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Statistics for Data Science, Winter 2023

Chapter 3:

Bootstrap and Jackknife

Overview

Bootstrap and Jackknife are simulation based methods for inference/uncertainty quantification.

CIs and testing

pros:

- Conceptually simple
- No need for mathematically complex probability calculations

cons:

- Computationally expensive
- Requires large sample size (as for the normal approximation)
- Can go wrong even in large samples!
- Use with care!

RECALL: SAMPLING DISTRIBUTION

$X_1, \ldots, X_n \overset{iid}{\sim} \text{Bernoulli}(\theta), \theta \in (0,1), \hat{\theta}_n = \frac{1}{n}\sum_{i=1}^n X_i$

$\frac{\hat{\theta}_n - \theta}{se_\theta} \xrightarrow[n\to\infty]{d.} N(0,1)$, $se_\theta = \sqrt{\text{Var}_\theta[\hat{\theta}_n]} = \sqrt{\frac{\theta(1-\theta)}{n}}$

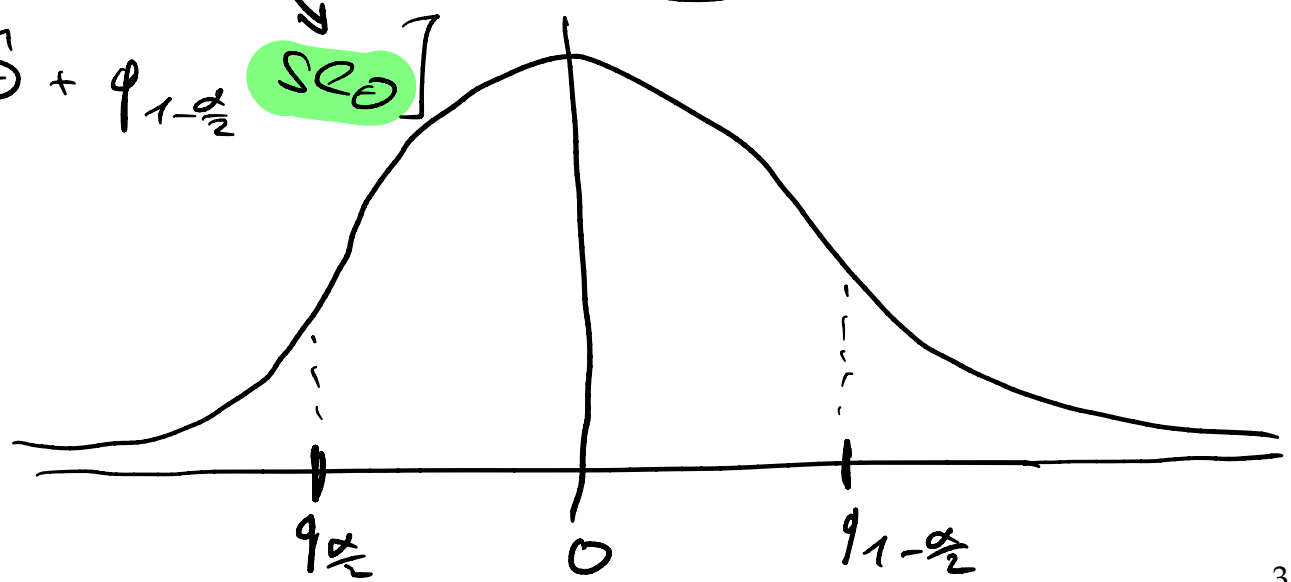
estimate se_θ by plug-in rule $se_{\hat{\theta}_n} = \sqrt{\frac{\hat{\theta}_n(1-\hat{\theta}_n)}{n}}$

$$P\left(q_{\frac{\alpha}{2}} \le \frac{\hat{\theta} - \theta}{se_\theta} \le q_{1-\frac{\alpha}{2}}\right) \approx 1-\alpha \qquad \left[\frac{\hat{\theta}_n - \theta}{se_\theta} \approx N(0,1)\right]$$

unknown

$$\left[\hat{\theta} - q_{1-\frac{\alpha}{2}} se_\theta,\ \hat{\theta} + q_{1-\frac{\alpha}{2}} se_\theta\right]$$

$$\hat{se} = se_{\hat{\theta}} = \sqrt{\frac{\hat{\theta}(1-\hat{\theta})}{n}}$$



In general

$X_1, \ldots, X_n \overset{iid}{\sim} f_\theta, \theta \in \Theta,$

We often have a CLT:

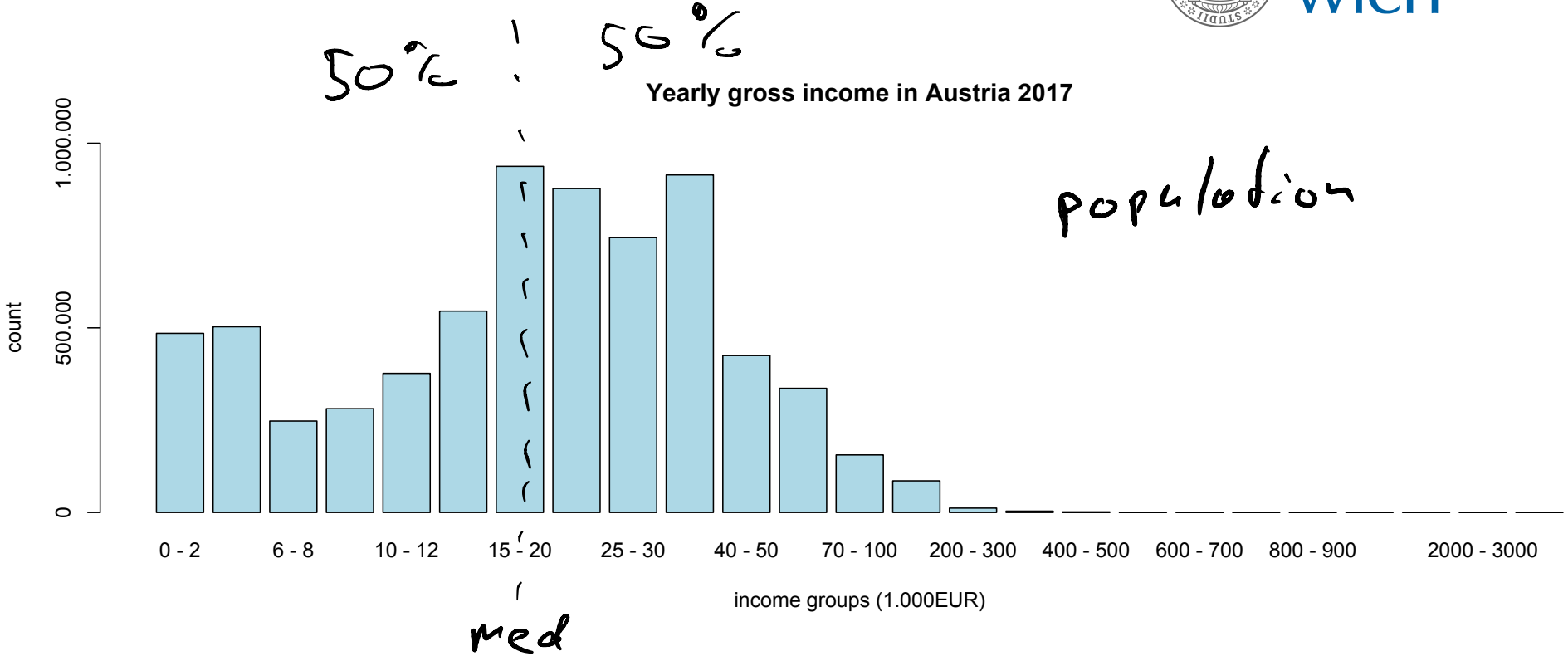
$$\frac{\hat{\theta}_n - \theta}{se_\theta} \xrightarrow[n\to\infty]{d.} N(0,1)$$

But the standard error $se_\theta := \sqrt{\mathrm{Var}_\theta[\hat{\theta}_n]}$ may be hard to compute or the plug-in idea may not be feasible.

First Bootstrap idea: se bootstrap
Estimate se_θ (without knowing its exact analytical form) and rely on the CLT.

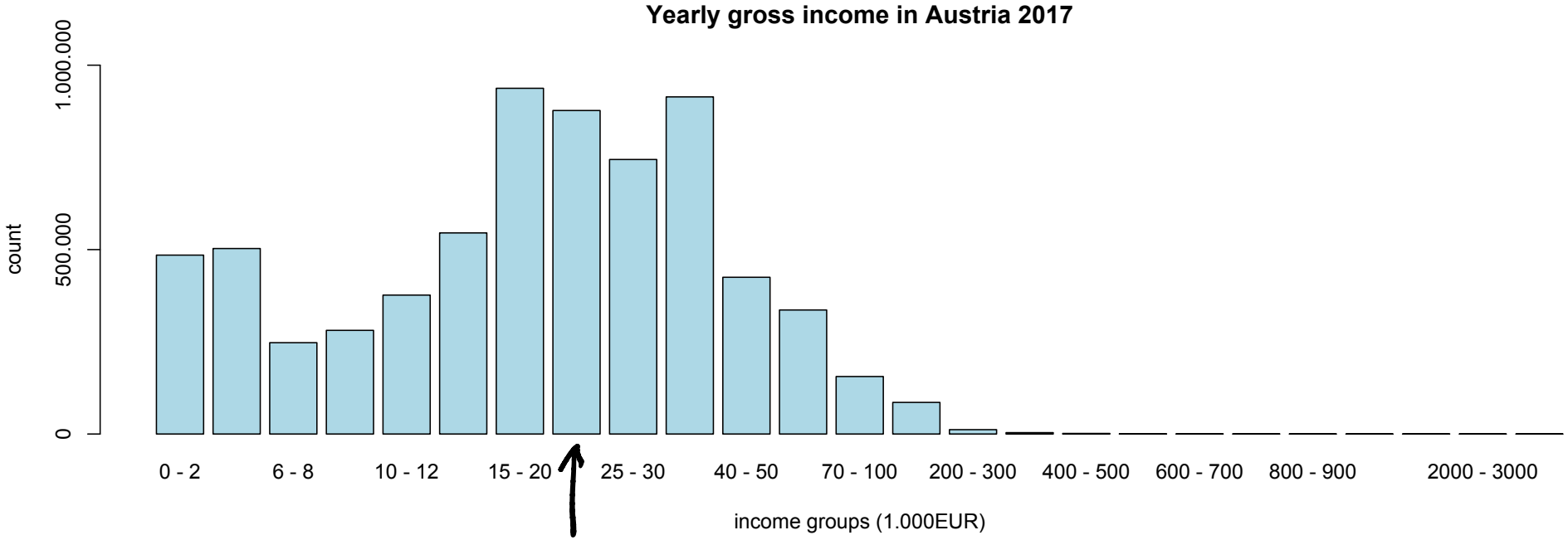
Second Bootstrap idea: pivotal bootstrap
Estimate quantiles of the sampling distribution of $\hat{\theta}_n - \theta$. No Gaussian approximation required.

EXAMPLE: MEDIAN INCOME



Recall: Median = 50% quantile = smallest number $m \in \mathbb{R}$ such that 50% of data are below or equal to m

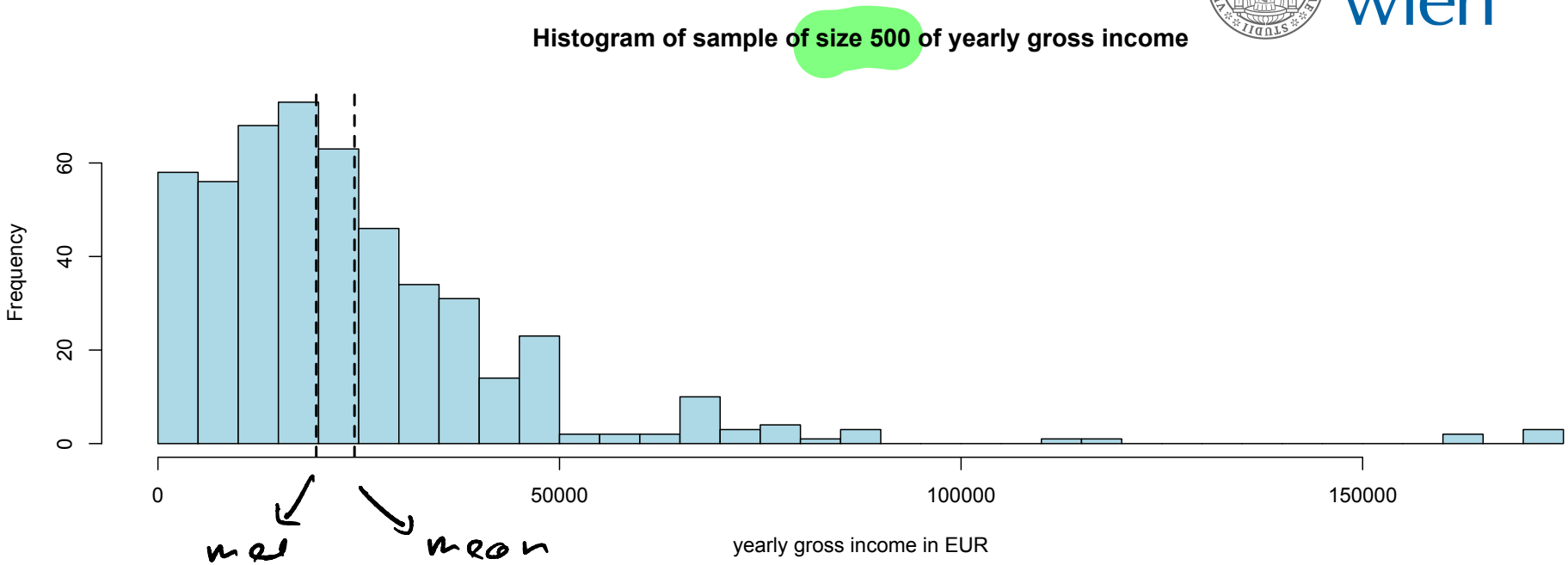
Example: median income



med 20k – 25k

```
> N/2
[1] 3466764
> cumsum(rev(dat$count))
 [1]  485050  987971 1235594 1516636 1893307 2438570
 [7] 3375906 4252996 4997282 5911340 6336321 6672594
[13] 6828489 6914181 6926012 6929730 6931288 6932039
[19] 6932500 6932774 6932960 6933085 6933416 6933475
[25] 6933529
```

EXAMPLE: MEDIAN INCOME



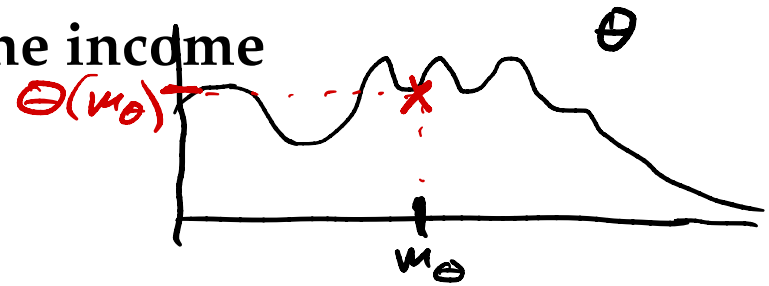
Min.	1st Qu.	Median	Mean	3rd Qu.	Max.
8	10716	19712	24475	31148	174629

$\hat{\theta}$

Median should be in the $20k$ – $25k$ group!?

EXAMPLE: MEDIAN INCOME

A realistic (nonparametric) model for the income distribution:



$$\mathcal{X} = [0, \infty)^n,$$

$$\Theta = \{\text{all pdfs } \theta \in C^1([0, \infty)) : \theta(m_\theta) > 0\}, \quad m_\theta := \text{med}(\theta)$$

$$f_\theta(x) = \prod_{i=1}^{n} \theta(x_i), \quad x = (x_1, \ldots, x_n)' \in \mathcal{X}, \theta \in \Theta.$$

True population is discrete! Should use pmfs?

$\rightarrow$ Model is an approximation/idealization!

EXAMPLE: MEDIAN INCOME

A realistic (nonparametric) model for the income distribution:

$$\mathcal{X} = [0, \infty)^n,$$

$$\Theta = \{\text{all pdfs } \theta \in C^1([0,\infty)) : \theta(m_\theta) > 0\}, m_\theta := \text{med}(\theta)$$

$$f_\theta(x) = \prod_{i=1}^{n} \theta(x_i), \quad x = (x_1, \ldots, x_n)' \in \mathcal{X}, \theta \in \Theta.$$

Use sample median $\hat{m}_n := \hat{F}_n^\dagger(1/2)$ to estimate population median $m_\theta := \psi(\theta) := F_\theta^\dagger(1/2)$, $F_\theta(x) := \int_{-\infty}^{x} \theta(y)dy$.

It is well known that for every $\theta \in \Theta$,

$$\frac{\hat{m}_n - m_\theta}{se_\theta} \xrightarrow[n\to\infty]{d.} N(0,1)$$

plug-in for Θ? estimate Θ non-parametrically

where $se_\theta = \frac{1}{2\sqrt{n}\theta(m_\theta)}$.

How do we estimate that?!

BOOTSTRAP ESTIMATION OF SE

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Given data $X = (X_1, \ldots, X_n)'$, $X_1, \ldots, X_n \overset{iid}{\sim} p_\theta$, $\theta \in \Theta$, and an estimator $\hat{\theta}_n : \mathcal{X}_0^n \to \mathbb{R}$ of θ (or $\psi(\theta)$), we want to estimate $se_\theta(\hat{\theta}_n) = \sqrt{\mathrm{Var}_\theta[\hat{\theta}_n]}$.

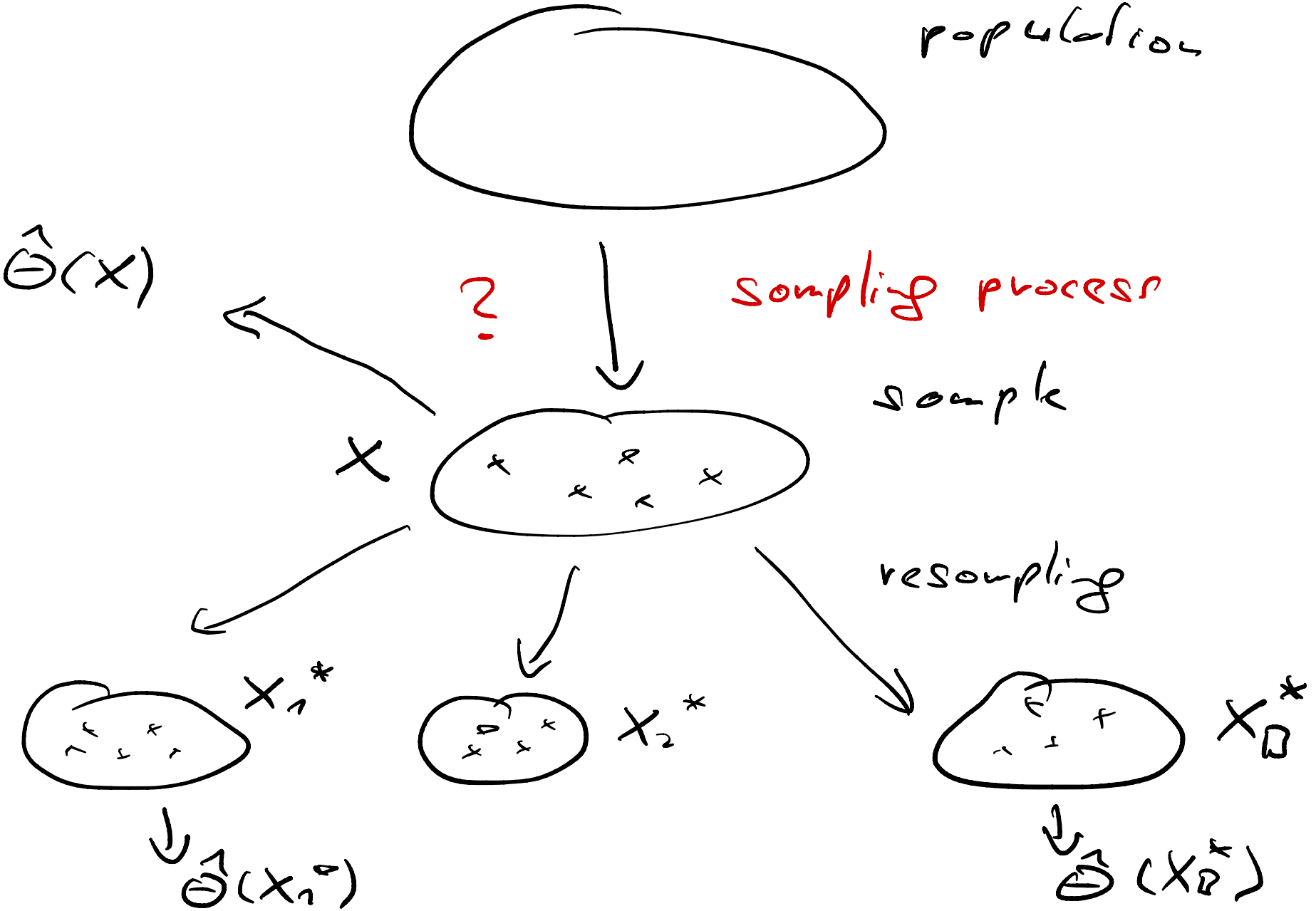
1. Draw a large number B of random samples of size n (with replacement) from the **sample!**

$$
\begin{aligned}
X_1^* &= (X_{1,1}^*, \ldots, X_{n,1}^*)' \\
X_2^* &= (X_{1,2}^*, \ldots, X_{n,2}^*)' \\
&\vdots \\
X_B^* &= (X_{1,B}^*, \ldots, X_{n,B}^*)'
\end{aligned}
$$

2. Compute $\hat{\theta}_n(X_1^*), \ldots, \hat{\theta}_n(X_B^*)$.
3. Approximate $\mathrm{Var}_\theta[\hat{\theta}_n]$ using the LLN (MC idea)

$$
\hat{se}_{boot}^2 = \frac{1}{B}\sum_{j=1}^{B} \hat{\theta}_n(X_j^*)^2 - \left(\frac{1}{B}\sum_{j=1}^{B} \hat{\theta}_n(X_j^*)\right)^2 .
$$

BOOTSTRAP ESTIMATION OF SE



General idea of the Bootstrap:

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Pretend that the sample is the population and simulate (imitate) the sampling process by 'resampling' from the sample.

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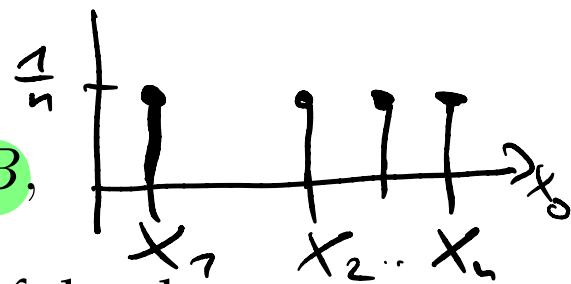
Why should this work?

Assume that the original data sample $X = (X_1, \ldots, X_n)'$ from sample space $\mathcal{X} = \mathcal{X}_0^n$ is **given and non-random**.

- Then the Bootstrap draws

$$X_{i,j}^*, \; i = 1, \ldots, n, \; j = 1, \ldots, B,$$



are iid from the **empirical distribution** $\hat{F}_n$ of the data, which has pmf

$$\hat{p}_n(x_0) := \frac{1}{n} \sum_{i=1}^{n} \mathbb{1}_{\{X_i\}}(x_0), \quad x_0 \in \{X_1, \ldots, X_n\}.$$

- Thus, also the $X_1^*, \ldots, X_B^*$ are iid from the n-fold product

$$\hat{f}_n(x) := \prod_{i=1}^{n} \hat{p}_n(x_i), \quad x = (x_1, \ldots, x_n)' \in \{X_1, \ldots, X_n\}^n.$$

Bootstrap estimation of SE

- But if $X_1^*, \ldots, X_B^* \overset{iid}{\sim} \hat{f}_n$, then (by the LLN)

$$\hat{se}^2_{boot} = \frac{1}{B}\sum_{j=1}^{B} \hat{\theta}_n(X_j^*)^2 - \left(\frac{1}{B}\sum_{j=1}^{B} \hat{\theta}_n(X_j^*)\right)^2 \xrightarrow[B\to\infty]{i.p.} \mathrm{Var}_{\hat{f}_n}[\hat{\theta}_n].$$

- Because $X_1^* = (X_{1,1}^*, \ldots, X_{n,1}^*)' \sim \hat{f}_n$ follows an iid model with marginal pmf $\hat{p}_n$, we also write $\mathrm{Var}_{\hat{f}_n}[\hat{\theta}_n] = \mathrm{Var}_{\hat{p}_n}[\hat{\theta}_n]$.
- Since the sample $X_1, \ldots, X_n \overset{iid}{\sim} p_\theta$, we have $\hat{F}_n \approx F_\theta$ (recall HW3), $\hat{p}_n \approx p_\theta$ and one can often show that

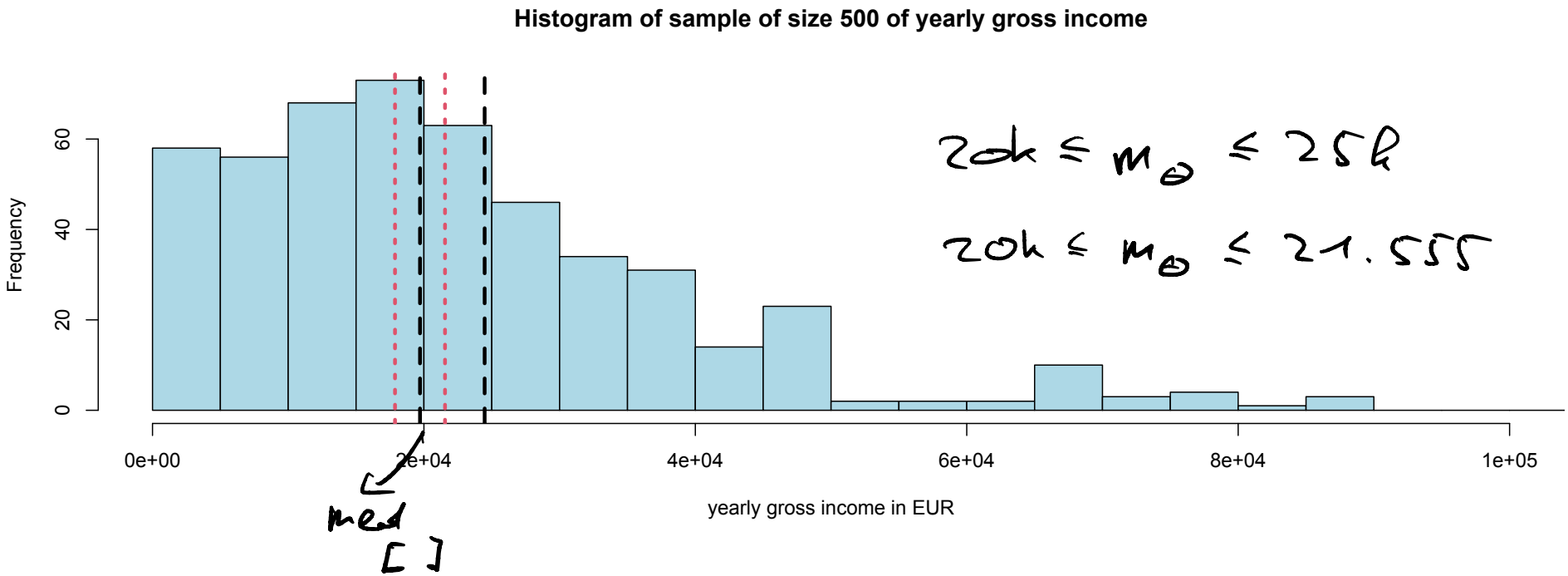
$$\mathrm{Var}_{\hat{p}_n}[\hat{\theta}_n] \approx \mathrm{Var}_{p_\theta}[\hat{\theta}_n] = \mathrm{Var}_\theta[\hat{\theta}_n], \quad \text{if } n \text{ is large.}$$

$$\underbrace{\hat{se}^2_{boot} \approx \mathrm{Var}_{\hat{p}_n}[\hat{\theta}_n]}_{\text{if B is large}}, \qquad \underbrace{\mathrm{Var}_{\hat{p}_n}[\hat{\theta}_n] \approx \mathrm{Var}_\theta[\hat{\theta}_n]}_{\text{if } n \text{ is large}} = se^2_\theta(\hat{\theta}_n)$$

EXAMPLE: MEDIAN INCOME

Compute an approximate 95% ($\alpha = 0.05$) bootstrap confidence interval (by bootstrap estimation of the standard error)

$$CI_\alpha = [\hat{m}_n - q^{(N)}_{1-\frac{\alpha}{2}} \hat{se}_{boot}, \hat{m}_n + q^{(N)}_{1-\frac{\alpha}{2}} \hat{se}_{boot}]$$



$20k \leq m_\Theta \leq 25k$

$20k \leq m_\Theta \leq 21.555$

```
> c(CI_l, CI_u)
[1] 17870 21555
```

```
> CI_u - CI_l
[1] 3685
```

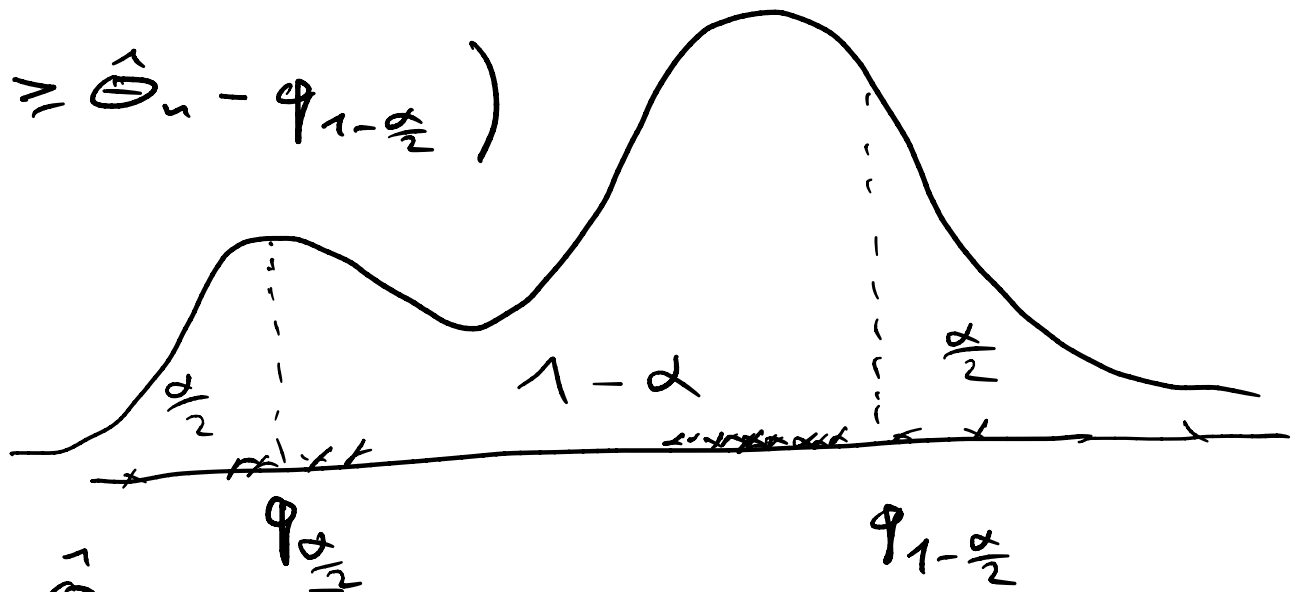
PIVOTAL BOOTSTRAP CI

Given data $X = (X_1, \ldots, X_n)'$, $X_1, \ldots, X_n \overset{iid}{\sim} p_\theta$, $\theta \in \Theta$, and an estimator $\hat{\theta}_n : \mathcal{X}_0^n \to \mathbb{R}$ of θ (or $\psi(\theta)$), we want to estimate the $\alpha/2$ and $1 - \alpha/2$ quantiles of the distribution of $\hat{\theta}_n(X) - \theta$.

Why? Say $\hat{\theta}_n - \theta \sim g_n$ is the unknown sampling distribution.

$$P_\theta\left(q_{\frac{\alpha}{2}} \le \hat{\theta}_n - \theta \le q_{1-\frac{\alpha}{2}}\right) = 1 - \alpha \qquad \hat{\theta}_n - \theta \sim g_n$$

$$= P_\theta\left(\hat{\theta}_n - q_{\frac{\alpha}{2}} \ge \theta \ge \hat{\theta}_n - q_{1-\frac{\alpha}{2}}\right)$$



$$CI_\alpha = \left[\hat{\theta}_n - q_{1-\frac{\alpha}{2}}, \hat{\theta}_n - q_{\frac{\alpha}{2}}\right]$$

PIVOTAL BOOTSTRAP CI

Given data $X = (X_1, \ldots, X_n)'$, $X_1, \ldots, X_n \overset{iid}{\sim} p_\theta$, $\theta \in \Theta$, and an estimator $\hat{\theta}_n : \mathcal{X}_0^n \to \mathbb{R}$ of θ (or $\psi(\theta)$), we want to estimate the $\alpha/2$ and $1 - \alpha/2$ quantiles of the distribution of $\hat{\theta}_n(X) - \theta$.

1. Draw a large number B of random samples of size n (with replacement) from the **sample!**

$$X_1^*, X_2^*, \ldots, X_B^*$$

2. Compute empirical (bootstrap) quantiles $\hat{q}^*_{\alpha/2}$ and $\hat{q}^*_{1-\frac{\alpha}{2}}$ of

$$\hat{\theta}_n(X_1^*) - \hat{\theta}_n(X), \ldots, \hat{\theta}_n(X_B^*) - \hat{\theta}_n(X).$$

3. $CI_\alpha = [\hat{\theta}_n(X) - \hat{q}^*_{1-\frac{\alpha}{2}}, \hat{\theta}_n(X) - \hat{q}^*_{\alpha/2}]$

EXAMPLE: MEDIAN INCOME

Comparison of 95% bootstrap CIs:

$B = 100$

method	lower	median	upper	length
bootstrap se	17870	19712	21555	3685
pivotal bootstrap	18074	19712	21452	3378

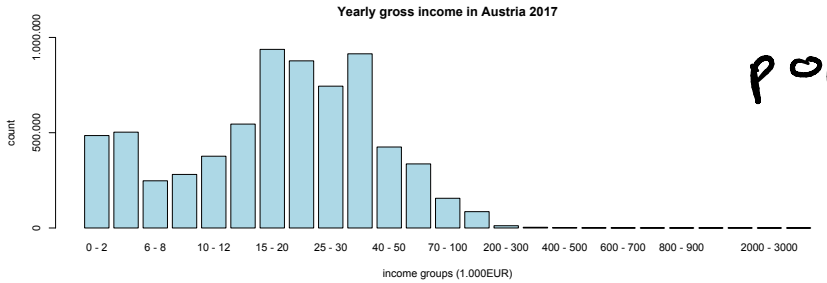
$B = 1000$

method	lower	median	upper	length
bootstrap se	18100	19712	21324	3224
pivotal bootstrap	18161	19712	21388	3227

EXAMPLE: MEDIAN INCOME

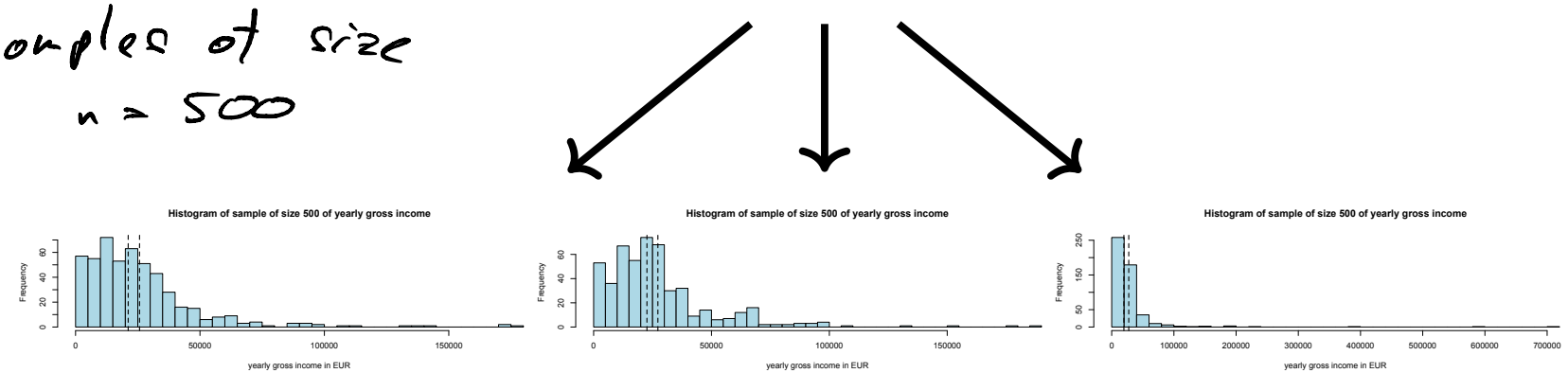
Can we actually trust this CI? Check by simulation!

$$m_\theta = F_\theta^\dagger(1/2)$$

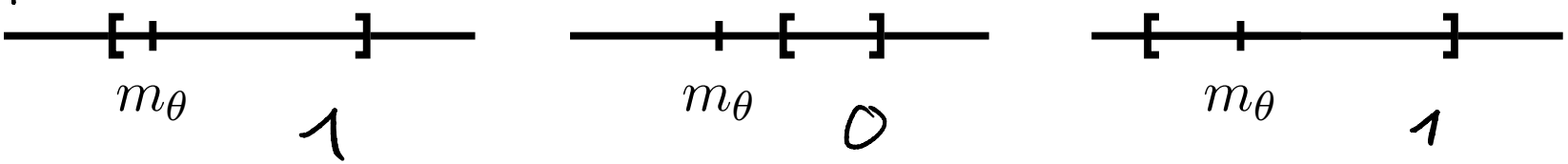


population

samples of size $n = 500$



Bootstrap samples



EXAMPLE: MEDIAN INCOME

Simulation results:

$1 - \alpha = 0.95$

number of (Montecarlo) samples drawn $= 1000$

$B = 1000$

sample size $n = 100$

method	coverage prob.	average length
se bootstrap	0.932	7601
pivotal bootstrap	0.871	7404

$\geq 1-\alpha = 0,95$

sample size $n = 1000$

method	coverage prob.	average length
se bootstrap	0.935	2412
pivotal bootstrap	0.917	2377

Failure of the Bootstrap

Recall: Bootstrap idea

- Regard your data sample as the population.
- Draw B iid random (bootstrap) samples from the sample (re-sample) like in a MC simulation.
- Compute your estimator on each of the bootstrap samples.
- Use this resulting 'bootstrap distribution' of your estimator as an approximation of its true unknown sampling distribution.

Recall

- In the median income example we simulated the actual coverage probability of the bootstrap CIs and found

$$P_\theta(m_\theta \in CI_\alpha) \approx 1 - \alpha.$$

- We did that for the true data generating parameter $\theta \in \Theta$. (we cheated!)
- We concluded that the bootstrap works relatively well for n large.
- In practice we would try many different choices for θ.

Failure of the Bootstrap

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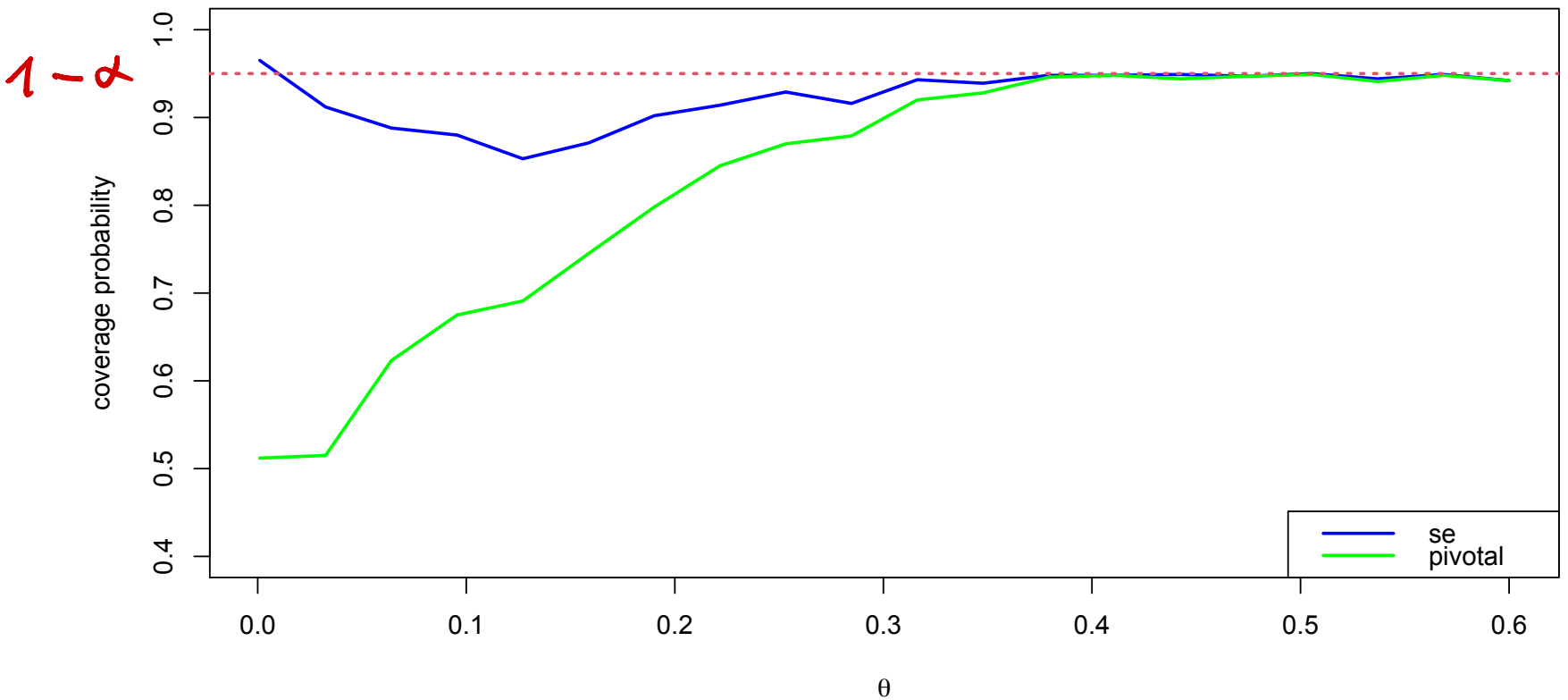
- Consider $X_1, \ldots, X_n \overset{iid}{\sim} N(\theta, 1)$, $\theta \in \Theta = [0, \infty)$.
- Goal: Bootstrap inference on θ.
- The classical estimator (MLE) is

$$\hat{\theta}_n = \max\{0, \bar{X}_n\}, \quad \bar{X}_n := \frac{1}{n} \sum_{i=1}^{n} X_i.$$

Failure of the Bootstrap

- $n = 100, \alpha = 0.05, B = 1000$
- 1000 MC iterations

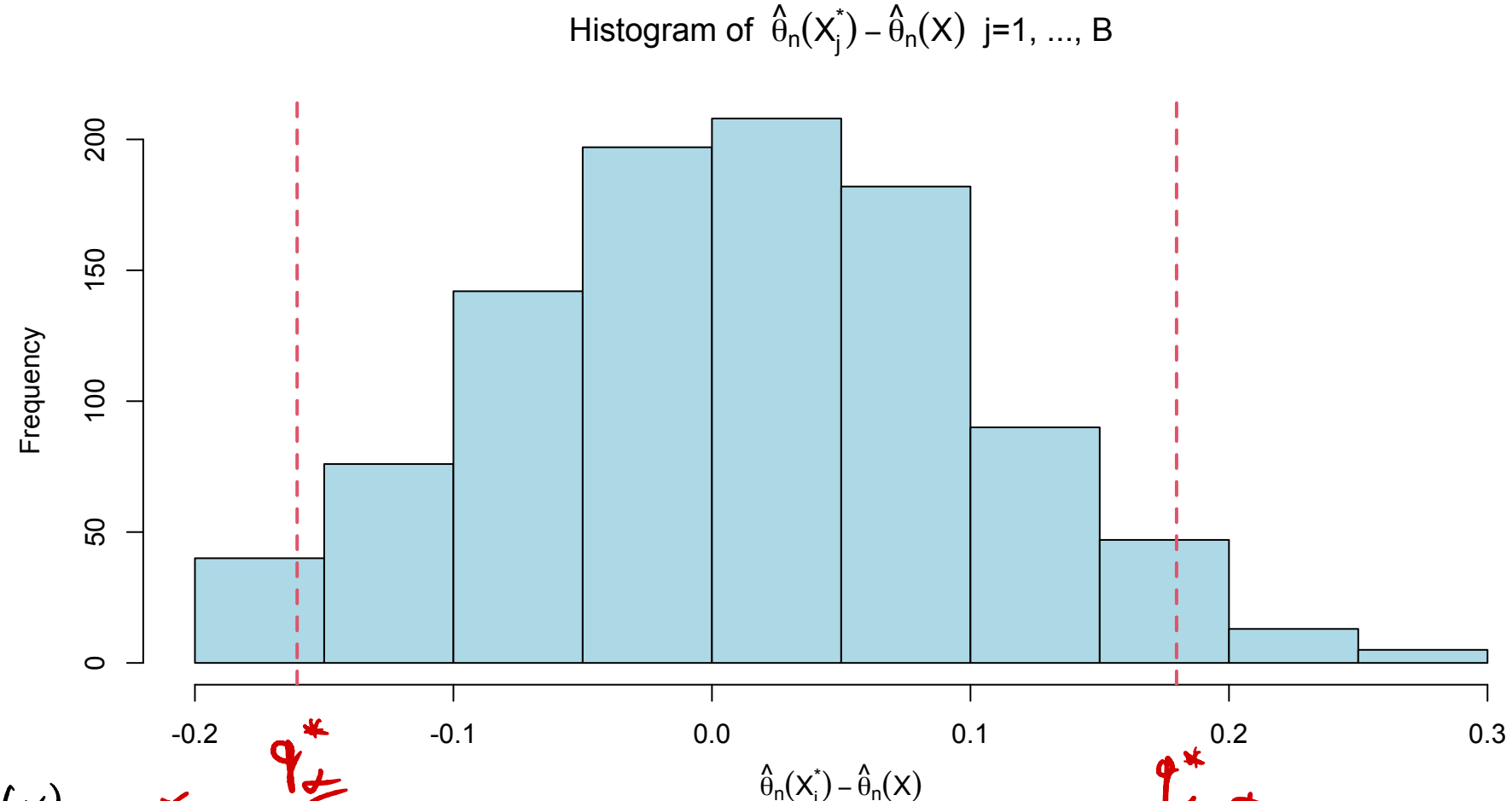


Failure of the Bootstrap

What went wrong?

Look at the 'bootstrap distribution' for a sample $X = (X_1, \ldots, X_n)$ with $\bar{X}_n = 0.185$.

$\hat{\theta}_n(X_j^*) = \max\{0, \bar{X}_j^*\}$

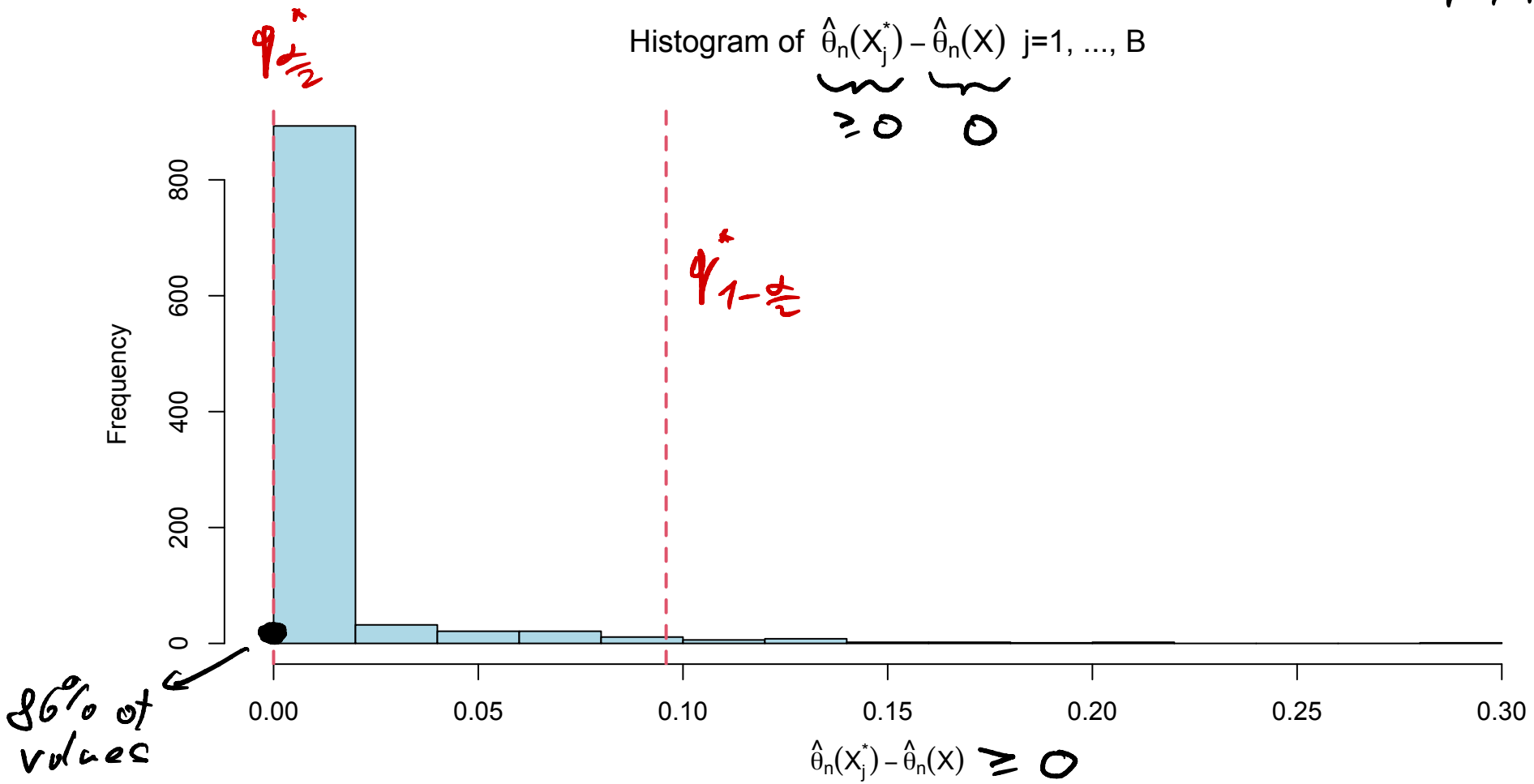


$q^*_{\alpha/2}$ $q^*_{1-\alpha/2}$

$\left[\hat{\theta}_n(X) - q^*_{1-\alpha/2},\ \hat{\theta}_n(X) - q^*_{\alpha/2}\right]$

Failure of the Bootstrap

Look at the 'bootstrap distribution' for a sample with $\bar{X}_n = -0.122$.



Here, actually 86% of bootstrap samples X_j^* produce $\hat{\theta}_n(X_j^*) - \hat{\theta}_n(X) = 0$.

Failure of the Bootstrap

- Look at the 'bootstrap distribution' for a sample with $\bar{X}_n = -0.122$.
- Notice: for every $j \in \{1, \ldots, B\}$, we have

$$\hat{\theta}_n(X_j^*) - \hat{\theta}_n(X) = \max\{0, \bar{X}_j^*\} - \max\{0, \bar{X}_n\} \geq 0,$$

$$\Rightarrow 0 \leq \hat{q}^*_{\alpha/2} \leq \hat{q}^*_{1-\alpha/2}.$$

- Therefore,

$$CI_\alpha = [\hat{\theta}_n(X) - \hat{q}^*_{1-\alpha/2}, \hat{\theta}_n(X) - \hat{q}^*_{\alpha/2}] \subseteq (-\infty, 0] \not\ni \theta > 0.$$

$= 0$ $= 0$

Failure of the Bootstrap

Recall: $X_1, \ldots, X_n \overset{iid}{\sim} N(\theta, 1)$

$\alpha = 0.05$

Thus, intuitively, for very small $\theta > 0$,

$$P_\theta(\theta \in CI_{0.05}) = P_\theta(\theta \in CI_{0.05} | \bar{X}_n < 0) P_\theta(\bar{X}_n < 0)$$

$= 0$ $\qquad \approx \frac{1}{2}$

$\bar{X}_n \sim N(\theta, \frac{1}{n})$

$$+ P_\theta(\theta \in CI_{0.05} | \bar{X}_n \geq 0) P_\theta(\bar{X}_n \geq 0)$$

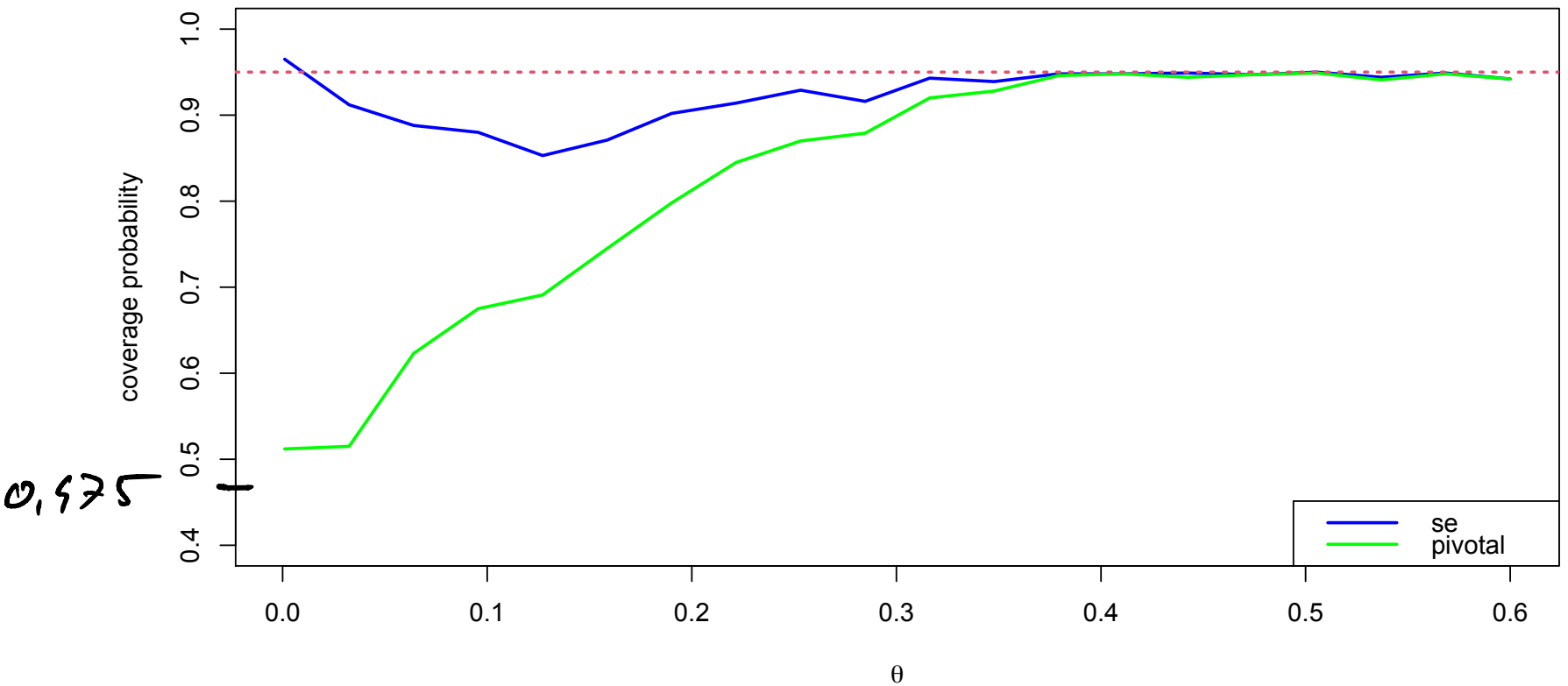
≈ 0.95 $\qquad \approx \frac{1}{2}$

≤ 1

$\approx \quad 0.475$

Failure of the Bootstrap

- $n = 100, \alpha = 0.05, B = 1000$
- 1000 MC iterations

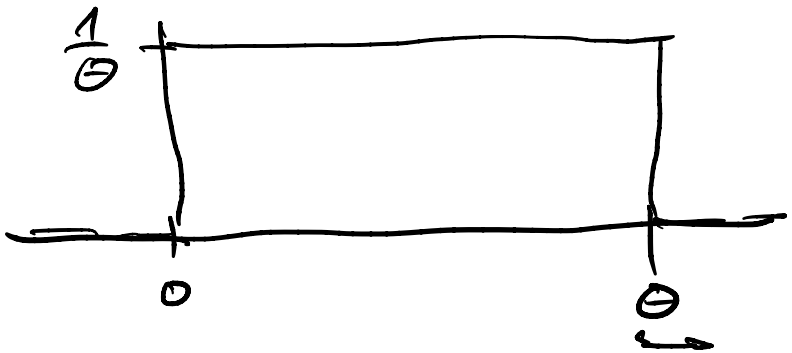


Failure of the Bootstrap

Is the se-bootstrap always superior to the pivotal method?

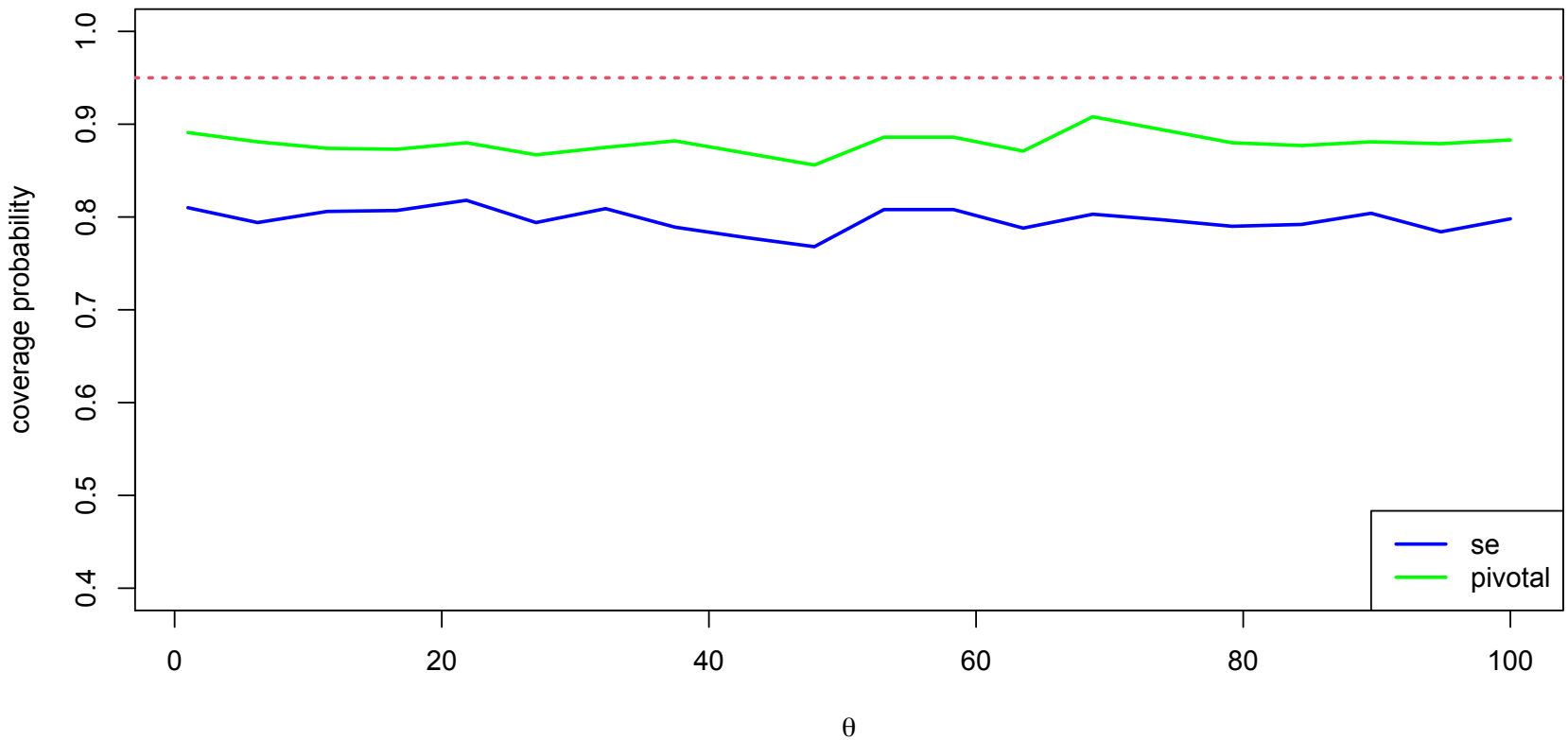
- Consider $X_1, \ldots, X_n \overset{iid}{\sim} \text{Unif}[0, \theta]$, $\theta \in \Theta = (0, \infty)$.
- Goal: Bootstrap inference on θ.
- The classical estimator (MLE) is

$$\hat{\theta}_n = \max\{X_1, \ldots, X_n\}.$$



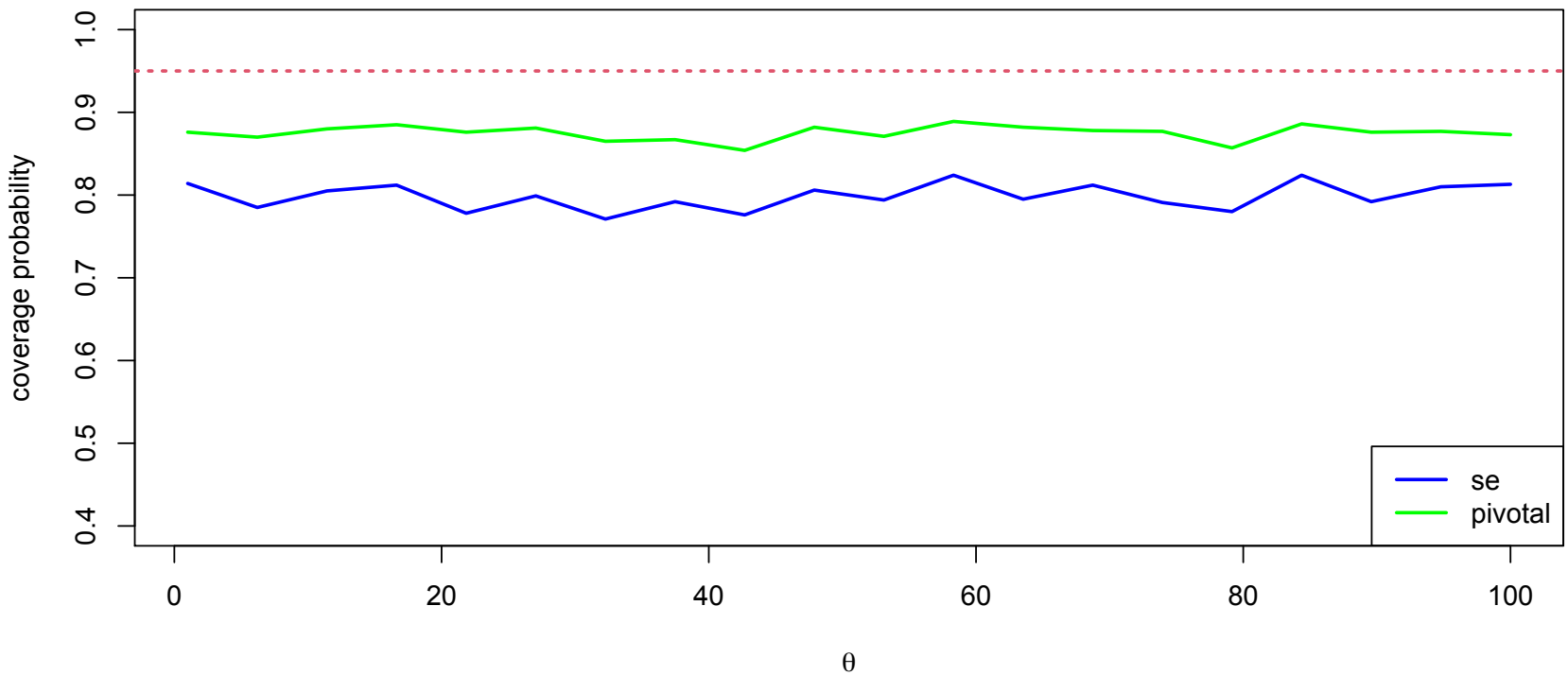
Failure of the Bootstrap

- $n = 100, \alpha = 0.05, B = 1000$
- 1000 MC iterations



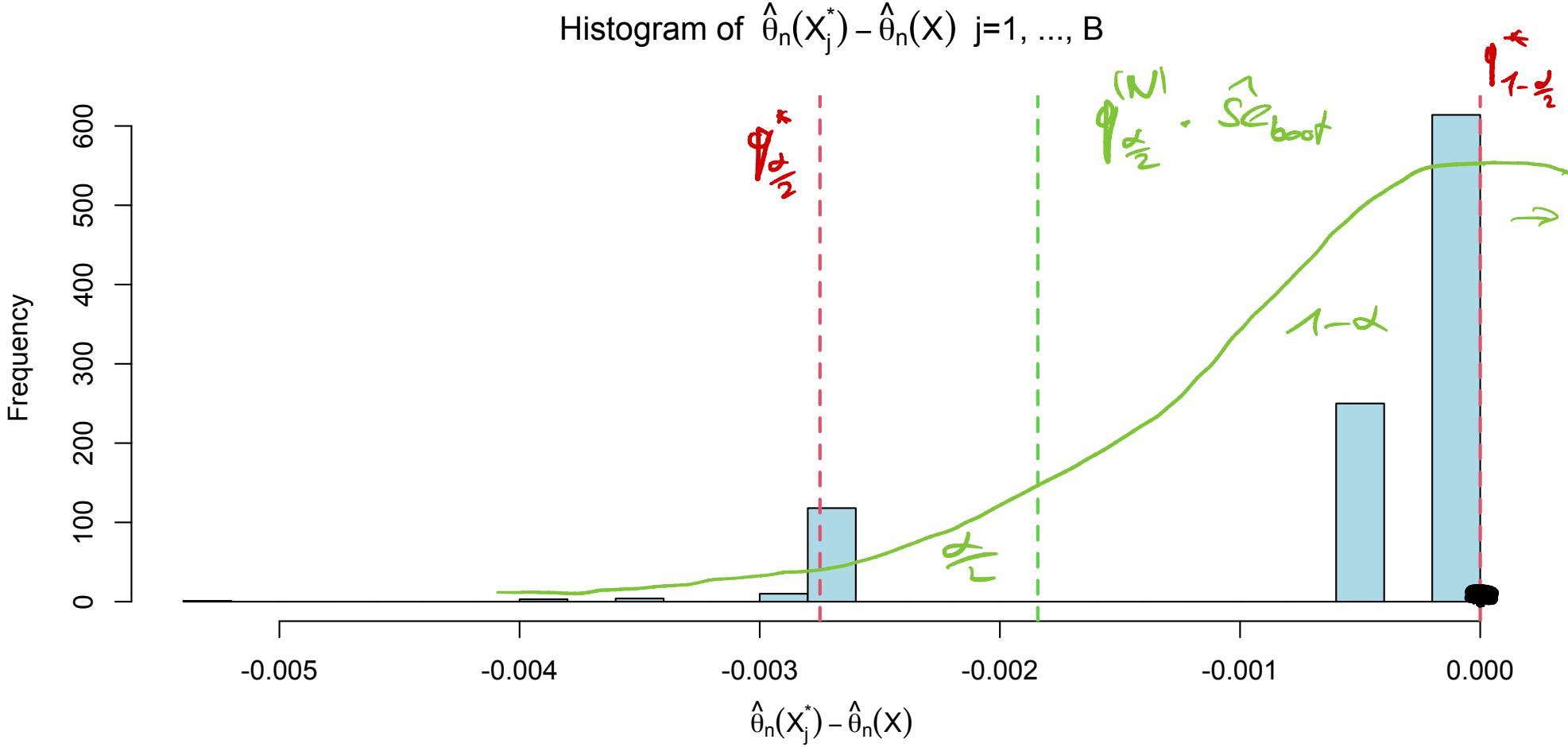
Failure of the Bootstrap

- $n = 1000$, $\alpha = 0.05$, $B = 1000$
- 1000 MC iterations



Failure of the Bootstrap

Look at the bootstrap distribution of one given sample of size $n = 1000$ with $\theta = 1$.



Here, 62% of all bootstrap samples X_j^* produce $\hat{\theta}_n(X_j^*) - \hat{\theta}_n(X) = 0$.

Failure of the Bootstrap

Here, 62% of all bootstrap samples X_j^* produce $\hat{\theta}_n(X_j^*) - \hat{\theta}_n(X) = 0$. Why?

assume no ties

$$\hat{\theta}_n(X_1^*) - \hat{\theta}_n(X) = \max\{X_{1,1}^*, \ldots, X_{n,1}^*\} - \max\{X_1, \ldots, X_n\}$$

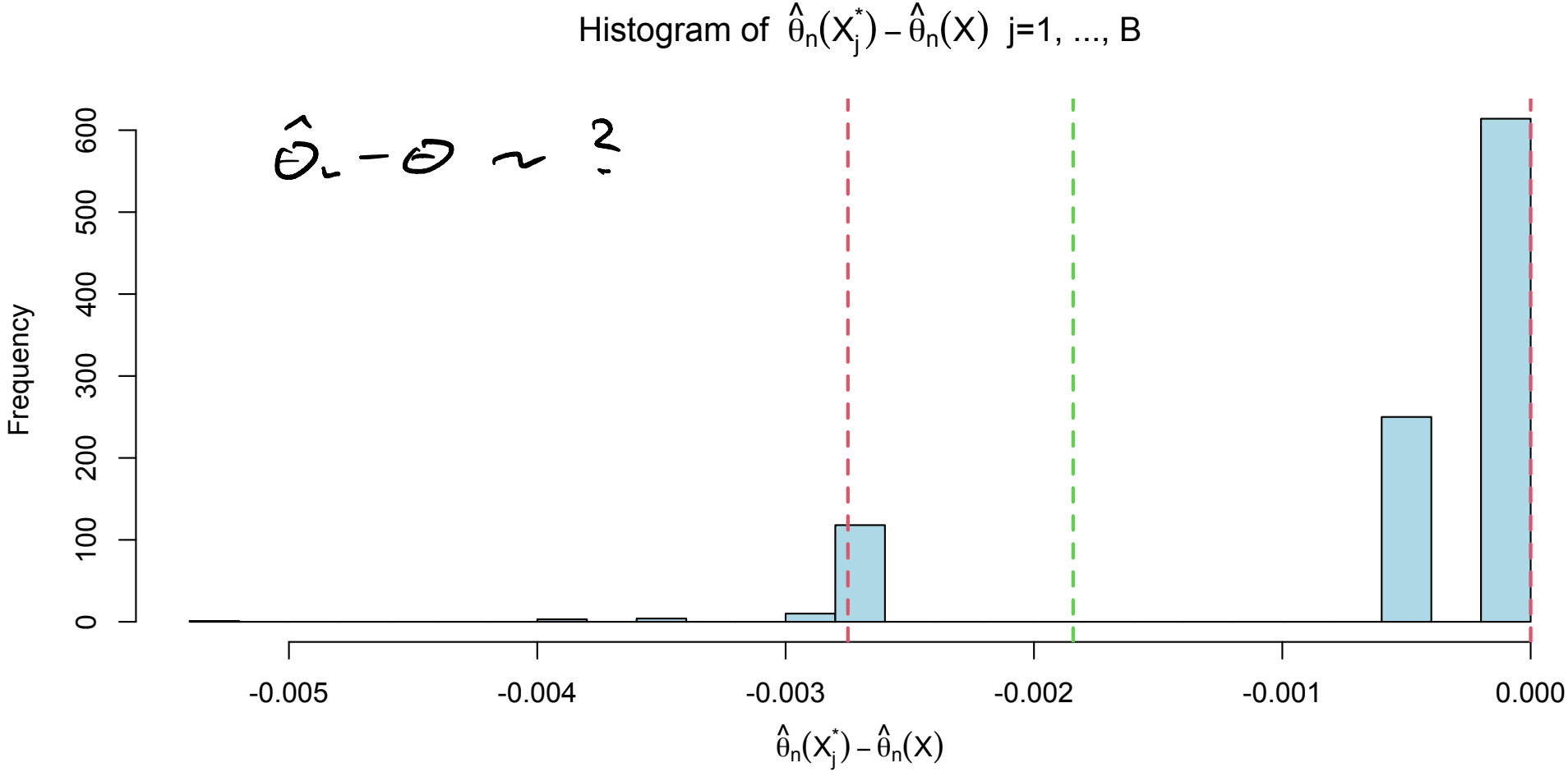
- This is equal to 0 if, and only if, in our bootstrap sample $X_{1,1}^*, \ldots, X_{n,1}^*$ we happen to draw the largest sample point from $\{X_1, \ldots, X_n\}$.
- What is the probability of that happening?

$$1 - \left(\frac{n-1}{n}\right)^n = 1 - \left(1 - \frac{1}{n}\right)^n \xrightarrow[n\to\infty]{} 1 - e^{-1}$$

$$\approx 0{,}63$$

Failure of the Bootstrap

Look at the bootstrap distribution of one given sample of size $n = 1000$ with $\theta = 1$.



Here, 62% of all bootstrap samples X_j^* produce $\hat{\theta}_n(X_j^*) - \hat{\theta}_n(X) = 0$.

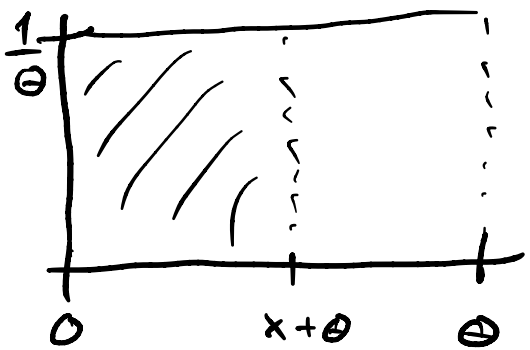
What is the actual sampling distribution of $\hat{\theta}_n - \theta$?

Recall:
$X_1, \ldots, X_n \overset{iid}{\sim} \text{Unif}[0, \theta], \theta \in \Theta = (0, \infty), \hat{\theta}_n = \max\{X_1, \ldots, X_n\}.$

$$P_\theta(\hat{\theta}_n - \theta \leq x) = P_\theta\left(\max\{X_1 \ldots X_n\} \leq x + \theta\right)$$

$$= P_\theta\left(X_1 \leq x+\theta \text{ and } X_2 \leq x+\theta \ldots \text{ and } X_n \leq x+\theta\right)$$

$$\overset{\text{indep.}}{=} \prod_{i=1}^{n} P_\theta(X_i \leq x+\theta)$$



$$= \begin{cases} 0 & \text{if } x+\theta < 0, \text{ if } x < -\theta \\ \frac{x+\theta}{\theta} & \text{if } 0 \leq x+\theta \leq \theta, -\theta \leq x \leq 0 \\ 1 & \text{if } x+\theta > \theta, x > 0 \end{cases}$$

$$P_\theta(\hat{\theta}_n - \theta \le x) = \begin{cases} 0 & x < -\theta \\ \left(1 + \frac{x}{\theta}\right)^n & -\theta \le x \le 0 \\ 1 & x > 0 \end{cases}$$

$$g_n(x) = \frac{d}{dx} P_\theta(\hat{\theta}_n - \theta \le x)$$

$$= \begin{cases} 0, & x < -\theta \\ n\left(1 + \frac{x}{\theta}\right)^{n-1} \frac{1}{\theta}, & -\theta \le x \le 0 \\ 0, & x > 0 \end{cases}$$

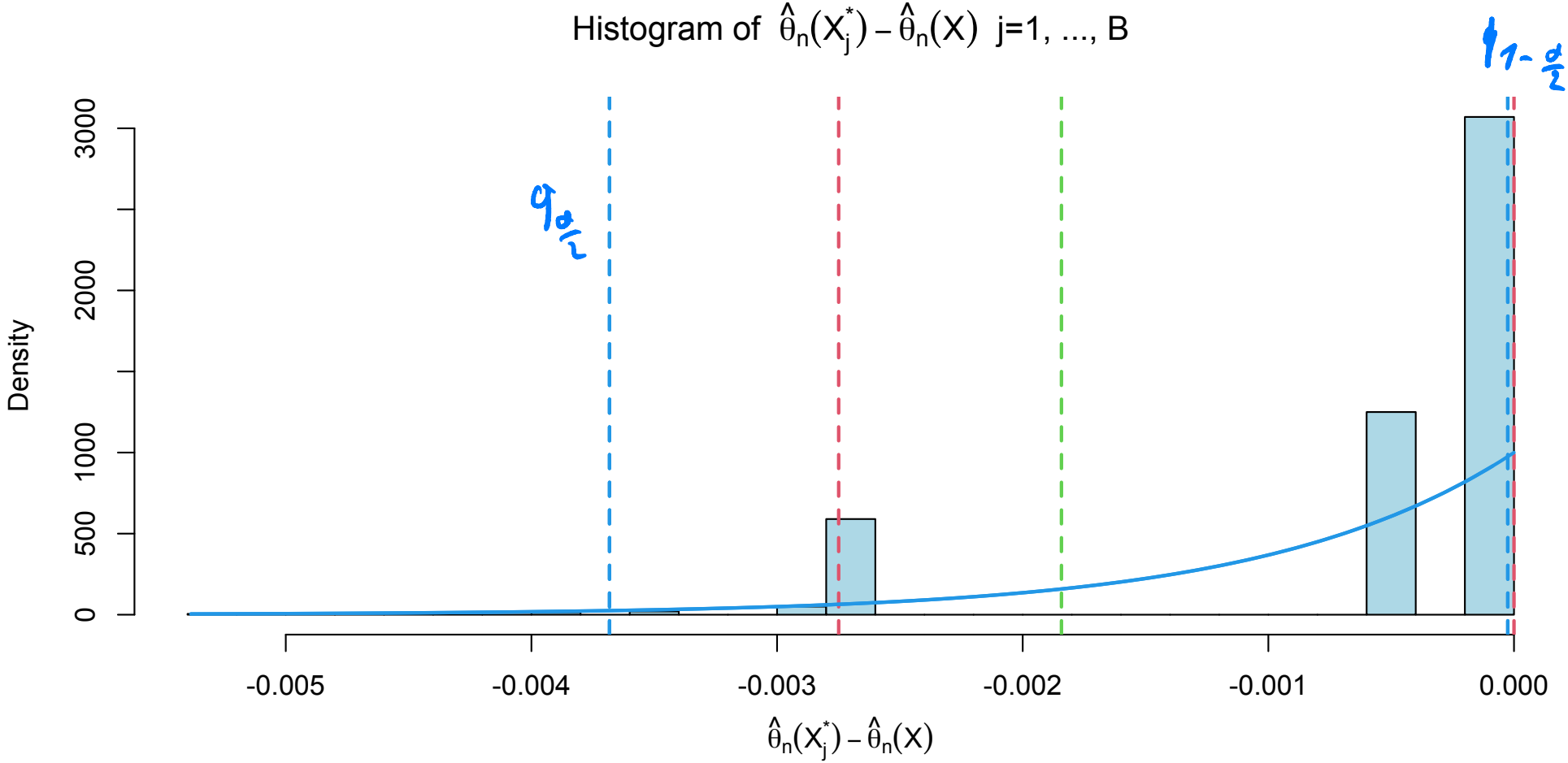
pdf of sampling distribution

$$q_\alpha^{(\hat{\theta}_n)} = \left[\alpha^{\frac{1}{n}} - 1\right]\theta$$

HW

Failure of the Bootstrap

Bootstrap vs. true sampling distribution of $\hat{\theta}_n - \theta$. $\theta = 1, n = 1000$.



Here, 62% of all bootstrap samples X_j^* produce $\hat{\theta}_n(X_j^*) - \hat{\theta}_n(X) = 0$.

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Always take a look at the bootstrap distribution!!!

Summing up:

- Computationally expensive simulation method.
- Very flexible, generic, no need for problem specific formulas.
- Produces only approximate inference; requires large samples.
- Can go wrong!
- In general: Works, if the normal approximation works.