Data Science School at DKE

Summer 2019

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Maastricht University, June 2019

About Me – My Background

- Assistant Professor (DKE, Maastricht University)
  - Teaching:
    - Statistics and Software Engineering courses
  - Research:
    - Statistical modeling of complex data
    - Omics (CyTOF and RNA-seq) and imaging data (2d and 3d)
    - Uncertainty quantification
    - Convergence of computer simulations
- Postdoc in **Statistics** (Stanford University)
- PhD in

  Computer Science (Inria, France) and

  Biomedical Engineering (University of Bern, Switzerland)

Topics of Today

1. What is Data Science?
2. Computer Simulations
3. The Bootstrap
4. Regularized Regression

What is Data Science?

What?

- Sciences are primarily defined by their **questions** not their tools

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- Example: **Astrophysics** is the discipline that
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What?

- Sciences are primarily defined by their **questions** not their tools
- Example: **Astrophysics** is the discipline that
  learns the composition of the stars,
  not the discipline that uses the spectroscope
- Definition: **Data science** is the discipline that
  describes,
  predicts, and
  makes causal inferences,
  not the discipline that uses machine learning algorithms or
  other technical tools

Classification of Tasks

	Data Science Task		
	Description	**Prediction**	**Causal inference**
Example of scientific question	How can women aged 60–80 years with stroke history be partitioned in classes defined by their characteristics?	What is the probability of having a stroke next year for women with certain characteristics?	Will starting a statin reduce, on average, the risk of stroke in women with certain characteristics?
Data	• Eligibility criteria • Features (symptoms, clinical parameters …)	• Eligibility criteria • Output (diagnosis of stroke over the next year) • Inputs (age, blood pressure, history of stroke, diabetes at baseline)	• Eligibility criteria • Outcome (diagnosis of stroke over the next year) • Treatment (initiation of statins at baseline) • Confounders • Effect modifiers (optional)
Examples of analytics	Cluster analysis …	Regression Decision trees Random forests Support vector machines Neural networks …	Regression Matching Inverse probability weighting G-formula G-estimation Instrumental variable estimation …

Source: Hernán, Hsu, and Healy (2019)

Why Now?

- **More data**
- **Cheaper computers**
- The field itself has existed for 50 years already (Donoho 2017)
- Two cultures (Breiman 2001)
  - Prediction: To be able to predict what the responses are going to be to future input variables
  - Inference: To [infer] how nature is associating the response variables to the input variables
- The predictive culture is currently winning because of **The Common Task Framework**

The Common Task Framework

Donoho (2017):

(a) A **publicly available training dataset** involving, for each observation, a list of (possibly many) feature measurements, and a class label for that observation.

(b) A set of enrolled **competitors** whose common task is to infer a class prediction rule from the training data.

(c) A **scoring referee**, to which competitors can submit their prediction rule. The referee runs the prediction rule against a testing dataset which is sequestered behind a Chinese wall. The referee objectively and automatically reports the score (prediction accuracy) achieved by the submitted rule.

The Common Task Framework: Netflix Prize

NETFLIX

Netflix Prize COMPLETED

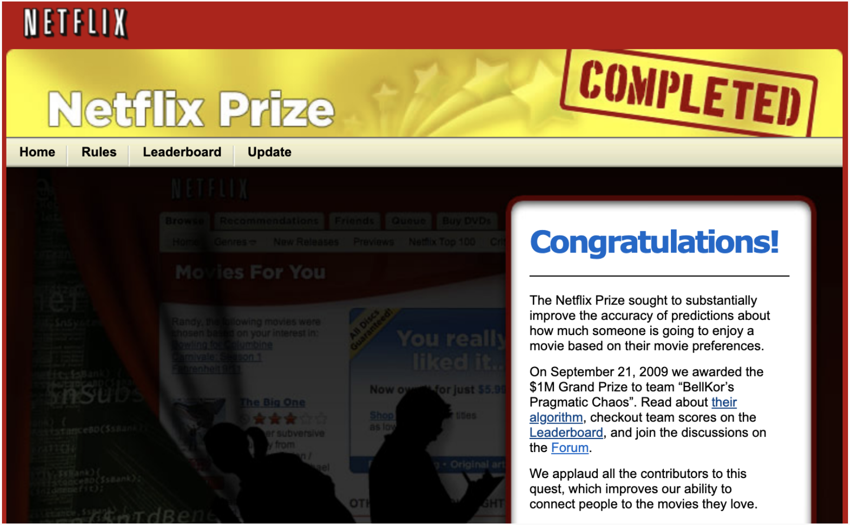
Home | Rules | Leaderboard | Update

Leaderboard

Showing Test Score. Click here to show quiz score

Rank	Team Name	Best Test Score	% Improvement	Best Submit Time
Grand Prize - RMSE = 0.8567 - Winning Team: BellKor's Pragmatic Chaos				
1	BellKor's Pragmatic Chaos	0.8567	10.06	2009-07-26 18:18:28
2	The Ensemble	0.8567	10.06	2009-07-26 18:38:22
3	Grand Prize Team	0.8582	9.90	2009-07-10 21:24:40
4	Opera Solutions and Vandelay United	0.8588	9.84	2009-07-10 01:12:31
5	Vandelay Industries !	0.8591	9.81	2009-07-10 00:32:20
6	PragmaticTheory	0.8594	9.77	2009-06-24 12:06:56
7	BellKor in BigChaos	0.8601	9.70	2009-05-13 08:14:09
8	Dace_	0.8612	9.59	2009-07-24 17:18:43
9	Feeds2	0.8622	9.48	2009-07-12 13:11:51
10	BigChaos	0.8623	9.47	2009-04-07 12:33:59
11	Opera Solutions	0.8623	9.47	2009-07-24 00:34:07
12	BellKor	0.8624	9.46	2009-07-26 17:19:11

The Common Task Framework: Netflix Prize

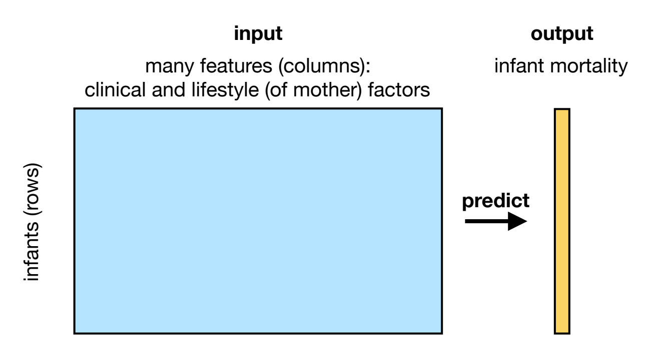


Prediction

- Google's algorithm to **diagnose** diabetic retinopathy (after 54 ophthalmologists classified more than 120,000 images)
- Microsoft's algorithm to **predict** pancreatic cancer months before its usual diagnosis (using the online search histories of 3,000 users who were later diagnosed with cancer), and
- Facebook's algorithm to **detect** users who may be suicidal (based on posts and live videos)

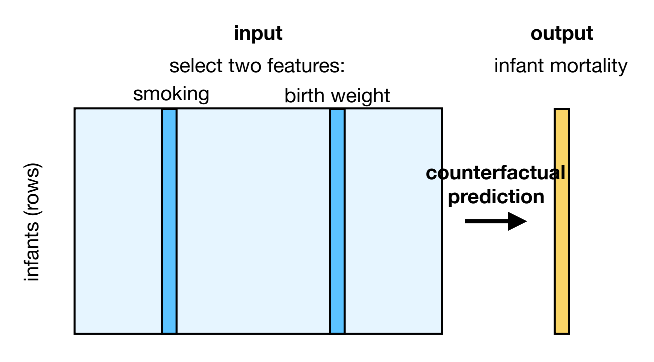
Prediction vs. Causal Inference

- Prediction: Large health records database to predict infant mortality from clinical and lifestyle factors

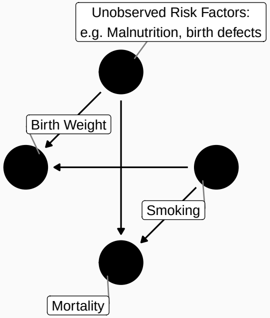


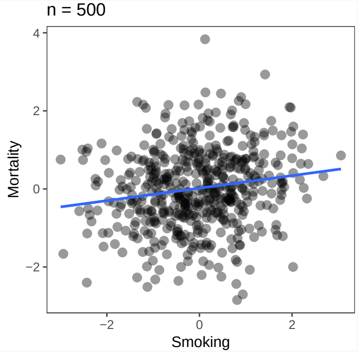
Prediction vs. Causal Inference: Birth Weight Paradox

- Causality: Answer what if statements, e.g. if a mother stops smoking during pregnancy does this reduce infant mortality



Prediction vs. Causal Inference: Birth Weight Paradox

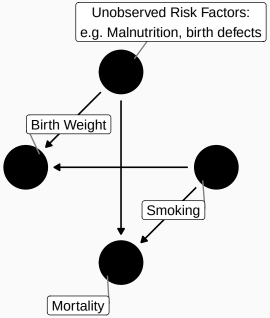


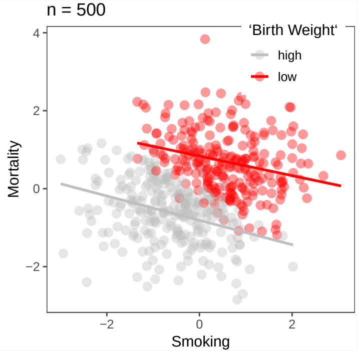



```
lm(formula = Mortality ~ Smoking,
   data = health_records) %>% tidy
```

```
## # A tibble: 2 x 5
##   term        estimate std.error statistic  p.value
##   <chr>          <dbl>     <dbl>     <dbl>    <dbl>
## 1 (Intercept)   0.0208    0.0453     0.460 0.646
## 2 Smoking       0.161     0.0429     3.75  0.000200
```

Prediction vs. Causal Inference: Birth Weight Paradox






```r
lm(formula = Mortality ~ Smoking + `Birth Weight`,
   data = health_records) %>% tidy
```

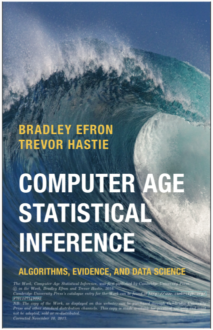
```
## # A tibble: 3 x 5
##   term              estimate std.error statistic  p.value
##   <chr>                <dbl>     <dbl>     <dbl>    <dbl>
## 1 (Intercept)         -0.795    0.0526    -15.1  1.01e-42
## 2 Smoking             -0.284    0.0387     -7.34 8.57e-13
## 3 `Birth Weight`low    1.65     0.0818     20.2  1.61e-66
```

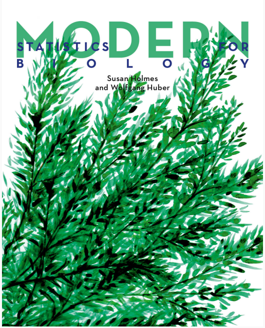
Prediction vs. Causal Inference: Birth Weight Paradox

- Birth weight is strongly associated with both maternal smoking and infant mortality
- Adjustment for it **induces bias**
- This bias is often referred to as the **“birth weight paradox”**:
    - Low birth weight babies from mothers who smoked during pregnancy have a lower mortality than those from mothers who did not smoke during pregnancy (Hernández-Díaz, Schisterman, and Hernán 2006)

Computer Simulations

Computer Age





Books freely available:

- Efron and Hastie (2016): website
- Holmes and Huber (2019): website

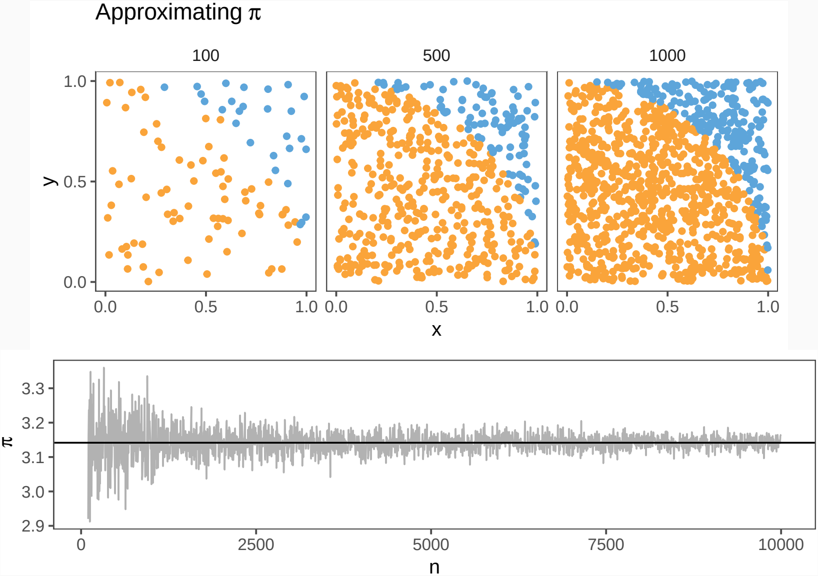
Modern Statistics

To quote Andrew Gelman (source):

```
"If you wanted to do foundational research in
statistics in the mid-twentieth century, you had to
be bit of a mathematician, ... if you want to do
statistical research at the turn of the twenty-first
century, you have to be a computer programmer."
```

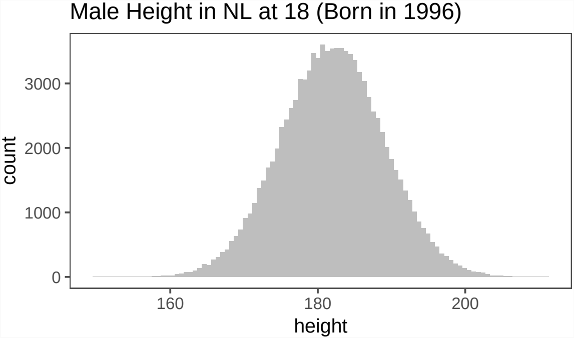
- RStudio Cloud for labs: https://rstudio.cloud/project/350555

Simulations Example



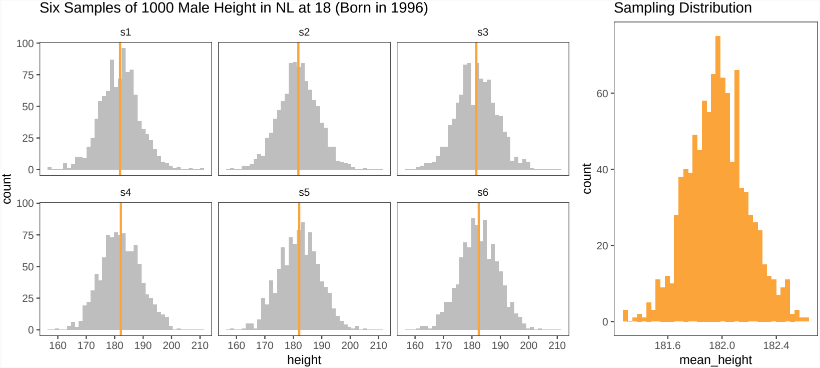
The Bootstrap

Height Example



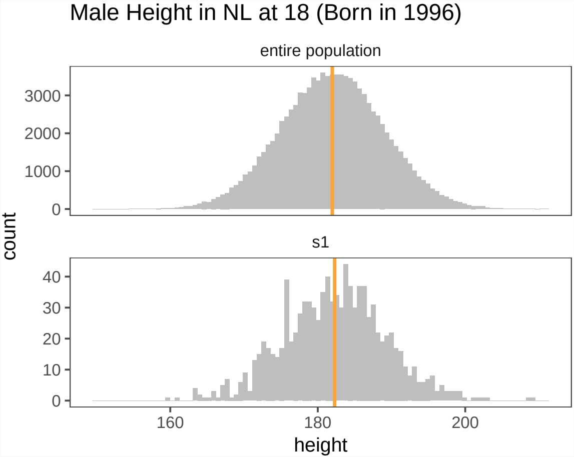
- Let's assume that we measured all 18 year old Dutch male born in 1996

Height Example



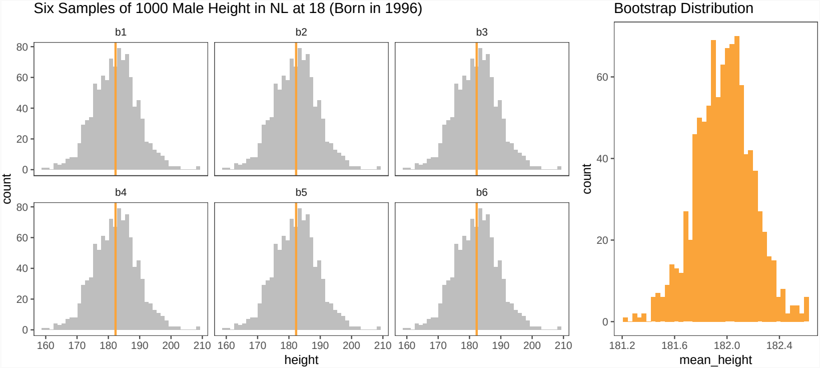
- In real life, too expensive
- We can only take samples from the population
- Sample surveys: **s1**, **s2**, **s3**, **s4**, **s5**, and **s6**

Height Example



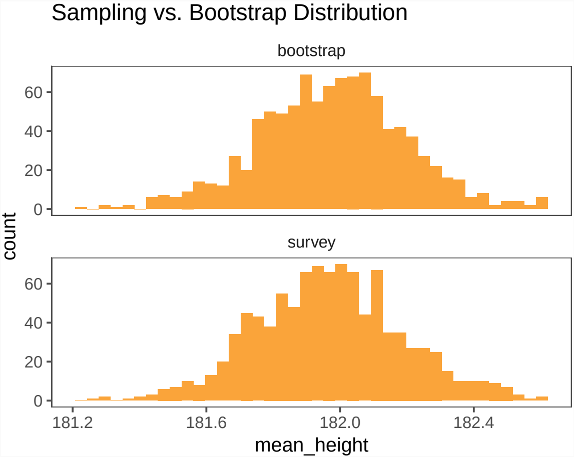
- Compare **population** with sample **s1**

Height Example



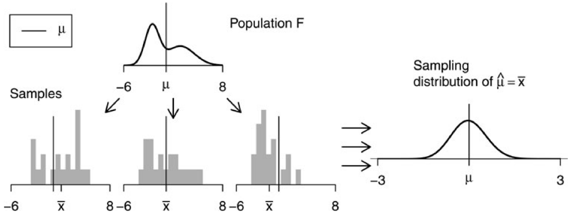
- Bootstrap samples: **b1**, **b2**, **b3**, **b4**, **b5**, and **b6**

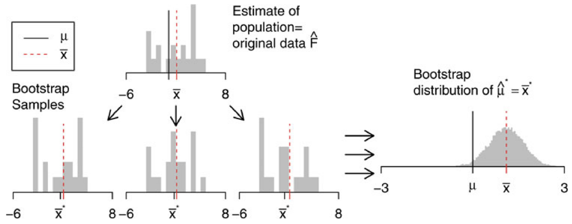
Height Example



- Compare distributions

Main Idea



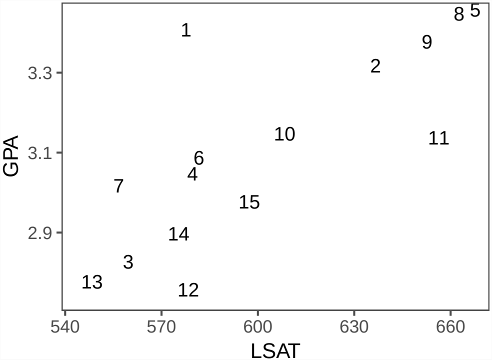


(Hesterberg 2015)

Monte Carlo Simulations

- If number of observations is **small**,
  then we can do **exhaustive bootstrap**
- If number of observations is **large**,
  then we can do **Monte Carlo simulations**

Law Schools Example



- Sample correlation coefficient:

```r
theta_hat = cor(law$LSAT, law$GPA)
theta_hat
```

```
## [1] 0.7763745
```

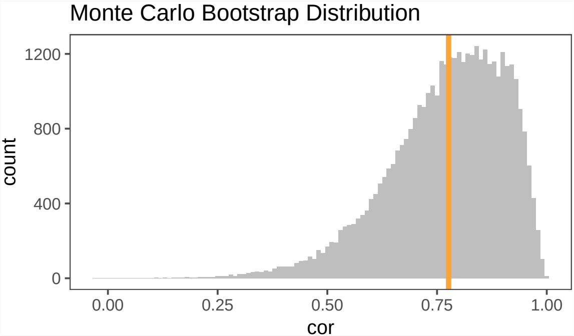
Law Schools Example

- How accurate is this estimate?
- Let's look at the bootstrap distribution:

```
draw_bootstrap_sample = function() {
  n = dim(law)[1]
  ind = sample(n, replace = TRUE)
  return(cor(law[ind,]$LSAT, law[ind,]$GPA))
}
B = 40000
theta_star = replicate(B, draw_bootstrap_sample())
```

Law Schools Example

- Evaluate the correlation coefficient using a Monte Carlo simulation:



Law Schools Example

- Create matrix of all
$$\binom{2n-1}{n-1}$$
enumerations
- Using R package `partitions`:

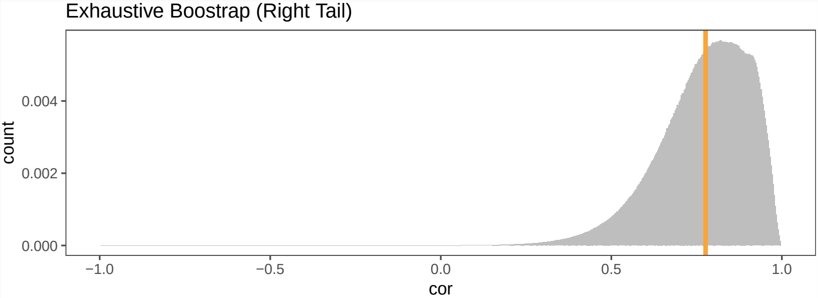
```
n = 15
allCompositions = compositions(n,n)
```

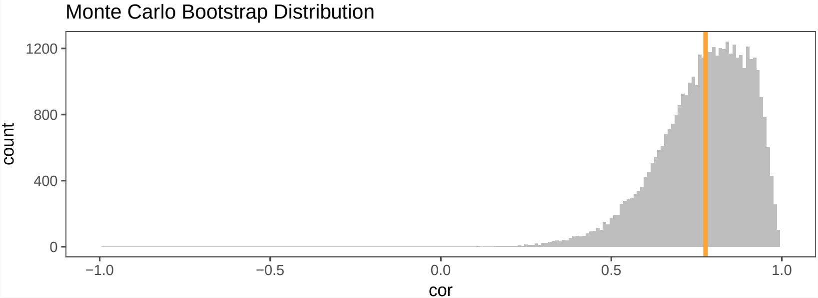
- Each bootstrap sample has weight according to
$$\text{Multinomial}\left(\#\text{trials } = n, \text{probabilities } = \frac{1}{n}, \ldots, \frac{1}{n}\right)$$
- For more details and background: Diaconis and Holmes (1994)

```r
allCompositions[,1:10]
```

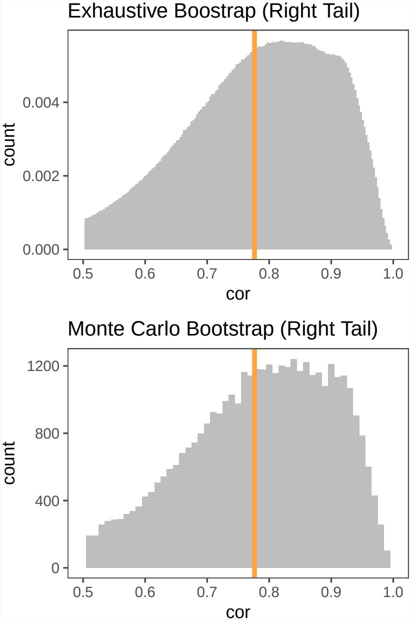
```
##       [,1] [,2] [,3] [,4] [,5] [,6] [,7] [,8] [,9] [,10]
##  [1,]   15   14   13   12   11   10    9    8    7     6
##  [2,]    0    1    2    3    4    5    6    7    8     9
##  [3,]    0    0    0    0    0    0    0    0    0     0
##  [4,]    0    0    0    0    0    0    0    0    0     0
##  [5,]    0    0    0    0    0    0    0    0    0     0
##  [6,]    0    0    0    0    0    0    0    0    0     0
##  [7,]    0    0    0    0    0    0    0    0    0     0
##  [8,]    0    0    0    0    0    0    0    0    0     0
##  [9,]    0    0    0    0    0    0    0    0    0     0
## [10,]    0    0    0    0    0    0    0    0    0     0
## [11,]    0    0    0    0    0    0    0    0    0     0
## [12,]    0    0    0    0    0    0    0    0    0     0
## [13,]    0    0    0    0    0    0    0    0    0     0
## [14,]    0    0    0    0    0    0    0    0    0     0
## [15,]    0    0    0    0    0    0    0    0    0     0
```

Law Schools Example



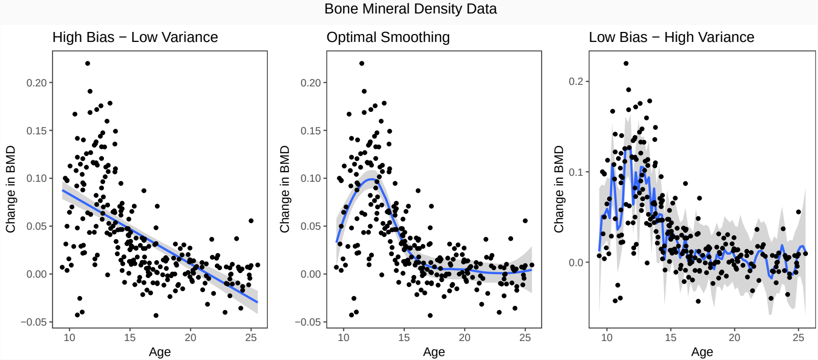


Law Schools Example

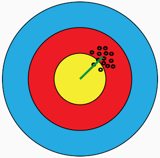


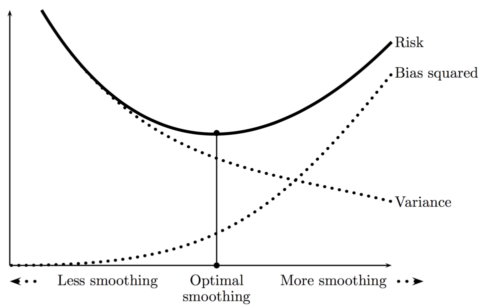
Regularized Regression

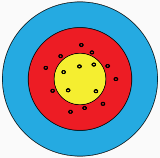
Smoothing



Bone Mineral Density Data
High Bias − Low Variance
Optimal Smoothing
Low Bias − High Variance
Change in BMD
Age
0.20
0.15
0.10
0.05
0.00
−0.05
0.2
0.1
0.0
10
15
20
25

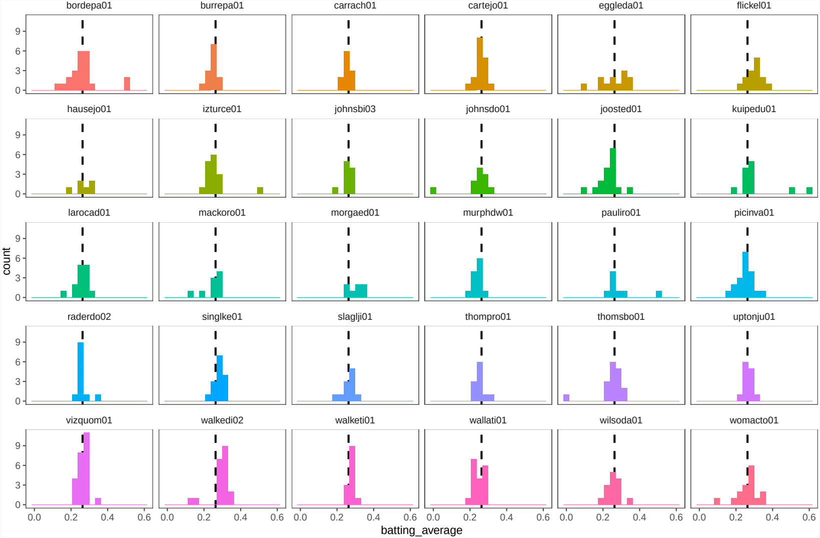






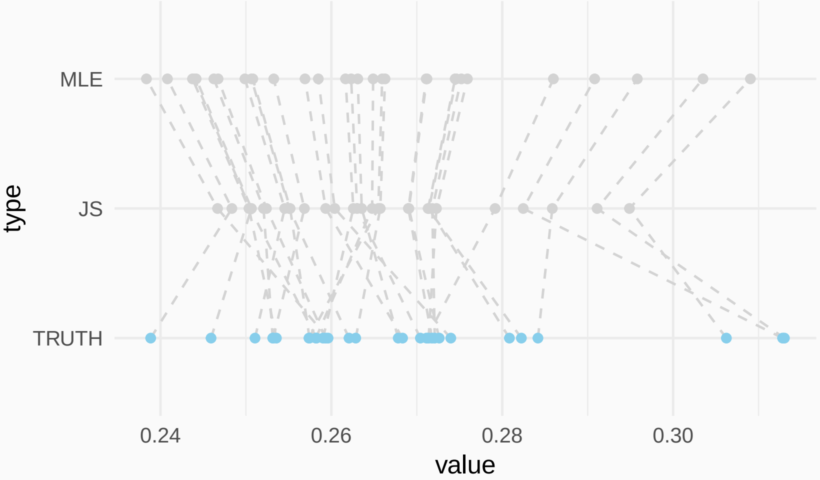
(Wasserman 2006)

Batting Average of Baseball Players



Batting Average of Baseball Players

- Here Maximum Likelihood Estimate (MLE) is the sample mean
- The James-Stein Estimator (JS) Shrinks the MLE



James-Stein Theorem

- For $d \geq 3$, the James-Stein estimator dominates the MLE in terms of expected total squared error; that is

$$E\left[\left\|\hat{\mu}^{\mathrm{JS}} - \mu\right\|^2\right] < E\left[\left\|\hat{\mu}^{\mathrm{MLE}} - \mu\right\|^2\right]$$

where $x_i|\mu_i$ is drawn from a distribution as follows

$$x_i|\mu_i \sim \mathrm{Normal}(\mu_i, 1).$$

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- In our baseball example:

$$3.0 \times 10^{-3} < 4.4 \times 10^{-3}$$

Thus a 31% improvement!

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  Thus a 31% improvement!
- For more R simulations: https://bookdown.org/content/922/james-stein.html

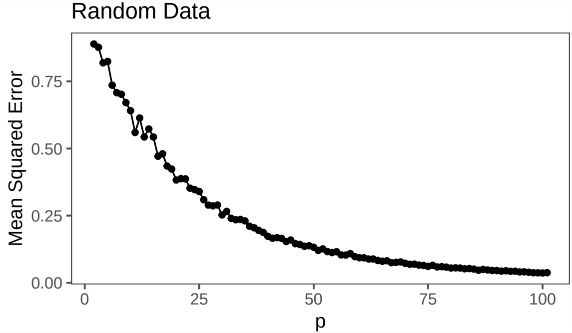
Ridge Regression

- Linear model

$$\mathbf{y} = \mathbf{X}\boldsymbol{\beta} + \boldsymbol{\epsilon}$$

- We observe or define $\mathbf{y}$ and $\mathbf{X}$
- Goal: Estimate $\hat{\boldsymbol{\beta}}$
- Idea: **shrink the coefficients** $\hat{\boldsymbol{\beta}}$ **to zero** (similarly to the Baseball example where we shrank the individual batting averages)
- The amount of shrinkage is controlled by a **tuning parameter** λ (thus estimate depends on it: $\hat{\boldsymbol{\beta}}_\lambda$)

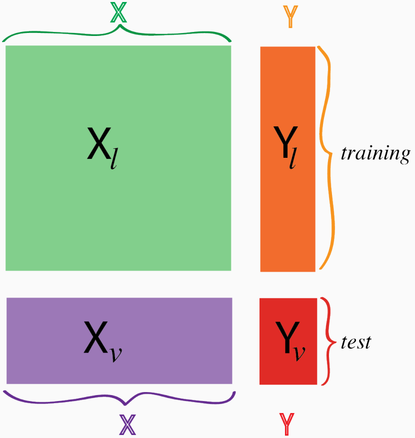
Ridge Regression: Computer Experiment



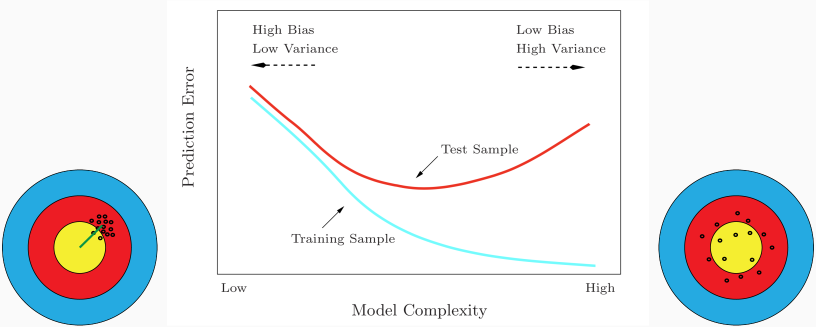
- Simulation setup:
  - Tuning parameter $\lambda = 1$
  - Number of observations $n = 20$
  - Let number of predictors p grow from 2 to 101
  - Both $\mathbf{y}$ and $\mathbf{X}$ are random (no relationship)

Cross-Validation

- **Problem**: model performance evaluated on training data
- **Solution**: train and evaluate on different data



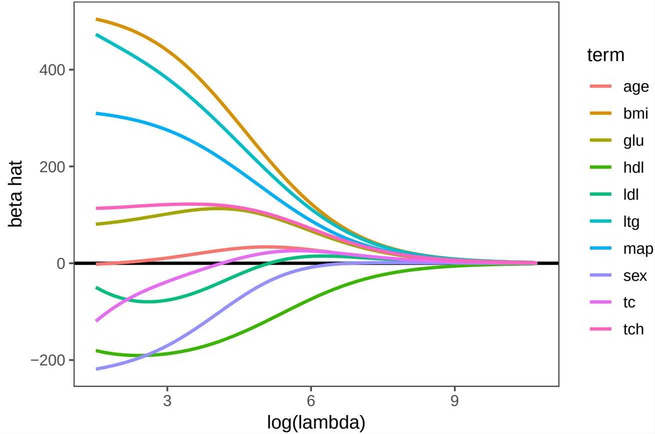
(Holmes and Huber 2019)



(Hastie, Tibshirani, and Friedman 2009)

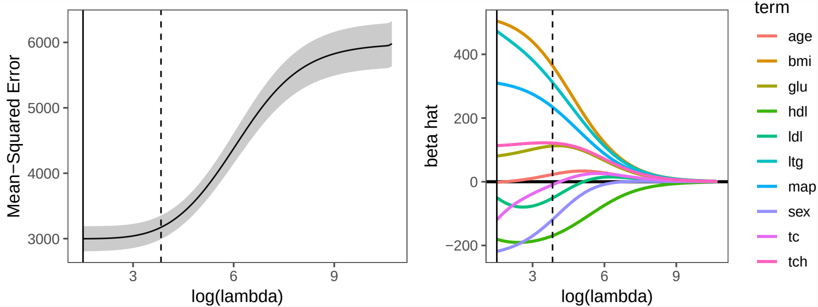
Ridge Regression: Example

- How to pick λ?



Ridge Regression: Example

- Use cross-validation:
  1. Split data in folds
  2. Fit model on all but one fold
  3. Calculate error on the left-out fold



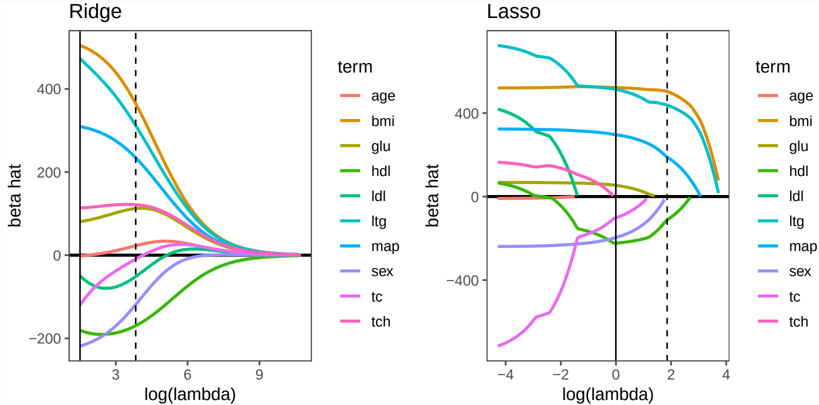
Lasso Regression

- Linear model

$$\mathbf{y} = \mathbf{X}\boldsymbol{\beta} + \boldsymbol{\epsilon}$$

- Idea: shrink the coefficients $\boldsymbol{\beta}$ to zero **and set some of them to zero completely** (similarly to the Baseball example where we shrank the individual batting averages)
- The amount of shrinkage is controlled by a **tuning parameter** λ (thus estimate depends on it: $\hat{\boldsymbol{\beta}}_\lambda$)

Lasso Regression: Example



Lab Session

- During the lab, we will get familiar with the following concepts:
  1. R and R markdown
  2. Plotting in R using package `ggplot2`
  3. Computer simulations in R using function `replicate`
  4. Construct bootstrap confidence intervals using function `quantile`
  5. Fitting regularized regression models in R using package `glmfit`
- We will use RStudio Cloud: https://rstudio.cloud/project/350555

References i

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