

## EE 046202 - Technion - Unsupervised Learning & Data Analysis

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## Tutorial 02 - Classical Methods in Statistical Inference - Confidence Intervals



## Agenda

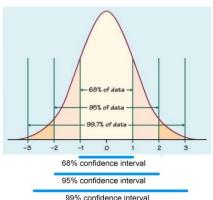
- Interval Estimation (Confidence Intervals))
  - Formulation
  - Finding Interval Estimators
- Bootstrap Approach
  - Boostrap for the Median Estimator ()
- · Confidence Interval with Chebyshev Inequality
- · Confidence Interval with DKW Inequality
- Recommended Videos
- · Credits

```
In [1]: # imports for the tutorial
        import numpy as np
        import pandas as pd
        from helpers.cdf_bounds import plot_cdf_confidence
        from scipy.stats import norm
        import time
        import matplotlib.pyplot as plt
        %matplotlib notebook
```



## **Confidence Intervals (Interval Estimation)**

- What is the problem with the **point estimation** for  $\theta$ ,  $\hat{\theta}$ ?
  - $\hat{\theta}$  alone does not give much information about  $\theta$ !
  - Without any additional information, we cannot tell how close is  $\hat{\theta}$  to the real  $\theta$ .
- Interval Estimation an interval that is *likely* to include the true value of  $\theta$ .
  - Instead of saying  $\hat{\theta} = 8.14$ , we report:  $[\hat{\theta}_p, \hat{\theta}_h] = [6.65, 9.87]$ , which we hope includes the real value of  $\theta$ .
  - We actually produce 2 estimates for  $\theta$ : high estimate  $\hat{\theta}_h$  and low estimate  $\hat{\theta}_l$ .
  - We define two important properties of a confidence interval:
    - **Length** the precision which we can estimate  $\theta$ . Defined as  $\hat{\theta}_h \hat{\theta}_l$ .
    - Confidence Level how confident are we in the interval. It is the *probability* that the real  $\theta$  lies in the interval. We wish to have high confidence (usually 90-95%).



## **Formulation**

Let  $X_1, X_2, \dots, X_n$  be a random sample from a distribution with a parameter  $\theta$  that is to be estimated.

**The goal** is to find *two* (point) estimators for  $\theta$ :

1. The low estimator:

$$\hat{\theta}_l = \hat{\theta}_l(X_1, X_2, \dots, X_n)$$

2. The high estimator:

$$\hat{\theta}_h = \hat{\theta}_h(X_1, X_2, \dots, X_n)$$

- The interval estimator is:  $[\hat{\theta}_l, \hat{\theta}_h]$ .
- Confidence Level defined to be  $1 \alpha$ .
- The estimators  $\hat{\theta}_l$ ,  $\hat{\theta}_h$  are chosen such that the **probability** that the interval  $[\hat{\theta}_l, \hat{\theta}_h]$  includes  $\theta$  is larger than the confidence level  $1 \alpha$ . Thus, we wish  $\alpha$  to be **small**.
  - lacktriangle Common values for lpha are: 0.1, 0.05, 0.01 which correspond to confidence levels 90%, 95% and 99% respectively.
- Formally: find  $\hat{\theta}_{l}, \hat{\theta}_{h}$  such that

$$P(\hat{\theta}_l \le \theta \le \hat{\theta}_h) \ge 1 - \alpha$$

or

$$P(\theta \in [\hat{\theta}_l, \hat{\theta}_h]) \ge 1 - \alpha$$



## **Finding Interval Estimators**

- Recall that for a continuous random variable X with **CDF** (Cumulative Distribution Function):  $F_X(x) = P(X \le x)$ .
- We wish to find probability between bounds such that:

$$P(x_l \le X \le x_h) = 1 - \alpha$$

We can choose (notice the different inequality signs):

$$P(X \le x_l) = \frac{\alpha}{2}$$
, and  $P(X \ge x_h) = \frac{\alpha}{2}$ 

Or, eqivalently

$$F_X(x_l) = \frac{\alpha}{2}$$
, and  $F_X(x_h) = 1 - \frac{\alpha}{2}$ 

$$\rightarrow x_l = F_X^{-1}(\frac{\alpha}{2}), x_h = F_X^{-1}(1 - \frac{\alpha}{2})$$

- Note: why do we divide α by 2 and not by 4 (and then pick α/4, 3α/4 instead of 2/2)?
   Since we are calculating both upper and lower bounds. Had we been interested in a single sided interval, then we would not have needed this division. Moreover, we would like our confidence level to be symmetrical in relation to both upper and lower bounds, there is no reason to give more weight to one over the other.

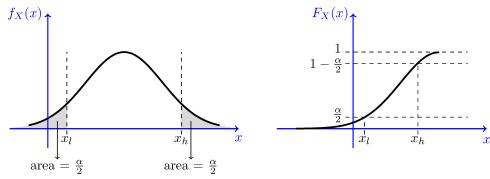


Image Source (https://www.probabilitycourse.com/chapter8/8 3 2 finding interval estimators.php)



## Exercise - Confidence Intervals for Normal Distribution (Using CLT)

1. (Probability Exercise) Let  $Z \sim \mathcal{N}(0, 1)$ . Find  $x_l, x_h$  such that

$$P(x_l \le Z \le x_h) = 0.95$$

- Normal Table (https://www.math.arizona.edu/~jwatkins/normal-table.pdf)
- 2. Let  $X_1, X_2, \dots, X_n$  be a random sample from a normal distribution  $\mathcal{N}(\theta, 1)$  ( $E[X] = \theta$ ). Find a 95% confidence interval for  $\theta$ .



#### Section 1

 $\alpha = 0.05$ , and  $\phi$  denotes the CDF of Z. Thus, we can choose:

$$x_l = \phi^{-1}(\frac{\alpha}{2}) = \phi^{-1}(0.025) = -1.96$$

$$x_h = \phi^{-1}(1 - \frac{\alpha}{2}) = \phi^{-1}(1 - 0.025) = 1.96$$

More generally, if we assume  $Z \sim \mathcal{N}(0,1)$ , for any  $p \in [0,1]$ , we define  $z_p$  as the real value for which  $P(Z > z_p) = p$ . Therfore,  $\phi(z_p) = 1 - p \rightarrow z_p = \phi^{-1}(1-p)$ . In our case

$$P(-z_{\frac{\alpha}{2}} \le Z \le z_{\frac{\alpha}{2}}) = 1 - \alpha$$

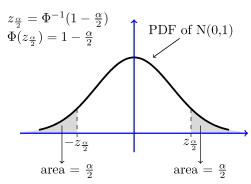


Image Source (https://www.probabilitycourse.com/chapter8/8 3 2 finding interval estimators.php)

## Section 2

We begin with finding the **point estimator** for  $\theta$ , which is the *mean* of the distribution. Recall from the previous tutorial that:  $\hat{\theta} = X = \frac{X_1 + X_2 + \ldots + X_n}{n}$  and since  $X_i \sim \mathcal{N}(\theta, 1)$  and the samples are i.i.d. then:  $X \sim \mathcal{N}(\theta, \frac{1}{n})$ . We now perform **standartization** (normalization in our case):

$$\frac{X-\theta}{\frac{1}{\sqrt{n}}} = \sqrt{n}(X-\theta) \sim \mathcal{N}(0,1)$$

- Why do we perform standartization? Because it is easier to work with  $\mathcal{N}(0, 1)$  and we are familiar with its CDF and can easily find the values with the table.
- Standartization in the general case where  $\sigma^2 \neq 1$ :

$$\frac{X-\theta}{\frac{\sigma}{\sqrt{n}}}$$

Thus:

$$P(-1.96 \le \sqrt{n(X-\theta)} \le 1.96) = 0.95$$

$$\to P\left(X - \frac{1.96}{\sqrt{n}} \le \theta \le X + \frac{1.96}{\sqrt{n}}\right) = 0.95$$

Therefore, the confidence interval is:

$$[\hat{\theta}_l, \hat{\theta}_h] = [X - \frac{1.96}{\sqrt{n}}, X + \frac{1.96}{\sqrt{n}}]$$

# Bootstrap

- · Bootstrap is a sampling method which we use to do estimations (and even train ML algorithms, as in Boosting/Bagging method).
- The bootstrap approach relies on the assumption that drawing random samples with replacement from the data, simulates well the actual distribution of the data.
- In that case, several statistics (e.g. the variance) can be calculated using random samples from the data.
- Motivation in general, we cannot compute the confidence interval. Thus, we need a numerical scheme to estimate it. This is where bootstrapping helps us.
- · In sampling with replacement, each sample unit of the population can occur one or more times in the sample.
  - In statistics, resampling with replacement is called bootstrapping.
- · Bootstrap Algorithm:
  - Denote the original sample:  $L_N = (x_1, x_2, \dots, x_N)$
  - Repeat M times:
    - $\circ$  Generate a sample  $L_k$  of size k from  $L_N$  by sampling with replacement (samples can contain multiple copies of the same point).
    - Compute h from  $L_k$  (that is, calculate an estimation h using  $L_k$ ).
  - Denote the bootstrap values  $H = (h^1, h^2, \dots, h^M)$ 
    - · Use these values for calculating all the quantities of interest.



#### Exercise - Bootstrap for the Median Estimator

Given n i.i.d. samples,  $\{X_i\}_{i=1}^n$ , from  $\mathcal{D}$  consider the median estimator denoted by  $\hat{\mu}_M$  and calculate the **standard deviation** using the bootstrap approach. Write down the boostrap algorithm for that case.



#### The algorithm:

- Denote the original sample:  $\mathcal{D} = X_n = (x_1, x_2, \dots, x_n)$
- Calculate the median estimator  $T: T \leftarrow median(\mathcal{D})$
- Repeat M times:
  - Generate a sample  $L_k$  of size k from  $L_N$  by sampling with replacement.
  - Compute  $T_{boot}^k$  from  $L_k$  (that is, calculate an estimation for the median  $T_{boot}$  using  $L_k$ ).

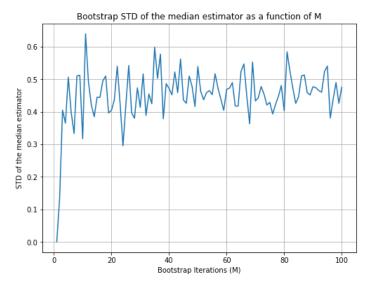
$$T_{boot}^k = median(L_k)$$

- Denote the bootstrap values  $\hat{T} = (T_{hoot}^1, T_{hoot}^2, \dots, T_{hoot}^M)$ 
  - Median ← T
  - $\hat{\sigma}^2 \leftarrow Variance(\hat{T})$

```
In [2]: # Let's see the magic
        def std_bootstrap(x, k, m, estimator=np.mean):
             estimate_value = estimator(x)
             estimations = []
            for _ in range(m):
    # sample K with replacement
                x_k = np.random.choice(x, size=k, replace=True)
                t_k = estimator(x_k)
                 estimations.append(t\_k)
             return estimate_value, np.std(estimations)
        # generate real data
        n = 300 # number of totals samples
        K = 100 # number of bootstrap samples
        mu , sigma = 1, 4
        x = np.random.normal(mu, sigma, size=n)
        M = np.arange(1, 101) # number of boostrap iterations
        stds = []
         for m in M:
            stds.append(std_bootstrap(x=x, k=K, m=m, estimator=np.median)[1])
            # [1] because we don't care about the estimate, just the std
```

```
In [3]: fig = plt.figure(figsize=(8, 6))
    ax = fig.add_subplot(1,1,1)
    ax.plot(M, stds)
    ax.grid()
    ax.set_xlabel("Bootstrap Iterations (M)")
    ax.set_ylabel("STD of the median estimator")
    ax.set_title("Bootstrap STD of the median estimator as a function of M")
```

Out[3]: Text(0.5, 1.0, 'Bootstrap STD of the median estimator as a function of M')



# <

## Confidence Interval with Chebyshev Inequality

• Recall the **Chebyshev Inequality**: if X is a random variable with finite mean and variance  $\sigma^2$ , then

$$P(|X - E[X]| \ge \epsilon) \le \frac{\sigma^2}{\epsilon^2}$$

for all  $\epsilon > 0$ .

• Also, letting  $\epsilon = k\sigma$ :

$$P(|X - E[X]| \ge k\sigma) \le \frac{1}{k^2}$$

- This is useful when we want to measure the distance in "standard deviations" (e.g., a confidence interval of 2 standard deviations).
- Chebyshev inequality allows us to calculate CIs given the variance (which can be estimated, for instance, with bootstrapping) of a random variable.

• For the sample mean  $X = \frac{1}{N} \sum_{k=1}^{N} X_{K}$ , Chebyshev inequality tells us:

$$P(|X - \mu| \ge \epsilon) \le \frac{\hat{\sigma}^2}{\epsilon^2} = \frac{\sigma^2}{N\epsilon^2}$$

- $\blacksquare$  Recall that  $\hat{\sigma}$  is the normalized empirical variance for a sample of size N
- For example, for a 95% CI,  $\frac{\sigma^2}{N\epsilon^2} = \alpha = 0.05 \rightarrow \epsilon = \frac{\sigma}{\sqrt{0.05N}}$ , which leads to:

$$X - \frac{\sigma}{\sqrt{0.05N}} \le \mu \le X + \frac{\sigma}{\sqrt{0.05N}}$$

with probability at least 0.95.

In practice, if you are not given σ, then you can't calculate the CI. But you can estimate it (wth Bootstrap for example).



## Confidence Interval with DKW Inequality

The **Dvoretzky–Kiefer–Wolfowitz** (DKW) inequality bounds how close an empirically determined distribution function will be to the distribution function from which the empirical samples are drawn.

Let  $X_1, X_2, ..., X_n$  be real-valued independent and identically distributed (i.i.d.) random variables with cumulative distribution function (CDF)  $F(\cdot)$  (that is, they are sampled from  $F: X_1, X_2, ..., X_n \sim F$ ). Let  $F_n$  denote the associated **empirical distribution** function defined by:

$$F_n(x) = \frac{1}{n} \sum_{i=1}^{n} 1_{\{X_i \le x\}}, x \in \mathbb{R}$$

- F(x) the probability that a *single* random variable X is smaller than x
- $F_n(x)$  the *fraction* of random variables that are smaller than x

The DKW inequality bounds the probability that the random function  $F_n$  differs from F by more than a given constant  $\epsilon > 0$  anywhere on the real line (R):

$$Pr(\sup_{x \in \mathbb{R}} |F_n(x) - F(x)| > \epsilon) \le 2e^{-2n\epsilon^2}, \forall \epsilon > 0$$

- This strengthens the Glivenko-Cantelli theorem by quantifying the rate of convergence as n tends to infinity.
  - But it holds for any n.

#### **Producing CDF-based Confidence Bounds**

- The DKW inequality is one method for generating CDF-based confidence bounds and producing a confidence band.
- $\bullet \ \ \, \text{The purpose of this confidence interval is to contain the entire CDF at the specified } \textbf{confidence level} \; .$ 
  - Alternative approaches attempt to only achieve the confidence level on each individual point which can allow for a tighter bound.
- The DKW bounds runs parallel to, and is equally above and below, the empirical CDF.

The interval that contains the **true CDF** F(x), with probability  $1 - \alpha$ :

$$F_n(x) - \epsilon \le F(x) \le F_n(x) + \epsilon$$

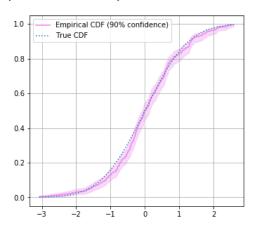
$$\alpha = 2e^{-2n\epsilon^2} \to \epsilon = \sqrt{\frac{\ln\frac{2}{\alpha}}{2n}}$$

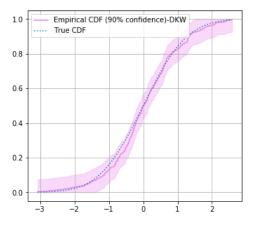
- · What is so special about the DKW condifence bounds?
  - It is distribution free therefore, it is very loose in comparison to the bootstrap estimates, which are usually tighter.
  - Faster to calculate.

```
In [4]: def compare_cdf_bounds():
                                        # generate random data
                                        x = np.random.randn(300)
                                         # plot
                                        fig = plt.figure(figsize=(12,5))
                                        ax1 = fig.add_subplot(1,2,1)
                                        ax1.grid()
                                        s_time = time.time()
                                        # Pointwise estimate (for each point!) confidence bounds using Beta distribution
                                        plot_cdf_confidence(data=x, confidence=0.9, color='violet', label='Empirical CDF (90% confidence)', ax=ax1)
                                        beta_time = time.time() - s_time
                                        x_sorted = np.sort(x)
                                        ax1.plot(x_sorted, norm.cdf(x_sorted), ':', label='True CDF')
                                        ax1.legend()
                                        ax2 = fig.add_subplot(1,2,2)
                                        ax2.grid()
                                        s_time = time.time()
                                        # DKW (not pointwise!) confidence bounds
                                        plot\_cdf\_confidence(data=x,\ confidence=0.9,\ color='violet',\ label='Empirical\ CDF\ (90\%\ confidence)-DKW',\ label='Empiri
                                                                                                         estimator_name='DKW', ax=ax2)
                                        dkw_time = time.time() - s_time
                                       x_sorted = np.sort(x)
ax2.plot(x_sorted, norm.cdf(x_sorted), ':', label='True CDF')
                                        ax2.legend()
                                        print("pointwise: {:.3} sec, DKW: {:.3} sec".format(beta_time, dkw_time))
```

In [5]: compare\_cdf\_bounds()

pointwise: 0.121 sec, DKW: 0.00598 sec







## Exercise - Confidence Intervals Calculation

• Reminder: **Hoeffding Inequality**: Let  $X_1, \ldots, X_n$  be i.i.d. random variables, bounded by the intervals  $a_i \le X_i \le b_i$ . Let the empirical mean be defined according to  $X = \frac{1}{n} \sum_{i=1}^{n} X_i$ . It holds that:

$$P(|X - E[X]| \ge \epsilon) \le 2e^{-\frac{2n^2\epsilon^2}{\sum_{i=1}^{n} (a_i - b_i)^2}}$$

Derive a 95% confidence band for the mean ( $E[X] = \mu$ ) using **DKW** (through the CDF bound) and **Hoeffding** inequalities.

#### Assume:

- True CDF: F(x), estimated CDF:  $F_n(x)$
- Estimated mean: X
- Number of samples n = 60
- Prior knowledge: the range of the random variables is  $X \in [0, 45]$ 
  - No specific distribution.



Section 1

Using DKW:

$$\begin{split} P(\sup_{x \in \mathbb{R}} |F_n(x) - F(x)| &> \epsilon) \leq 2e^{-2n\epsilon^2} = 0.05 \\ &\to \epsilon = \sqrt{\frac{-\ln(0.025)}{2*60}} = 0.175 \\ &\to F(x) \in [F_n(x) - 0.175, F_n(x) + 0.175] \end{split}$$

• Deriving a CI for the mean: we know that  $E[X] = \int_0^{45} (1 - F(x)) dx$  (from the Tail Sum formula), therefore:

$$\int_0^{45} (1 - F_n(x) \pm 0.175) dx = X \pm 7.875$$

• Why is  $E[X] = \int (1 - F(x))dx$ ? Recall the Tail Sum formula from previous tutorial ( $E[X] = \sum_{i=1}^{n} P(X \ge i)$ ). In the continuous space it is completely analogous!

$$E[X] = \int_{X} P(X \ge x) dx = \int_{X} (1 - P(X \le x)) dx = \int_{X} (1 - F(x)) dx$$

• Proof (https://en.wikipedia.org/wiki/Expected\_value#General\_case\_2)

Section 2

Using Hoeffding:

$$P(|X - E[X]| \ge \epsilon) \le 2e^{-\frac{2n^2\epsilon^2}{\sum_{i=1}^{n} (a_i - b_i)^2}} = 2e^{-\frac{2 \cdot 60^2\epsilon^2}{\sum_{i=1}^{60} (45 - 0)^2}} = 0.05$$

$$-$$

$$\rightarrow \epsilon = 7.89 \rightarrow E[X] \in [X - 7.89, X + 7.89]$$

• We see that both approaches yield similar CI (same range) for the mean. In this sense, the estimators are equivalent.



## **Recommended Videos**



- These videos do not replace the lectures and tutorials.
- · Please use these to get a better understanding of the material, and not as an alternative to the written material.

#### Video By Subject

- Confidence Intervals CrashCourse (https://www.youtube.com/watch?v=yDEvXB6ApWc&t=600s)
- Bootstrap Confidence Intervals: Intro to bootstrapping proportions (https://www.youtube.com/watch?v=655X9eZGxls)



- Examples, exercises and definitions from <a href="Introduction to Probability, Statistics and Random Processes">Introduction to Probability, Statistics and Random Processes</a> (<a href="https://probabilitycourse.com/">https://probabilitycourse.com/</a>) <a href="https://probabilitycourse.com">https://probabilitycourse.com</a>) (<a href="https://probabilitycourse.com"
- Icons from Icon8.com (https://icons8.com/) https://icons8.com (https://icons8.com)
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