Bootstrap Variations

Contents

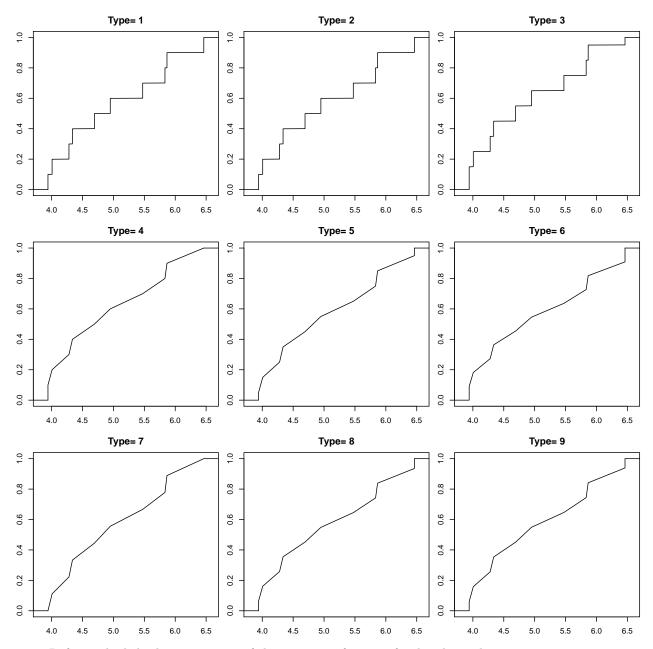
Bootstrap	2
Estimate for F	2
Parameteric Estimate	4
Non-parameteric Bootstrap	5
Parameteric Bootstrap	5
Agricultural census (USA): Parametric Example	6
	7
Agricultural census (USA): Non-parametric Example	
Comparing parametric and non-parametric results	7
Example - Median	8
Bootstrap in Regression	9
Iris Data	9
Resampling the Pairs: non-parametric bootstrap	11
Bootstrap the Regression Coefficients	12
Aside: Comparing Regression Models	13
Bootstrap Regression lines	13
Bootstrap Confidence Interval (Percentile Method)	14
Parametric Bootstrap	18
Illustration	18
Resampling the Errors	19
Illustration	20
Some other Examples	21
•	
Animals Data and LS	21
Animals Data and Robust Regression	22
Aircraft Data and LS	24
Quote	25
sharks <- read.csv("/Data/Sharks/sharks.csv") popSharks <- rownames(sharks)	
#samples <- combn(popSharks, 5)	
$\#N_s \leftarrow ncol(samples)$	
$N_s < 10^4$	
n = 6	
set.seed(341)	
<pre>samples <- sapply(1:N_s, FUN =function(b) sample(popSharks, n, replace = TRUE))</pre>	
<pre>avePop <- mean(sharks[, "Length"]) avesSamp <- apply(samples, MARGIN = 2,</pre>	
tmpAve <- mean(avesSamp)	
tmpSD <- sd(avesSamp)	

Bootstrap

- So far, to bootstrap we have been sampling with replacement from the sample \mathcal{S} .
 - Because the sample ${\mathcal S}$ was viewed as an estimate of the population ${\mathcal P}$
 - This sampling scheme is equivalent to sampling from the empirical distribution function, \hat{F} .
- In other words, we would like to sample from the distribution F, but instead,
 - we obtain a sample using an estimate \widehat{F} .
- What other possible estimates are there for the cumulative distribution function F?

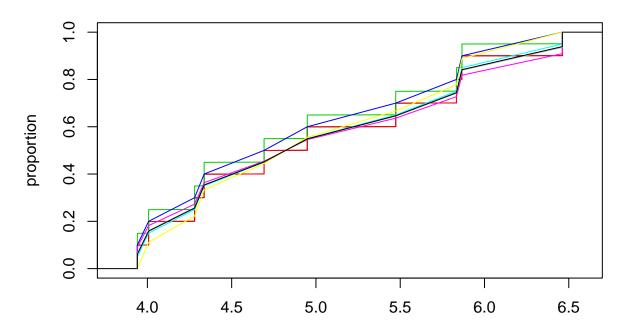
Estimate for F

- Varies empirical distribution functions using the argument type in the quantile function.
 - Generate 10 observations from G(5,1)



- Refer to the help documentation of the quantile function for details on the argument type.
- All on the quantile functions on one plot

Different Empirical Distribution Functions



Parameteric Estimate

- We can estimate the distribution function F(x) using a parametric model $F(x;\theta)$ which is indexed by some parameters.
- Generate 100 observations from $G(\mu = 5, \sigma = 1)$

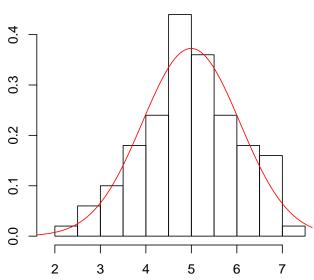
```
set.seed(341)
x = rnorm(100, mean=5)
c(mean(x), sd(x))
```

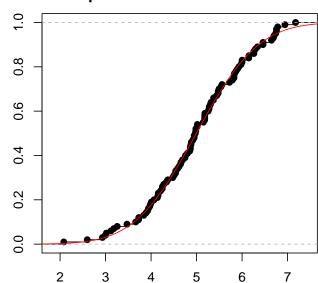
[1] 4.994535 1.070854

• Overlay the fitted Gaussian distribution $G(\mu = \hat{\mu}, \sigma = \hat{\sigma})$ on the empirical CDF.

Empirical Distribution Function

Empirical Distribution Function





Non-parameteric Bootstrap

- For a given sample ${\mathcal S}$ and non-parametric method
 - Obtain an estimate $\hat{F}(x)$ using the sample: this estimate is the empirical CDF
- Generate B bootstrap samples $\mathcal{S}_1^{\star}, \dots, \mathcal{S}_B^{\star}$ using $\widehat{F}(x)$
 - when you sample with replacement from \mathcal{S} , you are generating samples $\mathcal{S}_1^{\star}, \dots, \mathcal{S}_B^{\star}$ using $\widehat{F}(x)$
- Note: Alternatively, we could estimate the density function with some \hat{f} , and do the same thing.

Parameteric Bootstrap

- For a given sample S and parametric model $F(x;\theta)$
 - Obtain an estimate $\widehat{\theta}$ using the sample
- Generate B bootstrap samples $\mathcal{S}_1^{\star}, \dots, \mathcal{S}_B^{\star}$ using $F(x; \widehat{\theta})$.
 - Here, we will generate samples from the model, NOT through sampling with replacement from the sample.

Agricultural census (USA): Parametric Example

• Consider the West region and suppose we obtain a sample of size 50 from the 422 farms in Western region and measure the number of acres in 1987

```
set.seed(341)
acres87 = agpop[agpop$region == "W","acres87"]
N = length(acres87)
n =50
acres87Sam = acres87[sample(1:N, n)]
```

- From a the histogram and empirical distribution function, it seems an exponential distribution with rate equal to $1/\bar{x}$ fits the data well.
 - note that $1/\overline{x}$ is the maximum likelihood estimate of the parameter of the exponential distribution.

Acres from W region in 1987 **ECDF of Acres** 1.2e-06 0.8 9.0 Density 6.0e-07 Fn(x) 0.4 0.2 0.0e+00 0.0 500000 1500000 2500000 3500000 0e+00 1e+06 0 2e+06 3e+06 Acres from 1987 Acres

- The smooth curve is the fitted exponential model on the histogram/empirical CDF based on the data.
- Based on these graphs, exponential distribution seems to be a good fit for the data.
- This means that to repeat the experiment to get more samples each of size n, one can simply generate n random samples from $exp(1/\overline{x})$ distribution.

```
theta = 1/mean(acres87Sam)
B = 10<sup>4</sup>
```

```
Sstar <- sapply(1:B, FUN =function(b) rexp(n, rate=theta))
bootAvg = apply(Sstar,2,mean)</pre>
```

The summary statistics for the sample averages of the **parametric** bootstrap sample are

```
## [1] 99363.83

## Min. 1st Qu. Median Mean 3rd Qu. Max.

## 385665 644119 708854 713696 777726 1157148
```

sd(bootAvg) ; summary(bootAvg)

Agricultural census (USA): Non-parametric Example

- Consider the West region and suppose we obtain a sample of size 50 from the 422 farms in Western region and measure the number of acres in 1987
- From the sample of size 50 we take B samples with replacement, each of size n,
 - we calculate the average on each of the B sampels
 - then we look at the summary statistics of these averages

The summary statistics for the sample averages of the **non-parametric** bootstrap sample are

```
Sstar0 <- sapply(1:B, FUN =function(b) acres87Sam[sample(n,n, replace=TRUE)] )
bootAvg0 = apply(Sstar0,2,mean)
sd(bootAvg0) ; summary(bootAvg0)

## [1] 101643.7

## Min. 1st Qu. Median Mean 3rd Qu. Max.
## 369040 644437 709961 714699 780376 1183734</pre>
```

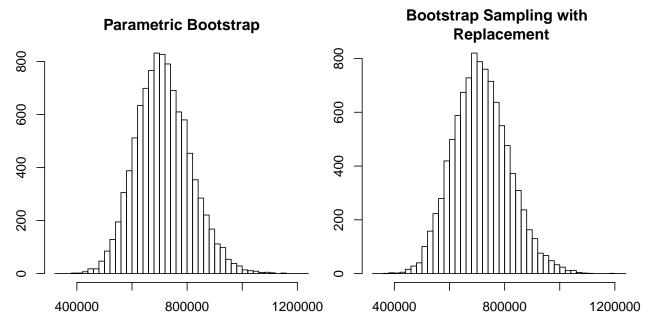
Comparing parametric and non-parametric results

• We can quantify estimating the standard error for the average, or other attributes, using the parametric and non-parametric bootstrap.

```
pseq = seq(0, 1, length.out=1000)
par(mfrow=c(1,2), mar=2.5*c(1,1,1,0.1))

hhPopAve <- hist(extendrange(c(bootAvg,bootAvg0)), breaks = 50, plot = FALSE)$breaks

hist(bootAvg, main="Parametric Bootstrap", breaks= hhPopAve)
hist(bootAvg0, main="Bootstrap Sampling with \n Replacement", breaks= hhPopAve)</pre>
```



- The histograms show very similar distributions for the sample average across the two methods.
- Compare the summary statistics of the parametric and non-parametric samples to see how close the findings of two methods are.
 - This is because the exponential distribution was a good fit to the data.
 - It may not work as well for statistics other than the sample average though (see example below)

Example - Median

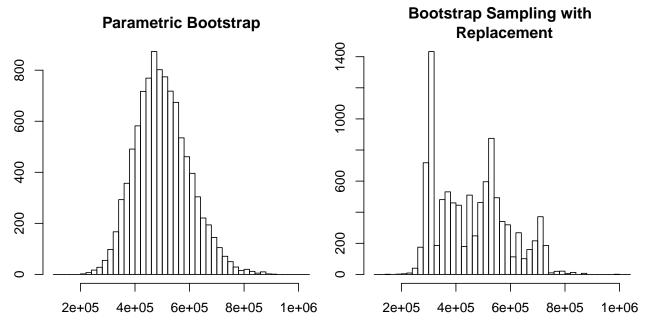
- Now consider the median for the same data, i.e.
 - the West region in the US agrical ture data, and suppose we obtain a sample of size 50 from the 422 farms in Western region and measure the number of acres in 1987.

```
bootMed = apply(Sstar,2, median)
bootMed0 = apply(Sstar0,2,median)

pseq = seq(0, 1, length.out=1000)
par(mfrow=c(1,2), mar=2.5*c(1,1,1,0.1))

hhPopMed <- hist(extendrange(c(bootMed,bootMed0)), breaks = 50, plot = FALSE)$breaks

hist(bootMed, main="Parametric Bootstrap", breaks= hhPopMed)
hist(bootMed0, main="Bootstrap Sampling with \n Replacement", breaks= hhPopMed)</pre>
```



- What do you observe?
- Try other attributes like IQR, min, max, midhinge, CV, etc.

Bootstrap in Regression

• For this section, for simplicity we will treat each data-set as a sample.

Iris Data

- Here we will explore the bootstrap in analyzing the famous Iris data-set.
 - Iris is a data set with 150 cases and 5 variables named Sepal.Length, Sepal.Width, Petal.Length,
 Petal.Width, and Species.
 - We will limit ourselves to the Setosa flower, in which Sepal. Length is our x-covariate and the Sepal. Width is our response.

The Iris data is built-in to R and a part of it is shown below:

```
data(iris)
head(iris)
```

##		Sepal.Length	Sepal.Width	Petal.Length	Petal.Width	Species
##	1	5.1	3.5	1.4	0.2	setosa
##	2	4.9	3.0	1.4	0.2	setosa
##	3	4.7	3.2	1.3	0.2	setosa
##	4	4.6	3.1	1.5	0.2	setosa

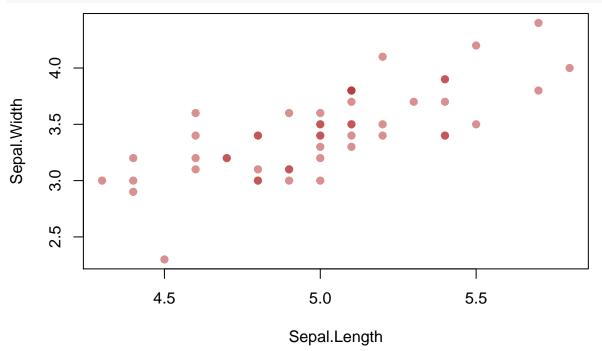


Figure 1: Iris Flower

```
## 5     5.0     3.6     1.4     0.2     setosa
## 6     5.4     3.9     1.7     0.4     setosa
iris.s = iris[iris[,5] == "setosa",-c(3,4,5)]
#head(iris.s)
```

The septal width and septal length seem to be correlated:

```
plot(iris.s, col=adjustcolor("firebrick", 0.5), pch=19)
```



- Here we assume that
 - $-\,$ sepal. Length is our x-covariate and

- the Sepal.Width is our response.

```
x = iris.s$Sepal.Length
y = iris.s$Sepal.Width
n = length(y)
```

• The assumed regression model is

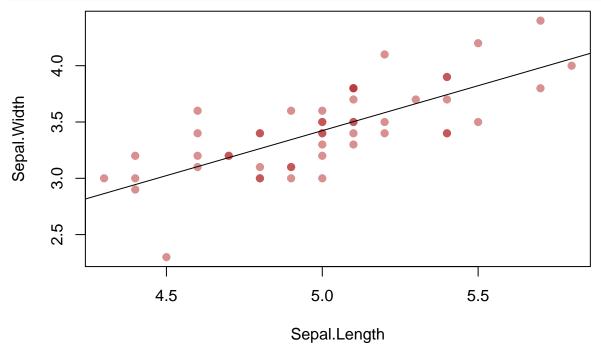
$$Y_i = \alpha + \beta \left(x_i - \overline{x} \right) + R_i$$

where $R_i \sim N(0, \sigma^2)$ and the least squares estimate of $(\widehat{\alpha}, \widehat{\beta})$ is

lm(y~x)\$coef

```
## (Intercept) x
## -0.5694327 0.7985283

data(iris)
iris.s = iris[iris[,5] == "setosa",-c(3,4,5)]
#head(iris.s)
plot(iris.s, col=adjustcolor("firebrick", 0.5), pch=19)
beta.hat = lm(y~ I(x-mean(x)))$coef
abline( beta.hat + c(-beta.hat[2]*mean(x),0) )
```



Resampling the Pairs: non-parametric bootstrap

- How can one assess the sampling variability of the regression line?
 - How can we assess the standard error of the regression line?

• The sample is

$$S = \{(x_1, y_1), (x_2, y_2), \dots, (x_n, y_n)\}\$$

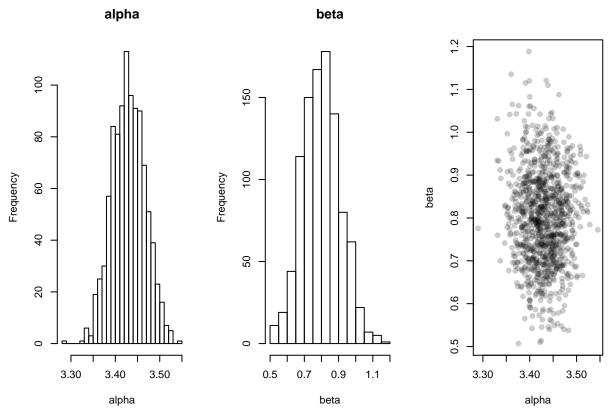
- We sample with replacement from the pairs of observations. i.e. sample (x_i, y_i) .

```
B = 1000;
beta.boot = t(sapply(1:B, FUN =function(b)
  lm(y~ I(x-mean(x)), subset=sample(n,n, replace=TRUE))$coef ))
```

• For each bootstrap sample \mathcal{S}_b^{\star} , we estimate the LS line to obtain $(\widehat{\alpha}_b^{\star}, \widehat{\beta}_b^{\star})$, for $b = 1, \dots, B$.

Bootstrap the Regression Coefficients

Plots of the boot estimates.



- Notice that the estimates seem to be generated from a bivariate normal (how so?)
 - which indicates that the bootstrap and the "theoretical" confidence intervals based on the errors being Gaussian should agree.

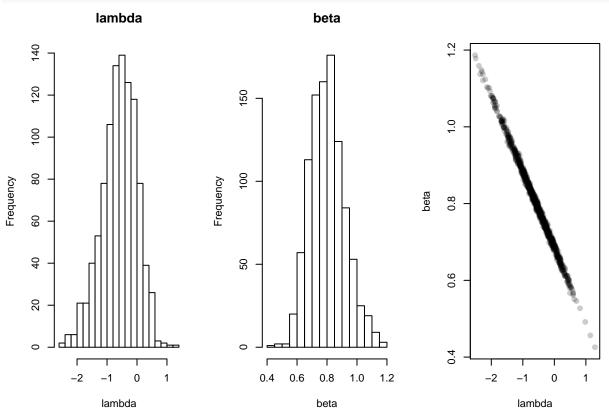
Aside: Comparing Regression Models

• Suppose we consider the alternative parameterization of the line.

$$Y_i = \alpha + \beta (x_i - \overline{x}) + R_i$$
 and $Y_i = \lambda + \beta x_i + R_i$

• The bootstrap replicates for this model are

```
beta.boot2 = t(sapply(1:B, FUN =function(b)
lm(y~ x, subset=sample(n,n, replace=TRUE))$coef ))
```



• Note the strong dependence between the estimates of the two parameters (negative correlation) which does not exist when using the centralized model, i.e. $Y_i = \alpha + \beta(x_i - \overline{x}) + R_i$.

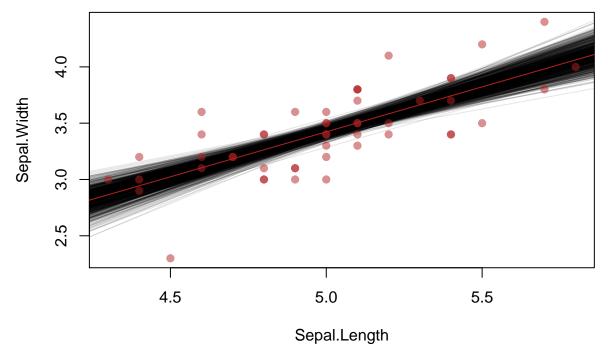
Bootstrap Regression lines

We can plot the data with the fitted model

$$y = \widehat{\alpha} + \widehat{\beta} \left(x - \overline{x} \right)$$

and all of the bootstrap regression lines.

$$y = \widehat{\alpha}_b^{\star} + \widehat{\beta}_b^{\star} (x - \overline{x})$$



• How can we construct a confidence interval for the regression line?

Bootstrap Confidence Interval (Percentile Method)

Suppose we want a confidence interval for the fitted line at the value x_0

• The fitted value is

$$\widehat{\mu}(x_0) = \widehat{\alpha} + \widehat{\beta} \left(x_0 - \overline{x} \right)$$

• The bootstrap replicates of \hat{y} are

$$\widehat{\mu}_b^{\star}(x_0) = \widehat{\alpha}_b^{\star} + \widehat{\beta}_b^{\star}(x_0 - \overline{x})$$
 where $b = 1, \dots, B$

 \bullet A 95% bootstrap confidence interval is the 2.5 and 97.5 quantiles from the bootstrap replicates (percentile interval)

$$\widehat{\mu}_{lower}(x_0) = Q_{\widehat{\mu}^*(x_0)}(0.025) \quad \text{ and } \quad \widehat{\mu}_{lower}(x_0) = Q_{\widehat{\mu}^*(x_0)}(0.975)$$
 x0 = 4.5
$$\text{mu0.hat} = \text{sum(beta.hat*c(1, x0 - mean(x)))}$$

$$\text{mu0.star.hat} = \text{apply(beta.boot, 1, function(z,a) { sum(z*a) }, \\ \text{a=c(1, x0 - mean(x)))}$$
 boot.ci0 = quantile(mu0.star.hat, prob= c(.025, .975))

• Using $x_0 = 4.5$ the fitted value, $\widehat{\mu}(x_0)$, is 3.02 and bootstrap confidence using the percentile method is 2.88, 3.15

Histogram of mu.star.hat(x0) 9 2 3.5 3 3.0 2.5 3.0 2.8 2.9 4.5 5.0 3.1 3.2 5.5

- To obtain a confidence interval for the whole regression line.
 - We vary x_0 , perform the bootstrap again and
 - $-\,$ connect the lower and upper confidence intervals

```
x.seq = c(4.5, 5.0, 5.6)
```

Using $x_0 = 4.5, 5, 5.6$, we obtain the following confidence intervals.

```
boot.ci = matrix(0, nrow=length(x.seq), 2)

for (i in 1:length(x.seq)) {
    y.hat = apply(beta.boot, 1, function(z,a) { sum(z*a) }, a=c(1, x.seq[i] - mean(x) ) )
```

```
boot.ci[i,] = quantile( y.hat, prob= c(.025, .975))
}
round(boot.ci,2)
##
        [,1] [,2]
## [1,] 2.88 3.15
## [2,] 3.35 3.50
## [3,] 3.76 4.05
par(mfrow=c(1,2), mar=2.5*c(1,1,1,0.1))
plot(iris.s, pch=19, col=adjustcolor("firebrick", 0.5))
abline(coef=beta.hat + c(-beta.hat[2]*mean(x),0) )
for (i in 1:length(x.seq)) lines( rep(x.seq[i],2), boot.ci[i,], col=4, lwd=2 )
plot(iris.s, pch=19, col=adjustcolor("firebrick", 0.5))
abline(coef=beta.hat + c(-beta.hat[2]*mean(x),0) )
lines( x.seq, boot.ci[,1], col=4, lwd=2 )
lines( x.seq, boot.ci[,2], col=4, lwd=2 )
4.0
                                           4.0
5
                                           S
                                           က
3.0
                                           3.0
2.5
                                           2
                                           ^{\circ}
         4.5
                    5.0
                              5.5
                                                    4.5
                                                               5.0
                                                                          5.5
```

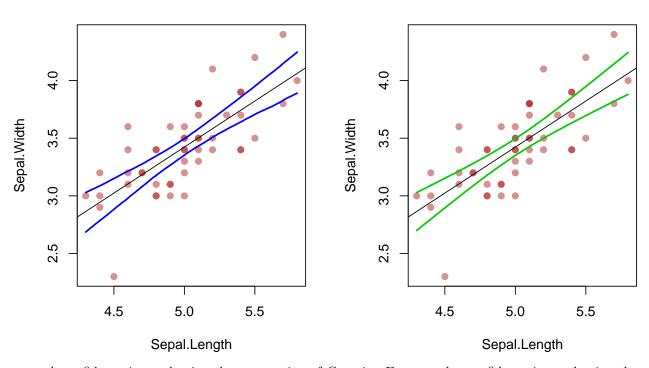
• We can add more x_0 values and then compare the bootstrap percentile interval to a confidence interval that uses the assumption of Gaussian errors.

```
x.seq = seq( min(x), max(x), length.out=100)
boot.ci = matrix(0, nrow=length(x.seq), 2)
```

```
for (i in 1:length(x.seq)) {
    y.hat = apply(beta.boot, 1, function(z,a) { sum(z*a) }, a=c(1, x.seq[i] - mean(x)))
    boot.ci[i,] = quantile( y.hat, prob= c(.025, .975))
}
## A CI using the assumption of Gaussian Errors
ci = predict( lm(y~x), newdata=data.frame(x=x.seq), interval="confidence")
par(mfrow=c(1,2))
plot(iris.s, pch=19, col=adjustcolor("firebrick", 0.5),
     main="Bootstrap Confidence Interval")
abline(coef=beta.hat + c(-beta.hat[2]*mean(x),0) )
lines(x.seq, boot.ci[,1], col=4, lwd=2)
lines(x.seq, boot.ci[,2], col=4, lwd=2)
plot(iris.s, pch=19, col=adjustcolor("firebrick", 0.5),
     main="Gaussian Confidence Interval")
abline(coef=beta.hat + c(-beta.hat[2]*mean(x),0) )
lines(x.seq, ci[,2], col=3, lwd=2)
lines(x.seq, ci[,3], col=3, lwd=2)
```

Bootstrap Confidence Interval

Gaussian Confidence Interval



- A confidence interval using the assumption of Gaussian Errors and a confidence interval using the bootstrap and the percentile method match.
- Important question: what does the coverage probability of 95% for a regression line mean?
 - note that a proper definition of a regression line is $E(Y \mid X = x) = \alpha + \beta x$

Parametric Bootstrap

- How would we apply the parametric bootstrap in the context of regression?
- The assumed regression model is

$$Y_i = \alpha + \beta (x_i - \overline{x}) + R_i$$

with $R_i \sim_{i.i.d} G(0, \sigma)$

- We fit the model to obtain the estimates $\widehat{\alpha}$, $\widehat{\beta}$, and $\widehat{\sigma}$
 - For thr Iris data above, these are $\hat{\alpha} = 3.428$, $\hat{\beta} = 0.7985$, and $\hat{\sigma} = 0.2565$.
 - Hence the fitted model is $Y_i = 3.428 + 0.7985 (x_i 5.006) + R_i$ with $R_i \sim_{i.i.d} G(0, 0.2565)$
- To obtain a bootstrap samples, we generate R_i^{\star} from $G(0,\widehat{\sigma})$ and set

$$y_i^{\star} = \widehat{\alpha} + \widehat{\beta} (x_i - \overline{x}) + R_i^{\star}$$

and then the bootstrap sample is

$$S_b^{\star} = \{(x_1, y_1^{\star}), (x_2, y_2^{\star}), \dots, (x_n, y_n^{\star})\}$$

• For each bootstrap sample S_b^{\star} we estimate the parameters to get the bootstrap replicates $\widehat{\alpha}_b^{\star}$, $\widehat{\beta}_b^{\star}$, and $\widehat{\sigma}_b^{\star}$

Illustration

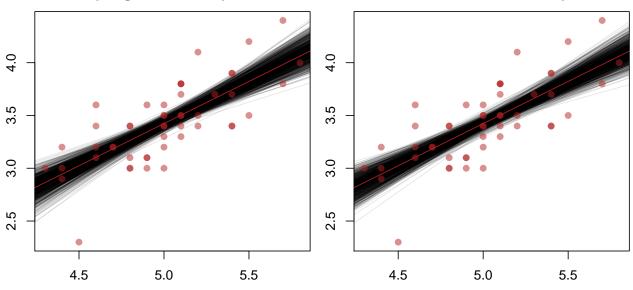
• Obtain the bootstrap samples using $\widehat{\alpha}=3.428,\,\widehat{\beta}=0.7985,\,$ and $\widehat{\sigma}=0.2565.$

```
B = 1000;
par.boot.sam = Map(function(b)
  { Rstar = rnorm(n, mean=0, sd= 0.2565)
    y = 3.428 + 0.7985*(x - mean(x)) + Rstar
    data.frame( x = x, y= y ) } , 1:B)

par.boot.coef = Map(function(sam)
    lm(y~I(x-mean(x)), data=sam )$coef, par.boot.sam)
```

Resampling Pairs: non-parametric

Parametric Bootstrap



- We notice that the results are very similar in this example.
- The parametric bootstrap motivates another way to re-sample data, i.e. sampling the errors.

Resampling the Errors

• Suppose the regression model is

$$Y_i = \alpha + \beta \left(x_i - \overline{x} \right) + R_i$$

where $R_i \sim F$, i.e. the errors come from some unknown density F.

- How might we estimate F?
- We fit the model to find $\widehat{\alpha},\,\widehat{\beta},\,$ and $\widehat{\sigma}$
 - then obtain the residuals $\hat{r}_i = y_i \hat{y}_i = y_i \left[\hat{\alpha} + \hat{\beta}(x_i \overline{x})\right]$ and
 - the sample of residuals or estimates of the errors is $\widehat{\mathcal{R}} = \{\widehat{r}_1, \dots, \widehat{r}_n\}$
- We can use the sample of residuals to estimate F using the empirical cdf.

$$\widehat{F}(t) = \frac{1}{n} \sum_{i=1}^{n} I\left(\widehat{r}_i \le t\right)$$

• We perform the bootstrap using \hat{F} , i.e. we generate a bootstrap sample of errors R_i^{\star} by resampling from $\hat{\mathcal{R}}$ and obtain

$$y_i^{\star} = \widehat{\alpha} + \widehat{\beta} (x_i - \overline{x}) + R_i^{\star}$$

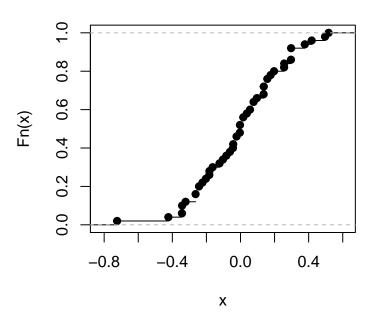
and then the bootstrap sample is

$$S_b^{\star} = \{(x_1, y_1^{\star}), (x_2, y_2^{\star}), \dots, (x_n, y_n^{\star})\}$$

Illustration

• The sample of residuals and the empirical cdf is

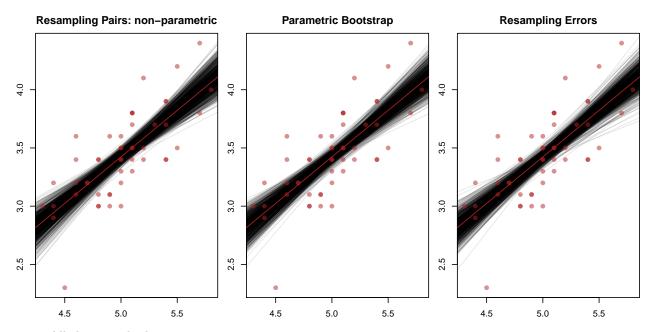
ecdf(R)



• Obtain the bootstrap samples

```
B = 1000;
nonpar.boot.sam = Map(function(b)
  { Rstar = R[sample(n,n,replace=TRUE)]
    y = 3.428 + 0.7985*(x - mean(x)) + Rstar
    data.frame( x = x, y= y ) } , 1:B)

nonpar.boot.coef = Map(function(sam)
    lm(y~I(x-mean(x)), data=sam )$coef, nonpar.boot.sam)
```

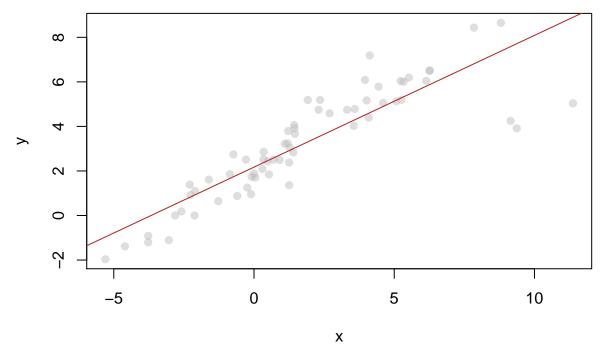


• All three methods agree

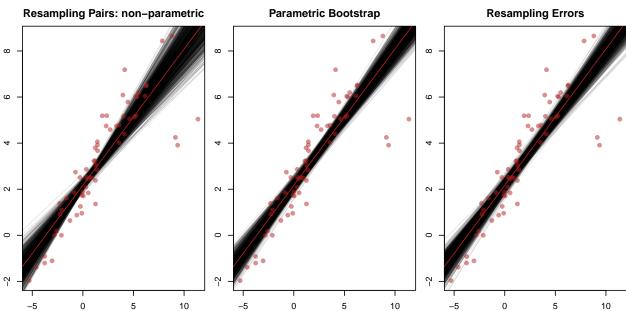
Some other Examples

Animals Data and LS

```
library(robustbase)
data(Animals2)
  #Animals2 = Animals2[-c(63,64,65),]
x = log(Animals2$body)
y = log(Animals2$brain)
n =length(y)
plot(x,y, pch=19, col=adjustcolor("grey", .5))
beta.hat = lm(y~ I(x-mean(x)))$coef
sd.hat = sqrt(sum(lm(y~ I(x-mean(x)))$residuals^2)/(n-2) )
abline(coef=beta.hat + c(-beta.hat[2]*mean(x),0), col=adjustcolor("firebrick", 1))
```







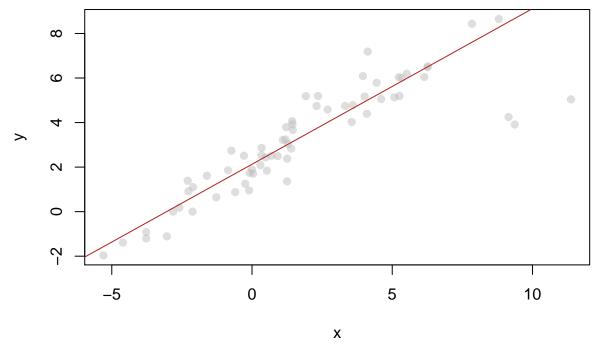
Animals Data and Robust Regression

• Let fit the robust regression line using the Huber function.

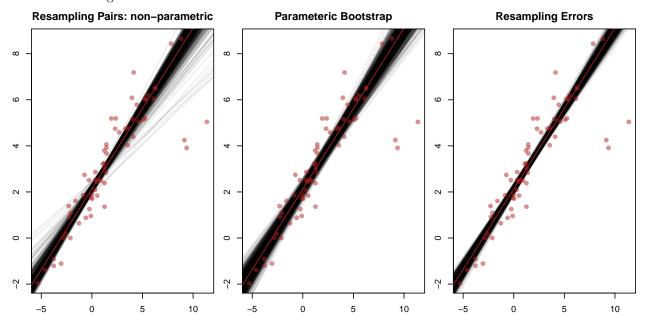
library(robustbase)
library(MASS)

```
data(Animals2)
#Animals2 = Animals2[-c(63,64,65),]
x = log(Animals2$body)
y = log(Animals2$brain)
n =length(y)
plot(x,y, pch=19, col=adjustcolor("grey", .5))
beta.hat = rlm(y ~ I(x-mean(x)), psi="psi.huber")$coef

sd.hat = sqrt(sum(rlm( y~ I(x-mean(x)), psi="psi.huber")$residuals^2)/(n-2) )
abline(coef=beta.hat + c(-beta.hat[2]*mean(x),0), col=adjustcolor("firebrick", 1))
```



• Robust Regression Confidence Intervals:

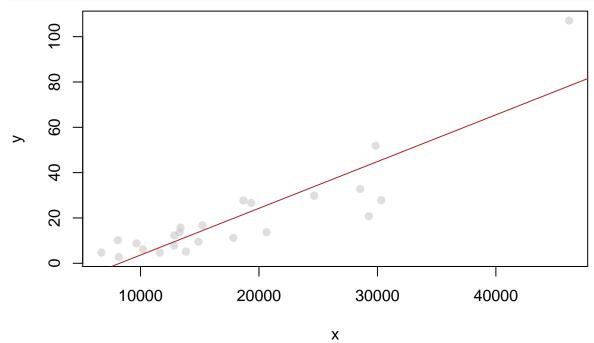


• What do you learn from these plots? Do they all agree?

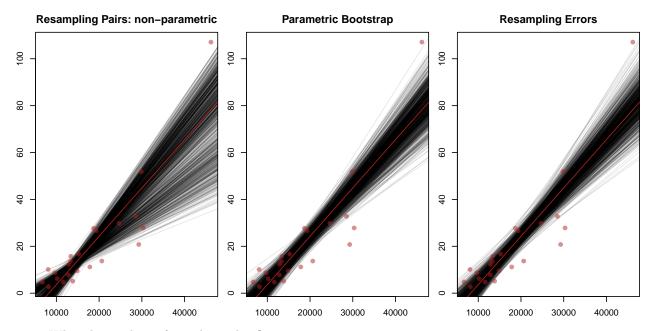
Aircraft Data and LS

- Aircraft Data deals with 23 single-engine aircraft built over the years 1947-1979, from Office of Naval Research.
 - x is the weight of the plane and
 - y is the cost in units of \$100,000

```
library(datasets)
x = aircraft$X3
y = aircraft$Y
n =length(y)
plot(x,y, pch=19, col=adjustcolor("grey", .5))
beta.hat = lm(y~ I(x-mean(x)))$coef
sd.hat = sqrt(sum(lm(y~ I(x-mean(x)))$residuals^2)/(n-2) )
abline(coef=beta.hat + c(-beta.hat[2]*mean(x),0), col=adjustcolor("firebrick", 1))
```



• Aircraft Data Confidence Intervals for the LS line:



- What do you learn from these plots?
- Do you think if robust regression would result in similar results?

Quote

The bootstrap "can blow the head off any problem if the statistican can stand the resulting mess."

– John Tukey