# What have we learned until now: Part 1

- Direct simulation from probability densities
- Several different methods
  - inversion sampling
  - methods based on relationship between RV
  - rejection sampling (*)
  - importance sampling (*)
- We get samples that are independent of each other

# What have we learned until now: Part 1 and 2

Bayesian paradigm

- Likelihood $\pi(y|x)$
- Prior $\pi(x)$
- Posterior $\pi(x|y) \propto \pi(y|x)\pi(x)$

# What have we learned until now: Part 2

Hierarchical models are an extremely useful tool in Bayesian model building.

Three parts:

- Observation model $\boldsymbol{y}|\boldsymbol{x}$: Encodes information about observed data.
- The latent model $\boldsymbol{x}|\boldsymbol{\theta}$: The unobserved process.
- Hyperpriors for $\boldsymbol{\theta}$: Models for all of the parameters in the observation and latent processes.

Note: here we indicate the observed data by $\boldsymbol{y}$ while $\boldsymbol{x}$ and $\boldsymbol{\theta}$ are parameters

# What have we learned untill now: Part 2

MCMC algorithm:

- Problem: Sample from $\pi(x)$, $x \in S$.
- MCMC idea:
  - Construct Markov chain with $\pi(x)$ as limiting distribution.
  - Simulate the Markov chain for a long time so that it has time to converge.
  - Most MCMC samplers are based on reversible Markov chains $\Rightarrow$ Their convergence is proved by checking the detailed balance equation.
- Can be applied to virtually any bayesian model
- Convergence and slow mixing can be a big issue

# What have we learned until now: Part 2

Integrated nested Laplace approximation:

- Can be applied only on a (large) class of models: Latent Gaussian models
- No sampling involved, based on numerical approximation
- The focus is on posterior marginals

# TMA4300 - Part 3

# TMA4300 - Part 3

*

*Slides are partially based on lecture notes kindly provided by Håkon Tjelmeland, Andrea Riebler, and Sara Martino.

# Last part of this course

$\Rightarrow$ Not closely related to the two first parts

- no more MCMC
- mostly non-Bayesian perspective

$\Rightarrow$ Two topics (not closely related to each other):

- Bootstrapping
- Expectation-Maximization algorithm

# Bootstrap

# Bootstrap

http://tradingconsequences.blogs.edina.ac.uk/files/2013/10/Dr_Martens_black_old.jpg

# An example for introduction

| Group | Survival Time | Sample size | Mean | Estimated SE |
|---|---|---|---|---|
| Treatment | 94,197,16,38<br>99,141,23 | 7 | 86.86 | |
| Control | 52,104,146,10,51,46<br>30,40,27,46 | 9 | 56.22 | |
| | | Differance: | 30.63 | |

- Is the difference in mean significant?
-

# An example for introduction

| Group | Survival Time | Sample size | Mean | Estimated SE |
|---|---|---|---|---|
| Treatment | 94,197,16,38<br>99,141,23 | 7 | 86.86 | 25.24 |
| Control | 52,104,146,10,51,46<br>30,40,27,46 | 9 | 56.22 | 14.14 |
| | | Differance: | 30.63 | 30.93 |

- Is the difference in mean significant?
-

# An example for introduction

| Group | Survival Time | Sample size | Mean | Estimated SE |
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| Treatment | 94,197,16,38<br>99,141,23 | 7 | 86.86 | 25.24 |
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| | | Differance: | 30.63 | 30.93 |

- Is the difference in mean significant?
- What if we want to compare the medians instead?

  Show code Bootstrap_intro.R

# . . . pull oneself up by one's bootstraps

> *To begin an enterprise or recover from a setback without any outside help; to succeed only on one's own effort or abilities.*
>
> Wiktionary


The term is sometimes attributed to Rudolf Erich Raspe's story "The Surprising Adventures of Baron Munchausen", where the main character pulls himself (and his horse) out of a swamp by his hair

http://redstateeclectic.typepad.com/redstate_commentary/2010/11/sustainability-isnt-sustainable.html

# The boostrap

- Bootstrap is a computer-based technique for doing statistical inference (usually with a minimum of assumptions)
- It is not Bayesian

# Important concepts

- empirical distribution function
- plug in estimator
- bootstrap sample

# Today's lecture

- Bootstrap
  - Non-parametric
  - Parametric
- Bootstrap estimate of SD
- Bootstrap estimate of bias

# Empirical distribution function

Assume we have iid observations from an (unknown) distribution $F$:

$$F \to (x_1, \ldots, x_n)$$

The empirical distribution function $\hat{F}$ is the CDF that puts mass $1/n$ at each data point $x_i$:

$$\hat{F}(x) = \frac{1}{n} \sum_{i=1}^{n} 1(x_i \leq x)$$

where $1(\cdot)$ denotes the indicator function.

For iid samples $\hat{F}$ is a sufficient estimator for $F$.

# Plug in estimator

Let $\theta$ be an interesting feature of $F$, $\theta = t(F)$.

For example:

$$\theta = \mathrm{E}(X) = \int x f(x) dx$$

$$\theta = \mathrm{Var}(X) = \int (x - \mathrm{E}(X))^2 f(x) dx$$

The plug-in estimator for $\theta$ is defined by:

$$\hat{\theta} = t(\hat{F})$$

The plug-in principle is quite good, if the only information about $F$, comes from the sample $x$.

# Examples

Thus

$$\theta = \mathsf{E}(X) \Rightarrow \hat{\theta} = \mathsf{E}_{\hat{F}}(X) = \sum_{i=1}^{n} x_i \frac{1}{n} = \bar{x}$$

# Examples

Thus

$$\theta = \mathsf{E}(X) \Rightarrow \hat{\theta} = \mathsf{E}_{\hat{F}}(X) = \sum_{i=1}^{n} x_i \frac{1}{n} = \bar{x}$$

$$\begin{aligned}\theta = \mathsf{Var}(X) \Rightarrow \hat{\theta} &= \mathsf{Var}_{\hat{F}}(X) = \mathsf{E}_{\hat{F}}[(X - \mathsf{E}_{\hat{F}}(X))^2] \\ &= \sum_{i=1}^{n} (x_i - \mathsf{E}_{\hat{F}}(X))^2 \frac{1}{n} = \frac{1}{n} \sum_{i=1}^{n} (x_i - \bar{x})^2\end{aligned}$$

# Examples

Thus

$$\theta = \mathrm{E}(X) \Rightarrow \hat{\theta} = \mathrm{E}_{\hat{F}}(X) = \sum_{i=1}^{n} x_i \frac{1}{n} = \bar{x}$$

$$\theta = \mathrm{Var}(X) \Rightarrow \hat{\theta} = \mathrm{Var}_{\hat{F}}(X) = \mathrm{E}_{\hat{F}}[(X - \mathrm{E}_{\hat{F}}(X))^2]$$
$$= \sum_{i=1}^{n} (x_i - \mathrm{E}_{\hat{F}}(X))^2 \frac{1}{n} = \frac{1}{n} \sum_{i=1}^{n} (x_i - \bar{x})^2$$

$$\theta = \mathrm{SD}(X) \Rightarrow \hat{\theta} = \mathrm{SD}_{\hat{F}}(X) = \sqrt{\mathrm{Var}_{\hat{F}}(X)}$$
$$= \sqrt{\frac{1}{n} \sum_{i=1}^{n} (x_i - \bar{x})^2}$$

# Example

$$E_F\left[\left(\frac{X-\mu}{\sigma}\right)^3\right] = \frac{E[X^3]-3\mu\sigma^2-\mu^3}{\sigma^3}$$

See notes

# Setting

Assume we have :

$$F \to (x_1, \ldots, x_n)$$

Thus $\hat{F}$ gives mass $\frac{1}{n}$ to each observed value.

A bootstrap sample is defined to be a random sample of size $n$ from $\hat{F}$, say $x^\star = (x_1^\star, \ldots, x_n^\star)$

$$\hat{F} \to (x_1^\star, \ldots, x_n^\star)$$

# Simple illustration

Suppose $n = 3$ univariate data points, namely

$$\{x_1, x_2, x_3\} = \{1, 2, 6\}$$

are observed as an iid sample from $F$ that has mean $\theta$ . At each observed data value, $\hat{F}$ places mass $1/3$. Suppose the estimator to be bootstrapped is the sample mean $\hat{\theta}$.

There are $3^3 = 27$ possible outcomes for $\mathcal{X}^\star = \{X_1^\star, X_2^\star, X_3^\star\}$.

# Simple illustration (II)

| $\mathcal{X}^\star$ | | | $\hat{\theta}^\star$ | $P^\star(\hat{\theta}^\star)$ | Observed frequency |
|---|---|---|---|---|---|
| 1 | 1 | 1 | 3/3 | 1/27 | 36/1000 |
| 1 | 1 | 2 | 4/3 | 3/27 | 101/1000 |
| 1 | 2 | 2 | 5/3 | 3/27 | 123/1000 |
| 2 | 2 | 2 | 6/3 | 1/27 | 25/1000 |
| 1 | 1 | 6 | 8/3 | 3/27 | 104/1000 |
| 1 | 2 | 6 | 9/3 | 6/27 | 227/1000 |
| 2 | 2 | 6 | 10/3 | 3/27 | 131/1000 |
| 1 | 6 | 6 | 13/3 | 3/27 | 111/1000 |
| 2 | 6 | 6 | 14/3 | 3/27 | 102/1000 |
| 6 | 6 | 6 | 18/3 | 1/27 | 40/1000 |

# Bootstrap estimate for standard error

- Parameter of interest: $\theta = t(F)$
- Our estimator for $\theta$: $\hat{\theta} = s(x)$
- Want (to estimate) $\text{SD}_F(\hat{\theta})$.

A bootstrap replication of $\hat{\theta}$ is

$$\hat{\theta}^\star = s(x^\star)$$

Use plug-in principle to estimate $\text{SD}_F(\hat{\theta})$.

The bootstrap estimate of the standard error of $\hat{\theta} = s(x)$ is $\text{SD}_{\hat{F}}(\hat{\theta}^\star)$.

This is called the ideal bootstrap estimate of standard error of $\hat{\theta}$.

# Ideal bootstrap estimate of standard error

- For the sample mean it can be computed analytically
- For (very) small sample sizes it can be computed using all the possible bootstrap replicates. (Number of possible bootstrap sample: $n^n$.)
- In other cases it can be approximated via Monte Carlo techniques

# Computational way of obtaining a good estimate

We can estimate $\text{SD}_{\hat{F}}(\hat{\theta}^\star)$ by simulation:

1. Generate $B$ bootstrap samples $x^{1\star}, \ldots, x^{B\star}$.
2. Evaluate the corresponding parameter estimates

$$\hat{\theta}^\star(b) = s(x^{b\star}), \quad b = 1, 2, \ldots, B$$

3. Estimate $\text{SD}_{\hat{F}}(\hat{\theta}^\star)$ by

$$\widehat{\text{SE}}_B = \sqrt{\frac{\sum_{b=1}^{B}(\hat{\theta}^\star(b) - \hat{\theta}^\star(\cdot))^2}{B-1}}$$

where

$$\hat{\theta}^\star(\cdot) = \frac{1}{B}\sum_{b=1}^{B}\hat{\theta}^\star(b)$$

Note

$$\lim_{B\to\infty}\widehat{\text{SE}}_B = \widehat{\text{SE}}_\infty = \widehat{\text{SD}}_{\hat{F}}(\hat{\theta}^\star)$$

# Example

Setting

$$\theta = \mathrm{E}(X)$$

$$\hat{\theta} = s(x) = \frac{1}{n}\sum_{i=1}^{n} x_i = \bar{x}$$

$$\hat{\theta^\star} = s(x^\star) = \frac{1}{n}\sum_{i=1}^{n} x_i^\star = \bar{x^\star}$$

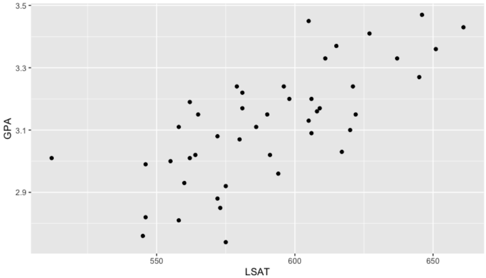
Here, the ideal bootstrap estimate exists

see blackboard

# Example: The correlation coefficient

Scores for 15 law schools in the USA

$$y_i = (LSAT_i, GPA_i), \ t = i \ldots, 15$$




The correlation between the two scores is estimated to be 0.78, but what is its standard error?

# Example: The correlation coefficient

- 1000 bootstrap replicates

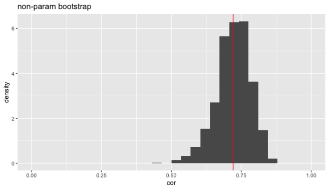
$$y^{1\star}, \ldots, y^{1000\star}$$

- For each replicates compute

$$\hat{\theta}^{i\star} = s(y^{i\star})$$

- Estimate bootstrap SE

$$\hat{SD}_{\hat{F}}(\theta) = 0.121$$



# How large do we need $B$?

Intuitively we understand that the $\widehat{\mathsf{SE}}_B$ has larger standard deviation than $\widehat{\mathsf{SE}}_\infty$.

Theory, not to be discussed here, gives the following rules of thumb:

1. Even a small $B$ is informative, say $B = 25$ or $B = 50$ is often enough to get a good estimate of $\mathsf{SE}_F(\hat{\theta})$.
2. Very seldomly more than $B = 200$ is necessary to estimate $\mathsf{SE}_F(\hat{\theta})$.

# The parametric bootstrap

When data are modeled to originate from a parametric distribution, so

$$X_1, \ldots, X_n \overset{\text{iid}}{\sim} F(x, \xi),$$

another estimate of $F$ may be employed.

Suppose that the observed data are used to estimate $\xi$ by $\hat{\xi}$. Then each parametric bootstrap pseudo-dataset $\mathcal{X}^\star$ can be generated by drawing $X_1^\star, \ldots, X_n^\star \overset{\text{iid}}{\sim} F(x, \hat{\xi}) = \hat{F}_{\text{par}}$.

# Again ...

... we can/must estimate $\mathrm{SD}_{\hat{F}_{\mathrm{par}}}(\hat{\theta}^\star)$ by simulation:

1. Generate $B$ bootstrap samples $x^{1\star}, \ldots, x^{B\star}$, where

$$x^{b\star} = (x_1^{b\star}, \ldots, x_n^{b\star})$$

   with $x_1^{b\star}, \ldots, x_n^{b\star} \stackrel{\text{iid}}{\sim} \hat{F}_{\mathrm{par}}$.

2. Evaluate the corresponding parameter estimates

$$\hat{\theta}^\star(b) = s(x^{b\star}), \quad b = 1, 2, \ldots, B$$

3. Estimate $\mathrm{SD}_{\hat{F}_{\mathrm{par}}}(\hat{\theta}^\star)$ by

$$\widehat{\mathrm{SE}}_B = \sqrt{\frac{\sum_{b=1}^{B}(\hat{\theta}^\star(b) - \hat{\theta}^\star(\cdot))^2}{B-1}}$$

   where

$$\hat{\theta}^\star(\cdot) = \frac{1}{B}\sum_{b=1}^{B}\hat{\theta}^\star(b)$$

# Example: Correlation coefficients

We assume now that

$$y_i = (LSAT_i, GPA_i) \sim \mathcal{N}(\boldsymbol{\mu}, \boldsymbol{\Sigma}), \text{ i.i.d}$$

where $\boldsymbol{\Sigma} = \left(\begin{smallmatrix} \sigma_1^2 & \sigma_{12} \\ \sigma_{12} & \sigma_2^2 \end{smallmatrix}\right)$ Estimate $\boldsymbol{\mu}$ and $\boldsymbol{\Sigma}$ and obtain:

$$\hat{F}_{(\hat{\boldsymbol{\mu}}, \hat{\boldsymbol{\Sigma}})}$$

# Example: The correlation coefficient

- 1000 bootstrap replicates

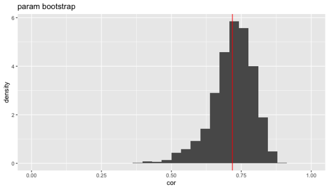
$$y^{1\star}, \ldots, y^{1000\star} \sim \hat{F}_{(\hat{\boldsymbol{\mu}}, \hat{\boldsymbol{\Sigma}})}$$

- For each replicates compute

$$\hat{\theta}^{i\star} = s(y^{i\star})$$

- Estimate bootstrap SE

$$\hat{SD}_{\hat{F}}(\theta)$$



# Bootstrapping regression

Consider the ordinary multiple regression model

$$Y_i = \boldsymbol{x}_i^\top \boldsymbol{\beta} + \epsilon_i, \quad \text{for } i = 1, \ldots, n,$$

where $\epsilon_i$ are iid mean zero random variables with constant variance.

- Parameters of interest $\boldsymbol{\beta}$
- Want to estimate $SD(\hat{\beta})$

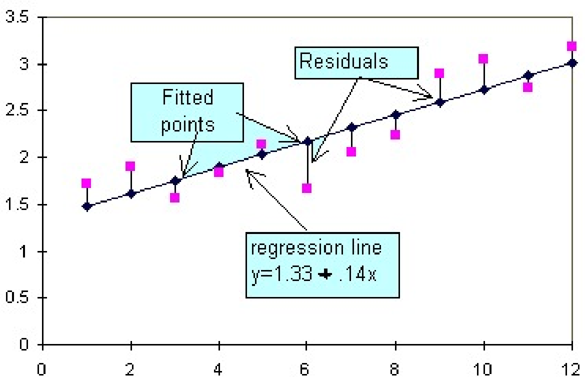
# Review: Linear Regression

- Least square estimate of $\boldsymbol{\beta}$

$$\hat{\boldsymbol{\beta}} = \text{argmin}\{\sum(Y_i - \boldsymbol{x}_i^\top \boldsymbol{\beta})^2\} \Rightarrow \hat{\boldsymbol{\beta}} = (\boldsymbol{X}^T\boldsymbol{X})^{-1}\boldsymbol{X}^T\boldsymbol{Y}$$

- Residuals

$$e_i = Y_i - \boldsymbol{x}_i^\top \hat{\boldsymbol{\beta}}$$



# Bootstrap regression

Alternative 1: Bootstrap the residuals $e_i = Y_i - \boldsymbol{x}_i^\top \hat{\boldsymbol{\beta}}$

Alternative 2: Bootstrap the pairs $\boldsymbol{Z}_i = (\boldsymbol{X}_i, Y_i)$

# Bootstrap the residuals

1. Fit the regression model to the observed data and obtain the fitted responses $\hat{y}_i$ and residuals $\hat{\epsilon}_i$.
2. Sample a bootstrap set of residuals $\hat{\epsilon}^\star_1, \ldots, \hat{\epsilon}^\star_n$ from the set of fitted residuals completely at random and with replacement.
3. Generate a bootstrap set of pseudo responses

$$Y^\star_i = \hat{y}_i + \hat{\epsilon}^\star_i, \quad \text{for } i = 1, \ldots, n.$$

4. Regress $Y^\star$ on $\boldsymbol{x}$ to obtain a bootstrap estimate $\hat{\boldsymbol{\beta}}^\star$.

Repeat this process to get an empirical distribution of $\hat{\boldsymbol{\beta}}^\star$.

# Bootstrapping residuals: Remarks

This approach is also used for autoregressive models, for example.

Note: Bootstrapping the residuals is reliant on

- The model provides an appropriate fit
- The residuals have a constant variance

Otherwise, a different scheme is recommended.

Comment: No need to bootstrap for linear regression model with least squares estimation, as analytical results are then available.

# Bootstrap the pair $\boldsymbol{Z}_i = (\boldsymbol{X}_i, Y_i)$

Suppose response and predictors are measured from a collection of individuals selected at random

$\Rightarrow$ Data pairs $\boldsymbol{z}_i = (\boldsymbol{x}_i, y_i)$ can be regarded as iid realisation from $\boldsymbol{Z}_i = (\boldsymbol{X}_i, Y_i)$ drawn from a joint response-predictor distribution.

Bootstrap:

- Sample $\boldsymbol{Z}_1^\star, \ldots, \boldsymbol{Z}_n^\star$ completely at random with replacement from $\boldsymbol{z}_1, \ldots, \boldsymbol{z}_n$.
- Apply regression model on pseudo dataset to get $\hat{\boldsymbol{\beta}}^\star$.

Repeat this approach many times.

Note: Paired bootstrap is less sensitive to violation of assumptions, e.g. adequacy of regression model, than bootstrapping the residuals.

# Copper-nickel alloy

Data: 13 measurements of corrosion loss ($y_i$) in copper-nickel alloys, each with a specific iron content ($x_i$).

Question: Change in corrosion loss in the alloys as the iron content increases, relative to corrosion loss where there is no iron, i.e. $\theta = \beta_1/\beta_0$.

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| $x_i$ | 0.01 | 0.48 | 0.71 | 0.95 | 1.19 | 0.01 | 0.48 |
| $y_i$ | 127.6 | 124.0 | 110.8 | 103.9 | 101.5 | 130.1 | 122.0 |
| $x_i$ | 1.44 | 0.71 | 1.96 | 0.01 | 1.44 | 1.96 | |
| $y_i$ | 92.3 | 113.1 | 83.7 | 128.0 | 91.4 | 86.2 | |

The observed data yield $\hat{\theta} = \hat{\beta}_1/\hat{\beta}_0 = -0.185$.

# Bias of an estimator

- We observe $X_1, X_2, \dots, X_n \sim F$ iid
- Parameter of interest $\theta = t(F)$
- Estimator $\hat{\theta} = s(X)$

  (may or may not be based on the plug-in principle)
- Bias definition

$$\text{bias}_F(\hat{\theta}, \theta) = \mathsf{E}_F[\hat{\theta}] - \theta = \mathsf{E}_F[s(\boldsymbol{x})] - t(F)$$

# Bootstrap estimate of bias

We want to estimate

$$\mathsf{bias}_F(\hat{\theta}, \theta) = \mathsf{E}_F[s(\boldsymbol{x})] - t(F)$$

Idea: Apply the plug-in principle and define the bootstrap estimate of bias as:

$$\mathsf{bias}_{\hat{F}} = \mathsf{E}_{\hat{F}}[s(\boldsymbol{x}^\star)] - t(\hat{F})$$

where $\hat{F}$ is an estimate of $F$ (for example the empirical distribution)

# Bias estimate of the bias

1. Generate $B$ bootstrap samples $x^{1\star}, \ldots, x^{B\star}$.
2. Evaluate the corresponding parameter estimates

$$\hat{\theta}^{\star}(b) = s(x^{b\star}), \quad b = 1, 2, \ldots, B$$

3. Approximate the bootstrap expectation $\mathrm{E}_{\hat{F}}[s(\boldsymbol{x}^{\star})]$ as:

$$\hat{\theta}^{\star}(\cdot) = \frac{1}{B}\sum_{b=1}^{B}\hat{\theta}^{\star}(b)$$

4. Approximate the ideal bootstrap estimate for bias as

$$\widehat{\mathrm{bias}}_B = \hat{\theta}^{\star}(\cdot) - t(\hat{F})$$

# Bias corrected estimate

One we have estimated the bias we can compute the bias-corrected estimator

$$\hat{\theta}_c = \hat{\theta} - \widehat{\text{bias}}_B = \hat{\theta} - [\hat{\theta}^{\star}(\cdot) - t(\hat{F})]$$

# Bias corrected estimate

One we have estimated the bias we can compute the bias-corrected estimator

$$\hat{\theta}_c = \hat{\theta} - \widehat{\text{bias}}_B = \hat{\theta} - [\hat{\theta}^\star(\cdot) - t(\hat{F})]$$

Note: Bias correction will not always give an improved estimator. We have that $\text{Var}(\hat{\theta}_c) \geq \text{Var}(\hat{\theta})$ so if the bias is small is better not to do bias correction.

# Bootstrap bias correction

## Copper-nickel alloy example

The mean value of

$$\hat{\theta}^{\star} - \hat{\theta}$$

among the pseudo datasets is about $-0.00125$.

The bias-corrected bootstrap estimate of $\beta_1/\beta_0$ is $-0.18507 - (-0.00125) = -0.184$.

# Confidence intervals (percentile method)

A "simple-minded" two-sided confidence interval with coverage $(1-\alpha)$ for a parameter $\alpha$ is given by

$$[q^{\star}_{\alpha/2}, q^{\star}_{1-\alpha/2}]$$

where $q^{\star}_{\alpha}$ is the $\alpha$-bootstrap quantile in the distribution of $\hat{\theta}^{\star}$.

Experience: Often good, but often too low coverage, i.e the true $\alpha$ for the interval is lower than the specified value.

Note: Better bootstrap confidence intervals exist and often have better coverage accuracy — at the price of being somewhat more difficult to implement

Show R-code bootstrap_regression.R