Model Selection and Hypothesis Testing

732A90
Computational Statistics

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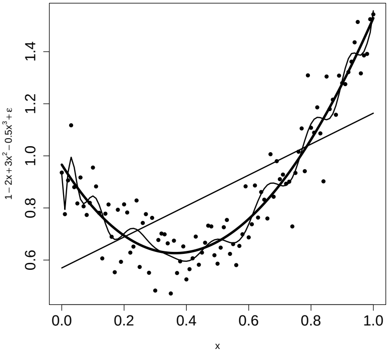
Model selection



Tools for model selection

- **Comparing different models**
- Information criteria (not this course)
- Cross–validation
- Hypothesis testing

- **Uncertainty estimation**
- Confidence intervals

Hypothesis testing: **Recap**

1. Assume a probabilistic model
State a null hypothesis (H_0 e.g. no difference) and alternative (H_1 difference)

2. Observe data X
3. Calculate a test statistic e.g. $T(X) = (\overline{X})/(\widehat{\mathrm{sd}(X)})$ (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

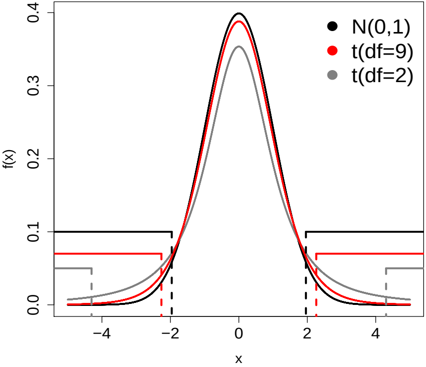
```
x<-rnorm(10,mean=4,sd=1)
```

Hypotheses:

$$H_0 : \mu = 4, X \sim \mathcal{N}(\mu, \sigma^2)$$
$$H_1 : \mu \neq 4, X \sim \mathcal{N}(\mu, \sigma^2)$$

Test statistic

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



```
tx<-(mean(x)-4)/(sqrt(var(x)/length(x)))
t0<-qt(0.975,df=length(x)-1)
(tx>t0)||(tx< (-t0)) ## reject if TRUE
```

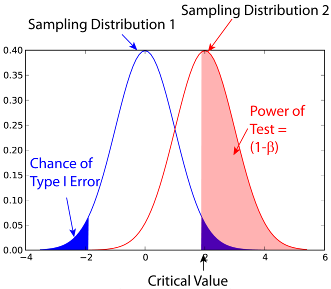
Hypothesis testing: Power

How does one compares different statistics?

POWER

Power = 1 − Type II error

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



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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.

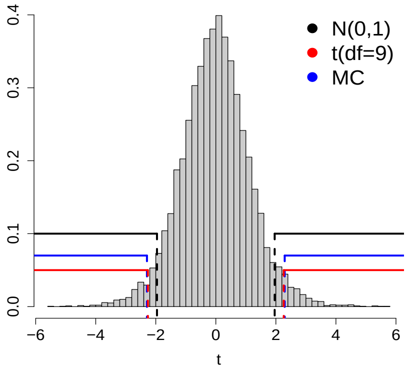
$H_0 : \mu = 4, X \sim \mathcal{N}(\mu, \sigma^2)$
$H_1 : \mu \neq 4, X \sim \mathcal{N}(\mu, \sigma^2)$

Test statistic

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

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

Monte Carlo Hypothesis testing



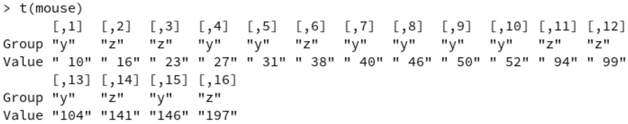
```
x<-rnorm(10,4,1)
s<-var(x)
B<-10000
n<-length(x)
tsamp<-rep(NA,B)
for (i in 1:B){
      Y<-rnorm(n,4,s)
      tsamp[i]<-(mean(Y)-4)/(sd(Y)/sqrt(length(Y)))
}
hist(tsamp,breaks=50,col=gray(0.8),main="",xlab="t"
   ,ylab="",freq=FALSE,cex.axis=1.5,cex.lab=1.5)
```

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:
  - Population 1 distributed as F
  - Population 2 distributed as G
  - $H_0 : F = G$
    $H_1 : F \neq G$

Permutation tests: mouse data

- Control group
- Treatment group
- Group variable g
- Values variable v

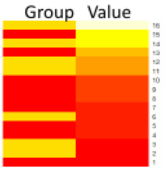


```
> t(mouse)
      [,1]  [,2]  [,3]  [,4]  [,5]  [,6]  [,7]  [,8]  [,9]  [,10] [,11] [,12]
Group "y"   "z"   "z"   "y"   "y"   "z"   "y"   "y"   "y"   "y"   "z"   "z"  
Value " 10" " 16" " 23" " 27" " 31" " 38" " 40" " 46" " 50" " 52" " 94" " 99"
      [,13] [,14] [,15] [,16]
Group "y"   "z"   "y"   "z"  
Value "104" "141" "146" "197"
```

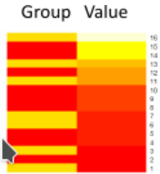
Do the values differ significantly between control and treatment groups?

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)



Before permutation



After permutation

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: $\hat{p} = \#\{T(X_{g_b^*}) \geq T(X)\}/B$
5: If test is two–sided: $\hat{p} = \#\{|T(X_{g_b^*})| \geq |T(X)|\}/B$
```

Permutation test: example

Data	Group	A	B	A	B	B	A	$\overline{\mathrm{A}} = 5/3$
	Value	1	2	2	1	1	2	$\overline{\mathrm{B}} = 4/3$
Set 1	Group	A	A	B	A	B	B	$\overline{\mathrm{A}} = 4/3$
	Value	1	2	2	1	1	2	$\overline{\mathrm{B}} = 5/3$
Set 2	Group	B	B	A	B	A	A	$\overline{\mathrm{A}} = 5/3$
	Value	1	2	2	1	1	2	$\overline{\mathrm{B}} = 4/3$
Set 3	Group	B	B	B	A	A	A	$\overline{\mathrm{A}} = 4/3$
	Value	1	2	2	1	1	2	$\overline{\mathrm{B}} = 5/3$

Observed difference is: $\overline{\mathrm{A}} - \overline{\mathrm{B}} = 5/3 - 4/3 = 1/3$
$\overline{\mathrm{A}} - \overline{\mathrm{B}}$ from permuted data: $\{-1/3,\ 1/3,\ -1/3\}$

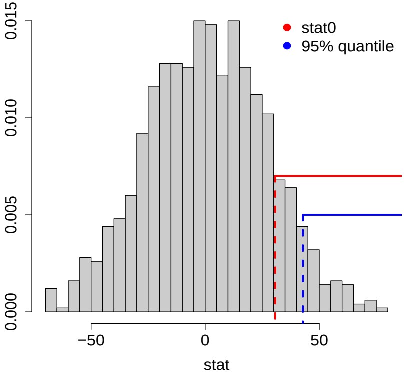
1/3 plausible based on background distribution?

Do conclusions differ between original and permuted data?

In permuted data: **NO SIGNAL!**

Permutation tests

Do we reject the null?



```
B=1000
stat=numeric(B)
n=dim(mouse)[1]
for(b in 1:B){
  Gb=sample(mouse$Group, n)
  stat[b]=mean(mouse$Value[Gb=='z'])-mean(mouse$
      Value[Gb=='y'])
}
stat0=mean(mouse$Value[mouse$Group=='z'])-mean(
    mouse$Value[mouse$Group=='y'])
print(c(stat0,mean(stat>stat0)))
## [1] 30.63492 0.12700
```

Resampling methods

Observed data:
75, 67, 89, 73, 59, 87, 76, 68, 77, 79, 74, 43, 88, 81, 78, 55, 44
$\overline{X} = 71.353$

Resampled data 1:
43, 59, 87, 75, 78, 89, 81, 77, 78, 68, 44, 43, 44, 89, 75, 73, 74
$\overline{X}_1^* = 69.235$

Resampled data 2:
88, 81, 74, 76, 77, 79, 75, 78, 68, 78, 87, 68, 76, 87, 67, 87, 44
$\overline{X}_2^* = 75.882$

Resampled data 3:
87, 68, 79, 75, 67, 43, 75, 73, 55, 59, 68, 88, 77, 79, 77, 89, 88
$\overline{X}_3^* = 73.353$

Jackknife and bootstrap

Theory **different**, coding **similar**

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

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

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

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

       $D_i^* = (X_1^*, \ldots, X_n^*)$ 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.}
```

Jackknife: Details

- Partition sample into r groups
- Group size $k \geq 1$
- For simplicity: $n = r \cdot k$
- $X_{[-i]}$ sample without group i, $i = 1, \ldots, r$

  $\rightarrow$ size of $X_{[-i]}$: $n - k$
- In step i compute estimation T from $X_{[-i]}$

  $\rightarrow$ $B \leq n$ (or $B \leq r$ if $k > 1$)

Nonparametric Bootstrap: example

Data: 1, 2, 2, 1, 3, 4, 1	$\overline{X} = 14/7 = 2$
Set 1: 1, 2, 2, 2, 3, 1, 1	$\overline{X}_1^* = 12/7$
Set 2: 1, 1, 1, 3, 3, 2, 2	$\overline{X}_2^* = 13/7$
Set 3: 4, 4, 4, 3, 1, 2, 1	$\overline{X}_3^* = 19/7$
Set 4: 2, 1, 1, 2, 1, 1, 4	$\overline{X}_4^* = 12/7$
Set 5: 3, 4, 4, 3, 2, 2, 4	$\overline{X}_5^* = 22/7$

Boostrap sample: $\{12/7, 13/7, 19/7, 12/7, 22/7\}$

$$\text{Var}\left[\overline{X}^*\right] = \text{Var}\left[\{12/7, 13/7, 19/7, 12/7, 22/7\}\right]$$

quantile: $P(\overline{X} \leq 3) \approx 4/5$
$P(\overline{X} \leq 2) \approx 3/5$

IDEA: Instead of working with the true (unknown) distribution underlying $\overline{X}$ we take the observed sample as a substitute.

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 $T(D_1^*), \ldots, T(D_B^*)$
2: Sort in ascending order, obtaining $y_1, \ldots, y_B$
   {percentile method} OR
   Compute $y_i = (T(D_i^*) - T(D))/(se(T(D_i^*)))$ $i = 1, \ldots, B$
   {t method}
3: Define $A_1 = \lceil (B\alpha/2) \rceil$, $A_2 = \lfloor (B - B\alpha/2) \rfloor$
4: Confidence interval is given by
   $(y_{A_1}, y_{A_2})$ {percentile method} OR
   $(T(D) - se(T(D^*)) \cdot y_{A_1}, T(D) + se(T(D^*)) \cdot y_{A_2})$
   {t method}
```

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

Uncertainty estimation: variance of estimator

Bootstrap

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

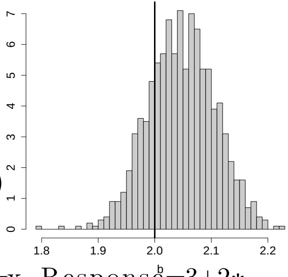
Jackknife $(n = B)$

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

where

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

Bootstrap in R



```
library(”boot”)
stat1<-function(data,vn){
    data<-as.data.frame(data[vn,])
    res<-lm(Response~Predictor ,data)
    res$coefficients[2]
}
x<-rnorm(100);data<-cbind(Predictor=x,Response=3+2*
   x+rnorm(length(x),sd=0.5))
res<-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

```
Observed data: $D = (X_1, \ldots, X_n)$, estimator $\widehat{w} = T(D)$
for $i = 1, \ldots, B$ do
    Generate

    $D_i^* = (X_1^*, \ldots, X_n^*)$ by sampling with replacement.
    Calculate $T_i^* = T(D_i^*)$.
end for
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 2016 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

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

Permutation tests for model selection: example

Data

Y	V_1^1	V_2^1	V_1^2	V_2^2
3	1	2	3	4
3	1	3	5	1
1	3	2	2	1
3	5	5	4	2
2	2	2	1	3
2	4	4	3	2

Data*

Y	V_2^1	V_1^1	V_1^2	V_2^2
3	2	1	3	4
3	3	1	5	1
1	2	3	2	1
3	5	5	4	2
2	2	2	1	3
2	4	4	3	2

Model: $Y = a_{11}V_1^1 + a_{12}V_2^1 + a_{21}V_1^2 + a_{22}V_2^2 + \epsilon$
Calculate some summary statistic, e.g. R^2

Model*: $Y = a_{11}V_2^1 + a_{12}V_1^1 + a_{21}V_1^2 + a_{22}V_2^2 + \epsilon$ with R^{*^2}

Compare R^2 and R^{*^2}
If R^{*^2} just as good, then V_1^1, V_2^1 are just *noise*.

Summary

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