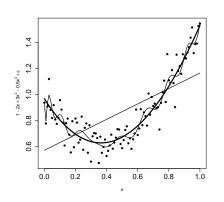
### Model Selection and Hypothesis Testing

732A90 Computational Statistics

Krzysztof Bartoszek (krzysztof.bartoszek@liu.se)

28 II 2017 Department of Computer and Information Science Linköping University

#### Model selection



#### Tools for model selection

- Comparing different models
- Information criteria (not this course)
- Cross-validation
- Hypothesis testing
- Uncertainty estimation
- Confidence intervals

# Hypothesis testing: Recap

- Assume a probabilistic model State a null hypothesis ( $H_0$  e.g. no difference) and alternative ( $H_1$  difference)
- Observe data X
- Calculate a test statistic e.g.  $T(X) = (\overline{X})/(\operatorname{sd}(X))$  (different statistics will have different **efficiency** (power, ability to distinguish between hypotheses) associated with them)
- 4 Under  $H_0$  T(X) has "known" distribution
- **5** Decision: Is the value of T(X) surprising (in the **critical** region)? If so reject  $H_0$  in favour of  $H_1$ .

## Hypothesis testing: Example

$$\begin{array}{c} \text{x} < -\mathbf{rnorm} \left( 10 \text{ ,mean} = 4, \mathbf{sd} = 1 \right) & \overset{\bullet}{\circ} & & & \\ \text{Hypotheses:} & & & & & \\ H_0 : \mu = 4, X \sim \mathcal{N}(\mu, \sigma^2) & & & & \\ H_1 : \mu \neq 4, X \sim \mathcal{N}(\mu, \sigma^2) & & & & \\ \text{Test statistic} & & & & \\ T(x) = \frac{\overline{x} - \mu}{s / \sqrt{n}} \sim t(n-1) & & & & \\ \end{array}$$

### Hypothesis testing: Power

How does one compares different statistics?

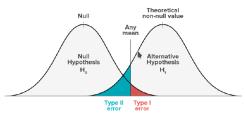
#### POWER

Power = 1 - Type II error

Ability to correctly identify surprise, i.e. indicate  $H_1$ .

How to compute power?

- Analytically (?)
- Generate data samples that satisfy  $H_1$ Compute percent of correct rejections



# Monte Carlo Hypothesis testing

We may use "any" test statistic.

We do **not** need to know its distribution.

$$H_0: \mu = 4, X \sim \mathcal{N}(\mu, \sigma^2)$$
  

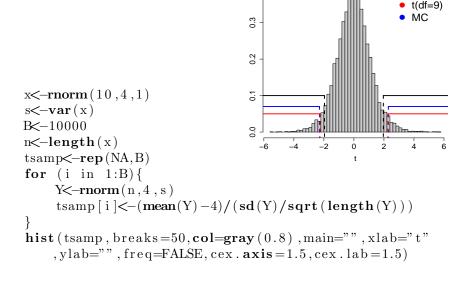
$$H_1: \mu \neq 4, X \sim \mathcal{N}(\mu, \sigma^2)$$

Test statistic

$$T(x) = \frac{\overline{x} - \mu}{s/\sqrt{n}} \sim t(n-1)$$

- 1: **for** i = 1 to B **do**
- 2: Generate  $Y_1, \ldots, Y_n$  i.i.d. from  $H_0$ , i.e.  $\mathcal{N}(\mathbf{4}, \sigma^2)$
- 3: Compute  $t_i$  from  $Y_1, \ldots, Y_n$
- 4: end for
- 5: Use  $t_1, \ldots, t_B$  to construct a histogram
- 6: Use the histogram as the distribution of T(x) under  $H_0$

# Monte Carlo Hypothesis testing



N(0,1)

## Permutation tests

- A. k. a. randomization tests
- One solution if we do not know the distribution under  $H_0$
- Computationally expensive
- Any sample size

- Two sample problem:
- I wo sample problem:
  Population 1 distributed as F

 $H_1: F \neq G$ 

Population 2 distributed as G
H<sub>0</sub>: F = G

#### Permutation tests: mouse data

- Control group
- Treatment group
- $\bullet$  Group variable g
- $\bullet$  Values variable v

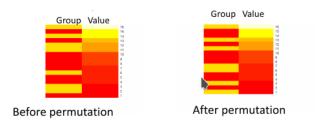
```
> t(mouse)

[,1] [,2] [,3] [,4] [,5] [,6] [,7] [,8] [,9] [,10] [,11] [,12] [,10] [,10] [,11] [,12] [,12] [,12] [,12] [,12] [,12] [,13] [,14] [,15] [,16] [,16] [,16] [,16] [,16] [,16] [,16] [,16] [,16] [,16] [,16] [,16] [,16] [,16] [,16] [,16] [,16] [,16] [,16] [,16] [,16] [,16] [,16] [,16] [,16] [,16] [,16] [,16] [,16] [,16] [,16] [,16] [,16] [,16] [,16] [,16] [,16] [,16] [,16] [,16] [,16] [,16] [,16] [,16] [,16] [,16] [,16] [,16] [,16] [,16] [,16] [,16] [,16] [,16] [,16] [,16] [,16] [,16] [,16] [,16] [,16] [,16] [,16] [,16] [,16] [,16] [,16] [,16] [,16] [,16] [,16] [,16] [,16] [,16] [,16] [,16] [,16] [,16] [,16] [,16] [,16] [,16] [,16] [,16] [,16] [,16] [,16] [,16] [,16] [,16] [,16] [,16] [,16] [,16] [,16] [,16] [,16] [,16] [,16] [,16] [,16] [,16] [,16] [,16] [,16] [,16] [,16] [,16] [,16] [,16] [,16] [,16] [,16] [,16] [,16] [,16] [,16] [,16] [,16] [,16] [,16] [,16] [,16] [,16] [,16] [,16] [,16] [,16] [,16] [,16] [,16] [,16] [,16] [,16] [,16] [,16] [,16] [,16] [,16] [,16] [,16] [,16] [,16] [,16] [,16] [,16] [,16] [,16] [,16] [,16] [,16] [,16] [,16] [,16] [,16] [,16] [,16] [,16] [,16] [,16] [,16] [,16] [,16] [,16] [,16] [,16] [,16] [,16] [,16] [,16] [,16] [,16] [,16] [,16] [,16] [,16] [,16] [,16] [,16] [,16] [,16] [,16] [,16] [,16] [,16] [,16] [,16] [,16] [,16] [,16] [,16] [,16] [,16] [,16] [,16] [,16] [,16] [,16] [,16] [,16] [,16] [,16] [,16] [,16] [,16] [,16] [,16] [,16] [,16] [,16] [,16] [,16] [,16] [,16] [,16] [,16] [,16] [,16] [,16] [,16] [,16] [,16] [,16] [,16] [,16] [,16] [,16] [,16] [,16] [,16] [,16] [,16] [,16] [,16] [,16] [,16] [,16] [,16] [,16] [,16] [,16] [,16] [,16] [,16] [,16] [,16] [,16] [,16] [,16] [,16] [,16] [,16] [,16] [,16] [,16] [,16] [,16] [,16] [,16] [,16] [,16] [,16] [,16] [,16] [,16] [,16] [,16] [,16] [,16] [,16] [,16] [,16] [,16] [,16] [,16] [,16] [,16] [,16] [,16] [,16] [,16] [,16] [,16] [,16] [,16] [,16] [,16] [,16] [,16] [,16] [,16] [,16] [,16] [,16] [,16] [,16] [,16] [,16] [,16] [,16] [,16] [,16] [,16] [,16] [,16] [,16] [,16] [,16] [,16] [,16] [,16] [,16] [,16] [,16] [,16] [,16] [,1
```

Do the values differ significantly between control and treatment groups?

#### Permutation tests

**IDEA**: If F = G then group label does not matter We may permute labels and still have a sample from F (or G)



Test statistic:

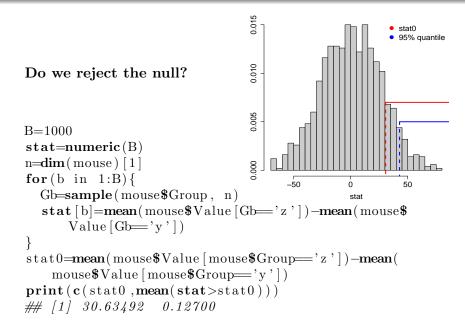
$$T(X) = \text{mean}(\text{values}|\text{group} = z) - \text{mean}(\text{values}|\text{group} = y)$$

#### Permutation test: scheme

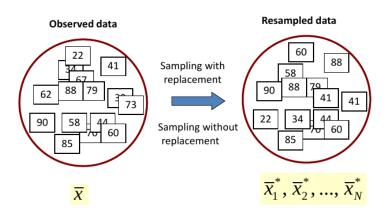
- 1: T(X) value of statistic from observed data
- 2: Create permutations  $g_1^*, \ldots, g_B^*$  of group variable {If the number of permutations is too large, sample B randomly **without** replacement. E.g. generate random permutations and keep only unique ones.}
- 3: Evaluate test statistic on each permutation

- 4: Estimate p-value:  $\hat{p} = \#\{T(X_{g_b^*}) \ge T(X)\}/B$
- 5: If test is two-sided:  $\hat{p} = \#\{|T(X_{g_h^*})| \ge |T(X)|\}/B$

#### Permutation tests



## Resampling methods



# Jackknife and bootstrap

Theory different, coding similar

Data (i.i.d.)  $X \sim F(\cdot, w)$ 

- 1: Observed data:  $D = (X_1, \dots, X_n)$ , estimator  $\widehat{w} = T(D)$ 
  - 2: for i = 1, ..., B { Jackknife  $B \le n$ } do
  - 3: Generate

$$D_i^* = (X_1^*, \dots, X_n^*)$$
 by sampling with replacement {Nonparametric Bootstrap,  $F$  unknown}

$$D_i^* = X[-i] \{$$
**Jackknife**,  $F$  unknown $\}$ 

$$D_i^* = (X_1^*, \dots, X_n^*)$$
 by generating from  $F(\cdot, \hat{w})$  {**Parametric Bootstrap**,  $F$  known}

- 4: end for
- 5: Distribution of  $\widehat{w}$  is estimated by  $T(D_1^*), \ldots, T(D_B^*)$  {The histogram based on resampled values is used in place of the true density.}

#### Uncertainty estimation: confidence intervals

Estimate  $100(1-\alpha)\%$  percentile confidence interval for w  $se(\cdot)$  is the square root of estimated variance (computationally heavy) **NOT** by jackknife **TOO DEPENDENT!!** 

```
1: Compute T(D_1^*), \ldots, T(D_R^*)
2: Sort in ascending order, obtaining y_1, \ldots, y_B
   {percentile method} OR
   Compute y_i = (T(D_i^*) - T(D))/(se(T(D_i^*))) \ i = 1, ..., B
   \{\mathbf{t} \text{ method}\}\
3: Define A_1 = [(B\alpha/2)], A_2 = |(B - B\alpha/2)|
4: Confidence interval is given by
   (y_{A_1}, y_{A_2}) {percentile method} OR
   (T(D) - se(T(D^*)) \cdot y_{A_1}, T(D) + se(T(D^*)) \cdot y_{A_2})
   \{\mathbf{t} \text{ method}\}\
```

Hypothesis testing: does statistic from observed data fall into CI  $(H_0)$  or not  $(H_1)$ 

### Uncertainty estimation: variance of estimator

#### Bootstrap

$$\widehat{\operatorname{Var}\left[T(\cdot)\right]} = \frac{1}{B-1} \sum_{i=1}^{B} \left( T(D_i^*) - \overline{T(D^*)} \right)^2$$

**Jackknife** (n = B)

$$\widehat{\operatorname{Var}\left[T(\cdot)\right]} = \frac{1}{n(n-1)} \sum_{i=1}^{n} (T_i^*) - J(T))^2,$$

where

$$T_i^* = nT(D) - (n-1)T(D_i^*)$$
  $J(T) = \frac{1}{n} \sum_{i=1}^n T_i^*$ 

# Bootstrap in R

```
library ("boot")
stat1<-function(data, vn){
    data < -as \cdot data \cdot frame(data[vn,])
    res<-lm(Response Predictor, data)
    res$coefficients[2]
                                                2.0
                                                    2.1
                                                        22
x \leftarrow rnorm(100); data \leftarrow cbind(Predictor=x, Response=3+2*)
   x+rnorm(length(x),sd=0.5))
res \leftarrow boot(data, stat1, R=1000)
print (boot.ci(res))
## BOOTSTRAP CONFIDENCE INTERVAL CALCULATIONS
##Based on 1000 bootstrap replicates
#Intervals:
\#Level Normal
                                   Basic
#95% (1.933, 2.164) (1.935, 2.162)
# Level Percentile
                                    BCa
#95\% (1.934, 2.161) (1.936, 2.166)
```

## Bootstrap bias correction

- 1: Observed data:  $D = (X_1, \dots, X_n)$ , estimator  $\widehat{w} = T(D)$
- 2: **for** i = 1, ..., B **do**
- 3: Generate

 $D_i^* = (X_1^*, \dots, X_n^*)$  by sampling with replacement.

- 4: Calculate  $T_i^* = T(D_i^*)$ .
- 5: **end for**
- 6: Bias corrected estimator is

$$T_1 := 2T(D) - \frac{1}{B} \sum_{i=1}^{B} T_i^*.$$

Jackknife also has a bias correction method (see last year's slides).

#### Comments

- Jackknife overestimate variance
- Bootstrap—t method is more accurate than percentile
- Permutations: sampling without replacement, bootstrap with
- Permutation p-value exact if all permutations used, bootstrap always approximate
- Bootstrap may be used for a wider class of problems
- Nonparametric bootstrap works badly for small samples (n < 40)
- Parametric bootstrap can work for small samples
- Bias corrections
- Methods do not require distributional assumptions

#### Permutation tests for model selection

**Data** predictors: X[,c(V1,V2)], response: Y **Model** M relating Y and X

#### Competing models

 $H_0$  variables V1 should not be in M (smaller model)  $H_1$  all variables are significant **Test statistic**: T(M)

#### Permutation test

- 1: **for** i = 1 ... B **do**
- Obtain V1\* by permuting order of columns in V1, fit model Y=M(X[,c(V1\*,V2)])
- 3: Compute test statistic  $T_i$  for this model
- 4: end for
- 5: Compute p-value using above distribution of T

# Summary

- Why are some models better than others?
- Hypothesis testing
- Monte Carlo hypothesis testing
- Resampling methods (permutations, jackknife, bootstrap)
- Simulation methods (parametric bootstrap)