The Bootstrap

Rizzo, Chapter 7

BTRY/STSCI 4520

Generating A Sample Distribution

- We have seen how to simulate in order to conduct tests in R.
- We can do the same thing for other measures of uncertainty.
- Eg: confidence intervals:
  - Simulate according to the model with parameters θ.
  - Estimate parameters.
  - Look at the distribution of parameter estimates over many simulations.

- Note: simulation depends on the parameters available.
- We can also evaluate bias.

Example: Estimating a Variance

Why we divide by $n-1$: consider $\hat{\sigma}^2 = \frac{1}{n}\sum_{i=1}^{n}(x_i - \bar{x})^2$ for $n = 4$:


```
nsim = 1000
sigest = rep(0,nsim)

for(i in 1:nsim){
  X = rnorm(4)
  sigest[i] = mean( (X-mean(X))^2 )
}
```


The expected value of the estimate is estimated by


```
mean(sigest)
```

and the bias (since the true variance is 1) is

```
> bias = 1-mean(sigest)
[1] -0.2484821
```

Working With Estimates

Simulation allows us to do a number of things

1. Bias correction: since we know the bias we can correct our estimate

$$\hat{\sigma}^{*2} = \hat{\sigma}^2 - bias$$

for one "real" sample giving $\hat{\sigma}^2$ (`sighat=sigest[1]`).

```
> sighat.nobias = sighat-bias
[1] 1.057343
```

2. Standard errors for estimate, from standard deviations of simulated samples

```
> sighat.sd = sd(sigest)
[1] 0.6474583
```

3. Confidence intervals based on normal theory:

```
> sighat.nobias + c(-1,1)*qnorm(0.975)*sighat.sd
[1] -0.2116517  2.3263383
```

Alternative Confidence Intervals

Distribution of `sigest` strongly skewed: symmetric confidence intervals not appropriate.

Defining a lower limit $b_{\alpha/2}$:

- We want $P(\hat{\sigma}^2 - b_{\alpha/2} > \sigma^2) = \alpha/2$.
- This is the same as $P(\hat{\sigma}^2 - \sigma^2 > b_{\alpha/2}) = \alpha/2$.
- Choose $b_{\alpha/2}$ to be the $1 - \alpha/2$ quantile of $\delta^2 = \hat{\sigma}^2 - \sigma^2$ from simulation

```
b.lower = quantile(sigest-sigma,0.975)
b.upper = quantile(sigest-sigma,0.025)
```

  Analogous for upper limit.

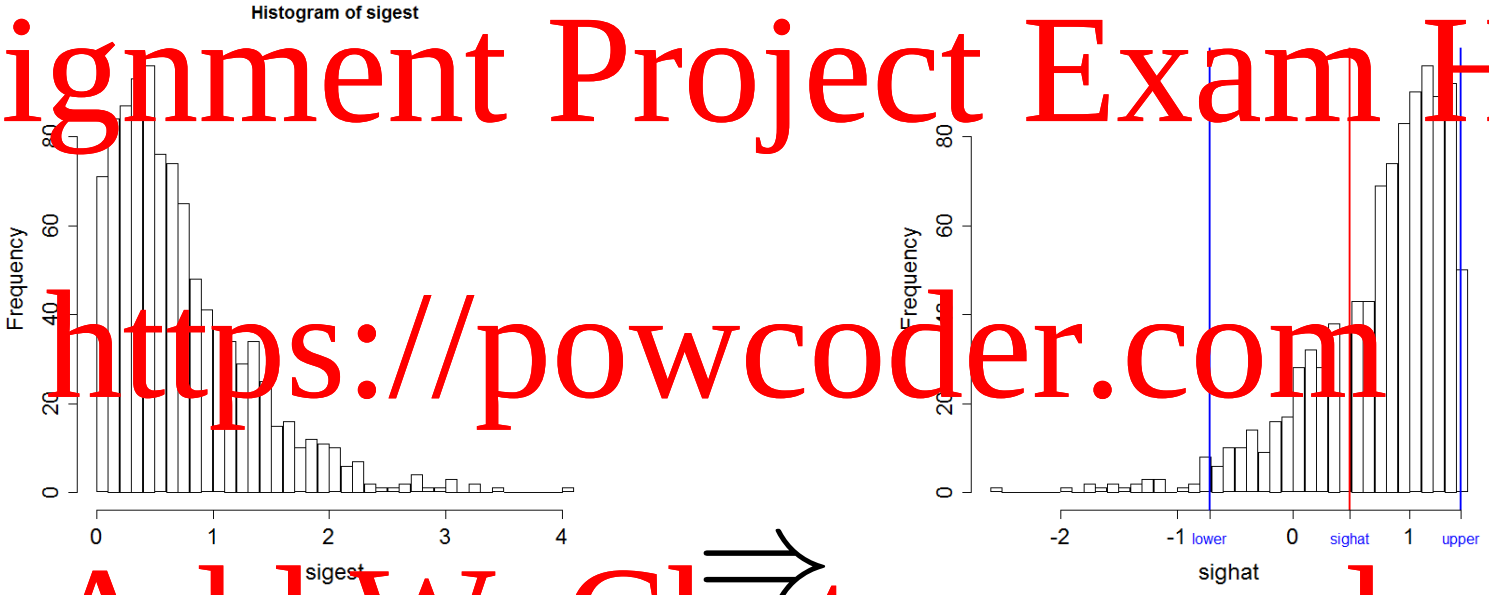
- Confidence interval is then

```
c(sighat - b.lower, sighat - b.upper)
```

Note: no bias correction (why?)

Confidence Intervals Continued

CI's *reverses* and shifts the distribution of $\hat{\sigma}^2$.



- $\hat{\sigma}^2$ has a long right tail (can be much too high)
- So lower side of confidence interval needs to be longer to include true σ^2.

Note: simulation procedure work for any statistic $t(X_1, \ldots, X_n)$ that estimates a parameter θ.

Making Fewer Assumptions

Some important limitations to value of simulation:

- Only valid under the parameters you use to simulate.
  - Bias of $\hat{\sigma}^2$ is σ^2/n – changes with σ^2.
  - But we don't know the parameters – we just have data.
  - Can always plug in our estimate, if that is biassed, our estimate of bias is also biassed.
- Only valid assuming the distribution you simulate from represents the data generating mechanism.
  - If our data isn't Gaussian, simulation above is not correct.

Maybe we could make more use of the data.

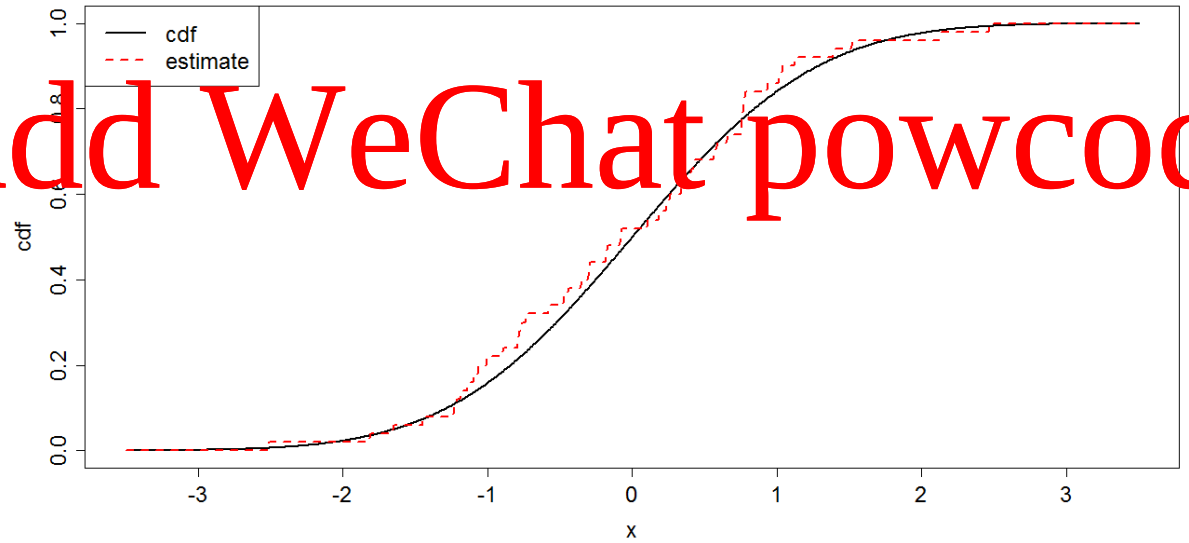
The Bootstrap

Introduced by Efron (1979), $>$ 26,000 citations from all of NSF's funding areas.

Arguably most important statistical development in last 50 years.

Simple idea:

- I want to simulate from distribution F, but I don't know it.
- However, I do have data $\Rightarrow$ use this as an estimate of F!



Empirical Estimates of a Distribution

- Cumulative distribution function: $F(x) = P(X \leq x)$
- Estimate from data:

$$F_n(x) = \frac{1}{n} \sum_{i=1}^{n} I(X_i \leq x)$$

"jumps" $1/n$ at each observation.

- $F_n(x)$ converges to $F(x)$ everywhere as $n \to \infty$.
- Interpretation of Y drawn from $F_n(x)$:
  For each i, Y takes value X_i with probability $1/n$.
- Practically: to sample from F_n, choose one X_i at random.
- To sample more "re-sample with replacement": *each time you choose an X_i, keep it in the data set for the next sample*.

Sampling Schemes

Some general terminology (informal)

sample from F generate a random variable X according to distribution F (later in 3520)

resample From a data set $X_1, \ldots, X_n$, choose one at random.

with replacement when I choose an X_i, keep it in the data for the next sample

without replacement when I choose an X_i, take it out of the data.

Different types of samples

bootstrap resample n observations with replacement

subsample resample $k < n$ observations without replacement.

Note: bootstrap samples will have repeated values; a subsample of size n is a permuation.

The Bootstrap Recipe

Given $X_1, \ldots, X_n$, and a statistic $t(X_1, \ldots, X_n)$ that estimates a parameter θ:

- Repeat B times:
  - Draw a bootstrap sample $X_1^*, \ldots, X_n^*$ by resampling $X_1, \ldots, X_n$ with replacement.
    - Record $T_b = t(X_1^*, \ldots, X_n^*)$.
- Use $T_1, \ldots, T_B$ to represent the sampling distribution of $T_o = t(X_1, \ldots, X_n)$.

sample

Will *resample* objects with or without replacement and will return a vector of required size.

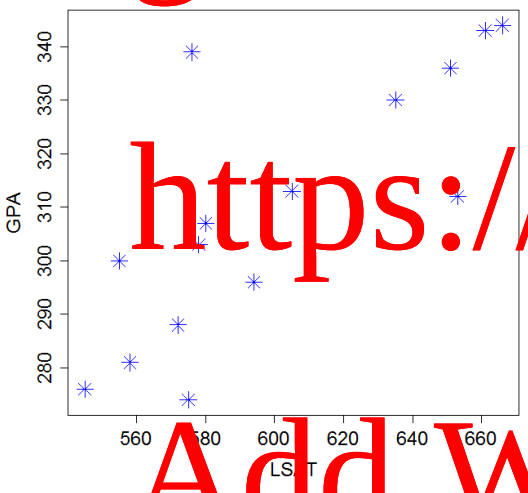

```
# A permutation of the numbers 5:10
sample(5:10)

# A subsample of size 3
sample(5:10,size=3)

# A bootstrap sample
sample(5:10,replace=TRUE)

# A subsample of size 3 with replacement
sample(5:10,size=3,replace=TRUE)
```

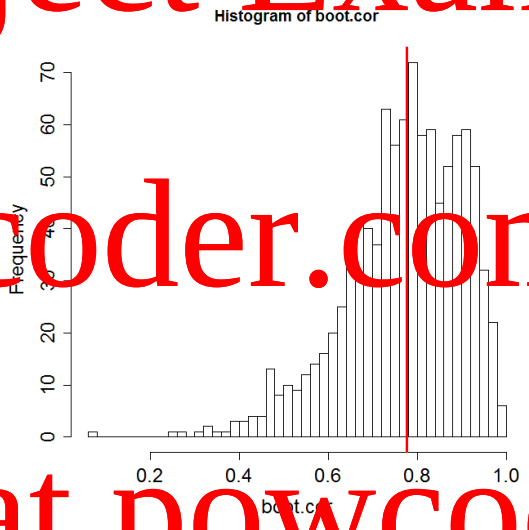

If `N` an integer `sample(N)` is the same as `sample(1:N)`.

Example

Law data: average LSAT and GPA for 15 law schools

Interest is in correlation between LSAT and GPA.






```
cor(law)
obs.cor = cor(law)[1,2]
```

```
nboot = 1000
boot.cor = rep(0,nboot)
n = nrow(law)
```

```
for(i in 1:nboot){
    boot.cor[i] = cor(law[sample(n,replace=TRUE),])[1,2]
}
```

Confidence Intervals

Number of possible ways to do confidence intervals.

Simplest: normal approximation

- Compute estimates $T_1, \ldots, T_B$.
- Obtain the standard deviation

$$\hat{se}(T) = \sqrt{\frac{1}{B}\sum_{b=1}^{B}(T_b - \bar{T})^2}$$

- Compute the confidence interval as

$$(T_o - z_{\alpha/2}\hat{se}(T),\ T_o + z_{\alpha/2}\hat{se}(T))$$

for $z_{\alpha/2}$ the normal critical value.

Assumes that T_o really is approximately normally distributed, but it does mean that you don't have to know its variance.

Bias Correction

Some statistics are biassed; to assess this we consider the average bootstrap replicate

$$\bar{T} = \frac{1}{B}\sum_{b=1}^{B} T_b$$

then we can measure the bias in T by

$$bias = \bar{T} - T_o$$

and we can even correct our estimate T_o by subtracting off the bias

$$T_o^c = T_o - bias = 2 * T_o - \bar{T}$$

and update confidence intervals

$$(T_o^c - z_{\alpha/2}\hat{se}(T),\ T_o^c + z_{\alpha/2}\hat{se}(T))$$

Example Continued

```
# Estimate the bias
> cor.bias = mean(boot.cor)-obs.cor
[1] -0.004983282

# Bias-Corrected Estimate
> obs.cor.c = obs.cor-cor.bias
[1] 0.7813578

# Boostrap Standard Error
> cor.se = sd(boot.cor)
[1] 0.1340546

# Bootstrap Corrected Confidence Interval
> obs.cor.c + c(-1,1)*qnorm(0.975)*cor.se
[1] 0.5186155 1.0441000
```

Confidence Intervals II

Can also use the empirical distribution of the bootstrap statistics.

Percentile bootstrap intervals:

$$(T_{(\alpha/2)}, T_{(1-\alpha/2)})$$

where $T_{(\alpha)}$ is the αth quantile in $T_1, \ldots, T_B$.

Alternatively, same recipe as for simulation confidence intervals:

- Lower bound is $b_{\alpha/2}$ such that $P(T - b_{\alpha/2} > \theta) = \alpha/2$.
- Use bootstrap sample for distribution of T, T_o in place of θ.
- Yields $b_{\alpha/2} = T_{(1-\alpha/2)} - T_o$ and confidence interval

$$(2T_o - T_{(1-\alpha/2)}, 2T_o - T_{(\alpha/2)})$$

  Same 'reverse the distribution' effect.
- Unlike simulation-based CIs, bias correction is important here. (Why?)

Continuing Example

```
# Quantiles of Bootstrap Distribution
b0.025 = quantile(boot.cor,0.025)
b0.975 = quantile(boot.cor,0.975)

# Percentile Bootstrap Confidence interval
> c(b0.025,b0.975)
0.4658674 0.9648874

# Standard Bootstrap Confidence Interval
> 2*obs.cor.c - c(b0.975, b0.025)
0.5978281 1.0968481
```


- Upper limit ≥ 1 can be thresholded (remember, this interval is just meant to capture the "truth", 95% of the time).
- Bootstrap test for $\rho \leq 0.5$ rejects – null hypothesis parameter is not within confidence interval.

Yet Further Intervals

Variants (increasingly elaborate) proposed to improve confidence intervals.

- Bootstrap t-interval

$$(t_0 - t^*_{1-\alpha/2}\hat{se}(t_0), (t_0 - t^*_{1\alpha/2}\hat{se}(t_0)$$

  - $\hat{se}(t_0)$: bootstrap estimate of standard error.
  - $t^*_{\alpha/2}$ quantiles of bootstrap t statistic: $t_b = (T_b - T_o)/\hat{se}(T_b)$.
  - $\hat{se}(T_b)$: estimate of standard error *for each* T_b; often a bootstrap within a bootstrap.
- Bias-corrected and accelerated bootstrap (BCa) corrects for both bias and skewness in bootstrap distribution.

Basic reasoning: using estimates of standard errors requires smaller B, and has better statistical properties than quantiles of bootstrap distribution.

Yet more variants: beyond this course.

When Bootstraps Break

Bootstrap doesn't work for all statistics

- $t(X_1, \ldots, X_n) = \min_j |X_i - X_j|$
  - Minimum distance between points in the data set.
  - Bootstrap sample: minimum distance is 0 (tied observations)
  - Real data = almost never ties for continuous variables.

Most cases of failure $t(X_1, \ldots, X_n)$ is not a smooth function of $X_1, \ldots, X_n$ (cannot differentiate with respect to X_i).

Subsampling often a good alternative (but $k < n$ might be an issue, as it is for this example).

Rare; most cases are pathological (although recent statistical methods are a problem).

Conditionally-Specified Models

Frequently we only describe part of the data generating mechanism.

Eg: regression models

$$y_i = \beta_0 + \beta_1 x_i + \epsilon_i$$
$$= \mathbf{x}_i \beta + \epsilon_i$$

with $\epsilon_i \sim N(0, \sigma^2)$.

- What about x_i? Treated as fixed (often chosen by experimenter)
- Or, frequently, $x_i \sim h(x)$, but h not specified.
- For large n (and in practice) very little variance in $\hat{\beta}$ due to randomness in x_i.

Example: Multiple Regression

In the lab, we looked at simple linear regression. For multiple regression

$$y_i = \beta_0 + \beta_1 x_{i1} + \beta_2 x_{i2} + \cdots + \epsilon_i$$

where the $\epsilon_i \sim N(0, \sigma^2)$. Also written as

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

Squared error is now represented by

$$SSE(\beta) = (\mathbf{y} - X\beta)^T(\mathbf{y} - X\beta)$$

so that the derivative of squared error is

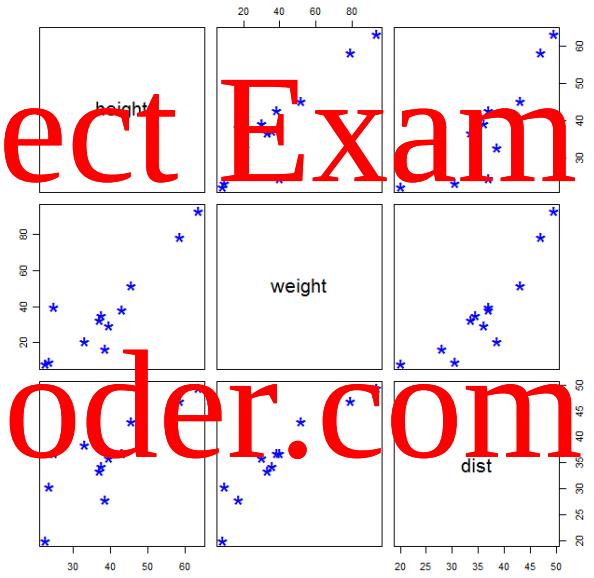
$$\frac{dSSE(\beta)}{d\beta} = 2(X^T X\beta - X^T \mathbf{y})$$

which is zero at

$$\beta = (X^T X)^{-1} X^T \mathbf{y}$$

A Data Set

- 12 children's height, weight and arterial distance from the wrist to the heart.
- Used as guidelines for inserting catheters.
- Model distance in terms of height and weights.




```
> mod = lm(dist~.,data=heart)
> summary(mod)

Coefficients:
            Estimate Std. Error t value Pr(>|t|)
(Intercept) 24.50804    5.12461   4.782 0.000998 ***
height       0.05091    0.21060   0.242 0.814396
weight       0.25495    0.10326   2.469 0.035624 *
```

A Simulation

We'll used the estimated coefficients and residual standard error to simulate at the observed covariates.

```
beta = mod$coef    # Start from observed coefficients

# Design matrix
X = as.matrix(cbind(rep(1,12),heart[,1:2]))

# Predicted values (also from mod$fit)
pred = X%*%beta

# Residual standard error
sigma = summary(mod)$sigma
```

Vectorizing A Simulation

Create a large matrix where response for each data set is in one column.

Recall that $\mathbf{y} = X\beta + \boldsymbol{\epsilon}$, repeat the same $X\beta$ over each column, but create a matrix of simulated $\boldsymbol{\epsilon}$.

```
nsim = 1000
Ysim = matrix(pred,12,nsim,byrow=FALSE) +
            matrix(rnorm(12*nsim,sd=sigma),12,nsim)
```

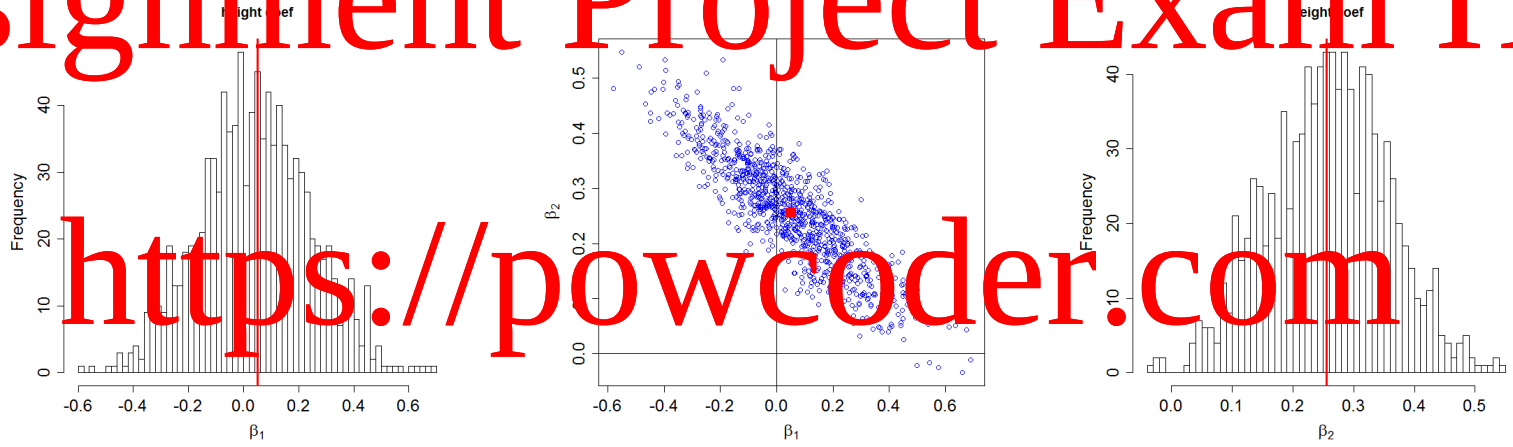
Now estimate β; the `solve` command inverts a matrix

```
beta.sim = solve( t(X)%*%X, t(X)%*%Ysim)
```

Because the estimate is linear in `Ysim` we can obtain them all at once.

Continuing

Simulation results:



Lovely Demonstration of effect of correlated covariates

Bootstrap options

- Re-sample (x_i, y_i) pairs and do standard bootstrap.
- Try to re-sample the ϵ_i – corresponds to our model.

Residual Bootstrap

Basically restricted to linear regression models:

$$y = X\beta + \epsilon$$

1. Estimate $\hat{\beta}$.
2. Estimate residuals $\hat{\epsilon}_i = y_i - \mathbf{x}_i\hat{\beta}$, $i = 1, \ldots, n$.
3. Bootstrap residuals to produce $\hat{\epsilon}_i^*$, $i = 1, \ldots, n$.
4. Add bootstrapped residuals back onto predictions $y_i^* = \mathbf{x}_i\hat{\beta} + \hat{\epsilon}_i^*$, $i = 1, \ldots, n$.
5. Estimate $\hat{\beta}_b$ for bootstrapped (x_i, y_i^*) for $b = 1, \ldots, B$.

Now all the bias, standard error, confidence interval statistics can be calculated with the same recipe.

Why Residual Bootstrap?

More stable, avoids ties in the $\mathbf{x}_i$, doesn't change a fixed design.

Continuing The Example


```
# Estimate errors
eps.hat = heart$dist - pred

# Now bootstrap residuals
eps.boot = eps.hat[sample(12,size=nsim*12,replace=TRUE)]
eps.boot = matrix(eps.boot,12,nsim)

# Create data
Y.boot = matrix(pred,12,nsim,byrow=FALSE) + eps.boot

# And re-estimate
beta.boot = solve( t(X)%*%X, t(X)%*%Y.boot)
```

Usual Statistics

Calculate the same statistics as before

```
# Bias
> biases = beta - apply(beta.boot,1,mean)
 (Intercept)        height        weight
 0.223436803 -0.007668818  0.002312965

# Standard Error
> se.boot = apply(beta.boot,1,sd)
(Intercept)        height        weight
 4.63035973 0.18945029 0.09076793
```

Biasses are probably not real but

```
> beta.c = beta-biases
24.28460334  0.05857949  0.25263440
```

Confidence Intervals

```
# Lower and Upper Bounds
>lb = apply(beta.boot,1,quantile,0.025)
>ub = apply(beta.boot,1,quantile,0.975)
                      lb          ub
(Intercept) 14.09073439 33.0530314
height      -0.30957338  0.4673601
weight       0.06940625  0.4273275


# Confidence Interval
>cbind(2*beta - ub, 2*beta-ub)
                    [,1]       [,2]
(Intercept) 15.96304893 34.9253459
height      -0.36603873  0.4113947
weight       0.08256726  0.4404885
```

Bootstrap Tests of Significance

We can also test how many times the bootstrap falls below 0

```
> pvals = apply(beta.boot<0,1,mean)
> pvals
(Intercept)      height      weight
      0.000       0.387       0.004
```

But note that this *does not* provide a global test for the significance of the regression.

More information: correlation of $\hat{\beta}$

```
> cor(t(beta.boot))
            (Intercept)     height     weight
(Intercept)   1.0000000 -0.9074095  0.6355241
height       -0.9074095  1.0000000 -0.8834964
weight        0.6355241 -0.8834964  1.0000000
```

Parametric Bootstrap

Residual bootstrap is not always applicable:

Eg: logistic regression;

$$y_i \in \{0, 1\},\ \log\left(\frac{P(y_i = 1)}{P(y_i = 0)}\right) = \mathbf{x}_i\beta$$

Doesn't make sense to do look at residuals.

Instead, estimate $\hat{\beta}$ and create a new data set by generating each y_i^* according to

$$P(y_i^* = 1) = \frac{e^{\mathbf{x}_i\hat{\beta}}}{1 + e^{\mathbf{x}_i\hat{\beta}}}$$

Isn't this just estimate parameters and then simulate data from the model?

Yes! But naming is part of good salesmanship.

Example

Linear regression simulation above, this is exactly a parametric bootstrap for linear regression.

Summary

- Simulation (parametric bootstrap) a tool for evaluating confidence intervals about estimated parameters.
- *Bootstrap*: avoids having to know distribution of data.
- Useful for
  - Bias Correction
  - Estimate standard errors
    - Confidence intervals
- Residual bootstrap for linear regression models.

But

- Justification is asymptotic: requires enough data that empirical distribution approximates truth.
- Won't work for every problem or every statistic (but most standard stats are OK).