Monte Carlo and Empirical Methods for Stochastic Inference (MASM11/FMSN50)

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Lecture 13
Introduction to the bootstrap
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Plan of today's lecture

1. Last time: MCMC methods for Bayesian inference
   - Korsbetningen (again)
2. The frequentist approach to inference
   - Statistics and sufficiency—small overview
   - Designing estimators
   - Uncertainty of estimators
3. Introduction to bootstrap (Ch. 9)
   - Empirical distribution functions
   - The bootstrap in a nutshell

We are here $\longrightarrow$ •

Example: Korsbetningen—background

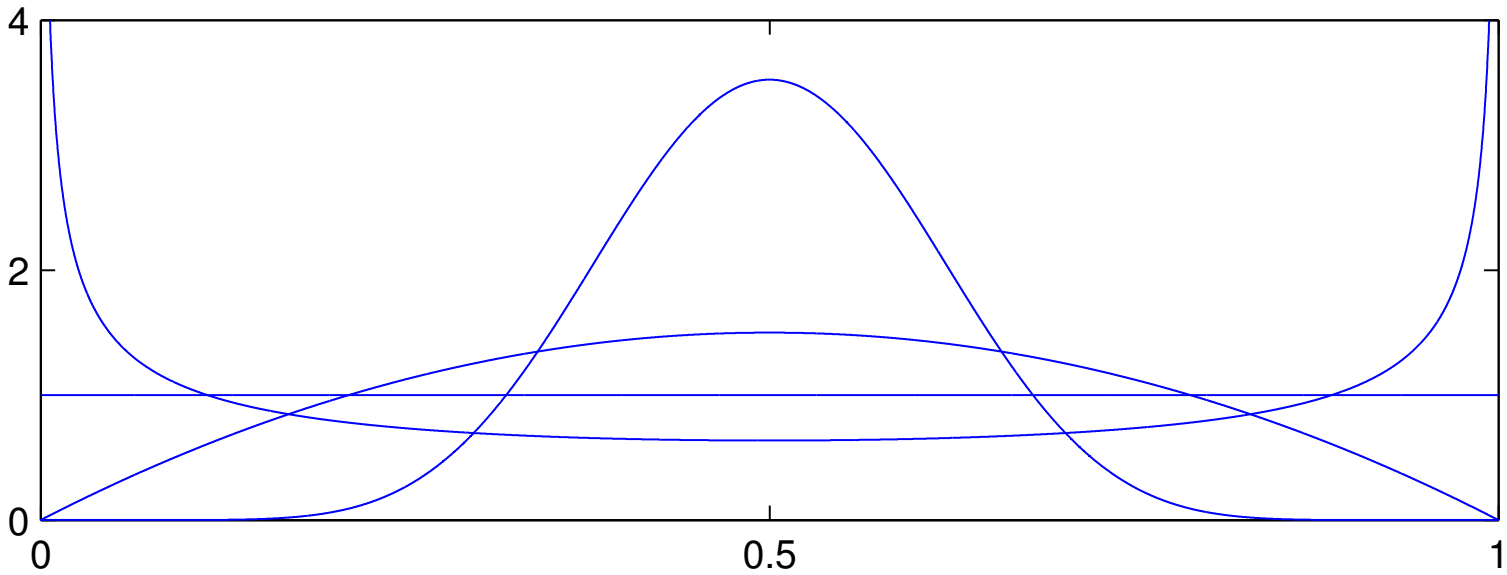
The background is the following.

- In 1361 the Danish king Valdemar Atterdag conquered Gotland and captured the rich Hanseatic town of Visby.
- Most of the defenders were killed in the attack and are buried in a field, Korsbetningen, outside of the walls of Visby.
- In 1929–1930 the gravesite (with several graves) was excavated . In grave one e.g. a total of 493 femurs, 237 right and 256 left, were found.
- We want to estimate the number of buried bodies.

Example: Korsbetningen—model

We set up the following model.

- Assume that the numbers y_1 and y_2 of left resp. right legs are two observations from a Bin(n, p) distribution.
- Here n is the total number of people buried and p is the probability of finding a leg, left or right, of a person.
- We put a conjugate Beta(a, b)-prior on p and a $\mathcal{U}(256, 2500)$ prior on n.



Example: Korsbetningen—a hybrid MCMC

We proceed as follows:

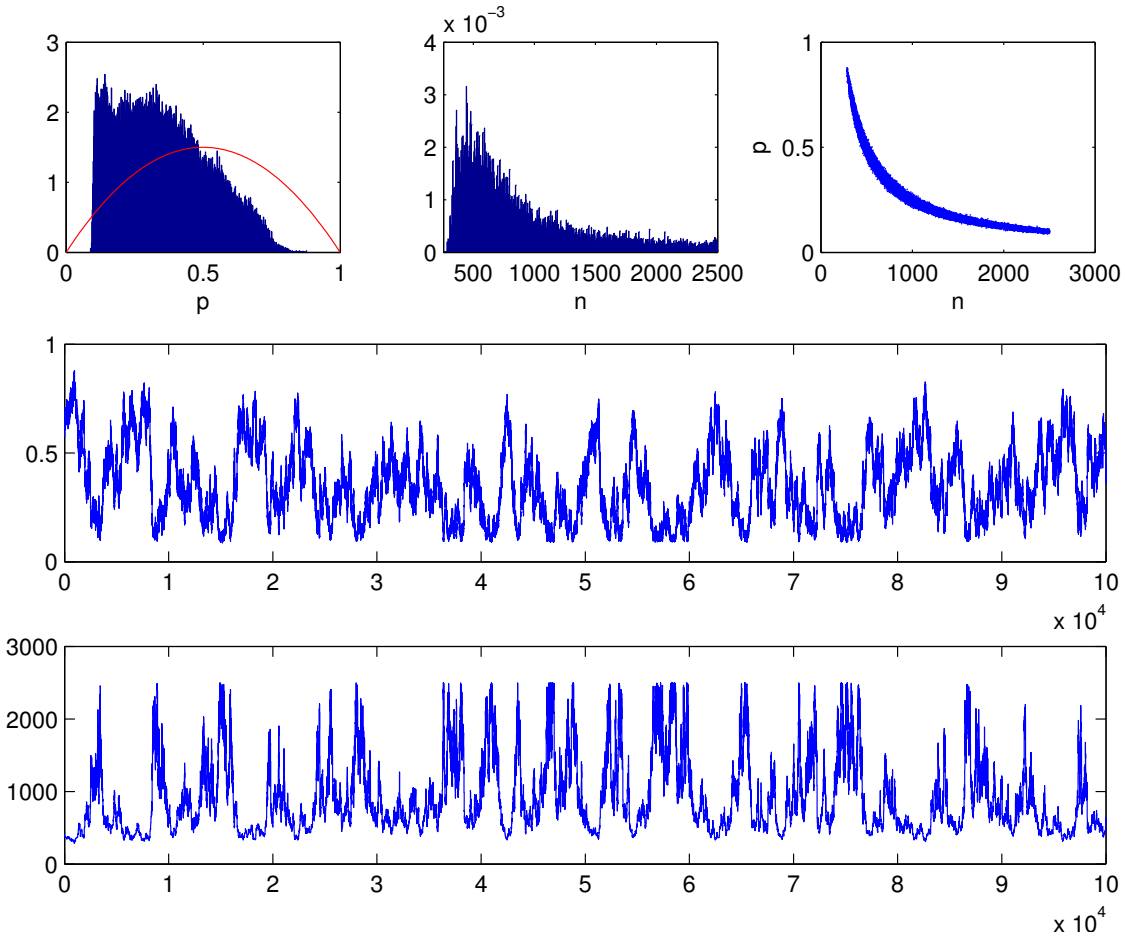
- A standard Gibbs step for

$$p|n, y_1, y_2 \sim \text{Beta}(a + y_1 + y_2, b + 2n - (y_1 + y_2)).$$

- MH for n, with a symmetric proposal obtained by drawing, given n, a new candidate n^* among the integers $\{n - R, \ldots, n, \ldots, n + R\}$.
- The acceptance probability becomes

$$\alpha(n, n^*) = 1 \wedge \frac{(1-p)^{2n^*}(n^*!)^2(n - y_1)!(n - y_2)!}{(1-p)^{2n}(n!)^2(n^* - y_1)!(n^* - y_2)!}.$$

Example: Korsbetningen—a hybrid MCMC



Example: Korsbetningen—an improved MCMC sampler

However, the previous algorithm mixes slowly. Thus, use instead the following scheme.

1. First draw a new n^* from the symmetric proposal as previously.
2. Then draw, conditional on n^*, also a candidate p^* from $f(p|n = n^*, y_1, y_2)$.
3. Finally, accept or reject both n^* and p^*.

This is a standard MH sampler!

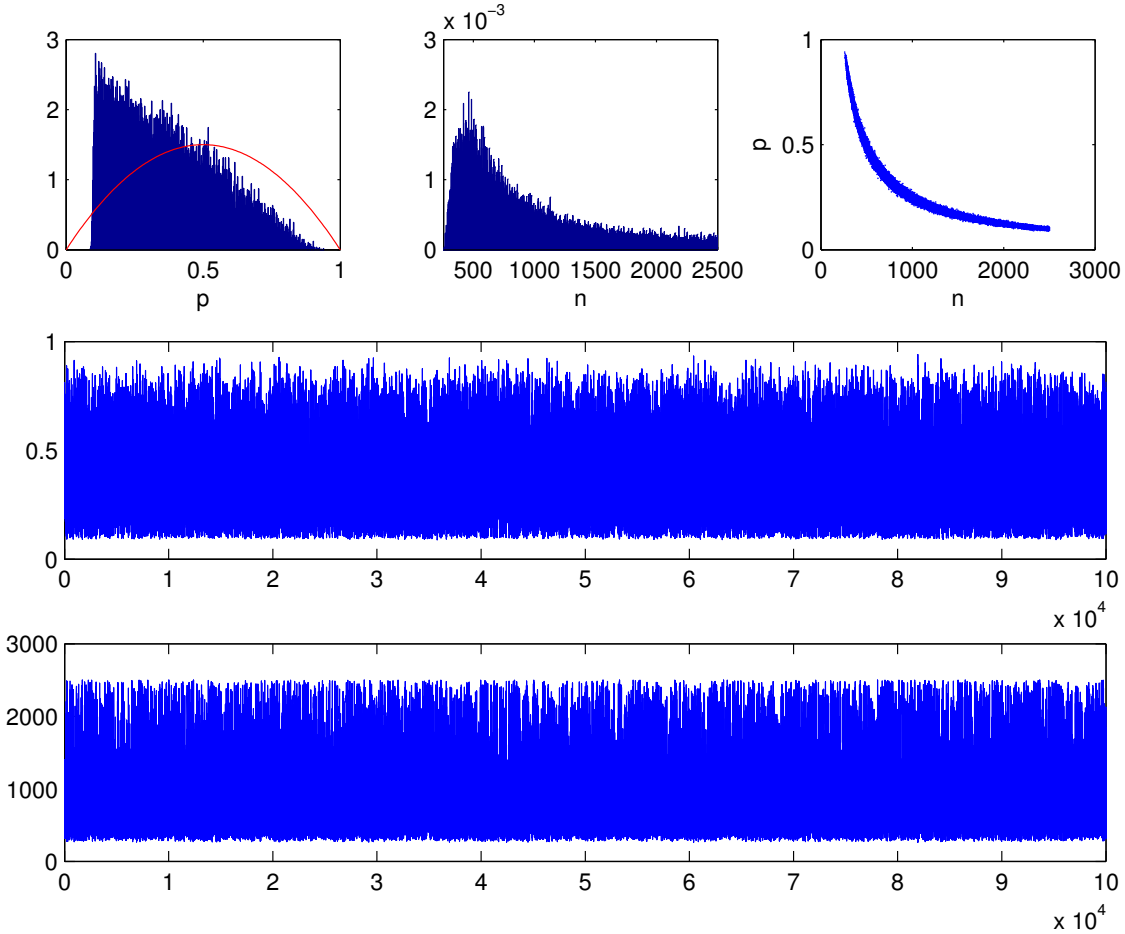
Example: Korsbetningen—an improved MCMC sampler

For the new sampler, the proposal kernel becomes

$$q(n^*, p^*|n, p) \propto \frac{(2n^* + a + b - 1)!}{(a + y_1 + y_2 - 1)!(2n^* + b - y_1 - y_2 - 1)!} \times (p^*)^{a+y_1+y_2-1}(1-p^*)^{b+2n^*-(y_1+y_2)-1}\mathbb{1}_{|n-n^*|\leq R},$$

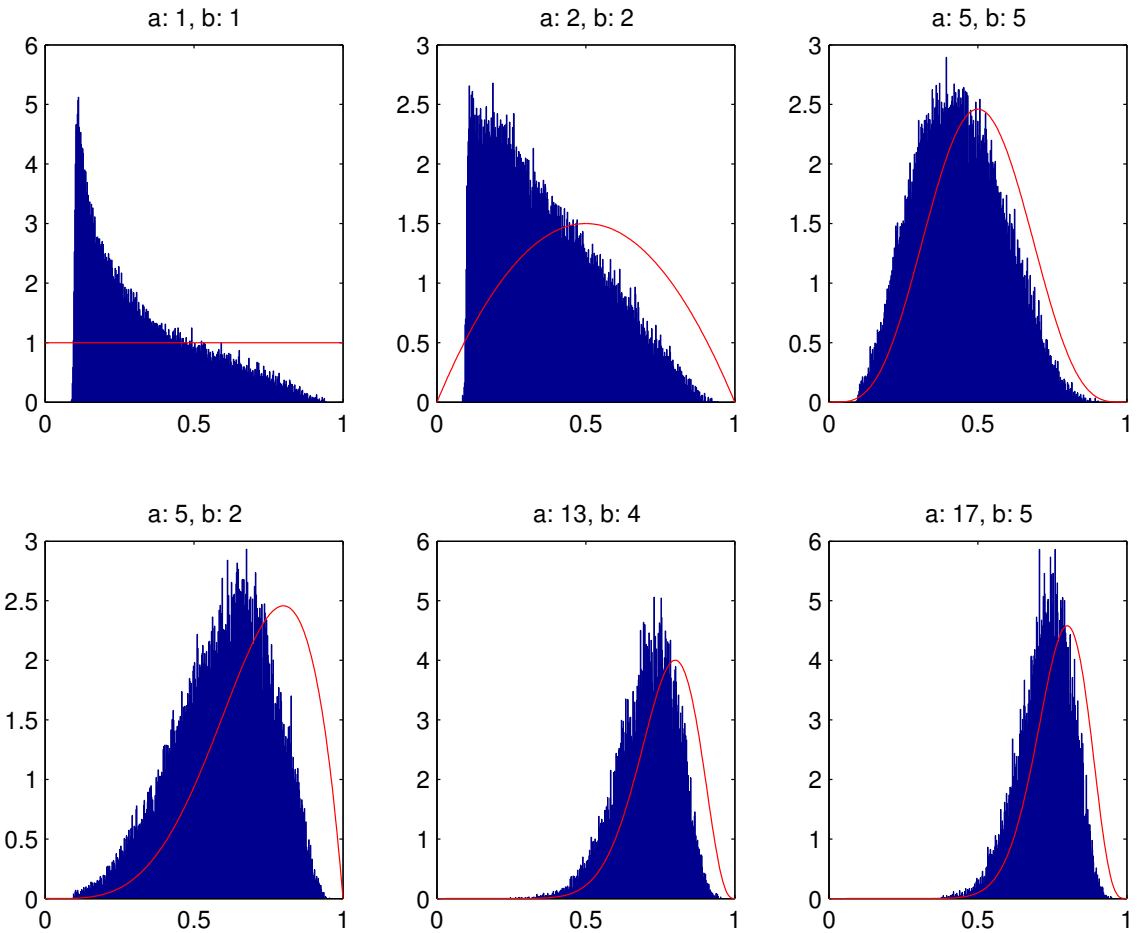
yielding the acceptance probability

$$\begin{aligned}\alpha((n,p),(n^*,p^*)) &= 1 \wedge \frac{f(n^*,p^*,y_1,y_2)q(n,p|n^*,p^*)}{f(n,p,y_1,y_2)q(n^*,p^*|n,p)} \\ &= 1 \wedge \left\{ \frac{(n^*!)^2(n-y_1)!(n-y_2)!}{(n!)^2(n^*-y_1)!(n^*-y_2)!} \right. \\ &\qquad \left. \times \frac{(2n+a+b-1)!(2n^*+b-y_1-y_2-1)!}{(2n^*+a+b-1)!(2n+b-y_1-y_2-1)!} \right\}.\end{aligned}$$

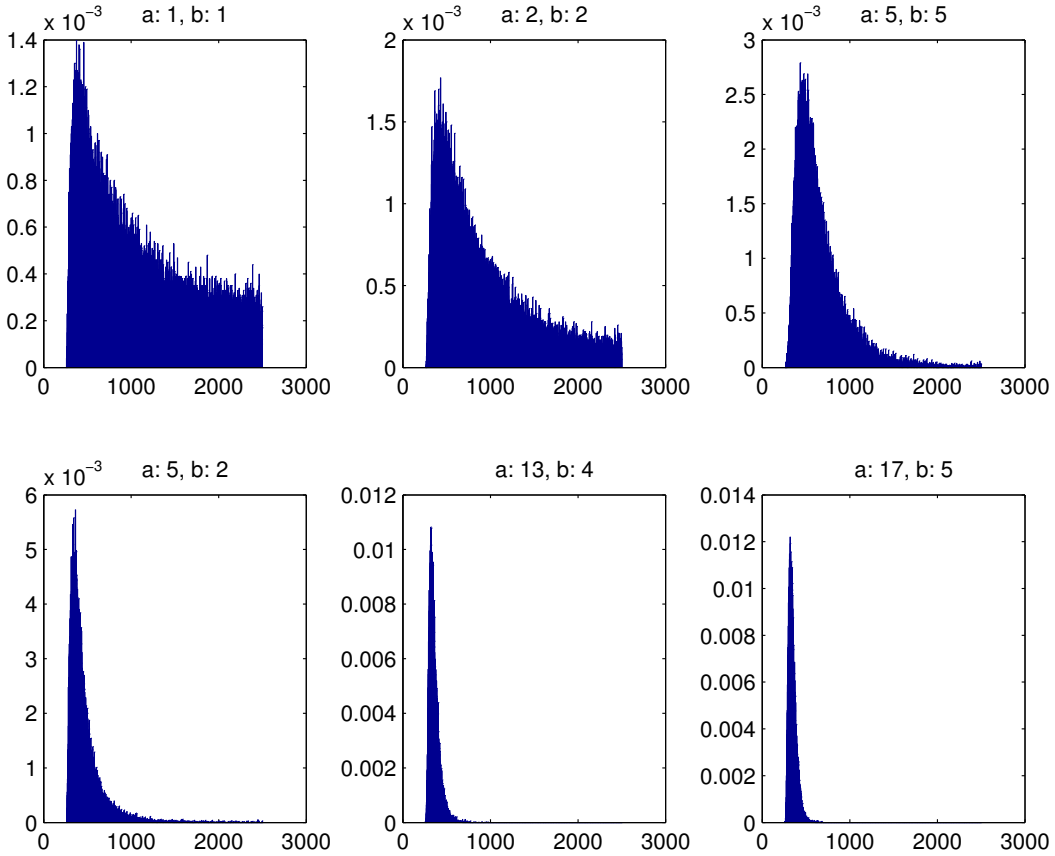


A one side 95% credible interval for n is $[343, \infty)$.

Korsbetningen—Effect of the prior



Korsbetningen—Effect of the prior



The lower side of a one sided 95% credible interval for n is $\{343, 346, 360, 296, 290, 289\}$. Posterior mean for n $\{1068, 883, 653, 453, 358, 346\}$.

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The frequentist approach (again)

The frequentist approach to statistics is characterized as follows.

- Data y is viewed as an observation of a random variable Y with distribution $\mathbb{P}_0$ which most often is assumed to be a member of a parametric family
$$\mathcal{P} = \{\mathbb{P}_\theta; \theta \in \Theta\}.$$
Thus, $\mathbb{P}_0 = \mathbb{P}_{\theta_0}$ for some $\theta_0 \in \Theta$.
- Estimates $\widehat{\theta}(y)$ are realizations of random variables.
- A 95% confidence interval is calculated to cover the true value in 95% of the cases.
- Hypothesis testing is made by rejecting a hypothesis $\mathcal{H}_0$ if $\mathbb{P}(\text{data}\|\mathcal{H}_0)$ is small.

The frequentist approach (again) (cont.)

Let us extend the previous framework somewhat: Given

- observations y
- and a model $\mathcal{P}$ for the data,

we want to make inference about some property (estimand) $\tau = \tau(\mathbb{P}_0)$ of the distribution $\mathbb{P}_0$ that generated the data. For instance,

$$\tau(\mathbb{P}_0) = \int x f_0(x)\, \mathrm{d}x, \quad \text{(mean)}$$

where f_0 is the density of $\mathbb{P}_0$.

The inference problem can split into two subproblems:

1. How do we construct a data-based estimator of τ?
2. How do we assess the uncertainty of the estimate?

Statistics

A statistic t is simply a (possibly vector-valued) function of data. Some examples:

1. The arithmetic mean: $t(y) = \bar{y} = \frac{1}{n}\sum_{i=1}^{n} y_i$.
2. The s^2-statistics: $t(y) = s^2(y) = \frac{1}{n-1}\sum_{i=1}^{n}(y_i - \bar{y})^2$.
3. The ordered sample (order statistics): $t(y) = \{y_{(1)}, y_{(2)}, \ldots, y_{(n)}\}$.
4. The maximum likelihood estimator (MLE): $t(y) = \text{argmax}_{\theta\in\Theta} f_\theta(y)$.

Sufficient statistics

A statistic that completely summarizes the information contained in the data about the unknown parameters θ is called a sufficient statistic for θ.

- Mathematically, t is sufficient if the conditional distribution of Y given $t(Y)$ does not depend on the parameter θ.
- This means that given $t(Y)$ we may, by simulation, generate a sample Y' with exact the same distribution as Y without knowing the value of the unknown parameter θ_0.
- The factorization criterion says that $t(y)$ is sufficient if and only if the density of Y can be factorized as

$$f_\theta(y) = h(y)g_\theta(t(y)).$$

Example: a simple sufficient statistic

For a simple example, let $y = (y_1, \ldots, y_n)$ be observations of n independent variables with $\mathcal{N}(\theta, 1)$-distribution. Then

$$f_\theta(y|\theta) = \prod_{i=1}^{n} f_\theta(y_i|\theta) = \prod_{i=1}^{n} \left(\frac{1}{\sqrt{2\pi}} \exp\left(-\frac{(y_i - \theta)^2}{2} \right) \right)$$
$$= \left(\frac{1}{\sqrt{2\pi}} \right)^n \exp\left(-\frac{1}{2} \sum_{i=1}^{n} y_i^2 \right) \exp\left(\theta n \bar{y} - \frac{1}{2} n \theta^2 \right).$$

We may now conclude that $t(y) = \bar{y}$ is sufficient for θ by applying the factorization criterion with

$$\begin{cases} t(y) \leftarrow \bar{y}, \\ g_\theta(t(y)) \leftarrow \exp\left(\theta n \bar{y} - \frac{1}{2} n \theta^2 \right), \\ h(y) \leftarrow \left(\frac{1}{\sqrt{2\pi}} \right)^n \exp\left(-\frac{1}{2} \sum_{i=1}^{n} y_i^2 \right). \end{cases}$$

Completeness

- A data dependent statistics V is called ancillary if its distribution does not depend on θ and first order ancillary if $\mathbb{E}_\theta(V) = c$ for all θ (note that the latter is weaker than the former).
- Since a good sufficient statistics $T = t(Y)$ provides lots of information concerning θ it should not—if T is good enough—be possible to form even a first order ancillary statistics based on T, i.e.

$$\mathbb{E}_\theta(V(T)) = c \; \forall \theta \Rightarrow V(t) \equiv c \text{ (a.s)}.$$

- Subtracting c leads to the following definition: A sufficient statistics T is called complete if

$$\mathbb{E}_\theta(f(T)) = 0 \; \forall \theta \Rightarrow f(t) \equiv 0 \text{ (a.s)}.$$

Completeness (cont.)

Theorem (Lehmann-Scheffé)

Let T be an unbiased complete sufficient statistics for θ, i.e. $\mathbb{E}_\theta(T) = \theta$. Then T is the (uniquely) best unbiased estimator of θ in terms of variance.

In the example above, where $y = (y_1, \ldots, y_n)$ were observations of n independent variables with $\mathcal{N}(\theta, 1)$-distribution, one may show that the sufficient statistics $t(y) = \bar{y}$ is complete. Thus, t is the uniquely best unbiased estimator of θ!

Maximum likelihood estimators

Our first task is to find a statistic that is a good estimate of the estimand $\tau = \tau(\mathbb{P}_0)$ of interest. Two common choices are

- the MLE and
- the least squares estimator.

As mentioned, the MLE is defined as the parameter value maximizing the likelihood function

$$\theta \mapsto f_\theta(y)$$

or, equivalently, the log-likelihood function

$$\theta \mapsto \log f_\theta(y).$$

Least square estimators

When applying least squares we first find the expectation as a function of the unknown parameter:

$$\mu(\theta) = \int x f_\theta(x) \, \mathrm{d}x.$$

After this, we minimize the squared deviation

$$t(y) = \operatorname{argmin}_{\theta \in \Theta} \sum_{i=1}^{n} (\mu(\theta) - y_i)^2$$

between our observations and the expected value.

Uncertainty of estimators

Some remarks:

- It is important to always keep in mind that the estimate $t(y)$ is an observation of a random variable $t(Y)$. If the experiment was repeated, resulting in a new vector y of random observations, the estimator would take another value.
- In the same way, the error $\Delta(y) = t(y) - \tau$ is a realization of the random variable $\Delta(Y) = t(Y) - \tau$.
- To assess the uncertainty of the estimator we thus need to analyze the distribution function F_Δ of the error $\Delta(Y)$ (error distribution) under $\mathbb{P}_0$.

Confidence intervals and bias

Assume that we have found the error distribution F_Δ. A confidence interval $(L(y), U(y))$ on level α for τ should fulfill

$$\begin{aligned} 1-\alpha &= \mathbb{P}_0\left(L(Y) \leq \tau \leq U(Y)\right) \\ &= \mathbb{P}_0\left(t(Y) - L(Y) \geq t(Y) - \tau \geq t(Y) - U(Y)\right) \\ &= \mathbb{P}_0\left(t(Y) - L(Y) \geq \Delta(Y) \geq t(Y) - U(Y)\right). \end{aligned}$$

Thus,

$$\begin{cases} t(Y) - L(Y) = F_\Delta^{-1}(1-\alpha/2) \\ t(Y) - U(Y) = F_\Delta^{-1}(\alpha/2) \end{cases} \Leftrightarrow \begin{cases} L(Y) = t(Y) - F_\Delta^{-1}(1-\alpha/2) \\ U(Y) = t(Y) - F_\Delta^{-1}(\alpha/2) \end{cases}$$

and the confidence interval becomes

$$I_\alpha = \left(t(y) - F_\Delta^{-1}(1-\alpha/2), t(y) - F_\Delta^{-1}(\alpha/2)\right).$$

Confidence intervals and bias

The bias of the estimator is

$$\mathbb{E}_0\left(t(Y)-\tau\right)=\mathbb{E}_0\left(\Delta(Y)\right)=\int z f_\Delta(z)\,\mathrm{d}z,$$

where $f_\Delta(z)=\frac{d}{dz}F_\Delta(z)$ denotes the density function of $\Delta(Y)$.

Consequently, finding the error distribution F_Δ is essential for making qualitative statements about the estimator.

In the previous normal distribution example,

$$\Delta(Y)=\bar{Y}-\theta_0\sim\mathcal{N}(0,1/n),$$

yielding $\mathbb{E}_0(\Delta(Y))=0$ and

$$\begin{cases}F_\Delta^{-1}(1-\alpha/2)=\lambda_{\alpha/2}\frac{1}{\sqrt{n}}\\ F_\Delta^{-1}(\alpha/2)=-\lambda_{\alpha/2}\frac{1}{\sqrt{n}}\end{cases}\quad\Rightarrow I_\alpha=\left(\bar{y}-\lambda_{\alpha/2}\frac{1}{\sqrt{n}},\bar{y}+\lambda_{\alpha/2}\frac{1}{\sqrt{n}}\right).$$

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Overview

So, we need $F_\Delta(z)$ (or $f_\Delta(z)$) to evaluate the uncertainty of t. However, here we generally face two obstacles:

1. We do not know $F_\Delta(z)$ (or $f_\Delta(z)$); these distributions may for instance depend on the quantity τ that we want to estimate.
2. Even if we knew $F_\Delta(z)$, finding the quantiles $F_\Delta^{-1}(p)$ is typically complicated as integration cannot be carried out on closed form.

The bootstrap algorithm deals with these problems by

1. replacing $\mathbb{P}_0$ by an data-based approximation resp.
2. analyzing the variation of $\Delta(Y)$ using MC simulation from the approximation of $\mathbb{P}_0$.

The empirical distribution function (EDF)

The empirical distribution (ED) $\widehat{\mathbb{P}}_0$ associated with the data $y = (y_1, y_2, \ldots, y_n)$ gives equal weight $(1/n)$ to each of the y_i's (assuming that all values of y are distinct).

Consequently, if $Z \sim \widehat{\mathbb{P}}_0$ is a random variable, then Z takes the value y_i with probability $1/n$.

The empirical distribution function (EDF) associated with the data y is defined by

$$\widehat{F}_n(z) = \widehat{\mathbb{P}}_0(Z \leq z)$$

$$= \frac{1}{n} \sum_{i=1}^{n} \mathbb{1}_{\{y_i \leq z\}} = \text{fraction of } y_i\text{'s that are less than } z.$$

Properties of the EDF

- It holds that

$$\lim_{z\to-\infty}\widehat{F}_n(z) = \lim_{z\to-\infty}F(z) = 0,$$
$$\lim_{z\to\infty}\widehat{F}_n(z) = \lim_{z\to\infty}F(z) = 1.$$

- In addition, trivially, $n\widehat{F}_n(z) \sim \text{Bin}(n, F(z))$.
- This implies the LLN (as $n \to \infty$)

$$\widehat{F}_n(z) \to F(z) \quad \text{(a.s.)}$$

- as well as the CLT

$$\sqrt{n}(\widehat{F}_n(z) - F(z)) \xrightarrow{\text{d.}} \mathcal{N}(0, \sigma^2(z)),$$

where

$$\sigma^2(z) = F(z)(1 - F(z)).$$

The bootstrap

- Having access to data y, we may now replace $\mathbb{P}_0$ by $\widehat{\mathbb{P}}_0$.
- Any quantity involving $\mathbb{P}_0$ can now be approximated by plugging $\widehat{\mathbb{P}}_0$ into the quantity instead. For instance,

$$\tau = \tau(\mathbb{P}_0) \approx \widehat{\tau} = \tau(\widehat{\mathbb{P}}_0).$$

- Moreover, the uncertainty of $t(y)$ can be analyzed by drawing repeatedly $Y^* \sim \widehat{\mathbb{P}}_0$ and looking at the variation (histogram) of $\Delta(Y^*) = t(Y^*) - \tau \approx \Delta(Y^*) = t(Y^*) - \widehat{\tau}$.
- Recall that the ED gives equal weight $1/n$ to all the y_i's in y. Thus, simulation from $\widehat{\mathbb{P}}_0$ is carried through by simply drawing, with replacement, among the values $y_1, \ldots, y_n$.

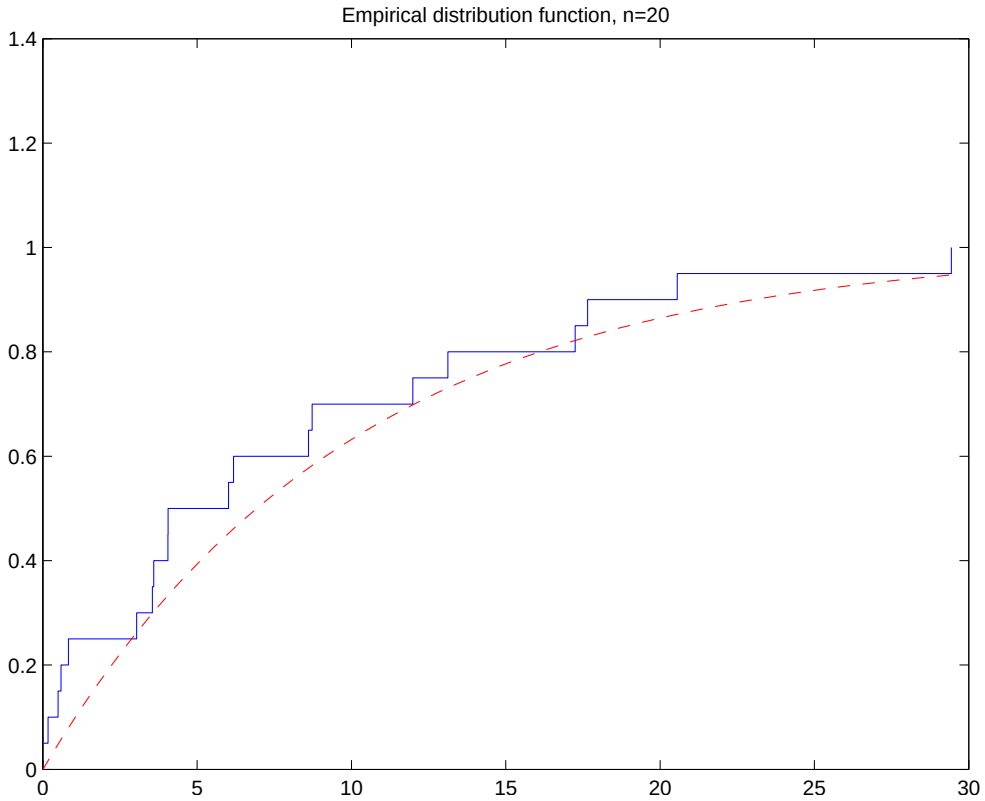
The bootstrap (cont.)

The algorithm goes as follows.

- Construct the ED $\widehat{\mathbb{P}}_0$ from the data y.
- Simulate B new data sets Y_b^*, $b \in \{1, 2, \ldots, B\}$, where each Y_b^* has the size of y, from $\widehat{\mathbb{P}}_0$. Each Y_b^* is obtained by drawing, with replacement, n times among the y_i's.
- Compute the values $t(Y_b^*)$, $b \in \{1, 2, \ldots, B\}$, of the estimator.
- By setting in turn $\Delta_b^* = t(Y_b^*) - \widehat{\tau}$, $b \in \{1, 2, \ldots, B\}$, we obtain values being approximately distributed according to the error distribution. These can be used for uncertainty analysis.

A Toy example: Exponential distribution

We let $y = (y_1, \ldots, y_{20})$ be i.i.d. observations of $Y_i \sim \text{Exp}(\theta)$, with unknown mean θ. As estimator we take, as usual, $t(y) = \bar{y}$ (which is an unbiased complete sufficient statistics also in this case).



A toy Example: Matlab implementation

In Matlab:

```
n = 20;
B = 200;
tau_hat = mean(y);
boot = zeros(1,B);
for b = 1:B, % bootstrap
    I =  randsample(n,n,true);
    boot(b) = mean(y(I));
end
delta = sort(boot - tau_hat); % sorting to obtain quantiles
alpha = 0.05; % CB level
L = tau_hat - delta(ceil((1 - alpha/2)*B)); % constructing CB
U = tau_hat - delta(ceil(alpha*B/2));
```

A Toy example: Exponential distribution