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UNIVERSITÀ
CATTOLICA
del Sacro Cuore

BOOTSTRAP CONFIDENCE INTERVALS AND TESTS

CONFIDENCE INTERVALS

INTRODUCTION

Interval estimation problem.

Assume that we observe a sample of size n of data following a certain (unknown) distribution F :

$$\mathbf{x} = (x_1, \dots, x_n), \text{ with } x_i \sim F \quad \forall i \in \{1, \dots, n\}$$

We focus on the problem of estimating one (or more) parameter θ of the distribution F . We denote it as $\theta = t(F)$.

Assume that $\hat{\theta} = t(\hat{F})$ is the plug-in estimator of θ .

Is it possible to build confidence intervals based on the Bootstrap estimate of the standard error?



DESIRED PROPERTIES OF CONFIDENCE INTERVALS

For ease of notation, we will define the properties for a one-tailed confidence interval of level $1 - \alpha$: $(\hat{\theta}_\alpha, +\infty)$.

Definition 1 *A confidence interval $(\hat{\theta}_\alpha, +\infty)$ of level $1 - \alpha$ for the parameter θ is said to be exact if, for all $\alpha \in (0, 1)$:*

$$\mathbb{P}(\theta \leq \hat{\theta}_\alpha) = \alpha.$$

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In general, we will work with asymptotic confidence intervals, i.e., confidence intervals for which exactness holds just asymptotically, for $n \rightarrow \infty$. For such intervals we can define the properties of accuracy and correctness:

DESIRED PROPERTIES OF CONFIDENCE INTERVALS

Definition 2 A confidence interval $(\hat{\theta}_\alpha, +\infty)$ of level $1 - \alpha$ for the parameter θ is said to be first-order accurate if, for all $\alpha \in (0, 1)$:

$$\mathbb{P}(\theta \leq \hat{\theta}_\alpha) = \alpha + \mathcal{O}(n^{-1/2}).$$

A confidence interval $(\hat{\theta}_\alpha, +\infty)$ of level $1 - \alpha$ for the parameter θ is said to be second-order accurate if, for all $\alpha \in (0, 1)$:

$$\mathbb{P}(\theta \leq \hat{\theta}_\alpha) = \alpha + \mathcal{O}(n^{-1}).$$

DESIRED PROPERTIES OF CONFIDENCE INTERVALS

Definition 3 Let $\hat{\theta}_{exact_\alpha}$ be the endpoint of an exact confidence interval of level $1 - \alpha$ for the parameter θ . A confidence interval $(\hat{\theta}_\alpha, +\infty)$ of level $1 - \alpha$ for the parameter θ is said to be first-order correct if, for all $\alpha \in (0, 1)$:

$$\hat{\theta}_\alpha = \hat{\theta}_{exact_\alpha} + \mathcal{O}(n^{-1}) = \hat{\theta}_{exact_\alpha} + \mathcal{O}(n^{-1/2}) \cdot \hat{\sigma}.$$

A confidence interval $(\hat{\theta}_\alpha, +\infty)$ of level $1 - \alpha$ for the parameter θ is said to be second-order correct if, for all $\alpha \in (0, 1)$:

$$\hat{\theta}_\alpha = \hat{\theta}_{exact_\alpha} + \mathcal{O}(n^{-3/2}) = \hat{\theta}_{exact_\alpha} + \mathcal{O}(n^{-1}) \cdot \hat{\sigma}.$$

BOOTSTRAP CONFIDENCE INTERVALS

- 1. Asymptotic normal confidence intervals.**
- 2. Bootstrap-t confidence intervals.**
- 3. Percentile intervals.**
- 4. BCa confidence intervals.**
- 5. ABC confidence intervals.**



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ASYMPTOTIC NORMAL CONFIDENCE INTERVAL

It is often possible to show asymptotic results on the estimator $\hat{\theta}$. In many cases we have that

$$\frac{\hat{\theta} - \theta}{\widehat{\text{se}}(\hat{\theta})} \rightarrow N(0, 1).$$

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Asymptotic confidence interval for theta with (asymptotic) coverage probability 1-alpha:

$$[\hat{\theta} - z_{\alpha/2} \widehat{\text{se}}_B, \hat{\theta} + z_{\alpha/2} \widehat{\text{se}}_B]$$

ASYMPTOTIC NORMAL CONFIDENCE INTERVAL

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Properties.

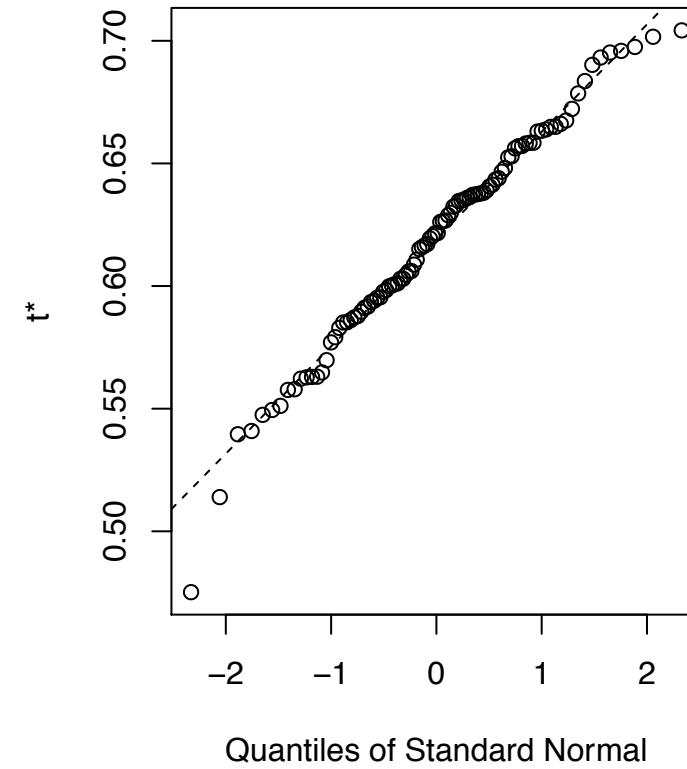
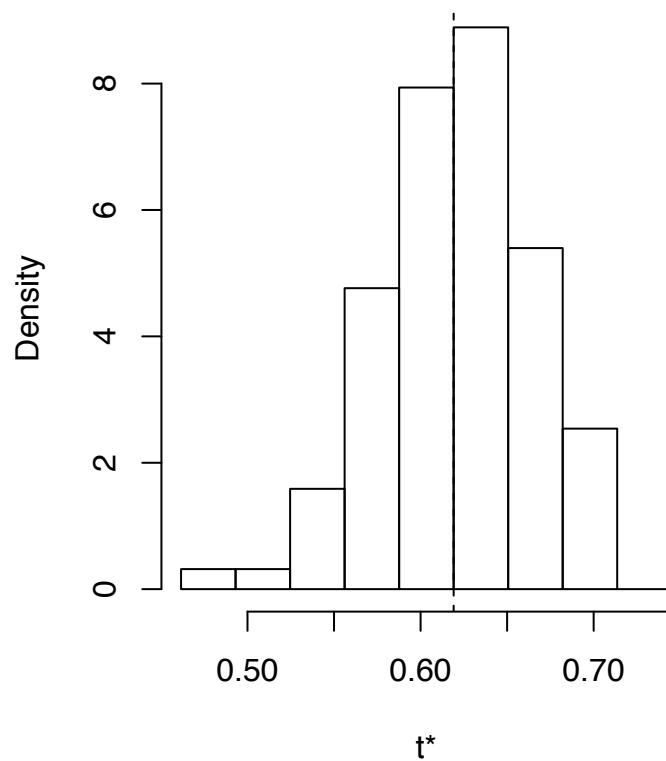
- If $x_i \sim N(\mu, \sigma^2)$ and $\theta = \mu$, the interval is exact.
- If $\frac{\hat{\theta} - \theta}{\widehat{se}(\hat{\theta})} \rightarrow N(0, 1)$, the interval is asymptotically exact.
- It is often possible to prove first order accuracy and correctness. However the properties of this interval strictly depend on the form of the estimator $\hat{\theta}$.

ASYMPTOTIC NORMAL CONFIDENCE INTERVAL

Example: test score data.

$B = 100$: $(0.5333, 0.7048)$

Histogram of t^*

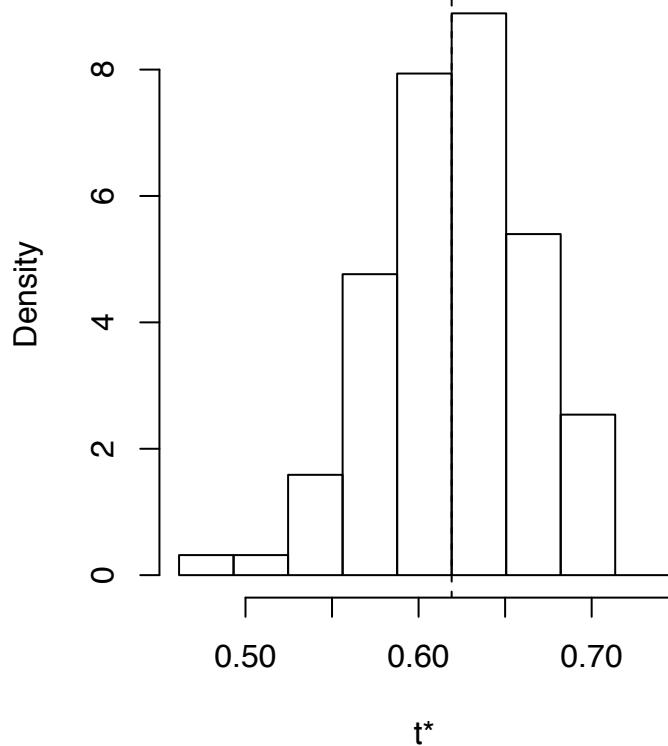


ASYMPTOTIC NORMAL CONFIDENCE INTERVAL

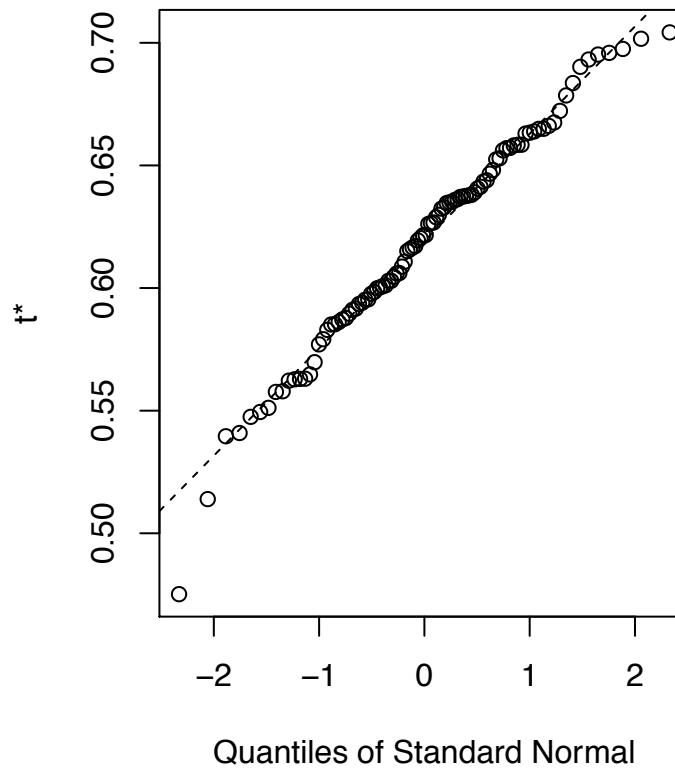
Example: test score data.

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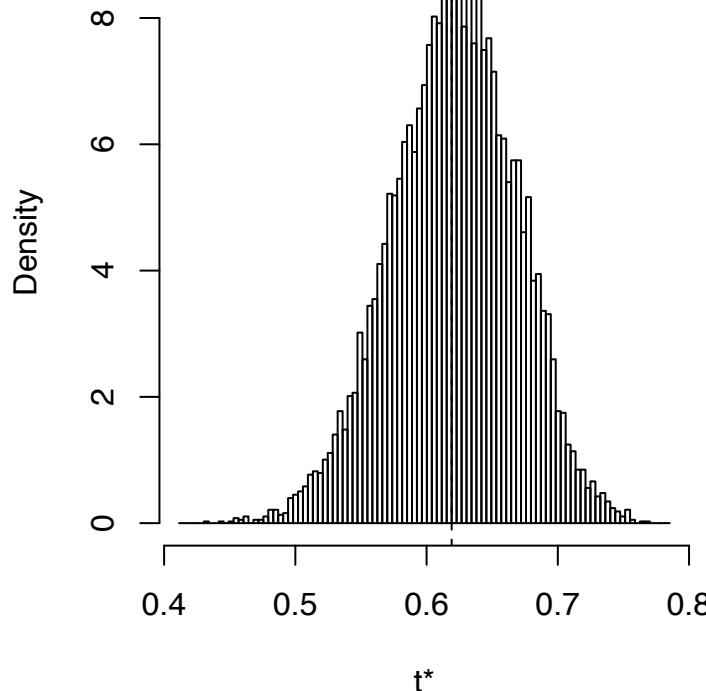
Here a low number of replications is ok, since we are using only the point estimate of sd to build the interval. However, it is difficult to understand from the QQplot if the distribution is approximately Normal.



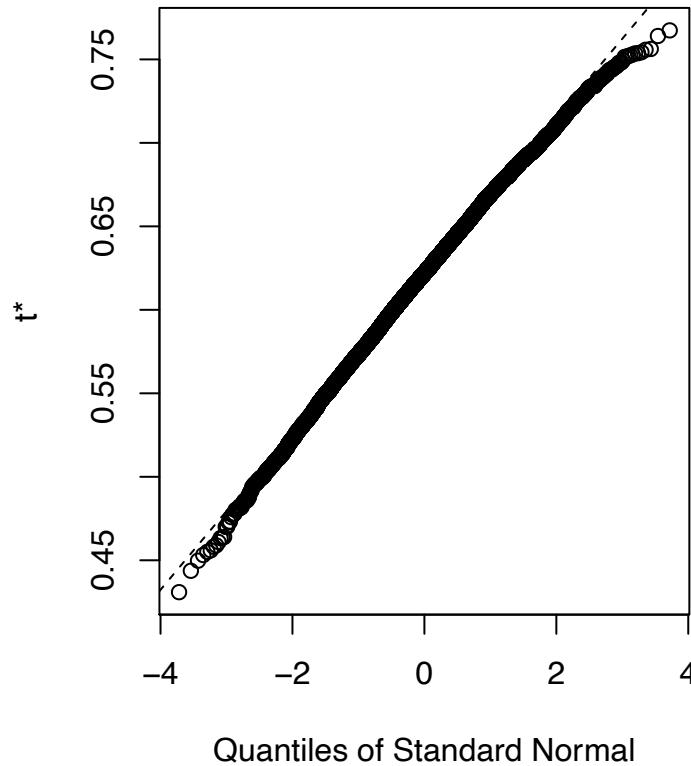
Example: test score data.

B = 10000: (0.5249, 0.7097)

Histogram of t^*



Here a low number of replications is ok, since we are using only the point estimate of sd to build the interval. However, it is difficult to understand from the QQplot if the distribution is approximately Normal.



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BOOTSTRAP-T INTERVAL

The idea of the Bootstrap- t interval is based on a Bootstrapped version of the Student- t pivotal statistic:

$$T = \frac{\hat{\theta} - \theta}{\text{se}(\hat{\theta})}.$$

The statistic T is used for building Normal-theory confidence interval, since its distribution does not depend on unknown parameters (Student- t distribution with $n - 1$ degrees of freedom).

Since the quantiles $t_{\alpha/2, n-1}$ of the t distribution are known, then:

$$\mathbb{P}(t_{1-\alpha/2, n-1} \leq T \leq t_{1-\alpha/2, n-1}) = 1 - \alpha$$

$$\mathbb{P}\left(\hat{\theta} - \text{se}(\hat{\theta})t_{1-\alpha/2, n-1} \leq \theta \leq \hat{\theta} + \text{se}(\hat{\theta})t_{1-\alpha/2, n-1}\right) = 1 - \alpha$$



$$\left(\hat{\theta} - \text{se}(\hat{\theta})t_{1-\alpha/2, n-1}, \hat{\theta} + \text{se}(\hat{\theta})t_{1-\alpha/2, n-1}\right)$$

Confidence interval for theta with coverage probability 1-alpha.

BOOTSTRAP-T INTERVAL



Idea. Instead of trying to elicit the distribution of T under parametric assumptions, we can generate a sample of B Bootstrap replications of the statistic T . In detail, As in the point estimation case, we can generate B Bootstrap samples $\mathbf{x}_1^*, \dots, \mathbf{x}_B^*$, which mimic sampling from the original model. Then, we can compute for each Bootstrap sample b the following quantity, mimicking the Student- t pivotal statistic T :

$$Z_b^* = \frac{\hat{\theta}_b^* - \hat{\theta}}{\widehat{\text{se}}_b^*}.$$

We have B Bootstrap copies Z_1^*, \dots, Z_B^* , and we can define the quantiles t_α such that:

$$\frac{\#\{Z_b^* \geq t_\alpha\}}{B} = \alpha.$$

Finally, the Bootstrap- t confidence interval of level $1 - \alpha$ is:

$$(\hat{\theta} - t_{\alpha/2} \widehat{\text{se}}_B, \hat{\theta} + t_{\alpha/2} \widehat{\text{se}}_B)$$

BOOTSTRAP-T INTERVAL

- We need to estimate \widehat{se}_b^* , that is the standard error of the b th Bootstrap sample: $\widehat{se}_b^* = \widehat{se}(\widehat{\theta}_b^*)$. If $\widehat{\theta}_b^*$ is simple, we usually have formulas that we can use (together with the plug-in estimates). Otherwise, we can apply another Bootstrap to compute it \Rightarrow two nested layers of Bootstrapping.
- To compute the point estimate \widehat{se}_b we can use around $B_1 \simeq 100$ replications. To compute the confidence interval, we need $B_2 \simeq 1000$ replications. This approach requires at least $B_1 \cdot B_2 \simeq 100000$ Bootstrap replications.
- This interval is not invariant under transformations: if we apply a non linear (monotone) function to the parameter, compute the CI, and then transform back the interval endpoints, we do not find necessarily the same result. In addition, some transformations have better properties than others, and we could use another Bootstrap layer to find the transformation itself ...

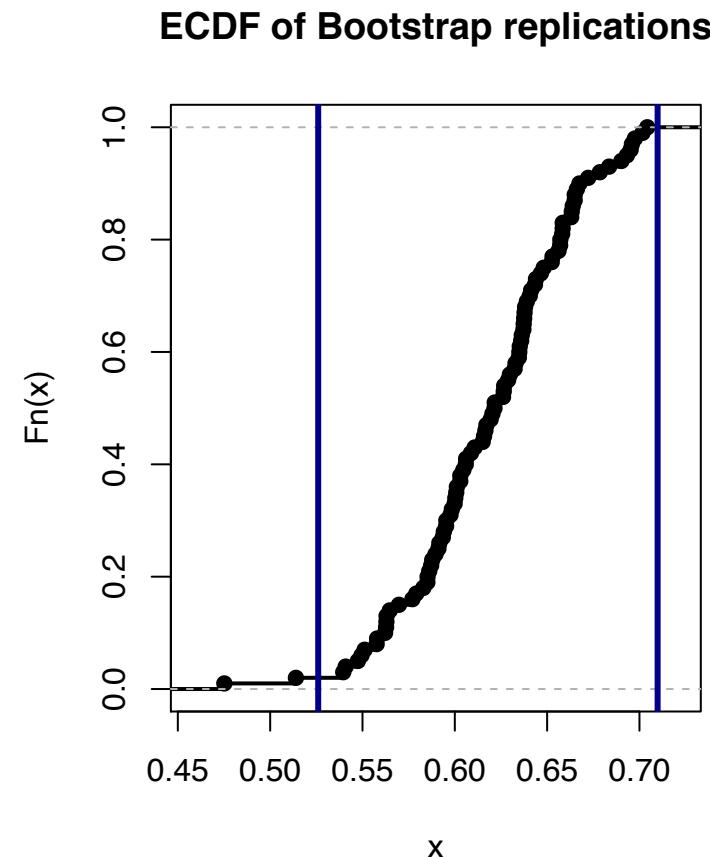
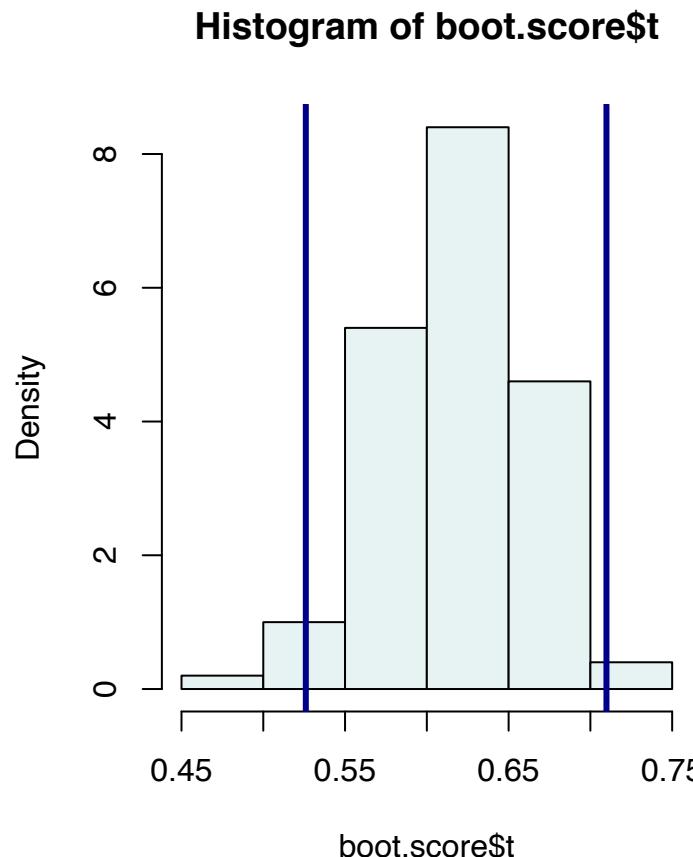


Properties.

- Not invariant under increasing transformations. If m is an increasing function and $(\hat{\theta}_{L_\alpha}, \hat{\theta}_{U_\alpha})$ is a Bootstrap- t confidence interval of level $1 - \alpha$ for θ , the confidence interval for $m(\theta)$ is not necessarily $(m(\hat{\theta}_{L_\alpha}), m(\hat{\theta}_{U_\alpha}))$.
- The Bootstrap- t interval is second-order accurate and second-order correct.
- To avoid computation of $\hat{s}e_b^*$, it is possible to use the non-studentized approximate pivot $\hat{\theta} - \theta$. This gives a confidence interval that is only first-order accurate and correct.

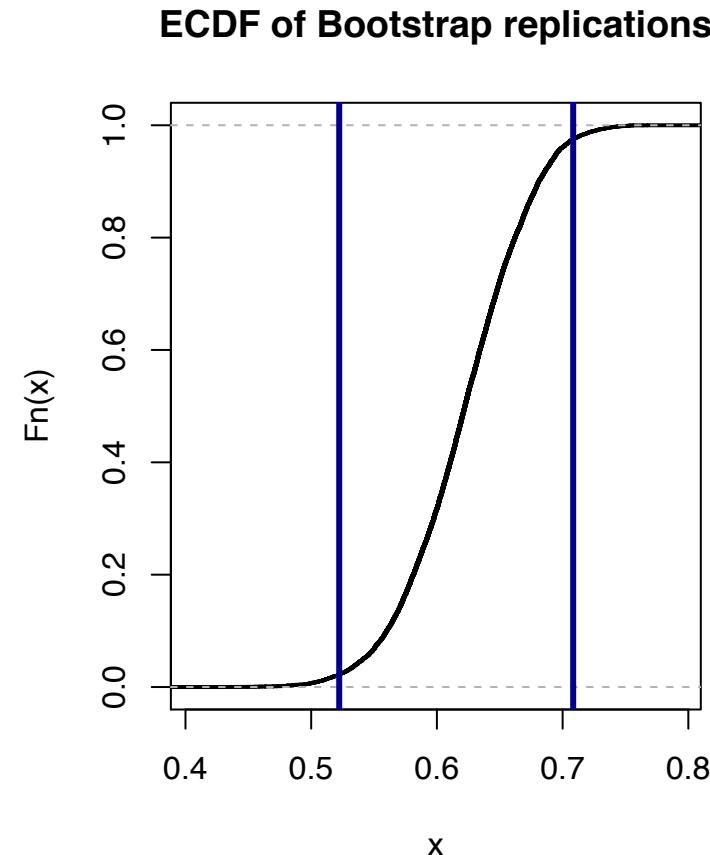
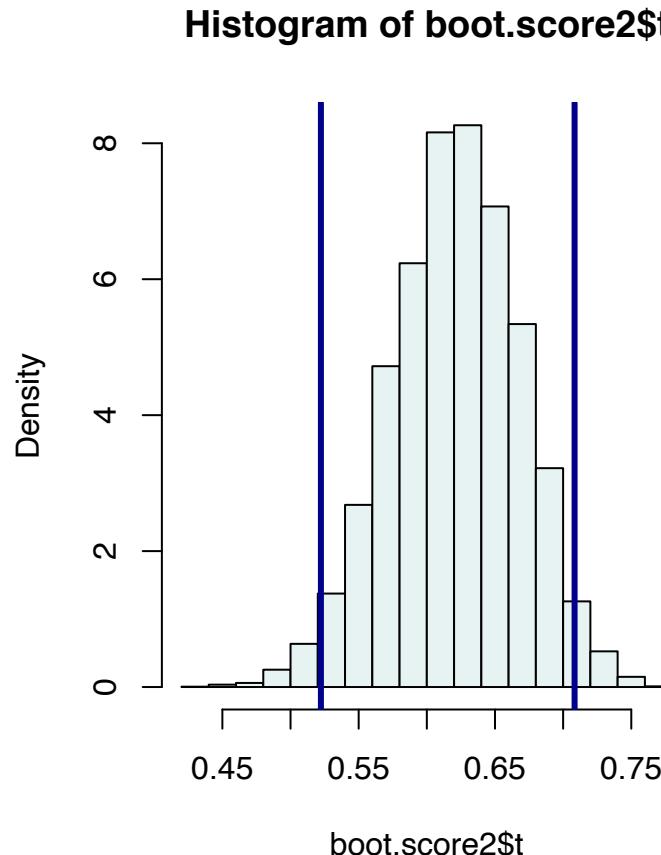
Example: test score data.

$B = 100: (0.5277, 0.7529)$



Example: test score data.

$B = 10000: (0.5226, 0.7165)$ **VERY LONG!!**



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PERCENTILE INTERVAL

For percentile intervals we use directly the empirical quantiles of $\hat{\theta}_1^*, \dots, \hat{\theta}_B^*$.
The $1 - \alpha$ confidence interval is then:

$$[\hat{\theta}_{(1-\alpha/2)}^*, \hat{\theta}_{(\alpha/2)}^*]$$



Empirical quantiles of the Bootstrap
replications distribution

PERCENTILE INTERVAL

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Properties:

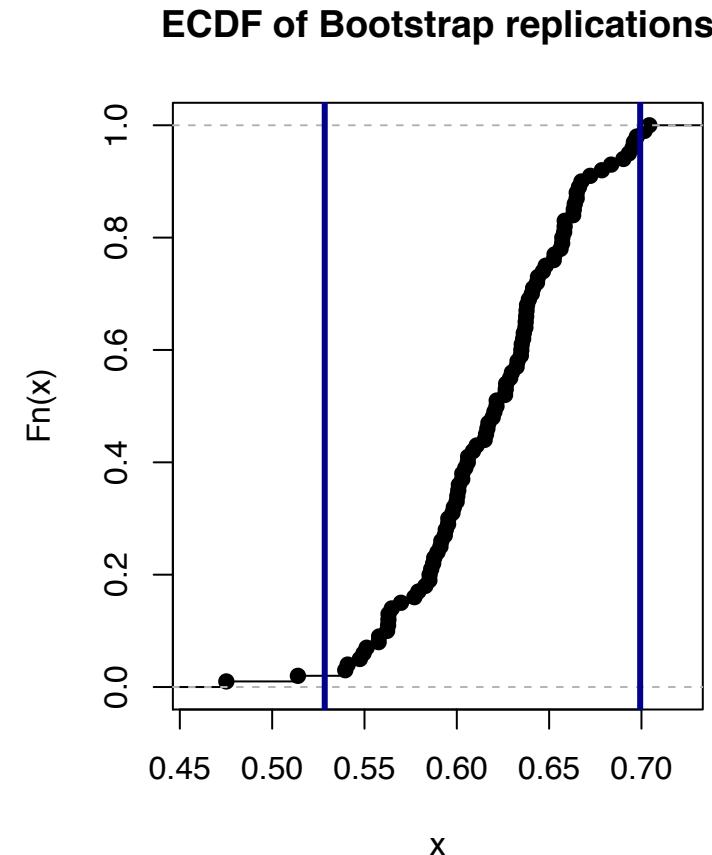
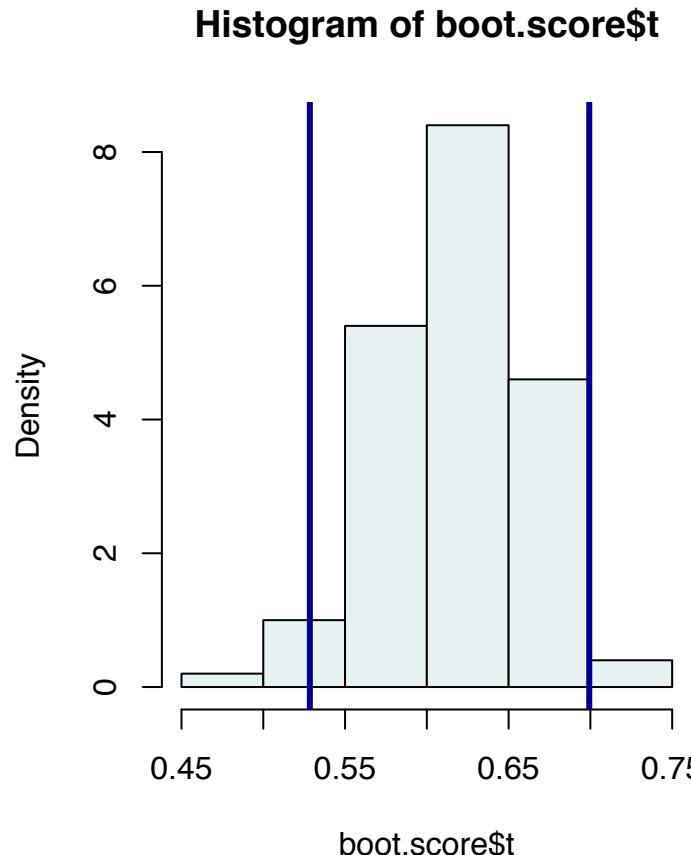
- It is invariant through monotone transformations (since any monotone transformation preserve the ordering of the quantities $\hat{\theta}_b^*$): for all increasing function m , if $(\hat{\theta}_{L_\alpha}, \hat{\theta}_{U_\alpha})$ is a Bootstrap- t confidence interval of level $1 - \alpha$ for θ , the confidence interval for $m(\theta)$ is $(m(\hat{\theta}_{L_\alpha}), m(\hat{\theta}_{U_\alpha}))$.
- It is first-order accurate and correct.
- In practice, if $\hat{\theta}$ is a biased estimator, for instance so that

$$\hat{\theta} \sim N(\theta + \text{Bias}, \text{Var}(\hat{\theta}))$$

the percentile interval (as well as the Bootstrap- t interval) does not generally behave well.

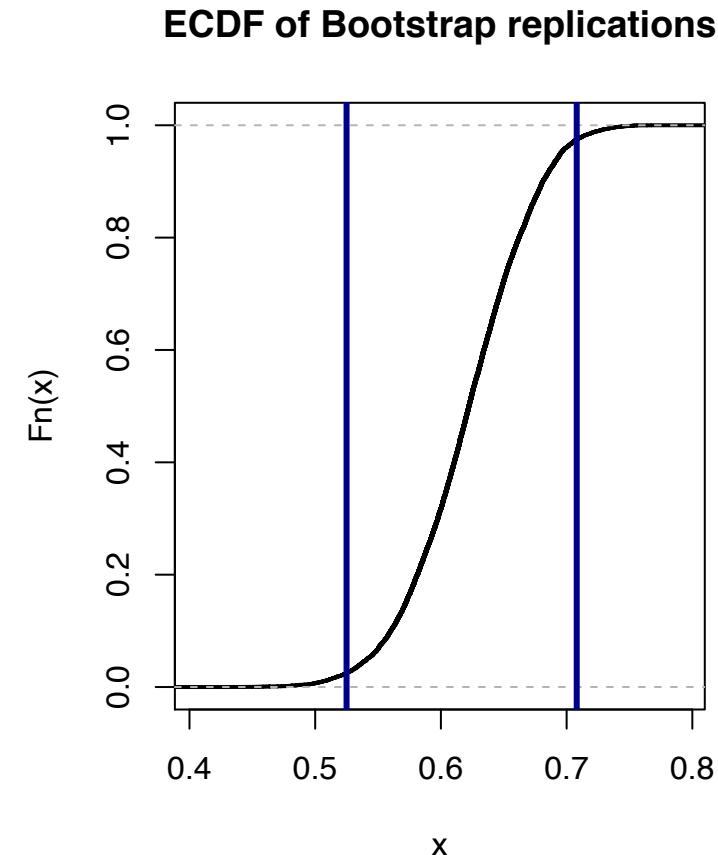
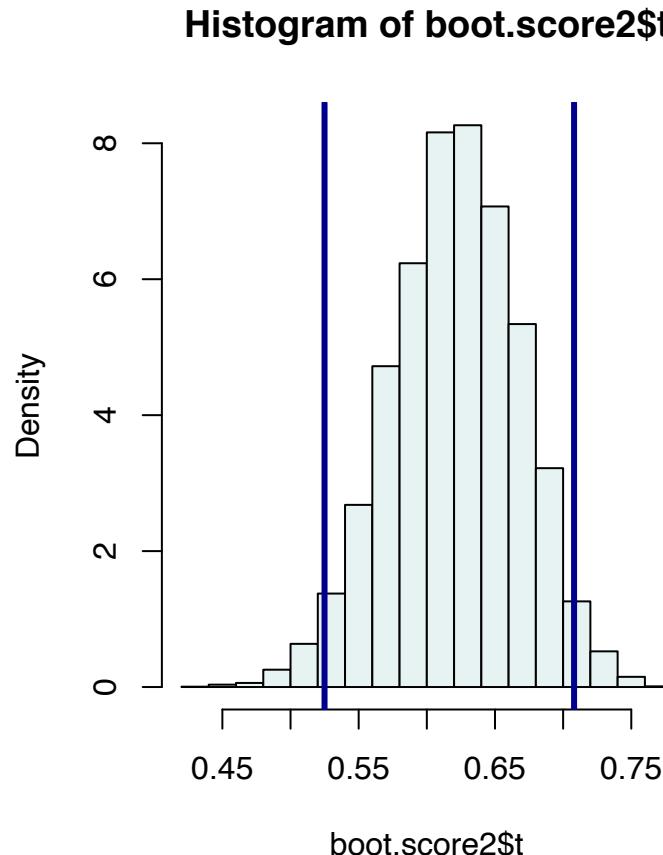
Example: test score data.

B = 100: (0.5285, 0.6993)



Example: test score data.

$B = 10000: (0.5249, 0.7080)$



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BC_A CONFIDENCE INTERVAL

BC_a confidence intervals: **Bias Corrected and Accelerated confidence intervals.**

Remember that percentile intervals are $\left[\hat{\theta}_{(1-\alpha/2)}^*, \hat{\theta}_{(\alpha/2)}^* \right]$.

The idea of BC_a confidence intervals is to introduce a correction to the previous interval to take into account that $\hat{\theta}$ might be biased. The interval is:

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where:

$$\begin{aligned}\alpha_1 &= 1 - \Phi \left(\hat{z}_0 + \frac{\hat{z}_0 + z_{1-\alpha/2}}{1 - \hat{a}(\hat{z}_0 + z_{1-\alpha/2})} \right) \\ \alpha_2 &= 1 - \Phi \left(\hat{z}_0 + \frac{\hat{z}_0 + z_{\alpha/2}}{1 - \hat{a}(\hat{z}_0 + z_{\alpha/2})} \right)\end{aligned}$$

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Cdf of the standard Normal distribution

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Quantiles of the standard Normal distribution

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\hat{z}_0 : bias correction parameter

\hat{a} : acceleration parameter

BC_A CONFIDENCE INTERVAL

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$$\alpha_2 = 1 - \Phi \left(\hat{z}_0 + \frac{\hat{z}_0 + z_{\alpha/2}}{1 - \hat{a}(\hat{z}_0 + z_{\alpha/2})} \right) \quad \hat{a}: \text{ acceleration parameter}$$

- If $\hat{a} = \hat{z}_0 = 0 \Rightarrow \alpha_1 = 1 - \Phi(z_{1-\alpha/2}) = 1 - \alpha/2$
 $\alpha_2 = 1 - \Phi(z_{\alpha/2}) = \alpha/2$
- In the general case:
 - $\hat{z}_0 = \Phi^{-1} \left(\frac{\#\{\hat{\theta}_b^* < \hat{\theta}\}}{B} \right)$. Measures the median bias of $\hat{\theta}$, that is the difference between the median of $\hat{\theta}^*$ and $\hat{\theta}$. If $\hat{\theta}^*$ is centered on $\hat{\theta}$: $\hat{z}_0 = \Phi^{-1}(0.5) = 0$.
 - $\hat{a} = \frac{\sum_{i=1}^n (\hat{\theta}_{(\cdot)_J} - \hat{\theta}_{(i)_J})^3}{6(\sum_{i=1}^n (\hat{\theta}_{(\cdot)_J} - \hat{\theta}_{(i)_J})^2)^{3/2}}$, where $\hat{\theta}_{(\cdot)_J}$ is the Jackknife estimate and $\hat{\theta}_{(i)_J}$ are the Jackknife replications. corrects from the fact that $\text{se}(\hat{\theta})$ can possibly depend on θ .

BC_A CONFIDENCE INTERVAL

Statistical model for BC_a confidence intervals.

Assume that there exists an increasing transformation m such that $\psi = m(\theta)$, and $\hat{\psi} = m(\hat{\theta})$ gives:

$$\frac{\hat{\psi} - \psi}{\text{se}_\psi} \sim N(-z_0, 1)$$

and assume that, for an appropriate reference point ψ_0 :

$$\text{se}_\psi = \text{se}_{\psi_0} (1 + a(\psi - \psi_0))$$

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and assume that, for an appropriate reference point ψ_0 :

$$\text{se}_\psi = \text{se}_{\psi_0}(1 + a(\psi - \psi_0))$$

If this model holds exactly, an exact upper $1 - \alpha$ limit (of a two-tailed interval) for ψ is:

$$\hat{\psi}_\alpha = \hat{\psi} + \text{se}_{\hat{\psi}} \frac{z_0 + z_{1-\alpha/2}}{1 - a(z_0 + z_{1-\alpha/2})}.$$

Mapping back this limit in the original θ parameter space we have the upper limit for θ :

$$\hat{\theta}_\alpha = G^{-1} \left(\Phi \left(z_0 + \frac{z_0 + z_{1-\alpha/2}}{1 - a(z_0 + z_{1-\alpha/2})} \right) \right).$$

This model also gives the estimates of $\hat{z}_0 = \mathbb{P}(\hat{\theta}^* < \theta)$ and \hat{a} .

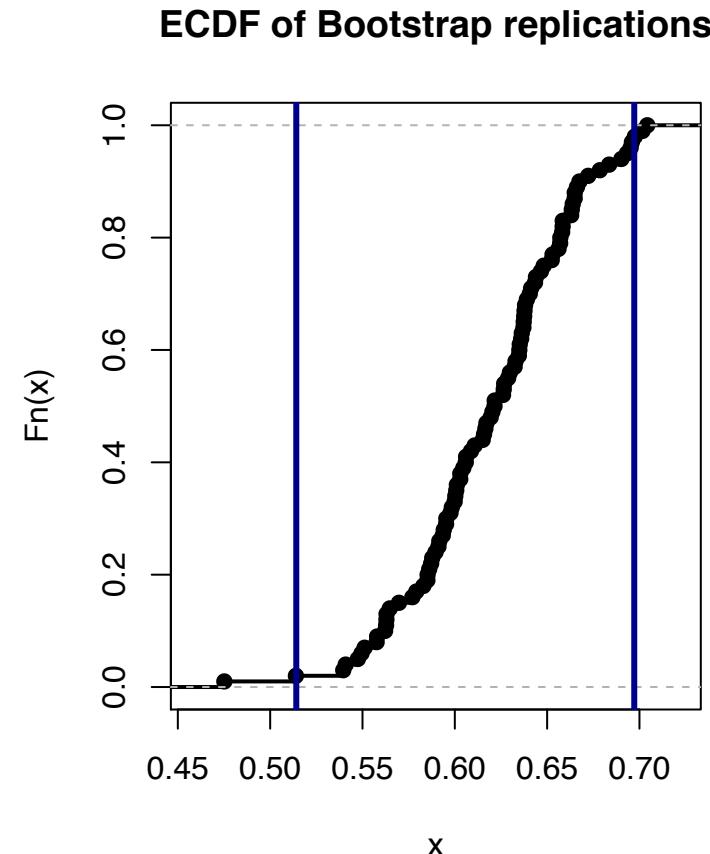
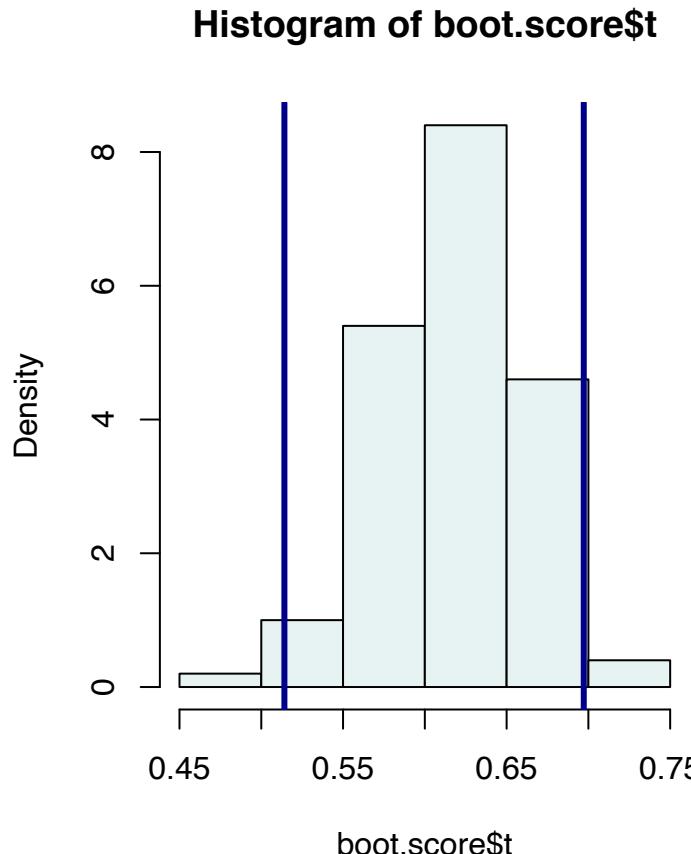
BC_A CONFIDENCE INTERVAL

Properties.

- It is invariant through monotone transformations: for all increasing function m , if $(\hat{\theta}_{L_\alpha}, \hat{\theta}_{U_\alpha})$ is a BC_a confidence interval of level $1 - \alpha$ for θ , the confidence interval for $m(\theta)$ is $(m(\hat{\theta}_{L_\alpha}), m(\hat{\theta}_{U_\alpha}))$.
- It is second-order accurate and correct.
- It requires a large number of Bootstrap replications to be computed with a low approximation error.

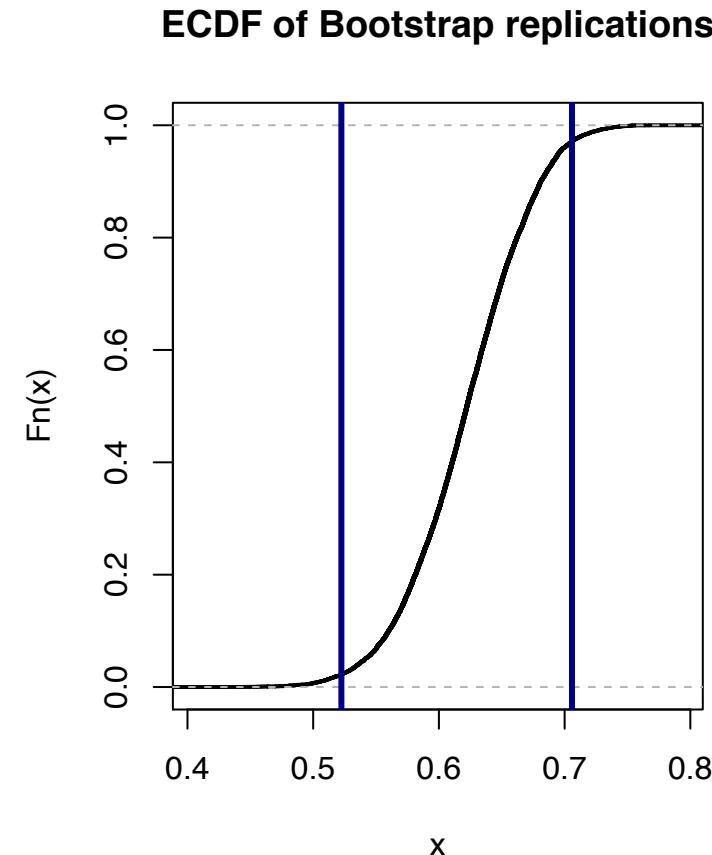
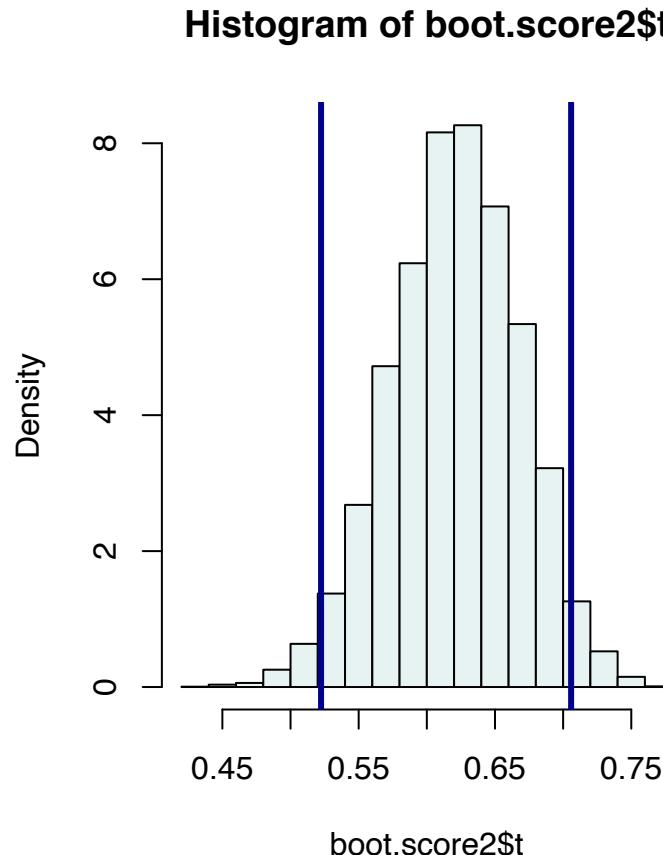
Example: test score data.

B = 100: (0.5141, 0.6972)



Example: test score data.

B = 10000: (0.5224, 0.7059)



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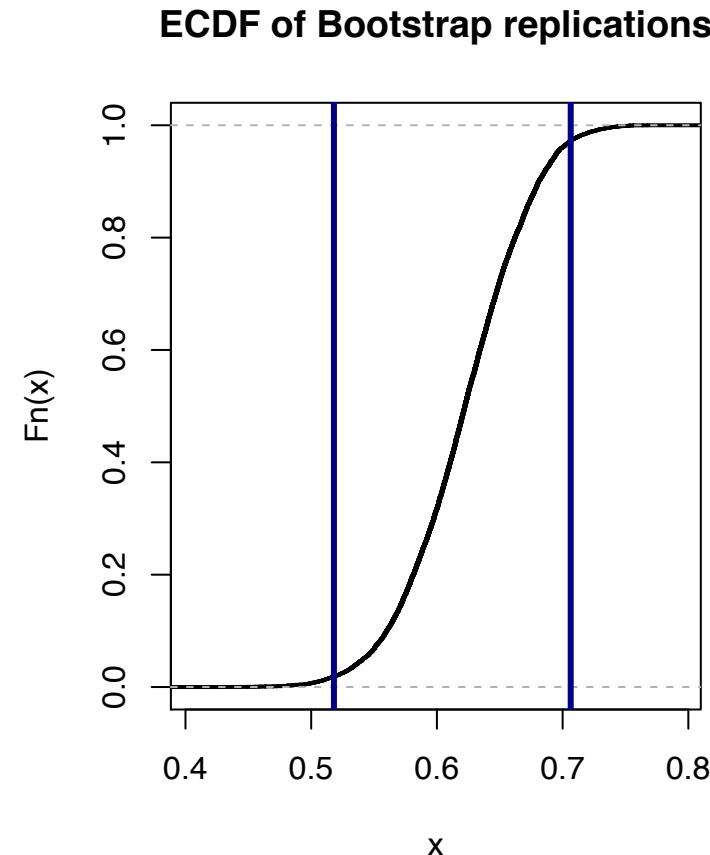
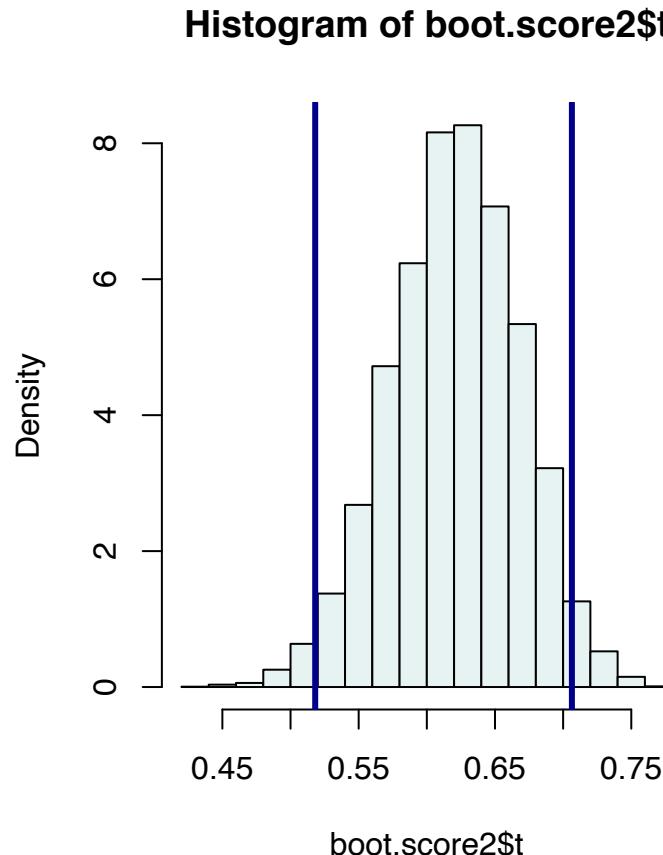


ABC CONFIDENCE INTERVAL

- Based on an analytical approximation of the BC_a confidence intervals (instead of MC replications).
- Requires that the estimator of theta is smooth (is first and second order differentiable).
- Uses Taylor expansion to approximate the endpoints.
- It is invariant under monotone transformations.
- It is second-order accurate and correct (if the estimator is smooth).
- In order to use it, it is necessary to find the expression of theta as a function of the vector \mathbf{P}^* , collecting the proportion of units in the bootstrap sample that equals the j th original data point.

Example: test score data.

The result does not depend on B: (0.5180939, 0.7064266)



TESTS

TESTING THE MEAN OF ONE SAMPLE

Let us assume that we observe a sample \mathbf{x} of size n from unknown F . Define $\mu_x = \mathbb{E}[X_i]$. We now want to test the following hypotheses:

$$H_0 : \mu_x = \mu_0$$

$$H_1 : \mu_x \neq \mu_0$$

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Classical approach: under the assumption of normality of data or of large sample size, we find the (eventually approximate) distribution F_0 of a test statistic $t(\mathbf{X})$ under the null hypothesis H_0 . Using such distribution, we find the level α rejection region of the test, or the test p -value:

$$p = \mathbb{P}_{H_0}(t(\mathbf{X}) \geq t(\mathbf{x})).$$

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Bootstrap approach: approximate the distribution F_0 using an empirical estimate \hat{F}_0 and compute the p -value by drawing data sets from \hat{F}_0 .

TESTING THE MEAN OF ONE SAMPLE

Problem: the empirical distribution \hat{F} is not a good candidate for estimating F_0 , since it does not obey to H_0 . We first have to impose that H_0 is true, that is $\mu_x = \mu_0$.



TESTING THE MEAN OF ONE SAMPLE

Problem: the empirical distribution \hat{F} is not a good candidate for estimating F_0 , since it does not obey to H_0 . We first have to impose that H_0 is true, that is $\mu_x = \mu_0$.

However, we can first translate data so that their sample mean is exactly μ_0 . Then, we compute the empirical distribution \hat{F}_0 of translated data, and use it to generate Bootstrap replications and to approximate the null distribution of the test statistic.

We find a procedure for testing H_0 against H_1 with an approximate level α .

The level of the test is asymptotically correct (thanks to convergence of \hat{F}_0 to F_0).



TESTING THE MEAN OF ONE SAMPLE

Algorithm for testing the mean of one population.

- Translate the data so that their sample mean is μ_0 :

$$z_i = x_i - \bar{x} + \mu_0$$

- Approximate F_0 with \hat{F}_0 , that is the empirical distribution of data z_i .
- Repeat B times:
 - Draw a sample \mathbf{z}_b^* from \hat{F}_0 .
 - Evaluate the test statistic on \mathbf{z}_b^* :

$$t(\mathbf{z}_b^*) = \frac{\mathbf{z}_b^* - \mu_0}{\sqrt{\hat{\sigma}_b^2/n}}$$

- Finally, evaluate the p -value of the test as:

$$\hat{p}_B = \frac{\#\{t(\mathbf{z}_b^*) \geq t(\mathbf{x})\}}{B}.$$

TESTING MEAN DIFFERENCES BETWEEN TWO SAMPLES

Assume that we observe two independent samples:

- \mathbf{z} : sample of size m drawn from the unknown distribution F , $\mu_z = \mathbb{E}[F]$.
- \mathbf{y} : sample of size n drawn from the unknown distribution G , $\mu_y = \mathbb{E}[G]$.

We now want to test mean differences between the two groups, that is testing the hypotheses:

$$H_0 : \mu_z = \mu_y$$

$$H_1 : \mu_z \neq \mu_y$$

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$$\begin{aligned} H_0 &: \mu_z = \mu_y \\ H_1 &: \mu_z \neq \mu_y \end{aligned}$$

Estimating F_0 and G_0 : under H_0 , F and G have the same mean. So, we estimate the sample distributions \hat{F}_0 and \hat{G}_0 by first translating both samples so that they have a common mean, and then computing separately the two empiric distributions:

$$\begin{aligned} \tilde{z}_i &= z_i - \bar{z} + \bar{x} \\ \tilde{y}_i &= y_i - \bar{y} + \bar{x} \\ \bar{x} &= \left(\sum_{i=1}^m z_i + \sum_{i=1}^n y_i \right) / (n + m) \end{aligned}$$

TESTING MEAN DIFFERENCES BETWEEN TWO SAMPLES

Bootstrap data sets: We draw a sample of size n from F_0 and a sample of size n from \hat{G}_0 .

Test statistic: The test statistic can be borrowed from the classical parametric case (studentized statistic, similar to the one used for the construction of Bootstrap-t confidence intervals).

In the case of assuming equal variances:

$$t(\mathbf{x}) = \frac{\bar{z} - \bar{y}}{\sqrt{s_p^2 \left(\frac{1}{m} + \frac{1}{n} \right)}}$$

with s_p^2 is the pooled estimate of the variance.

In the case of assuming unequal variances:

$$t(\mathbf{x}) = \frac{\bar{z} - \bar{y}}{\sqrt{\left(\frac{s_z^2}{m} + \frac{s_y^2}{n} \right)}}$$

TESTING HYPOTHESES ON LINEAR REGRESSION PARAMETERS

Assume that we observe pairs (\mathbf{c}_i, y_i) for $i = 1, \dots, n$. We assume that data follow the linear regression model

$$y_i = \mathbf{c}_i \boldsymbol{\beta}' + \varepsilon_i = \sum_{j=1}^p c_{ij} \beta_j + \varepsilon_i$$

where ε_i is an i.i.d. sample from an unknown distribution F with $\mathbb{E}[\varepsilon_i] = 0$, $\text{Var}[\varepsilon_i] = \sigma^2 \forall i$.

We want to test, for $j = 1, \dots, p$:

$$H_0 : \beta_k = 0$$

$$H_1 : \beta_k \neq 0$$

TESTING HYPOTHESES ON LINEAR REGRESSION PARAMETERS

Estimating the null distribution.

Under the null hypothesis, the model reduces to:

$$y_i = \sum_{j \neq k} c_{ij} \beta_j + \varepsilon_i = [\mathbf{c}_i]_{(k)} \boldsymbol{\beta}_0 + \varepsilon_i.$$

Null model:
model under the
null hypothesis

So, the null model $P_0 = (\boldsymbol{\beta}_0, F_0)$ can be estimated with $\hat{P}_0 = (\hat{\boldsymbol{\beta}}_0, \hat{F}_0)$ where $\hat{\boldsymbol{\beta}}_0$ is the OLS estimator of $\boldsymbol{\beta}_0$ and \hat{F}_0 the empirical distribution of the residuals of the null model.

TESTING HYPOTHESES ON LINEAR REGRESSION PARAMETERS

Bootstrap data sets.

Bootstrap data sets are generated sampling the residuals ε^* from \hat{F}_0 , and then plugging-them in the null model:

$$y_i^* = \sum_{j \neq k} c_{ij} \hat{\beta}_{j_0} + \varepsilon_i^* = [\mathbf{c}_i]_{(k)} \hat{\boldsymbol{\beta}}_0 + \varepsilon_i^*.$$

Test statistic.

As test statistic we can use the classical t -test statistic:

$$t(\mathbf{x}) = \frac{\hat{\beta}_k}{\text{se}(\hat{\beta}_k)}.$$

OLS estimate on the
original model.