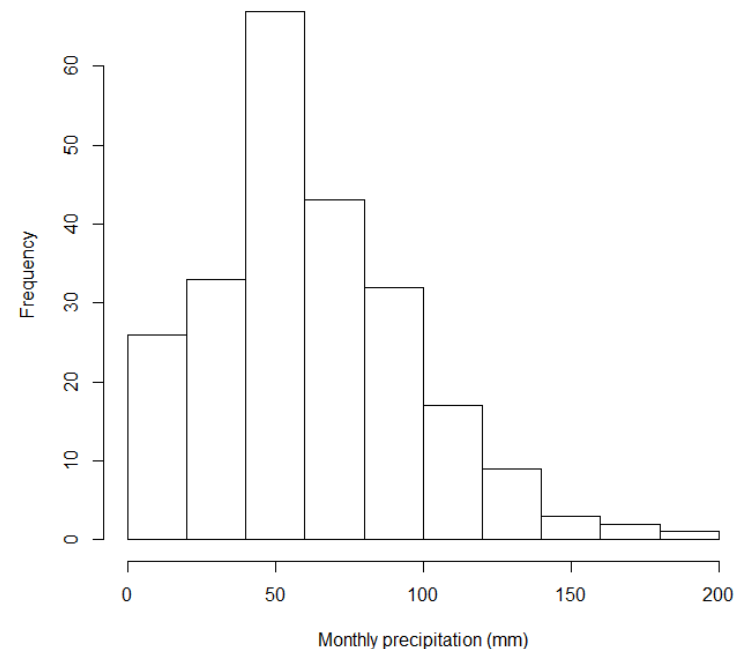




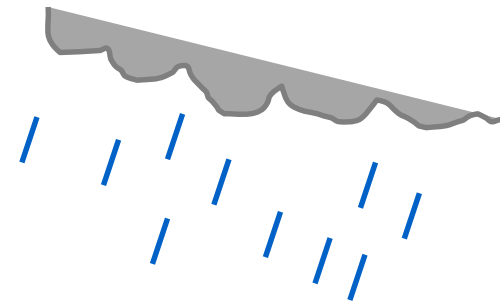
Analysis of precipitation data

- Rainfall data from July in 233 years in Stockholm
- What is the mean and a 95%-CI for the mean?
- With methods from earlier in course, we can calculate CI:
 $\bar{x} = 62.6\text{mm}$, $s = 35.0$, $n = 233$,
 $s_{\bar{x}} = s/\sqrt{n} = 2.29$,
 $t_{0.025,233} = 1.970$
- 95%-CI: (58.1, 67.1)
- But: normal distribution assumed

Precipitation in Stockholm, July, 1786-2018



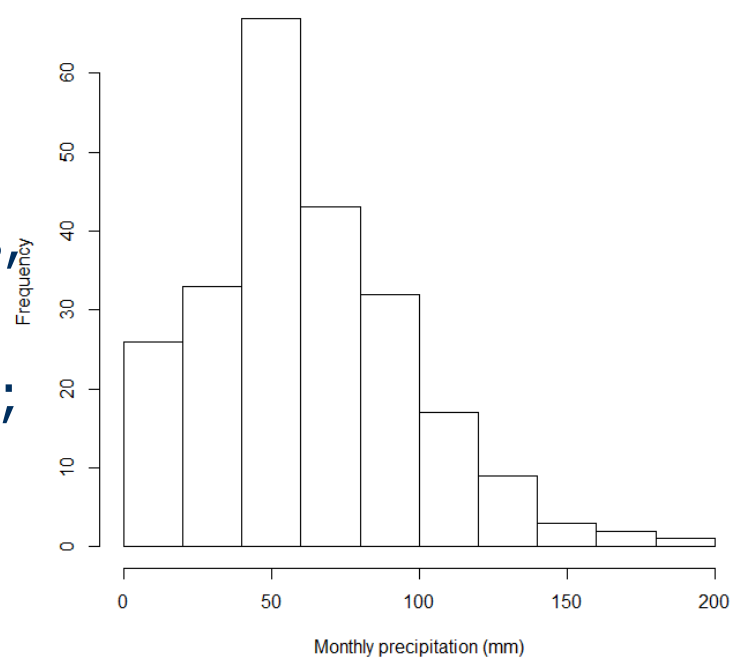
Data source: SMHI



Analysis of 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

Precipitation in Stockholm, July, 1786-2018



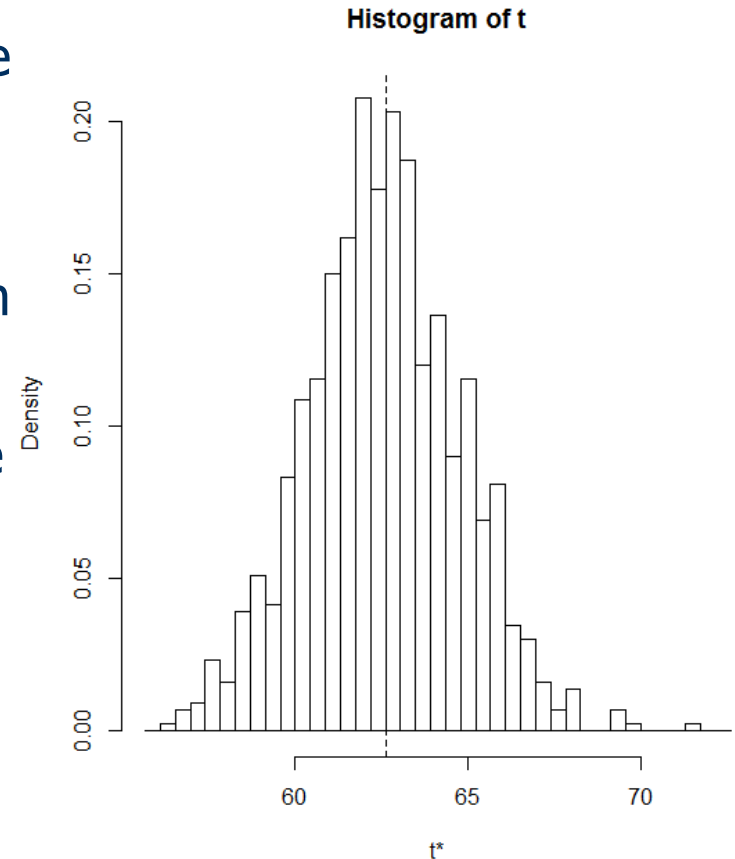
Analysis of precipitation data

- 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

Analysis of 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 (e.g. mean, variance, ...) is of interest and its uncertainty should be quantified (e.g. CI)
- 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

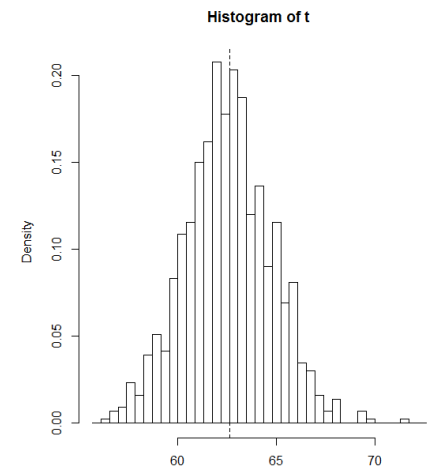
- Usually, there are repetitions in a resample
- Calculate the property of interest for each resample – you have now B of them; the distribution of these B values (“bootstrap distribution”) can be used e.g. to compute a CI
- Advantage: no assumption for distribution of original data

Bootstrap in R

- R code using a loop for bootstrap replicates:

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

```
bss <- boot(mrain, bootmean, R=1000)
```
- You can plot a histogram of the bootstrap distribution:

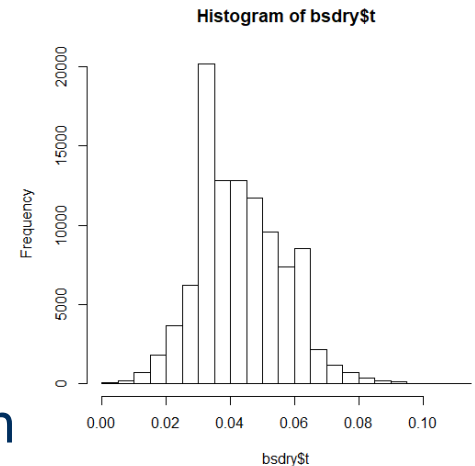
```
hist(bss$t)
```
- A 95%-CI is between the 2.5%- and 97.5%-percentile of the bootstrap distribution:

```
boot.ci(bss, type="perc")
```



Analysis of 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 its 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

- Now function of interest: proportion of cases below 10mm

```
bootdry <- function(x,i) mean((x[i]<10))
```

- Generate B=100000 bootstrap resamples: 0's or 1's

```
bsdry <- boot(mrain, bootdry, R=100000)
```

- Plot a histogram of bootstrap distribution:

```
hist(bsdry$t)
```

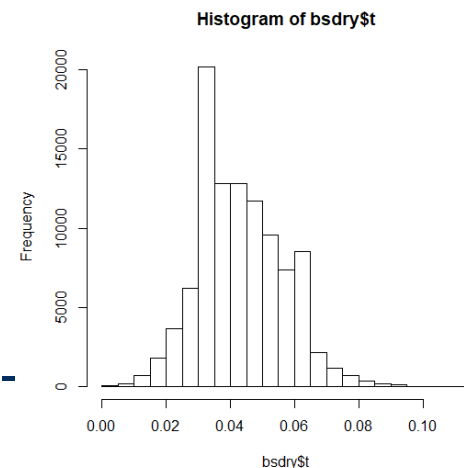
- Estimate proportion:

```
bootdry(mrain) 0.0429
```

- A 95%-CI is between the 2.5%- and 97.5%-percentile of the bootstrap distribution:

```
boot.ci(bsdry, type="perc")
```

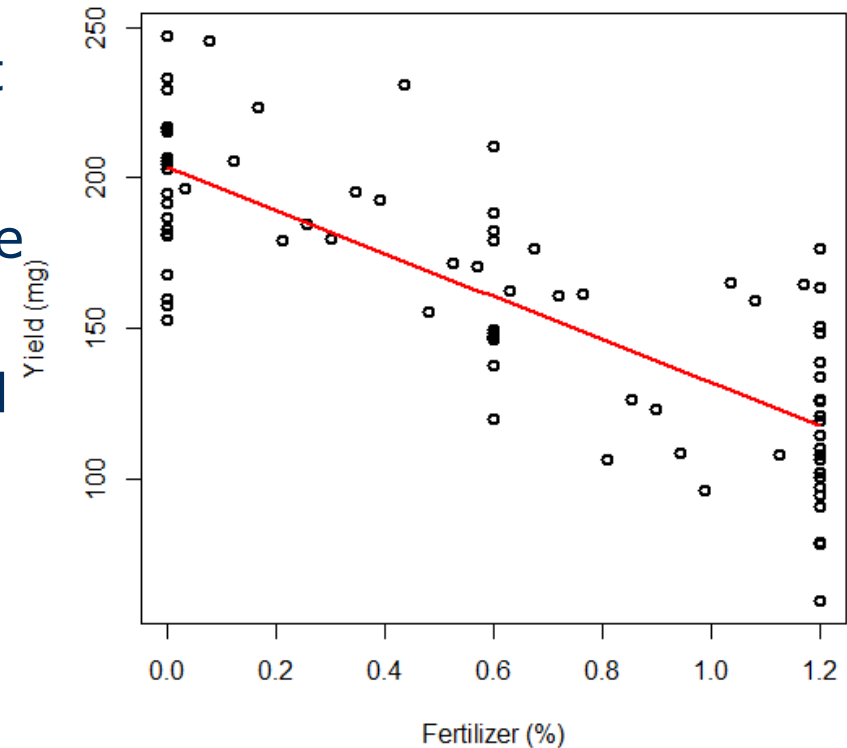
| Level | Percentile |
|-------|------------------|
| 95% | (0.0172, 0.0687) |



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 for R^2**
- 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 $R^2=0.63$
- CI for slope? CI for R^2 ?

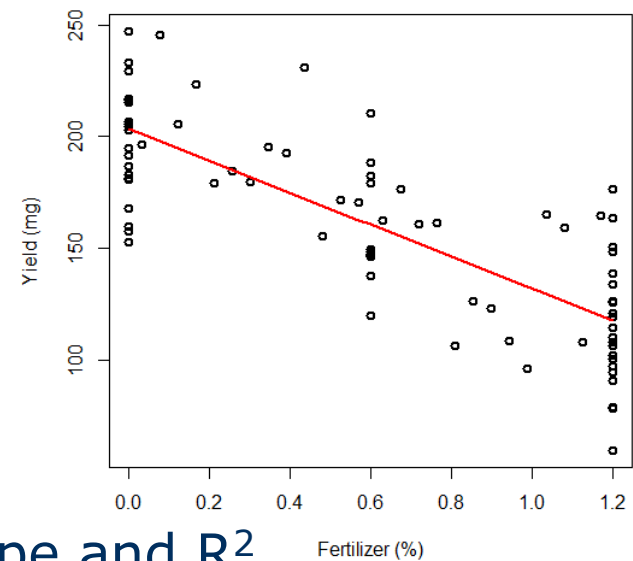


Bootstrap for regression models

- The dataset has $n=81$ pairs of fertilizer-yield-values
- The bootstrap resamples **n pairs** with replacement, computes regression-slope and R^2
- 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

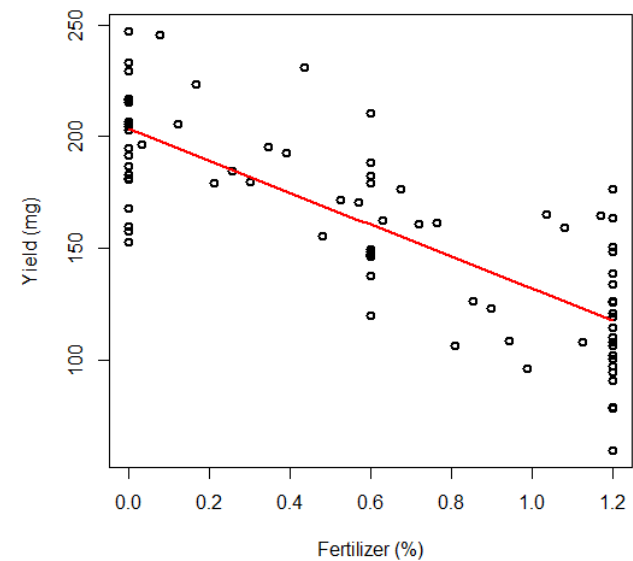


Bootstrap for regression models

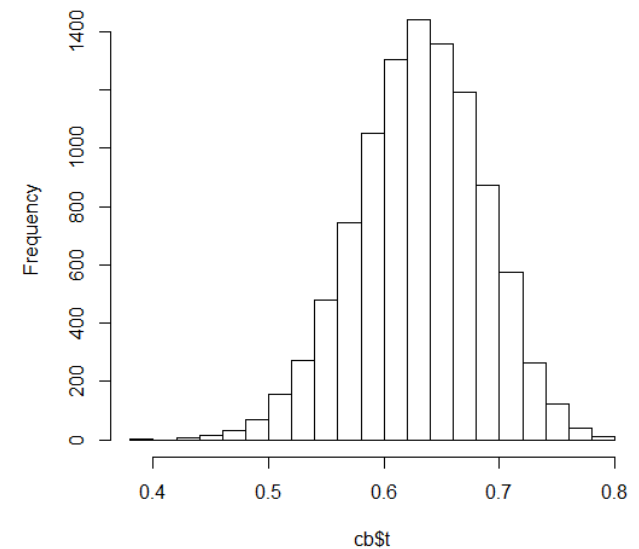
- Function to analyse regression- R^2 instead of slope:

```
cmr2 <- function(dat, i)
{
  cm <- lm(yield~fertilizer, subset=i, data=dat)
  summary(cm)$r.squared
}
```

- Result for CI-limits: 0.518, 0.733

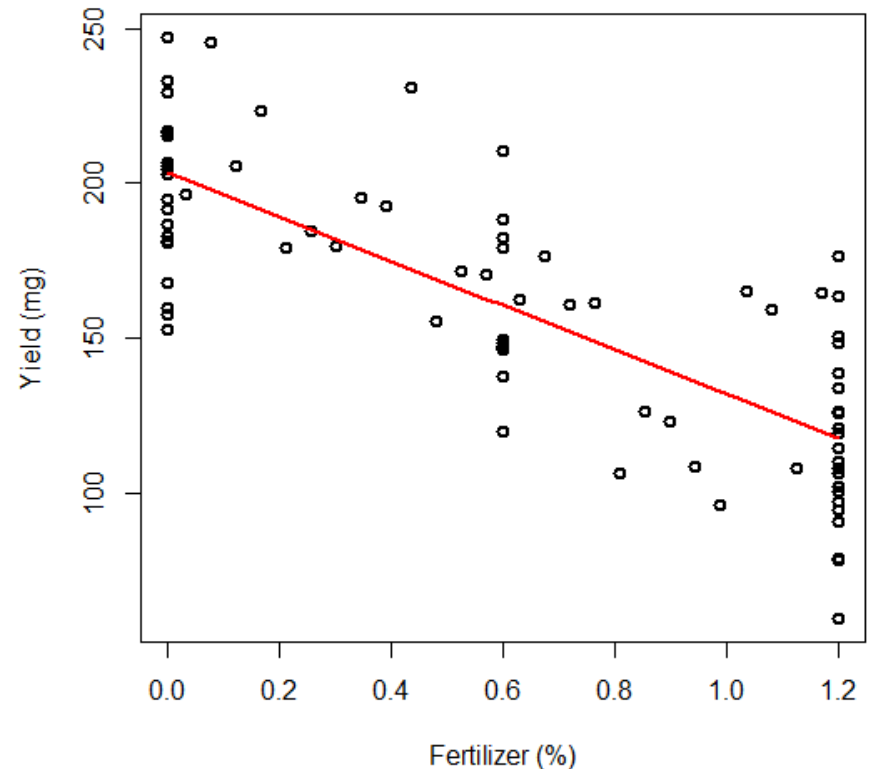


Histogram of cb\$t



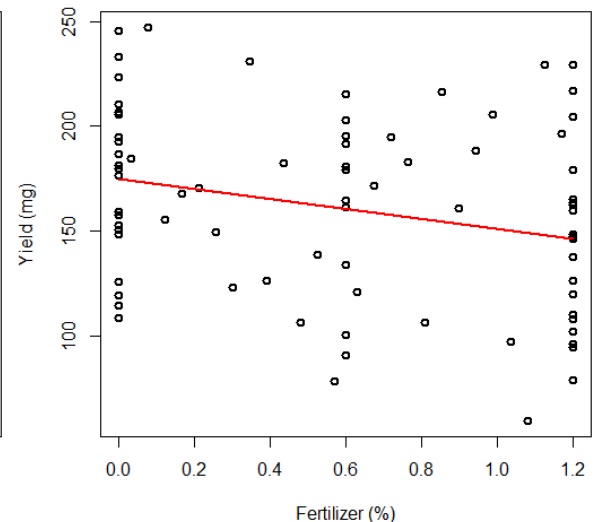
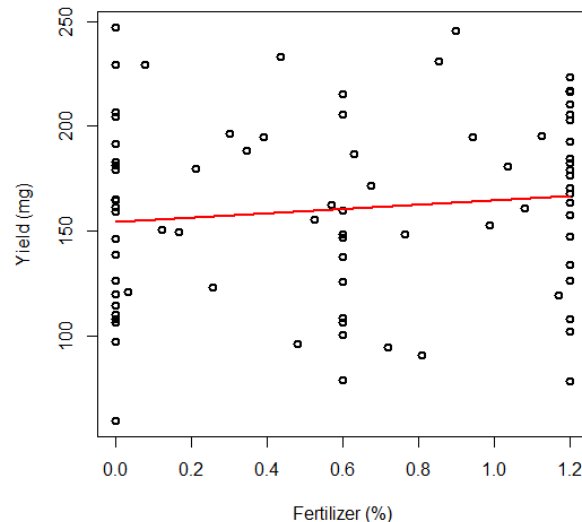
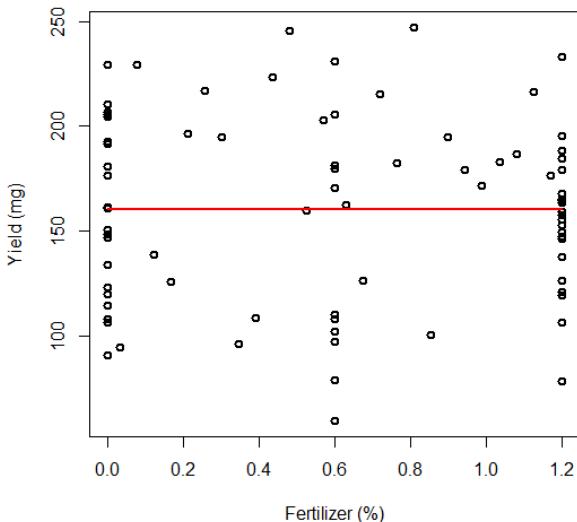
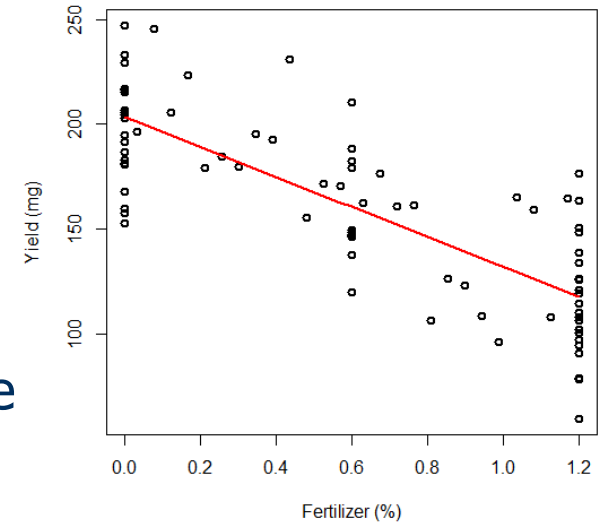
Permutation tests

- Want to **test if there is association between two variables**
- Example: Is there an association between amount of fertilizer and cress yield?
 - Is the *slope* significantly different from 0?
 - Alternative: Is the *correlation* significantly different from 0?
- We could perform t-test from linear regression, but we want to **avoid the assumptions** (here avoid normality assumption, in other examples independence)



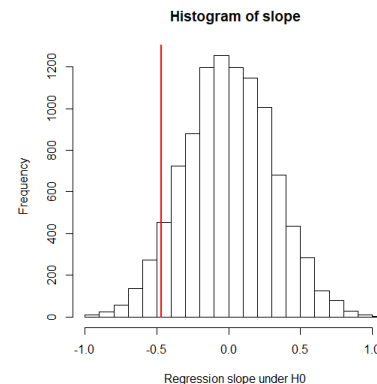
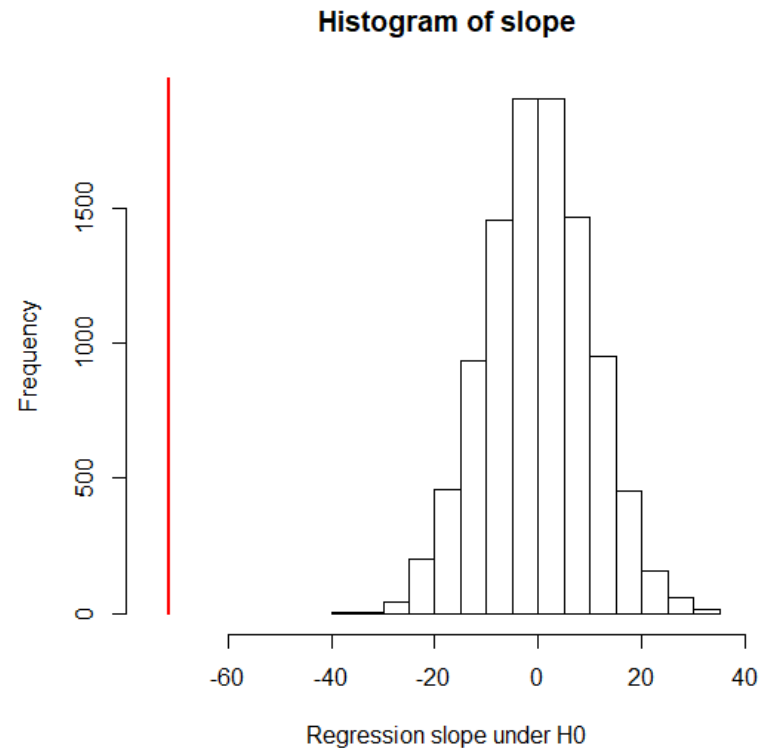
Permutation tests

- Idea: If we permute yield-results (assign them randomly to fertilizer-values), we have no association, but we compute a slope (=chance-slope)
- We do this repeated times (e.g. 10000) and obtain a distribution for chance-slopes; three of the chance-slopes:



Permutation tests

- If observed slope different from chance-slopes, conclude that association is real
- Here: Evident that real slope (-71.3) not by chance
- In general: We calculate proportion of resamples which give a more extreme slope than the real one
- Proportion is the p-value: conclude that there is an association if $p < 0.05$



Permutation tests – analysis with R

- The function `independence_test` in the package `coin` can be used:

```
library(coin)
independence_test(yield ~ fertilizer,
alternative="less")
```

- **Result:**

Asymptotic General Independence Test

```
data: yield by fertilizer
Z = -7.0994, p-value = 6.265e-13
alternative hypothesis: less
```

- **Conclusion:** Since $p\text{-value} < 0.05$, we conclude that there is an association between fertilizer and yield

Permutation tests: The Mantel test

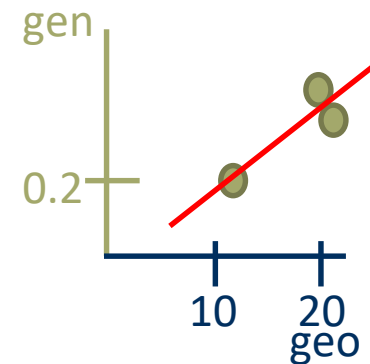
- Association between genetic and geographic distances?

- Genetic distances:

| | A | B | C |
|---|------|-----|------|
| A | | 0.2 | 0.35 |
| B | 0.2 | | 0.4 |
| C | 0.35 | 0.4 | |

- Geographic distances:

| | A | B | C |
|---|----|----|----|
| A | | 12 | 20 |
| B | 12 | | 19 |
| C | 20 | 19 | |



- Compute correlation between genetic and geographic dist.
- Permute one of the distance matrices e.g. 10000 times; compute correlation for all of them (=chance-correlations)
- Is real correlation different from chance-correlations?
- This specific permutation test is the Mantel test



Permutation tests: The Mantel test

- Why do we not just compute the correlation for the real data and test by “usual” test if it is 0 or not?
 - Assumption of independence is violated
 - Usually also normality questionable
- The Mantel test avoids these problems

- To read more about the Mantel test:
 - p.597-608 in Legendre P, Legendre L (2012). Numerical Ecology. 3rd edition.

The Mantel test – analysis with R

- Function `mantel.randtest` in package `ade4` can be used:

```
gen <- as.dist(geneticdist)
geo <- as.dist(geographicdist)
gg <- mantel.randtest(geo, gen, nrepet = 10000)
gg
plot(gg, main = "Mantel test")
```

- Example: distance matrices for 19 villages of Yanomama Indians in `ade4`; can be analysed by running first following:

```
data(yanomama)
geneticdist <- yanomama$gen
geographicdist <- yanomama$geo
```

