Nonparametric Bootstrapping

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January, 12, 2016

Overview

Origin of the Term "Bootstrap"

- derives from "to pull oneself up by one's bootstrap"
- widely thought to be based on 18th century adventures of Baron Munchausen by R. E. Raspe
- Baron had fallen to bottom of deep lake and rescued himself by picking up himself by his own bootstraps
- however, it appears that this is a misattribution: in the original story, he picks up himself by his hair

Bootstrapping in Statistics

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- when it is very hard or impossible to obtain formulas for standard error of estimator analytically, we can still use bootstrapping to assess the accuracy of the estimator
- to motivate the bootstrapping algorithm, we will briefly review the "plug-in" principle

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- this is the Riemann-Stieltjes integral notation
- if cdf F differentiable everywhere, i.e., a pdf f exists, equivalent to $\int x \, f(x) \mathrm{d}x$
- advantage of the Riemann-Stieltjes integral notation: also holds when only valid cdf, but no pdf which will be handy for the following

The "Plug-In" Principle: Continued 1

More generally, most quantities we are interested in can be written in the form:

$$\mathbb{E}_F(g(x)) = \int g(x)\,\mathrm{d}F(x). \tag{2}$$

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- "plug-in" principle simply replaces the unknown distribution F with the empirical distribution function $\hat{F}_n$ which assigns probability $\frac{1}{n}$ to each observed data point x_i

$$\hat{F}_n(x) = \frac{\text{number of } x_i \leq x}{n} = \frac{1}{n}\sum_{i=1}^{n} I(x_i \leq x). \tag{3}$$

The "Plug-In" Principle: Continued 3

Then the estimator for the population mean is:

$$\bar{x} = \mathbb{E}_{\hat{F}_n}(x) = \int x \, \mathrm{d}\hat{F}_n(x) = \frac{1}{n} \sum_{i=1}^{n} x_i. \tag{4}$$

The "Plug-In" Principle: Continued 3

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More generally:

$$\mathbb{E}_{\hat{F}_n}(g(x)) = \int g(x) \, \mathrm{d}\hat{F}_n(x) = \frac{1}{n}\sum_{i=1}^{n} g(x_i). \tag{5}$$

Bootstrapping: Using the "Plug-In" Principle to Approximate the Sampling Distribution

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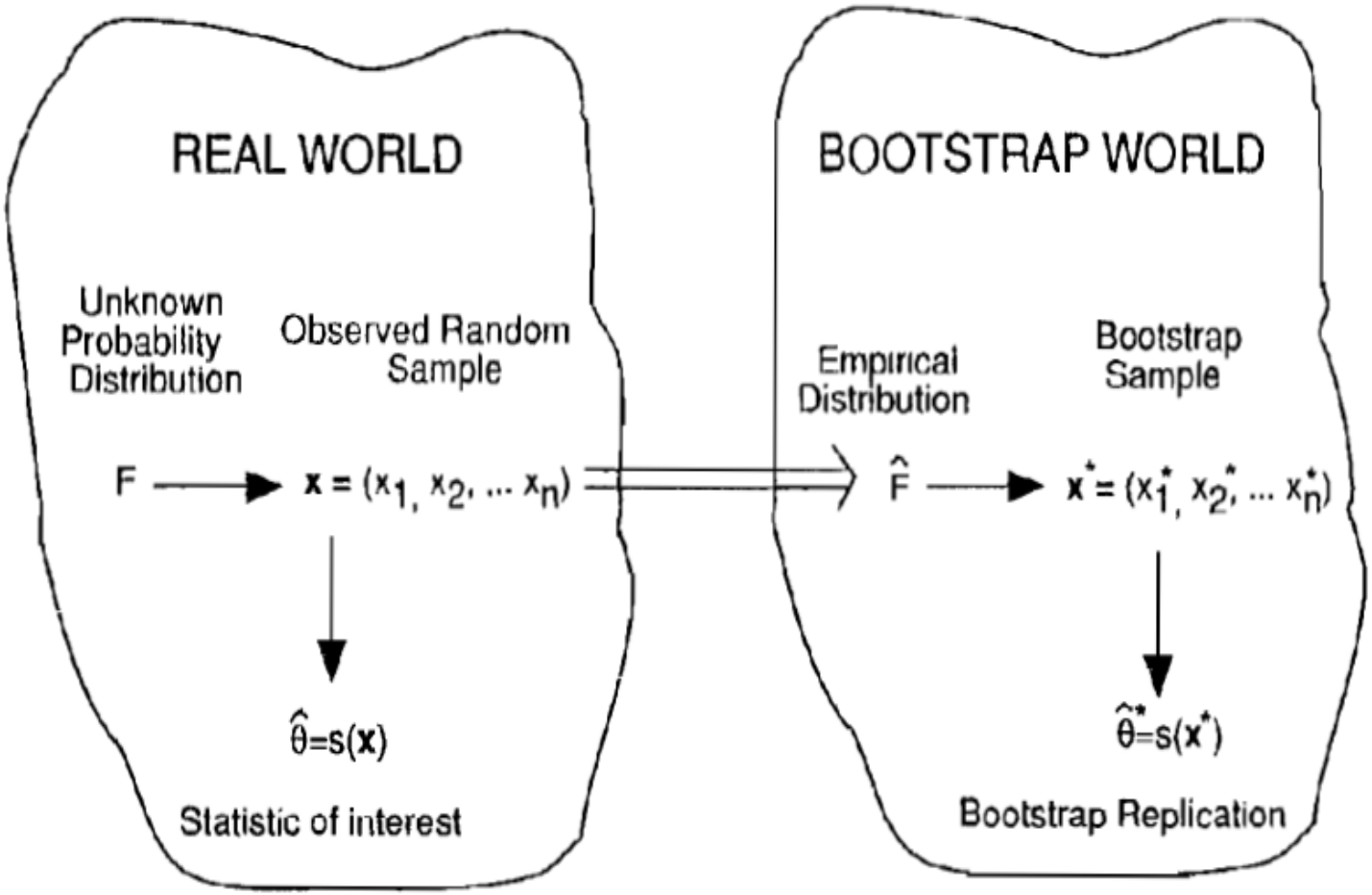
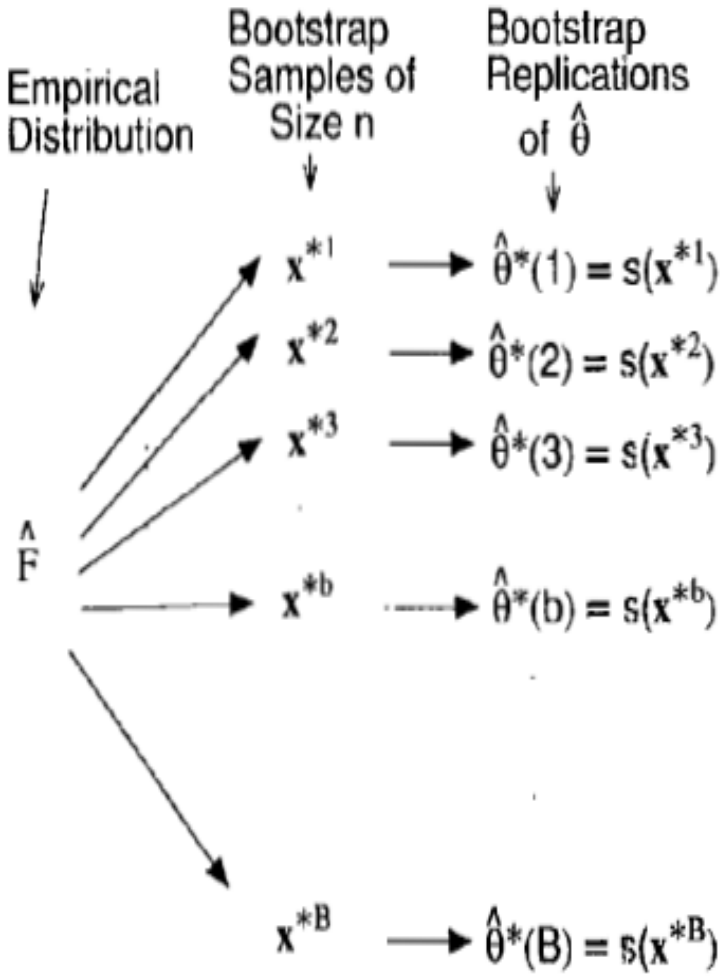
- suppose we knew population distribution F
- then, we could construct sampling distribution by repeatedly sampling from the population and calculating the statistic of interest for each sample
- bootstrapping simply replaces the population distribution F by the empirical distribution $\hat{F}_n$ ("plug-in" principle)

Bootstrapping: Using the "Plug-In" Principle to Approximate the Sampling Distribution Continued



The Bootstrap Algorithm

1. Obtain B independent bootstrap samples each of size n by sampling from $\hat{F}_n$. This simply means, sampling *with replacement* from the observed data values.
2. Calculate the statistic of interest for each of the B bootstrap samples.



Why does it work? – A Little Intuition

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- why possible to replace unknown population distribution F with empirical distribution $\hat{F}_n$?
- one reason: has been proven that empirical distribution function $\hat{F}_n$ converges to population distribution F

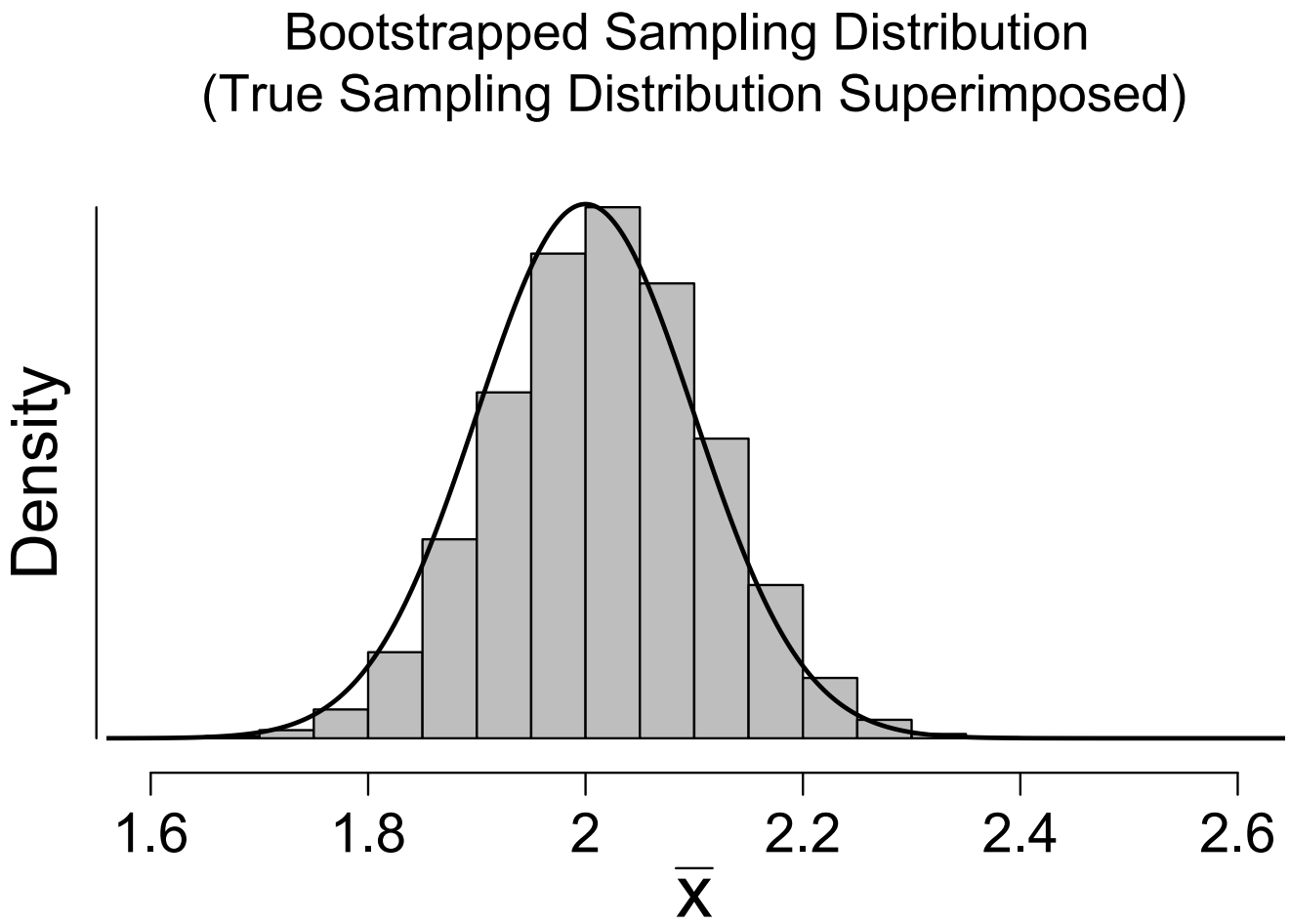
Theorem (Glivenko-Cantelli theorem)

$\sup_{x \in \mathbb{R}} |\hat{F}_n(x) - F(x)| \longrightarrow 0$ *almost surely as* $n \longrightarrow \infty$.

A Toy Example: Bootstrapping the Mean

```r
### generate data ###

set.seed(123456)

n <- 100 # number of observations
data <- rnorm(n, mean = 2)

### bootstrapping ###

B <- 100000 # number of bootstrap replicates

boot.means <- numeric(B)

for (i in seq_len(B)) {

        indices <- sample(seq_len(n), n, replace = TRUE)
        boot.data <- data[indices]
        boot.means[i] <- mean(boot.data)

}
```

A Toy Example: Bootstrapping the Mean Continued



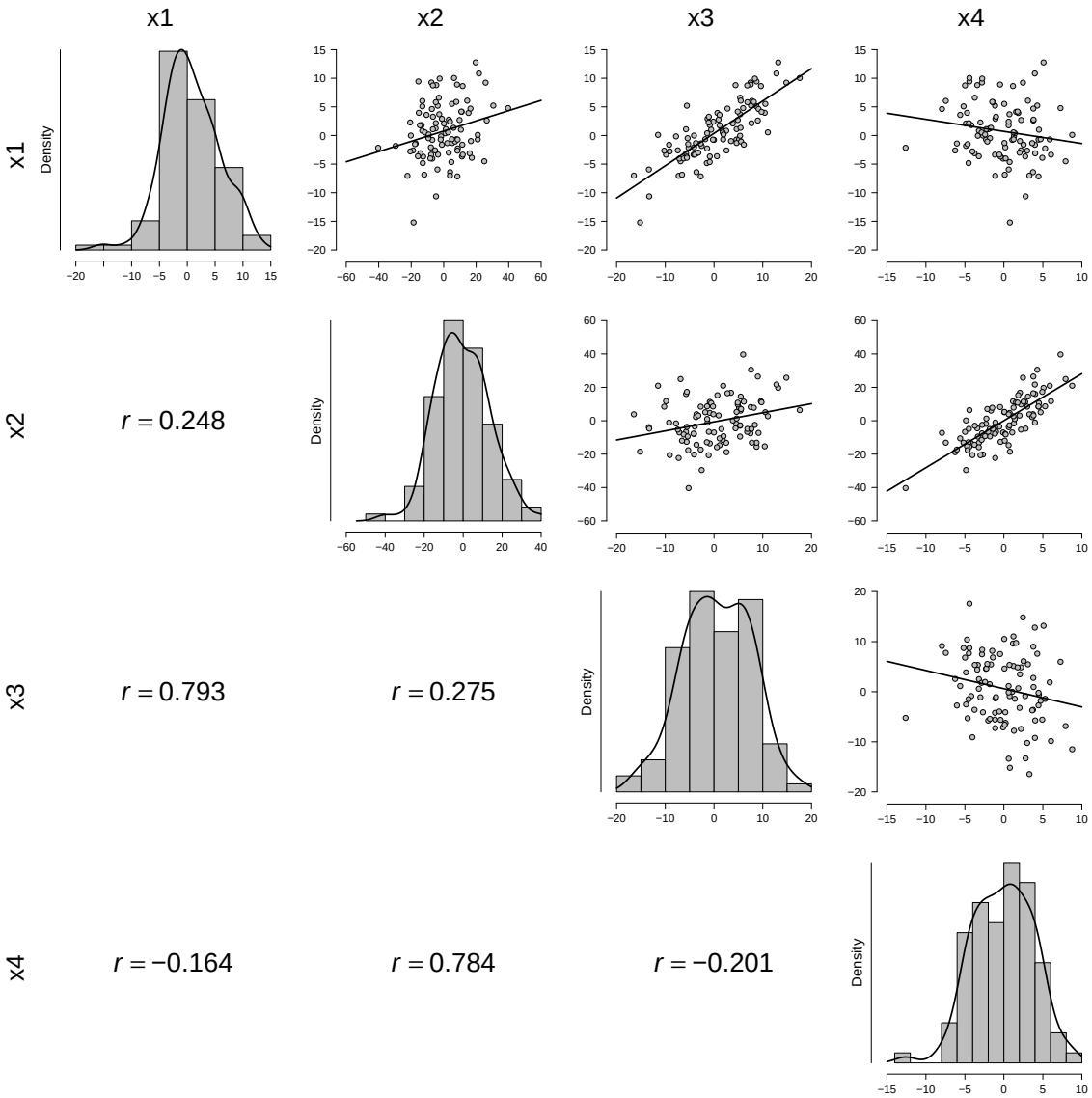
Bootstrapping Confidence Intervals in Principle Component Analysis

- assume we are interested in assessing accurracy of proportion of variance explained by principle components via confidence intervals
- to the best of my knowledge, no easy formula for doing this exists
- we can use bootstrapping to obtain approximate confidence intervals

Data Generation

```r
### generate data ###

library(mvtnorm)

# standard deviations

sds <- c(5, 15, 7, 4)

# correlation matrix

R <- matrix(c(

          1, .2,  .8, -.2,
         .2,  1,  .2,  .8,
         .8, .2,   1, -.2,
        -.2, .8, -.2,   1

        ), 4, 4, byrow = TRUE)

# covariance matrix

Sigma <- diag(sds) %*% R %*% diag(sds)

# data

set.seed(2343457)

n <- 100
data <- rmvnorm(n, mean = rep(0, 4), sigma = Sigma)
```

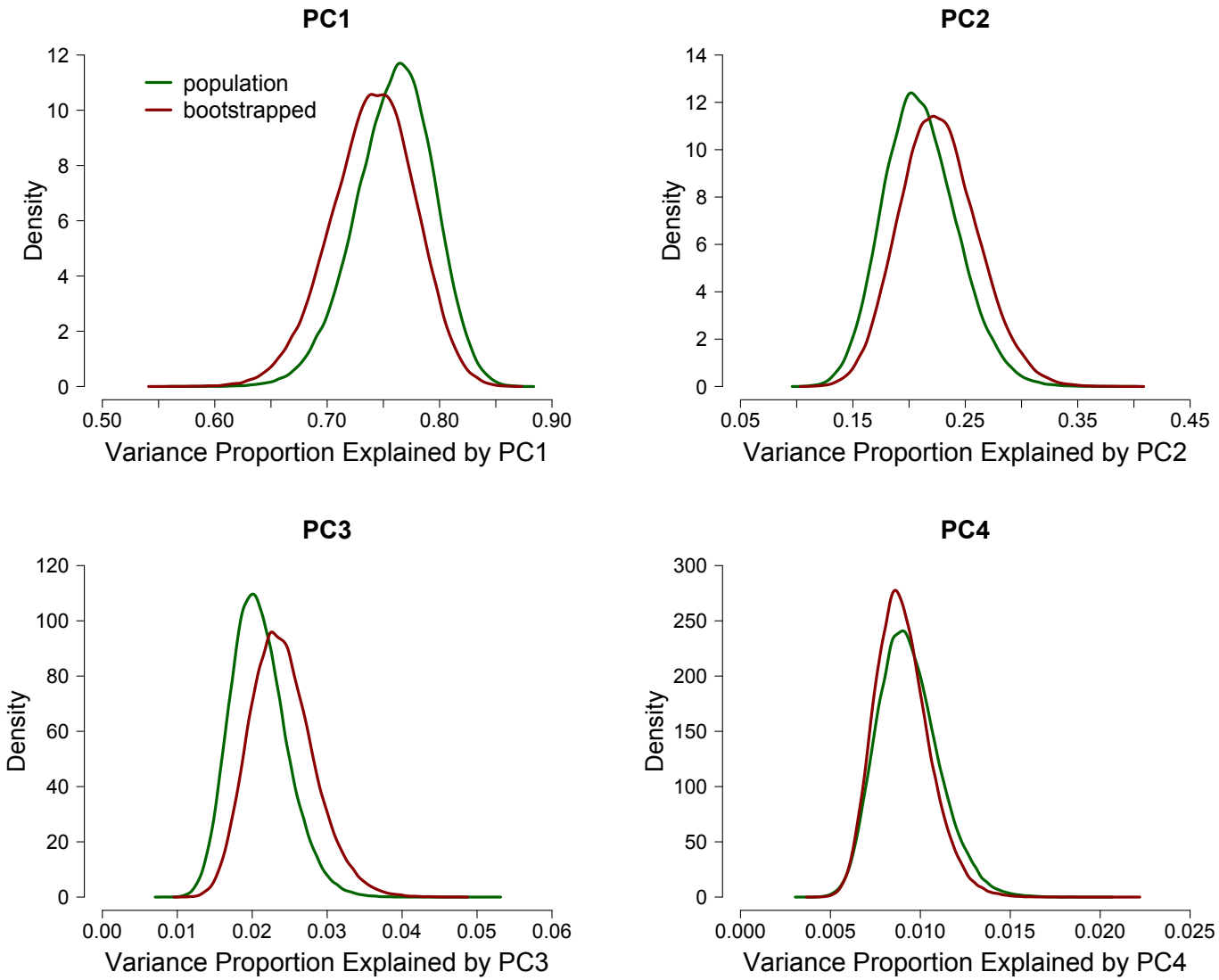
Data Visualization



Bootstrapping: R Code

```
### bootstrapping ###

library(boot)

B <- 100000 # number of bootstrap replicates

boot.func <- function(data, indices) {

        pca <- prcomp(data[indices, ])

        summary(pca)$importance["Proportion of Variance", ]

}

boot.result <- boot(data, boot.func, B)
boot.samples <- boot.result$t
```

Population and Bootstrapped Sampling Distribution



Eigendecomposition of Covariance Matrix to Obtain True Variance Proportions

$$\mathbf{\Sigma} = \mathbf{V}\mathbf{\Lambda}\mathbf{V}^{\mathsf{T}} = \sum_i \lambda_i \mathbf{v}_i \mathbf{v}_i^{\mathsf{T}} \tag{6}$$

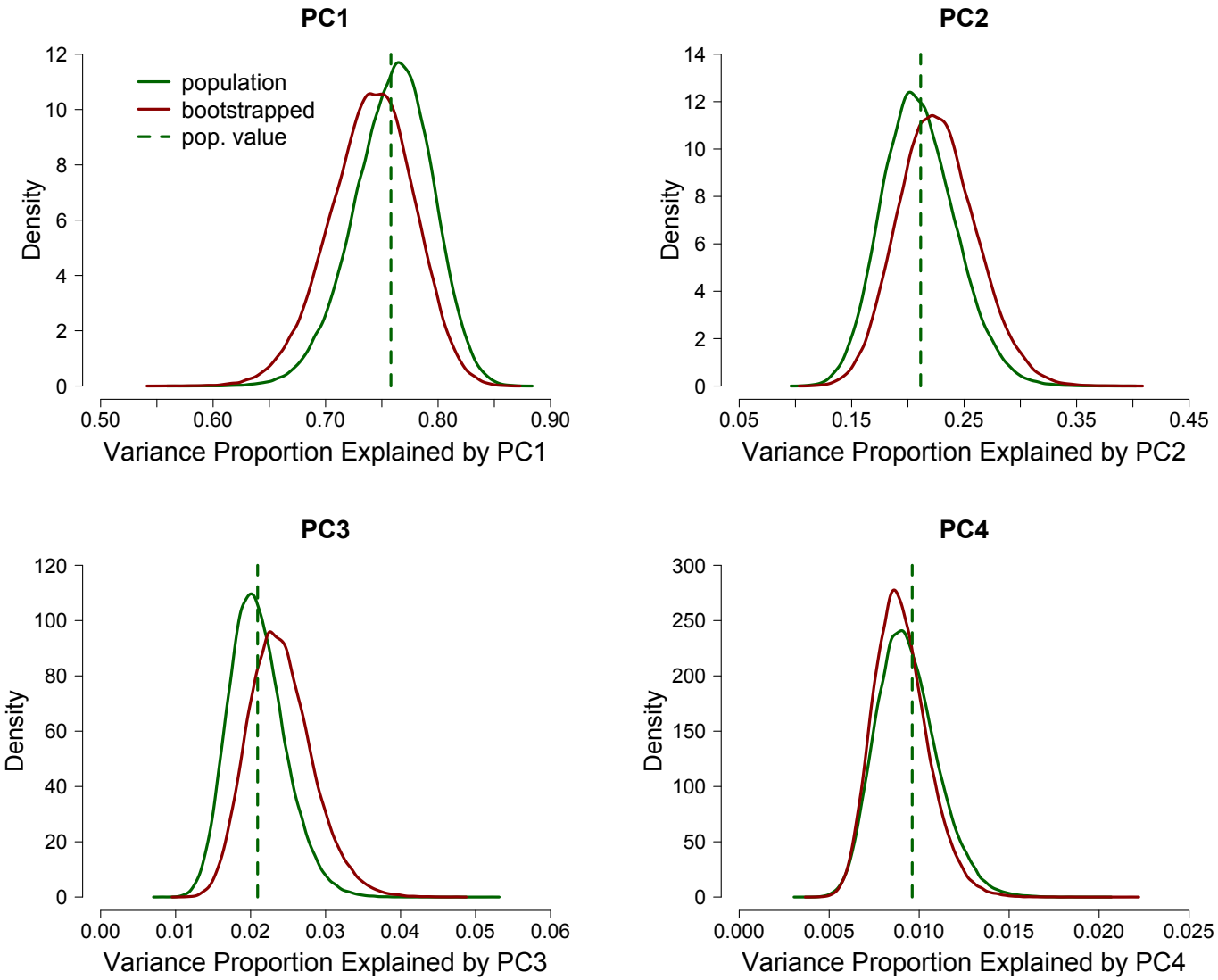
Eigenvalues λ_i correspond to variances explained by different components. Hence, proportion of variance explained by i-th component is given by

$$\frac{\lambda_i}{\sum_i \lambda_i}. \tag{7}$$

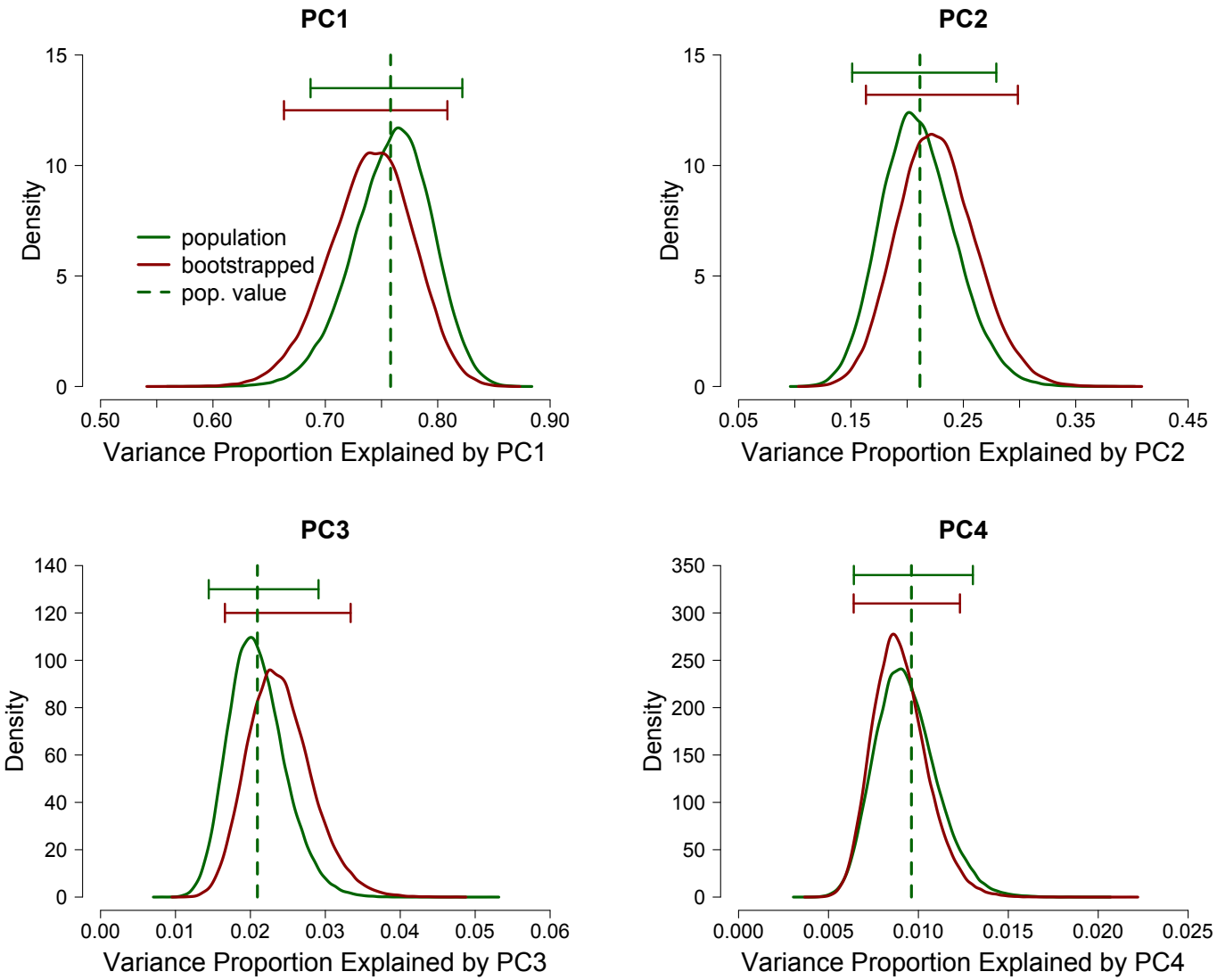
```
eigen(Sigma)$values / sum(eigen(Sigma)$values)
```

```
## [1] 0.758087539 0.211362100 0.020937298 0.009613063
```

Population and Bootstrapped Sampling Distribution with "True" Value



Population CI and Percentile Bootstrapped CI



Bootstrapping Confidence Intervals in Principle Component Analysis: BC_a Intervals

Also use percentiles of bootstrap distribution, but they are *acceleration* and *bias*-corrected.

$$p_1 = \Phi\left(\hat{z}_0 + \frac{\hat{z}_0 + z^{\alpha/2}}{1 - \hat{\alpha}(\hat{z}_0 + z^{\alpha/2})}\right) \tag{8}$$

$$p_2 = \Phi\left(\hat{z}_0 + \frac{\hat{z}_0 + z^{1-\alpha/2}}{1 - \hat{\alpha}(\hat{z}_0 + z^{1-\alpha/2})}\right) \tag{9}$$

where Φ is the standard normal cdf and z^{α} is the 100αth percentile of a standard normal distribution. $\hat{\alpha}$ is the acceleration and $\hat{z}_0$ is the bias correction.

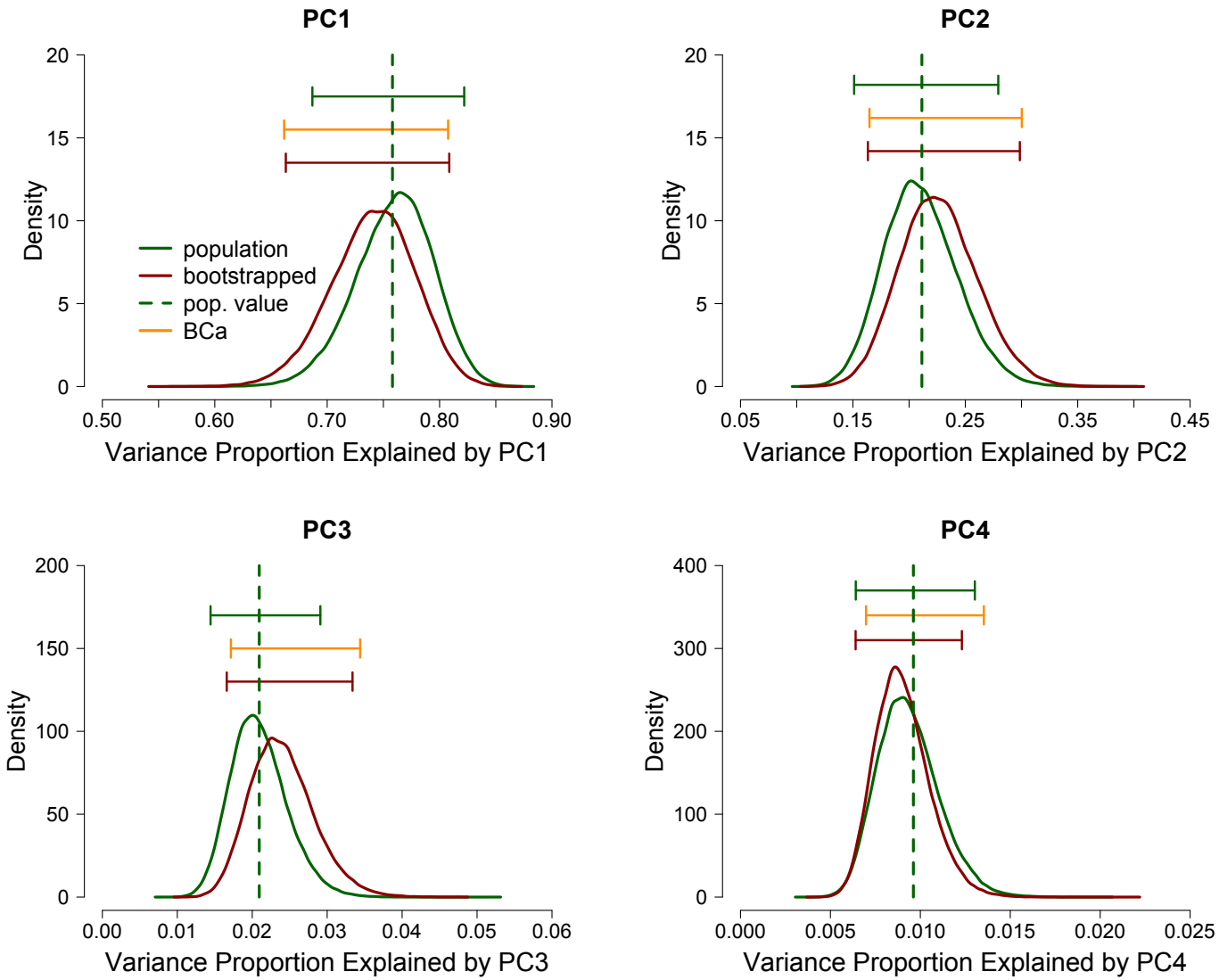
Bootstrapping Confidence Intervals in Principle Component Analysis: BC_a Intervals Continued

- *acceleration* $\hat{\alpha}$ corrects for fact that standard error might be different for different population values
- $\hat{z}_0$ corrects for *bias* by considering proportion of bootstrap samples smaller than original estimate
- if 50% of bootstrapped values smaller than original estimate, no bias correction

In R:

```
# bias-corrected and accelerated bootstrapped confidence intervals

boot.ci.bca <- matrix(ncol = 4, nrow = 2)

boot.ci.bca[ ,1] <- boot.ci(boot.out = boot.result, type = "bca", index = 1)$bca[4:5]
boot.ci.bca[ ,2] <- boot.ci(boot.out = boot.result, type = "bca", index = 2)$bca[4:5]
boot.ci.bca[ ,3] <- boot.ci(boot.out = boot.result, type = "bca", index = 3)$bca[4:5]
boot.ci.bca[ ,4] <- boot.ci(boot.out = boot.result, type = "bca", index = 4)$bca[4:5]
```

Population CI, Percentile Bootstrapped CI, and BC_a CI




Thanks!