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

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Lecture 14
Bootstrap and MC tests
March 5, 2020

Plan of today's lecture

1. Last time: Introduction to bootstrap (Ch. 9)
2. More on the bootstrap (Ch. 9)
   - Example: law schools
   - Parametric bootstrap
   - Semi-parametric bootstrap
3. MC methods for hypothesis testing (Ch. 9)
   - Preliminaries
   - MC tests
   - Permutation tests

We are here $\longrightarrow \bullet$

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The frequentist approach to statistical inference

We assume that we have at hand

- observations y
- and a (possibly parametric) model $\mathcal{P}$ for the data.

In this setting 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 estimand τ is estimated using a statistic $t(y)$.

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 of the error $\Delta(Y)$ (error distribution).

Bootstrap in a nutshell

Using the bootstrap algorithm we deal with this matter by

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

A generic way to obtain the approximation $\widehat{\mathbb{P}}_0$ is to use the empirical distribution.

The empirical distribution (ED)

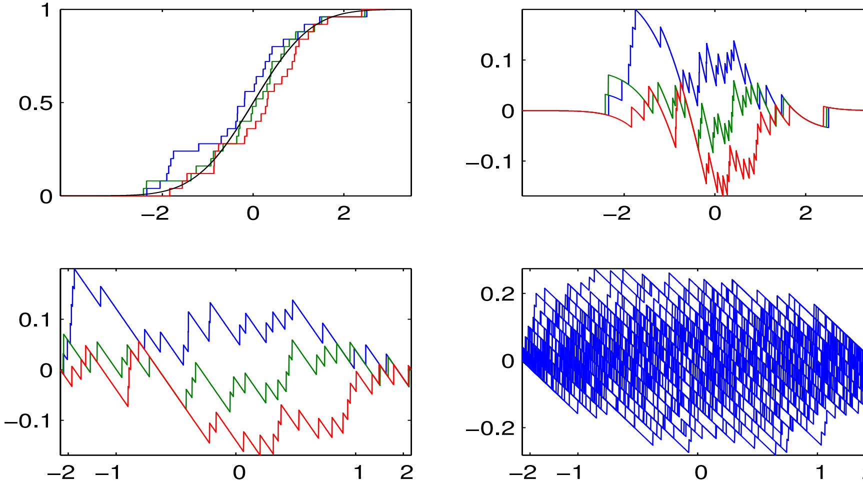
The empirical distribution (ED) $\widehat{\mathbb{P}}_0$ associated with the data $y = (y_1, y_2, \ldots, y_n)$ gives equal weight $(1/n)$ to each of the y_i's (assuming that all values of y are distinct).

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

$$
\begin{aligned}
\widehat{F}_n(z) &= \widehat{\mathbb{P}}_0(Z \le z) \\
&= \frac{1}{n}\sum_{i=1}^{n} \mathbb{1}_{\{y_i \le z\}} = \text{fraction of } y_i\text{'s that are less than } z.
\end{aligned}
$$

The EDF



Generating samples from the ED

Consequently a sample Y^* of size n from the empirical distribution $\widehat{\mathbb{P}}_0$ associated with the observations $y = (y_1, y_2, \ldots, y_n)$ is generated by

1. drawing indices $I_1, I_2, \ldots, I_n$ independently from the uniform distribution on the integers $\{1, 2, \ldots, n\}$, and
2. letting $Y^* = (y_{I_1}, y_{I_2}, \ldots, y_{I_n})$.

Note that this algorithm draws n values from the set $\{y_1, y_2, \ldots, y_n\}$ with replacement.

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. In particular,

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

  which, e.g., in the case of the mean, becomes

$$\tau = \int y f_0(y)\,\mathrm{d}y \approx \frac{1}{n}\sum_{i=1}^{n} y_i.$$

- Moreover, the uncertainty of $t(y)$ can be analyzed by drawing repeatedly $Y^* \sim \widehat{\mathbb{P}}_0$ and look at the variation (histogram) of $\Delta(Y^*) = t(Y^*) - \tau \approx= t(Y^*) - \widehat{\tau}$.
- In the case of the empirical distribution, 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 an approximation $\widehat{\mathbb{P}}_0$ of $\mathbb{P}_0$ 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 $\widehat{\mathbb{P}}_0$.
- 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.

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Non-parametric Bootstrap

- The bootstrap algorithm considered above is non-parametric in the sense that we have no assumptions on the distribution $\mathbb{P}_0$ apart from the samples being i.i.d.; in particular, we do not assume that $\mathbb{P}_0$ belongs to a certain parametric family.
- Our approximation $\widehat{\mathbb{P}}_0$ of $\mathbb{P}_0$ is the empirical distribution function.
- The simulation step boils down to drawing from the empirical distribution, i.e. drawing from the data with replacement.

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Example: law schools

We have average test scores (LSAT and GPA) from 15 american law schools and want to investigate if the two scores are correlated, i.e. τ is the correlation between the two datasets.

1. Our data consists of pairs $(x, y) = ((x_1, y_1), \dots, (x_{15}, y_{15}))$.
2. Estimate the correlation of the data using the sample correlation

$$\widehat{\tau} = t(x, y) = \frac{n \sum_i x_i y_i - \sum_i x_i \sum_i y_i}{\sqrt{n \sum_i x_i^2 - (\sum_i x_i)^2} \sqrt{n \sum_i y_i^2 - (\sum_i y_i)^2}} \approx 0.776.$$

3. Create bootstrap samples $(X, Y)_b^*$, $b \in \{1, 2, \dots, B\}$, where each sample $(X, Y)_b^*$ is generated by drawing 15 times with replacement from the pairs (x_i, y_i), $i \in \{1, \dots, 15\}$.
4. Calculate the correlation $t((X, Y)_b^*)$ for each random sample.

Example: law schools (cont.)

- Given the $(X, Y)_b^*$'s we create variables $\Delta_b^* = t((X, Y)_b^*) - \widehat{\tau}$, $b \in \{1, 2, \ldots, B\}$, being approximately distributed according to the error distribution.
- This gives that the bias of our estimate is approximately $\mathbb{E}(\Delta(X, Y)) \approx \overline{\Delta^*} = -0.0057$.
- The bias-corrected estimate is $t(x, y) - \overline{\Delta^*} = 0.783$.
- A one-sided 95%-confidence interval for the correlation is consequently

$$\begin{aligned} I_{0.05} &= \left(\widehat{\tau} - F_{\Delta}^{-1}(0.95), 1\right) \\ &\approx \left(\widehat{\tau} - \Delta^*_{\lceil 0.95B \rceil}, 1\right) \\ &= (0.614, 1). \end{aligned}$$

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Parametric bootstrap

In the non-parametric bootstrap we had no assumptions on the distribution function apart from the observed data y being i.i.d.

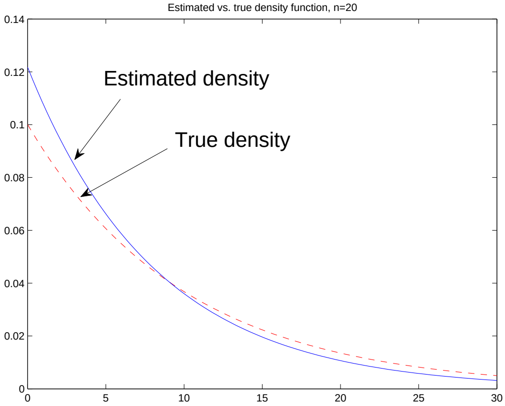
In the parametric bootstrap we assume that data comes from a distribution $\mathbb{P}_0 = \mathbb{P}_{\theta_0} \in \{\mathbb{P}_\theta; \theta \in \Theta\}$ belonging to some parametric family.

Instead of using the ED, we find an estimate $\widehat{\theta} = \widehat{\theta}(y)$ of θ_0 from our observations and

1. generate new bootstrapped samples Y_b^*, $b \in \{1, 2, \ldots B\}$, from $\widehat{\mathbb{P}}_0 = \mathbb{P}_{\widehat{\theta}}$.
2. After this we form, as usual, bootstrap estimates $\widehat{\theta}(Y_b^*)$ and errors $\Delta_b^* = \widehat{\theta}(Y_b^*) - \widehat{\theta}$, $b \in \{1, 2, \ldots B\}$.

A toy example: exponential distribution

We let $y = (y_1, \ldots, y_{20})$ be i.i.d. observations of $Y_i \sim \text{Exp}(\theta_0)$, with unknown mean θ_0. The MLE of θ_0 is $\widehat{\theta}(y) = \bar{y}$ and following plot displays $\text{Exp}(\widehat{\theta}(y))$ vs. $\text{Exp}(\theta_0)$.

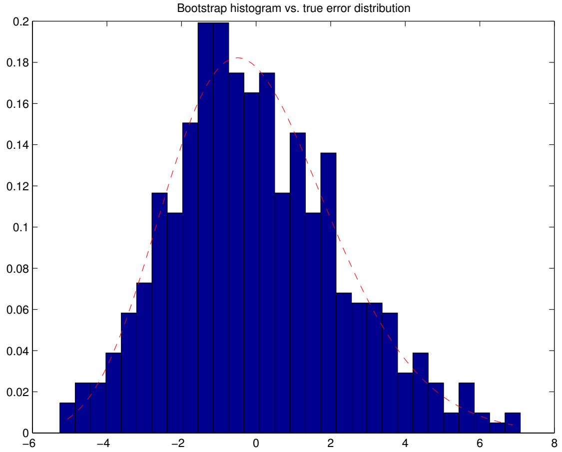


A toy example: exponential distribution (cont.)

In Matlab:

```
n = 20;
B = 500;
theta_hat = mean(y);
boot = zeros(1,B);
for b = 1:B, % bootstrap
    y_boot = exprnd(theta_hat,1,n);
    boot(b) = mean(y_boot);
end
delta = sort(boot - theta_hat); % sorting to obtain quantiles
alpha = 0.05; % CB level
L = theta_hat - delta(ceil((1 - alpha/2)*B)); % forming CB
U = theta_hat - delta(ceil(alpha*B/2));
```

A toy example: exponential distribution (cont.)



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Semi-parametric bootstrap

- We assume a parametric model for the data, for instance

$$Y_i = kx_i + m + \epsilon_i, \quad i \in \{1, 2, \dots n\},$$

  and a non-parametric model for the residuals ϵ_i.
- Our only assumption on the residuals is that they are i.i.d.
- Given data $y = (y_1, \dots, y_n)$ we want to construct estimators $\widehat{k}(y)$ and $\widehat{m}(y)$ of the parameters k and m and assess the uncertainty of the estimates.
- To do the latter, we would generate bootstrap samples Y_b^* and parameter estimates $\widehat{k}(Y_b^*)$ and $\widehat{m}(Y_b^*)$ and study the variation of e.g. $\Delta_b^* = \widehat{k}(Y_b^*) - \widehat{k}(y)$.
- A confidence interval for k is then given by

$$\left(\widehat{k}(y) - \Delta^*_{\lceil B(1-\alpha/2)\rceil}, \widehat{k}(y) - \Delta^*_{\lceil B\alpha/2\rceil}\right).$$

Semi-parametric bootstrap (cont.)

We proceed as follows:

- Find estimators $\widehat{k} = \widehat{k}(y)$ and $\widehat{m} = \widehat{m}(y)$ for the parameters using least squares.
- Estimate the residuals as

$$\widehat{\epsilon}_i = y_i - \widehat{k}x_i - \widehat{m}, \quad i \in \{1, 2, \dots, n\}.$$

- Now, the $\widehat{\epsilon}_i$'s approximately form an i.i.d. sample from an unknown distribution. For $b = 1, 2, \dots, B$,
  1. resample the residuals to generate a bootstrap sample $\epsilon_b^* = (\epsilon_1, \dots \epsilon_n)_b^*$ and
  2. Use the bootstrapped residuals to generate bootstrapped observations

$$(Y_i)_b^* = \widehat{k}x_i + \widehat{m} + (\epsilon_i)_b^*.$$

  3. Given the bootstrapped observations, estimate the parameters to obtain $\widehat{k}(Y_b^*)$ and $\widehat{m}(Y_b^*)$.

Example: linear regression

As an example,

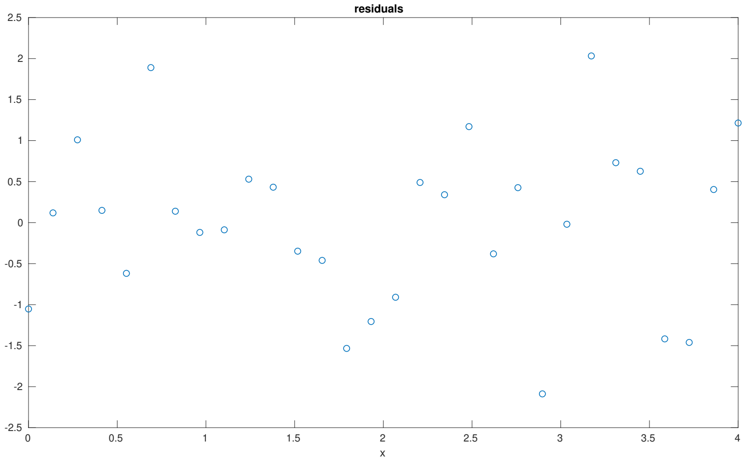
- assume that $Y_i = kx_i + m + \epsilon_i$, with standard Gaussian residuals.
- To test the semi-parametric bootstrap we simulate a data set with $m = 3$ and $k = 4$.
- Given data, the parameters are estimated using least squares estimation.
- For comparison, we know from the theory of linear regression that an exact confidence interval for k is given by

$$I_\alpha = \left(\widehat{k} - t_{\alpha/2}(n-2)s_b, \widehat{k} + t_{\alpha/2}(n-2)s_b\right).$$

where

$$s_b^2 = \frac{\frac{1}{n-2}\sum_i \widehat{\epsilon}_i^2}{\sum_i (x_i - \bar{x})^2}.$$

Check residuals



Example: Simple regression

Applying this to the given data set yields

$$I_{0.05} = (3.56, 4.20)\,.$$

For a comparison we applied semi-parametric as well as parametric bootstrap to the same data set.

- Using semi-parametric bootstrap, where we resample the estimated residuals, we obtain the interval

$$I_{0.05} = (3.57, 4.18)\,.$$

- Instead using parametric bootstrap, where we draw new residuals from $\mathcal{N}(0, \hat{\sigma}^2)$, we obtain

$$I_{0.05} = (3.57, 4.20)\,.$$

Summary: Different types of bootstrap

- Non-parametric bootstrap
  - makes no assumptions on the distribution apart from i.i.d.
  - needs more data than parametric.
- Parametric bootstrap
  - assumes that data comes from a parametric family of distributions.
  - needs less data to get good estimates due to stronger assumptions.
  - may however be sensitive to assumptions.
- Semi-parametric bootstrap
  - assumes a parametric model, coupled with non-parametric nuisance variables, often residuals.
  - is typically used for regression.

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Statistical hypotheses

- A statistical hypothesis is a statement about the distributional properties of data.
- The goal of a hypothesis test is to see if data agrees with the statistical hypothesis.
- Rejection of a hypothesis indicates that there is sufficient evidence in the data to make the hypothesis unlikely.
- Strictly speaking, a hypothesis test does not accept a hypothesis; it fails to reject it.

Testing hypotheses

The basis of a hypothesis test consist of

- a null hypothesis $\mathcal{H}_0$ that we wish to test.
- a test statistic $t(y)$, i.e. a function of the observed data y.
- a critical region R.

If the test statistic falls into the critical region, then we reject the null hypothesis $\mathcal{H}_0$.

Important concepts

Significance The probability (risk) that the test incorrectly rejects the null hypothesis.

Power The probability that the test correctly rejects the null hypothesis. Is a function of the true, unknown parameter.

p-value The probability, given the null hypothesis, of observing a result at least as extreme as the test statistic.

Type I error Incorrectly rejecting the null hypothesis=False positive.

Type II error Failing to reject the null hypothesis=False negative.

Testing simple hypotheses

- A simple hypothesis specifies completely a single distribution for the data, e.g. $Y \sim \mathcal{N}(\theta, 1)$ with $\mathcal{H}_0 : \theta = 0$.
- We construct/define a test statistic $t(y)$ such that large values of $t(y)$ indicate evidence against $\mathcal{H}_0$.
- The p-value of the test is now $p(y) = \mathbb{P}(t(Y) \geq t(y) \| \mathcal{H}_0)$.
- The rejection region is $\mathsf{R} = \{y : p(y) \leq \alpha\}$, where α is the level of the test.
- Thus, to evaluate the p-value we need to find the distribution of $t(Y)$ under $\mathcal{H}_0$.

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MC test of a simple hypothesis

An MC-based algorithm for testing simple hypotheses is as follows:

1. Draw N samples, $Y_1, \ldots, Y_N$, from the distribution specified by $\mathcal{H}_0$.
2. Calculate the test statistic $t_i = t(Y_i)$ for each sample.
3. Estimate the p-value using MC integration by letting

$$\widehat{p}(y) = \frac{1}{N} \sum_{i=1}^{N} \mathbb{1}_{\{t_i \geq t(y)\}}.$$

4. If $\widehat{p}(y) \leq \alpha$, reject $\mathcal{H}_0$.

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Permutation tests

- The random variables of a set Y is said to be exchangeable if they have the same distribution for all permutations.
- The distribution of Y given the ordered sample is then the uniform distribution on the set of all permutations of Y.
- Conditioning on the ordered variables leads to permutation tests.
- Permutation tests can be very efficient in testing an exchangeable null-hypothesis against a non-exchangeable alternative, e.g. for testing if two samples differ in some way.

MC permutation test

An MC-based permutation test can be implemented as follows.

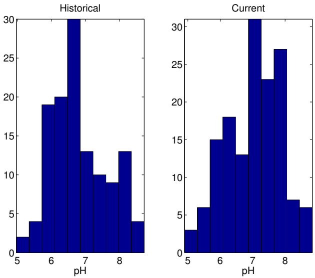
1. Draw N permutations, $Y_1, \ldots, Y_N$, of the vector y.
2. Calculate the test statistic $t_i = t(Y_i)$ for each permutation.
3. Estimate the p-value using MC integration according to

$$\widehat{p}(y) = \frac{1}{N} \sum_{i=1}^{N} \mathbb{1}_{\{t_i \geq t(y)\}}.$$

4. If $\widehat{p}(y) \leq \alpha$, reject $\mathcal{H}_0$.

Example: pH data

- We have 273 historical and current pH-measurements of 149 lakes in Wisconsin and want to test if the pH-levels have increased.
- We assume that all measurements are independent and that historical measurements have a distribution F_0 and that new measurements have a distribution G_0.
- We want to test $\mathcal{H}_0 : F_0 = G_0$ against $\mathcal{H}_1 : F_0 \neq G_0$



Example: pH data (cont.)

- Assume that the distribution for current data can be written as $G_0(y) = F_0(y - \theta)$. That is, the mean of the current data is the mean of the historical data plus θ.
- We now want to test $\mathcal{H}_0 : \theta = 0$ against $\mathcal{H}_1 : \theta > 0$.
- Under $\mathcal{H}_0$, all data are i.i.d. and thus exchangeable.
- We use the difference in the sample means as a test statistic.
- A permutation test using 10000 random permutations gives $p = 0.0185$