Estimating the Mean from Data: Introduction to Estimation Theory

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April 2, 2023

Outline

Mean Estimation Problem and Motivations

The Data Generation Process Matters

Preliminaries: Key Properties of Expectation and Variance

Statistical Estimators

Mean Square Error and Bias-Variance Decomposition

Bias-Variance Decomposition in Mean Estimation

Consistency and Unbiasedness

Variance Reduction by Introducing a Bias

Estimation of the Mean

- Let X be a random variable taking values in \mathbb{R} with probability distribution P.

(Note: In the previous lecture, P is used to denote the distribution of the underlying probability space, but here P denotes the distribution of X).

- The mean (or the expected value) of X is defined by

$$\mu := \mathbb{E}_{X \sim P}[X] = \int x \ dP(x) \in \mathbb{R}.$$

Assume that we don't know P, and thus we don't know μ .

Estimation of the Mean

- Assume instead that we are given some data:

$$X_1,\ldots,X_n\in\mathbb{R}$$

- These are assumed to be random variables taking values in \mathbb{R} .
- The task of mean estimation is estimating the unknown mean μ from the data X_1, \ldots, X_n .
- This is one of the most ubiquitous and fundamental problems in statistics.
- In this lecture, we look at this problem in details.

Motivation 1: Relation to Many Problems

Many problems can be formulated as estimation of the mean.

Examples:

- Monte Carlo: Simulation-based mean estimation.
- Design of experiments: Average treatment (causal) effect.
- Regression: Estimation of the conditional mean.
- Supervised machine learning:
 - Risk = the mean of a loss function.
 - ► Stochastic gradient = approximation of the expected gradient.

Motivation 2: Different Statistical Approaches

Mean estimation can be used for illustrating different approaches.

- The "frequentist" approach maximum likelihood estimation.
- The "Bayesian" approach posterior inference.
- The "empirical Bayes" the mixed approach.

Motivation 3: Key Notions

We can learn key notions in statistics.

- Estimator and consistency.
- Bias-variance decomposition/trade-off
- Law of large numbers and the central limit theorem.

Most importantly,

- The key is how data are generated/obtained.

Is the Empirical Average a Good Approach?

A standard approach is to take the empirical average of data points:

$$\hat{\mu} := \frac{1}{n} \sum_{i=1}^{n} X_i.$$

In this lecture, we will address questions like:

- When is the empirical average a good estimate, and when is it not?
- When can we justify the use of the empirical average?
- What conditions do we need for the data X_1, \ldots, X_n ?

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Population and Data

In the mean estimation problem, we have two kinds of random variables:

[Population] Random variable X represents the hypothetical population of interest, with P being its probability distribution.

[Data] Random Variables X_1, \ldots, X_n represent the given data.

- The data X_1, \ldots, X_n are assumed to provide information about the population random variable X (or its distribution P).
- Otherwise, we cannot estimate the population mean $\mu = \mathbb{E}_{X \sim P}[X]$ from the data X_1, \dots, X_n .
- Therefore, how the data are generated/obtained becomes very important.

Example: Estimating the Average Income in France

- Assume that $X \in \mathbb{R}$ represents the income of a randomly sampled French person, with P being its distribution.
- The population mean $\mu = \mathbb{E}_{X \sim P}[X]$ represents the average income of French people.
- The data X_1, \ldots, X_n are the incomes of n French people randomly selected from the French population.
- Then, is the empirical average

$$\hat{\mu} := \frac{1}{n} \sum_{i=1}^{n} X_i$$

a good estimate of the true average income $\mu = \mathbb{E}_{X \sim p}[X]$?

Example: Estimating the Average Income in France

- Assume that data X_1, \ldots, X_n are the incomes of randomly sampled French persons in French Riviera.
- Then, the empirical average

$$\hat{\mu} := \frac{1}{n} \sum_{i=1}^{n} X_i$$

would be higher than the average income of the French population.

Example: Estimating the Average Income in France

- Assume that the data X_1, \ldots, X_n are the incomes of randomly sampled French people between age 20 and 30.
- Then, the empirical average

$$\hat{\mu} := \frac{1}{n} \sum_{i=1}^{n} X_i$$

would give an estimate lower than the true average income.

The Data Generating Process Matters

These examples indicate that how the data are generated/obtained strongly affects the validity of the empirical average.

- We need to make sure that data X_1, \ldots, X_n are sampled from the same population as that of the target random variable $X \sim P$.
- This requirement is mathematically formulated by assuming that random variables X_1, \ldots, X_n are independently and identically distributed (i.i.d.) with $X \sim P$.

Independently and Identically Distributed (i.i.d.)

Recall that random variables X_1, \ldots, X_n are i.i.d. with a random variable $X \sim P$ if they satisfy the following:

- Independence:
 - ▶ X_i and X_i are independent for all $i \neq j$.
 - \triangleright X_i and X are independent for all $i=1,\ldots,n$;
 - ► Recall that *X* represents the hypothetical population (e.g., randomly selected French person).
- Identity:
 - X_i follows the same probability distribution P of X (for all i = 1, ..., n).

We often write $X_1, \ldots, X_n \sim P$ (i.i.d.).

See also the lecture slides on Probability Theory.

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Preliminaries

Before going further, we collect here some key properties of Expectation and Variance of random variables.

Some Key Properties of Expectation

- For any real-valued random variable X and a constant $c \in \mathbb{R}$, we have

$$\mathbb{E}[cX] = c\mathbb{E}[X].$$

- For any real-valued random variables X and Y, we have

$$\mathbb{E}[X+Y] = \mathbb{E}[X] + \mathbb{E}[Y].$$

- If X and Y are independent,

$$\mathbb{E}[XY] = \mathbb{E}[X]\mathbb{E}[Y]$$

Variance of a Random Variable

In statistics, the variance of a random variable plays a key role.

- Let X be a real-valued random variable with probability distribution P.

Then the variance of X is defined by

$$\mathbb{V}[X] := \mathbb{E}[(X - \mathbb{E}[X])^2] = \int (x - \mathbb{E}[X])^2 dP(x) \ge 0.$$

- Note that the mean $\mathbb{E}[X] \in \mathbb{R}$ is a constant.

Let X be a real-valued random variable.

Then we have

$$\mathbb{V}[X] = \mathbb{E}[X^2] - (\mathbb{E}[X])^2$$

Proof:

$$V[X] = \mathbb{E}[(X - \mathbb{E}[X])^2]$$

$$= \mathbb{E}[X^2 - 2X\mathbb{E}[X] + (\mathbb{E}[X])^2]$$

$$= \mathbb{E}[X^2] - 2(\mathbb{E}[X])^2 + (\mathbb{E}[X])^2$$

$$= \mathbb{E}[X^2] - (\mathbb{E}[X])^2$$

Let X be a real-valued random variable. Then for any constant $c \in \mathbb{R}$, we have

$$\mathbb{V}[cX] = c^2 \mathbb{V}[X].$$

Proof:

$$V[cX] := \mathbb{E}[(cX - \mathbb{E}[cX])^2]$$
$$= c^2 \mathbb{E}[(X - \mathbb{E}[X])^2] = c^2 V[X].$$

In particular, by setting c = 1/n, we have

$$\mathbb{V}\left[\frac{X}{n}\right] = \frac{1}{n^2} \mathbb{V}[X].$$

Let X and Y be real-valued random variables.

If X and Y are independent, then

$$\mathbb{V}[X+Y] = \mathbb{V}[X] + \mathbb{V}[Y].$$

Proof:

$$V[X + Y] := \mathbb{E}[(X + Y - \mathbb{E}[X + Y])^{2}]$$

$$= \mathbb{E}[(X - \mathbb{E}[X] + Y - \mathbb{E}[Y])^{2}]$$

$$= \mathbb{E}[(X - \mathbb{E}[X])^{2} + 2(X - \mathbb{E}[X])(Y - \mathbb{E}[Y]) + (Y - \mathbb{E}[Y])^{2}]$$

$$= \mathbb{E}[(X - \mathbb{E}[X])^{2}] + 2\mathbb{E}[(X - \mathbb{E}[X])(Y - \mathbb{E}[Y])] + \mathbb{E}[(Y - \mathbb{E}[Y])^{2}]$$

$$= \mathbb{E}[(X - \mathbb{E}[X])^{2}] + \mathbb{E}[(Y - \mathbb{E}[Y])^{2}] = \mathbb{V}[X] + \mathbb{V}[Y],$$

where we used

$$\mathbb{E}[(X - \mathbb{E}[X])(Y - \mathbb{E}[Y])] = \mathbb{E}[(X - \mathbb{E}[X])]\mathbb{E}[(Y - \mathbb{E}[Y])] = 0,$$

which follows from the independence of X and Y.

By recursive applications of the previous result, we have the following useful result:

Let $X_1, X_2, ..., X_n$ are independent real-valued random variables (note: they don't necessary identically distributed).

Then we have

$$\mathbb{V}[\sum_{i=1}^{n} X_i] = \sum_{i=1}^{n} \mathbb{V}[X_i]$$

Corollary:

- ▶ Let $X_1, ..., X_n$ be independent real-valued random variables.
- ▶ Let $c_1, \ldots, c_n \in \mathbb{R}$ be constants.

Then

$$\mathbb{V}[\sum_{i=1}^{n} c_i X_i] = \sum_{i=1}^{n} \mathbb{V}[c_i X_i] = \sum_{i=1}^{n} c_i^2 \mathbb{V}[X_i].$$

In particular, assuming that X_1, \ldots, X_n are i.i.d. with a random variable X, and setting $c_i := 1/n$, we have

$$\mathbb{V}[\frac{1}{n}\sum_{i=1}^{n}X_{i}] = \frac{1}{n^{2}}\sum_{i=1}^{n}\mathbb{V}[X_{i}] = \frac{1}{n}\mathbb{V}[X].$$

- Thus, the variance of the empirical average $\frac{1}{n} \sum_{i=1}^{n} X_i$ is n times smaller than the variance of X.
- By taking the average over independent observations, the variance can be reduced.

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Estimators and Estimates

In statistics, the procedure of estimating a quantity of interest is formulated as a function of data.

- This function is called an estimator.
- The output from the estimator is called an estimate.

Estimators and Estimates

- Let $\theta^* \in \Theta$ be an unknown quantity of interest that we want to estimate (Θ is an appropriate set) (θ^* is also called an estimand).
- Assume that we are given some data D_n of size $n \in \mathbb{N}$ of the form

$$D_n := (X_1, \ldots, X_n) \in \mathcal{X}^n$$

where each $X_i \in \mathcal{X}$ is a random variable (\mathcal{X} is a measurable space.).

Definition: a map

$$F_n: \mathcal{X}^n \to \Theta$$

is called an estimator (of θ^*).

- The estimator should be designed so that the estimate will be close to θ^* .
- $\hat{\theta}_n := F_n(D_n)$ is called an estimate (of θ^*).

Estimators and Estimates: Mean Estimation

Let's consider the mean estimation problem as an example.

The quantity of interest is the mean of the random variable $X \sim P$:

$$\theta^* := \mu := \mathbb{E}[X] \in \mathbb{R} =: \Theta.$$

Assume that *n* random variables X_1, \ldots, X_n are given as data:

$$D_n = (X_1, \dots, X_n) \in \mathcal{X}^n, \quad \mathcal{X} := \mathbb{R}.$$

Then one can define an estimator $F_n: \mathcal{X}^n \to \Theta$ of the mean θ^* by

$$F_n(D_n) := \frac{1}{n} \sum_{i=1}^n X_i = \hat{\mu} =: \hat{\theta}.$$

i.e., the empirical average of X_1, \ldots, X_n .

Which Estimator Should We Choose?

Note that the empirical average is not the only choice.

For instance, we can define various estimators for the mean estimation problem; e.g.,

- 1. $F_n(D_n) := (X_1 + \cdots + X_n)/n$.
- 2. $F_n(D_n) := X_1$ (i.e., discarding $X_2, ..., X_n$).
- 3. $F_n(D_n) := 0$ (i.e., always outputs constant 0, no matter what D_n is).
- 4. $F_n(D_n) := c_0 + c_1 X_1 + \cdots + c_n X_n$ for some $c_0, c_1, \dots, c_n \ge 0$.
- Which estimator should we choose?
- When is the empirical average a good choice, and when is it not?

(Actually we'll see that the empirical average is not always a good choice).

Which Estimator Should We Choose?

To investigate these questions, we need to introduce criteria for comparing different estimators.

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Mean Square Error (MSE)

To discuss the quality of a statistical estimator, we need a certain error criterion.

Here we consider the mean square error (MSE), one of the most standard criteria.

- Let $\theta^* \in \Theta \subset \mathbb{R}$ be the unknown quantity of interest.
- We assume $\Theta \subset \mathbb{R}$ for simplicity, but the following argument also holds for more general situations.
- Consider an estimator $F_n: \mathcal{X}^n \to \Theta$ such that

$$\hat{\theta}_n := F_n(D_n) \in \Theta, \quad D_n := (X_1, \dots, X_n) \in \mathcal{X}^n.$$

- Note that the estimate $\hat{\theta}_n = F_n(D_n) = F_n((X_1, \dots, X_n))$ is a random variable, since X_1, \dots, X_n are random variables.

Mean Square Error (MSE)

- Then we can consider the squared error between the target θ^* and estimate $\hat{\theta}_n$:

$$(\hat{\theta}_n - \theta^*)^2 = (F_n(D_n) - \theta^*)^2.$$

- This error is also a random variable, because the estimate $\hat{\theta}_n = F_n(D_n)$ is a random variable.
- Then the mean square error (MSE) of the estimator F_n is defined as the expectation of the squared error:

$$\mathbb{E}[(\hat{\theta}_n - \theta^*)^2] = \mathbb{E}[(F_n(D_n) - \theta^*)^2]$$

where the expectation is with respect to the data $D_n = (X_1, \dots, X_n)$.

- The MSE quantifies how the estimate $\hat{\theta}_n$ is close to (or far from) the target θ^* on average.

Mean Square Error (MSE)

Note that the MSE

$$\mathbb{E}[(\hat{\theta}_n - \theta^*)^2] = \mathbb{E}[(F_n(D_n) - \theta^*)^2]$$

depends on

- 1. the target quantity θ^*
- 2. the estimator F_n
- 3. the distribution of the data X_1, \ldots, X_n

By theoretically studying the MSE, we can study

- which estimator F_n is good for estimating the target θ^* ,
- \blacktriangleright when the data X_1, \ldots, X_n are distributed in an assumed way.

Probabilistic Error Bound from MSE

- A general fact: For any non-negative real-valued random variable Z, Markov's inequality states that

$$\Pr(Z \ge c) \le \frac{\mathbb{E}[Z]}{c}, \quad \forall c > 0.$$

- By setting $Z:=(\hat{\theta}_n-\theta^*)^2$, we then have

$$\Pr((\hat{\theta}_n - \theta^*)^2 \ge c) \le \frac{\mathbb{E}[(\hat{\theta}_n - \theta^*)^2]}{c}, \quad \forall c > 0.$$

- Thus, if the MSE $\mathbb{E}[(\hat{ heta}- heta^*)^2]$ is small, then the probability of

$$(\hat{\theta}_n - \theta^*)^2 > c$$

becomes small for any c > 0.

Bias-Variance Decomposition

- The following is a very important result concerning the MSE.

Theorem: The MSE can be decomposed into the bias and the variance of the estimator, as follows:

$$\mathbb{E}[(\hat{\theta}_n - \theta^*)^2] = \underbrace{\mathbb{E}[(\hat{\theta}_n - \mathbb{E}[\hat{\theta}_n])^2]}_{Variance} + \underbrace{(\mathbb{E}[\hat{\theta}_n] - \theta^*)^2}_{Bias}$$

This is called the bias-variance decomposition.

- The bias of the estimator $F_n: \mathcal{X}^n \to \Theta$ is defined as the difference between the expectation of the estimate $\mathbb{E}[\hat{\theta}_n]$ and the target θ^* :

$$\mathbb{E}[\hat{\theta}_n] - \theta^* = \mathbb{E}[F_n(D_n)] - \theta^*.$$

where the expectation is with respect to the data $D_n = (X_1, \dots, X_n)$.

Bias-Variance Decomposition

$$\mathbb{E}[(\hat{\theta}_n - \theta^*)^2] = \underbrace{\mathbb{E}[(\hat{\theta}_n - \mathbb{E}[\hat{\theta}_n])^2]}_{Variance} + \underbrace{(\mathbb{E}[\hat{\theta}_n] - \theta^*)^2}_{Bias}$$

- The variance of the estimator $F_n: \mathcal{X}^n \to \Theta$ is defined as

$$\mathbb{E}[(\hat{\theta}_n - \mathbb{E}[\hat{\theta}_n])^2] = \mathbb{E}[(F_n(D_n) - \mathbb{E}[F_n(D_n)])^2].$$

- ▶ i.e., the average deviation of the estimate $\hat{\theta}_n := F_n(D_n)$ from its mean $\mathbb{E}[\hat{\theta}_n]$.
- ▶ Recall again that the estimate $\hat{\theta}_n$ is a random variable.
- To make the mean-square error small, both the bias and variance need to be small!

Proof of Bias-Variance Decomposition

- The mean square error can be expanded as

$$\begin{split} &\mathbb{E}[(\hat{\theta}_{n} - \theta^{*})^{2}] \\ =& \mathbb{E}[(\hat{\theta}_{n} - \mathbb{E}[\hat{\theta}_{n}] + \mathbb{E}[\hat{\theta}_{n}] - \theta^{*})^{2}] \\ =& \mathbb{E}[(\hat{\theta}_{n} - \mathbb{E}[\hat{\theta}_{n}])^{2}] + \mathbb{E}[(\mathbb{E}[\hat{\theta}_{n}] - \theta^{*})^{2}] + 2\mathbb{E}[(\hat{\theta}_{n} - \mathbb{E}[\hat{\theta}_{n}])(\mathbb{E}[\hat{\theta}_{n}] - \theta^{*})] \\ =& \mathbb{E}[(\hat{\theta}_{n} - \mathbb{E}[\hat{\theta}_{n}])^{2}] + (\mathbb{E}[\hat{\theta}_{n}] - \theta^{*})^{2}, \end{split}$$

where the last line follows from $\mathbb{E}[\hat{\theta}_n]$ being a constant:

$$\begin{split} &\mathbb{E}[(\mathbb{E}[\hat{\theta}_n] - \theta^*)^2] = (\mathbb{E}[\hat{\theta}_n] - \theta^*)^2, \\ &\mathbb{E}[(\hat{\theta}_n - \mathbb{E}[\hat{\theta}_n])(\mathbb{E}[\hat{\theta}_n] - \theta^*)] = \mathbb{E}\left[(\hat{\theta}_n - \mathbb{E}[\hat{\theta}_n])\right](\mathbb{E}[\hat{\theta}_n] - \theta^*) = 0. \end{split}$$

Remarks on the Bias-Variance Decomposition

- The bias-variance decomposition holds under a very generic situation.
 - ▶ This is because the proof does not require any assumption about the joint distribution of the data X_1, \ldots, X_n (essentially).
 - ▶ The only assumption is that the MSE is finite.
- Thus, for instance, we can consider cases like:
 - \triangleright where X_1, \ldots, X_n are not independently distributed
 - where X_1, \ldots, X_n are not identically distributed.
- By considering a different setting for the distribution of the data X_1, \ldots, X_n , we can study when a certain estimator is a good choice, when it is not.
- This is done by analyzing the bias and variance of the estimator.

Bias-Variance Decomposition: Multivariate Case

- Let $\theta^* \in \Theta \subset \mathbb{R}^d$ be the quantity of interest.
- Let $\hat{\theta}_n$ be any estimate of θ^* (you can just think of $\hat{\theta}_n$ as a random variable in \mathbb{R}^d).
- Define the mean square error by

$$\mathbb{E}[\|\hat{\theta}_n - \theta^*\|^2],$$

where $\|\cdot\|$ is the norm of \mathbb{R}^d .

Theorem. - Assume that

$$\|\mathbb{E}[\hat{\theta}_n]\| < \infty, \quad \mathbb{E}[\|\hat{\theta}_n\|^2] < \infty.$$

Then the following bias-variance decomposition holds:

$$\mathbb{E}[\|\hat{\theta}_n - \theta^*\|^2] = \underbrace{\mathbb{E}[\|\hat{\theta}_n - \mathbb{E}[\hat{\theta}_n]\|^2]}_{\textit{Variance}} + \|\underbrace{\theta^* - \mathbb{E}[\hat{\theta}_n]}_{\textit{Bias}}\|^2$$

Bias-Variance Decomposition: Multivariate Case

Exercise: Prove the above bias-variance decomposition.

Hint: for any $a, b \in \mathbb{R}^d$,

$$||a-b||^2 = \langle a-b, a-b \rangle$$

where $\langle \cdot, \cdot \rangle$ is the inner product in \mathbb{R}^d .

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Mean Estimation Problem: Setup

- Now consider the mean estimation problem.
- Let $X \sim P$ be the random variable of interest, whose mean

$$\mu_P := \mathbb{E}[X] = \int x \ dP(x)$$

is the estimand.

- To deal with a generic situation, we assume that i.i.d. data X_1, \ldots, X_n are generated from a probability distribution Q, which can be different from P:

$$X_1,\ldots,X_n\sim Q,i.i.d.$$

- Let $Y \sim Q$ be a random variable, with distribution Q;
- Then X_1, \ldots, X_n are i.i.d. with Y.

Bias-Variance Decomposition in Mean Estimation

- Assume that the mean and the variance of $Y \sim Q$ are finite:

$$|\mu_Q| < \infty, \quad \mu_Q := \mathbb{E}_{Y \sim Q}[Y]$$

 $\sigma_Q^2 < \infty, \quad \sigma_Q^2 := \mathbb{V}_{Y \sim Q}[Y] := \mathbb{E}_{Y \sim Q}[(Y - \mu_Q)^2].$

Theorem: The mean square error of the empirical average estimator

$$\hat{\mu} := \frac{1}{n} \sum_{i=1}^{n} X_i$$

is given by

$$\mathbb{E}[(\hat{\mu} - \mu_P)^2] = \mathbb{E}[(\hat{\mu} - \mathbb{E}[\hat{\mu}])^2] + (\mathbb{E}[\hat{\mu}] - \mu_P)^2$$
$$= \frac{\sigma_Q^2}{n} + (\mu_Q - \mu_P)^2.$$

Proof: Bias-Variance Decomposition in Mean Estimation

Proof:

- The first identity follows from the bias-variance decomposition.
- Thus, we show the second identity.

Variance term.

Because X_1, \ldots, X_n are i.i.d. with $Y \sim Q$, the variance term can be expressed as

$$\mathbb{E}[(\hat{\mu} - \mathbb{E}[\hat{\mu}])^{2}] = \mathbb{V}[\hat{\mu}] = \mathbb{V}[\frac{1}{n} \sum_{i=1}^{n} X_{i}]$$

$$= \sum_{i=1}^{n} \mathbb{V}[\frac{1}{n}X_{i}] = \frac{1}{n^{2}} \sum_{i=1}^{n} \mathbb{V}[X_{i}] = \frac{1}{n} \mathbb{V}[Y] = \frac{\sigma_{Q}^{2}}{n}.$$

Proof: Bias-Variance Decomposition in Mean Estimation

Bias term. On the other hand,

$$\mathbb{E}[\hat{\mu}] = \mathbb{E}\left[\frac{1}{n}\sum_{i=1}^{n}X_{i}\right] = \frac{1}{n}\sum_{i=1}^{n}\mathbb{E}[X_{i}] = \mathbb{E}[Y] = \mu_{Q}.$$

Therefore, the bias term is

$$(\mathbb{E}[\hat{\mu}] - \mu_P)^2 = (\mu_Q - \mu_P)^2.$$

46 / 84

We proved the bias-variance decomposition:

$$\mathbb{E}[(\hat{\mu} - \mu_P)^2] = \frac{\sigma_Q^2}{n} + (\mu_Q - \mu_P)^2.$$

Let's study what this means.

- The bias of the estimator $\hat{\mu} = \frac{1}{n} \sum_{i=1}^n X_i$ is

$$\mathbb{E}[\hat{\mu}] - \mu_P = \mu_Q - \mu_P$$

i.e., the difference between

- ▶ the mean μ_Q of the data distribution Q, and
- ▶ the mean μ_P of the target distribution P.

Therefore,

- ▶ if the data $X_1, ..., X_n$ are independently generated from a distribution Q, and
- ▶ if the mean μ_Q of Q is different from the mean μ_P of the target random variable $X \sim P$,

then the use of the empirical average

$$\hat{\mu} = \frac{1}{n} \sum_{i=1}^{n} X_i,$$

causes a non-zero bias, $\mu_Q - \mu_P \neq 0$.

Note that in this case, since $(\mu_Q - \mu_P)^2 > 0$, the mean square error

$$\mathbb{E}[(\hat{\mu} - \mu_P)^2] = (\mu_Q - \mu_P)^2 + \frac{\sigma_Q^2}{n} \ge (\mu_Q - \mu_P)^2 > 0$$

does not decrease to 0, even when $n \to \infty$.

This example shows the importance of the data distribution Q.

- If possible, we should collect data X_1, \ldots, X_n generated from the same distribution P as the target random variable X, i.e., Q = P.
- In this case, the bias becomes 0: $(\mu_Q \mu_P)^2 = 0$, and the MSE is

$$\mathbb{E}[(\hat{\mu} - \mu_P)^2] = \frac{\sigma_P^2}{n},$$

where $\sigma_P^2 = \mathbb{V}[X]$ is the variance of $X \sim P$.

- Thus, the MSE decreases as the sample size *n* increases.

- On the other hand, the variance term

$$\mathbb{E}[(\hat{\mu} - \mathbb{E}[\hat{\mu}])^2] = \frac{\sigma_Q^2}{n}$$

depends only on the data X_1, \ldots, X_n , and not on the target μ_P .

- Therefore, whatever the data distribution Q is, the variance term converges to 0 as $n \to \infty$:

$$\lim_{n\to\infty} \mathbb{E}[(\hat{\mu} - \mathbb{E}[\hat{\mu}])^2] = \lim_{n\to\infty} \frac{\sigma_Q^2}{n} = 0.$$

- Note that in the derivation of the variance term, we used

$$\mathbb{V}[\frac{1}{n}\sum_{i=1}^{n}X_{i}] = \sum_{i=1}^{n}\mathbb{V}[\frac{1}{n}X_{i}].$$

- This follows from the independence between X_1, \ldots, X_n . (see pp.21-22)
- Therefore, if the independence between X_1, \ldots, X_n does not hold, the variance may not decrease to 0 (we'll see an example later).

- For example, recall the example where $X \sim P$ represents the income of a randomly picked-up French person.
- Assume that data $X_1, \ldots, X_n \sim Q$ (i.i.d.) are the incomes of randomly picked-up French persons in French Riviera.
- Then we would have

$$\mu_Q := \mathbb{E}_{Y \sim Q}[Y] > \mathbb{E}_{X \sim P}[X] =: \mu_P$$

i.e., the average income of French Riviera people μ_Q is higher than the average income of the whole population μ_P .

- Thus, the empirical average of the data

$$\hat{\mu} := \frac{1}{n} \sum_{i=1}^{n} X_i$$

has a non-zero bias:

$$\mathbb{E}[\hat{\mu}] - \mu_P = \mu_Q - \mu_P \neq 0.$$

- Therefore, the MSE of the empirical average

$$\mathbb{E}[(\hat{\mu} - \mu_P)^2] = (\mu_Q - \mu_P)^2 + \frac{\sigma_Q^2}{n}$$

does not decrease to 0, even when n is very large.

- Thus, we should make sure that data X_1, \ldots, X_n are randomly picked-up from the whole French population. (i.e., Q = P).

Mean Estimation in the Multivariate Case

- Let $X \sim P$ be a random vector in \mathbb{R}^d . Define

$$\mu_P := \mathbb{E}_{X \sim P}[X] \in \mathbb{R}^d$$

- Let $X_1, \ldots, X_n \sim Q$ (i.i.d.) be random vectors in \mathbb{R}^d , and let $Y \sim Q$. Define

$$\mu_Q := \mathbb{E}_{Y \sim Q}[Y] \in \mathbb{R}^d, \quad \sigma_Q^2 := \mathbb{E}_{Y \sim Q}[\|Y - \mu_Q\|^2] \ge 0.$$

Theorem. Assume that

$$\|\mu_P\| < \infty$$
, $\|\mu_Q\| < \infty$, $\sigma_Q^2 < \infty$.

Then, the empirical average estimator $\hat{\mu} = \frac{1}{n} \sum_{i=1}^{n} X_i$ satisfies

$$\mathbb{E}[\|\hat{\mu} - \mu_P\|^2] = \mathbb{E}[\|\hat{\mu} - \mathbb{E}[\hat{\mu}]\|^2] + \|\mathbb{E}[\hat{\mu}] - \mu_P\|^2$$
$$= \frac{\sigma_Q^2}{n} + \|\mu_Q - \mu_P\|^2.$$

Exercise. Prove this. (The first identity is the bias-variance decomposition)

How Large should the Sample Size be?

- In the mean estimation problem, when $X_1,\dots,X_n\sim P$ i.i.d., the MSE is given by

$$\mathbb{E}[(\hat{\mu} - \mu_P)^2] = \frac{\sigma_P^2}{n}, \quad \sigma_P^2 := \mathbb{V}[X].$$

for the empirical average estimate $\hat{\mu} := \frac{1}{n} \sum_{i=1}^{n} X_i$.

- Assume that one wants to make the MSE small in that sense that

$$\mathbb{E}[(\hat{\mu} - \mu_P)^2] \le \varepsilon^2,$$

for some $\varepsilon > 0$. Then the sample size n should satisfy

$$\mathbb{E}[(\hat{\mu} - \mu_P)^2] = \frac{\sigma_P^2}{n} \le \varepsilon^2$$

or equivalently

$$n \geq \frac{\sigma_P^2}{\varepsilon^2}$$
.

How Large should the Sample Size be?

For instance, consider the example of estimating the average income.

- Assume $\mu_P=2,000$ EUR/month (mean) and $\sigma_P=500$ (standard deviation).

Then, the sample size n should satisfy

$$n\geq\frac{500^2}{\varepsilon^2}.$$

For instance,

- to achieve the precision of $\varepsilon = 10$, we need $n \ge 2500$.
- to achieve the precision of $\varepsilon = 1$, we need $n \ge 250,000$.

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Consistency

- Let $\theta^* \in \Theta \subset \mathbb{R}$ be an estimand (i.e., the quantity of interest).
- Let X_1, \ldots, X_n be random variables such that $X_i \in \mathcal{X}$, and define the data as

$$D_n := (X_1, \ldots, X_n) \in \mathcal{X}^n$$

- Let $F_n: \mathcal{X}^n \to \mathbb{R}$ be an estimator, and let $\hat{\theta}_n:= F_n(D_n)$ be an estimate.

Definition. We call F_n a consistent estimator of θ^* , if the estimate $\hat{\theta_n}$ converges to θ^* as $n \to \infty$ in an appropriate sense, e.g.,

$$\mathbb{E}[(\hat{\theta}_n - \theta^*)^2] \to 0$$
 as $n \to \infty$.

- The consistency means that, as we have more data X_1, \ldots, X_n , the estimate $\hat{\theta}_n$ becomes more accurate (in estimating θ^*).
- Consistency is one of the most important concepts in statistics.

Unbiasedness

Definition. We call F_n an unbiased estimator of θ^* , if the bias is zero for every $n \in \mathbb{N}$, i.e.,

$$\mathbb{E}[F_n(D_n)] - \theta^* = \mathbb{E}[\hat{\theta}_n] - \theta^* = \mathbf{0}, \quad \forall n \in \mathbb{N}.$$

- If this is not satisfied, we call F_n a biased estimator of θ^* .

Unbiasedness

For instance, consider the mean estimation problem.

- If the data X_1, \ldots, X_n are i.i.d. with $X \sim P$, then the empirical average $\hat{\mu} := \frac{1}{n} \sum_{i=1}^{n} X_i$ satisfies

$$\mathbb{E}[\hat{\mu}] = \mathbb{E}[\frac{1}{n} \sum_{i=1}^{n} X_i] = \frac{1}{n} \sum_{i=1}^{n} \mathbb{E}[X_i] = \frac{1}{n} \sum_{i=1}^{n} \mathbb{E}[X] = \mathbb{E}[X] = \mu_P.$$

- So, in this case, the empirical average $\hat{\mu}$ is an unbiased estimator of the mean μ_P .
- If X_1, \ldots, X_n are i.i.d. with $Y \sim Q$, and if $\mu_Q \neq \mu_P$, then

$$\mathbb{E}[\hat{\mu}] = \mu_{Q} \neq \mu_{P}.$$

- So, in this case, the empirical average $\hat{\mu}$ is a biased estimator of the mean μ_P .

Unbiasedness

- If F_n is an unbiased estimator, then the MSE is given by

$$\mathbb{E}[(\hat{\theta}_n - \theta^*)^2] = \mathbb{E}[(\hat{\theta}_n - \mathbb{E}[\hat{\theta}_n])^2] = \mathbb{V}[\hat{\theta}_n]$$

i.e., the MSE is equal to the variance of the estimate $\hat{\theta}_n$.

Some important consequences of unbiasedness:

- If the variance $\mathbb{V}[\hat{\theta}_n]$ decreases to 0 as $n \to \infty$, then $\hat{\theta}_n$ converges to θ^* ; thus F_n becomes a consistent estimator.
- If we can estimate the variance $\mathbb{V}[\hat{\theta}_n]$, then we can estimate the amount of error (MSE):
 - ▶ In other words, we can estimate how far the estimate $\hat{\theta}_n$ is from the target θ^* .
 - Thus, an estimate of the variance $\mathbb{V}[\hat{\theta}_n]$ can be used for constructing a confidence interval for θ^* (not covered in the course).

Unbiasedness and Consistency

Note that

- the unbiasedness does not imply the consistency;
 - ► An unbiased estimator can be inconsistent.
- the consistency does not require the unbiasedness;
 - ► A biased estimator can be consistent (we'll see this later).

Example of an Unbiased Estimator that is not Consistent

Consider the mean estimation problem.

- Let $X \sim P$, and assume that $X_1, \ldots, X_n \sim P$ (i.i.d.).
- Define an estimator F_n by

$$\hat{\mu}:=F_n(X_1,\ldots,X_n):=X_1.$$

- i.e., we only use X_1 , and discard X_2, \ldots, X_n .
- Then, this estimator is unbiased: In fact,

$$\mathbb{E}[\hat{\mu}] = \mathbb{E}[X_1] = \mathbb{E}[X] = \mu_P.$$

Example of an Unbiased Estimator that is not Consistent

- However, the variance of the estimate $\hat{\mu}$ is a constant:

$$\mathbb{V}[\hat{\mu}] = \mathbb{E}[(\hat{\mu} - \mathbb{E}[\hat{\mu}])^2] = \mathbb{E}[(X_1 - \mu_P)^2] = \mathbb{E}[(X - \mu_P)^2] = \sigma_P^2.$$

- Thus, the MSE of this estimator is

$$\mathbb{E}[(\hat{\mu} - \mu_P)^2] = \mathbb{E}[(\hat{\mu} - \mathbb{E}[\hat{\mu}])^2] = \sigma_P^2.$$

- Thus, the MSE does not decrease to 0, even if $n \to \infty$, i.e., the estimator is not consistent.

This example demonstrates that the unbiasedness does not imply consistency.

- For consistency, we need to make sure that the variance of the estimate decreases to 0 as $n \to \infty$.

Consider again the mean estimation problem.

- Let $X \sim P$, and assume $X_1, \ldots, X_n \sim Q$ (i.i.d.).
- Assume that the data distribution Q is different from the target P.
- We show here that we can still construct an unbiased estimator of the mean

$$\mu_P = \mathbb{E}_{X \sim P}[X]$$

from the data $X_1, \ldots, X_n \sim Q$ (i.i.d.).

- To this end, assume that distributions P and Q have density functions p and q, respectively.
- Define a weight function by

$$w(x) := \frac{p(x)}{q(x)}, \quad x \in \mathbb{R}$$

- Assume that this weight function is well-defined and bounded:

$$\max_{x\in\mathbb{R}}w(x)=:C<\infty.$$

- Note that this requires p(x)/q(x) < C, and thus

$$p(x) < Cq(x)$$
 for all $x \in \mathbb{R}$.

- Thus, if the target density has a positive value p(x) > 0, then the data density should also have a positive value q(x) > 0.

- We assume for simplicity that this weight function w(x) = p(x)/q(x) is known.
 - ▶ Otherwise we need to estimate it from data.
- Define an estimator F_n of the mean μ_P as:

$$\hat{\mu} := F_n(X_1, \dots, X_n) := \frac{1}{n} \sum_{i=1}^n w(X_i) X_i.$$

- This is an unbiased estimator of the mean μ_P of P: This can be shown as follows.

- Recall that X_1, \ldots, X_n are i.i.d. with $Y \sim Q$. Therefore,

$$\mathbb{E}[\hat{\mu}] = \mathbb{E}\left[\frac{1}{n}\sum_{i=1}^{n}w(X_{i})X_{i}\right]$$

$$= \frac{1}{n}\sum_{i=1}^{n}\mathbb{E}[w(X_{i})X_{i}] = \frac{1}{n}\sum_{i=1}^{n}\mathbb{E}[w(Y)Y]$$

$$= \mathbb{E}[w(Y)Y] = \int x \ w(x)dQ(x) = \int x \ \frac{p(x)}{q(x)}q(x)dx$$

$$= \int x \ p(x)dx = \int x \ dP(x) = \mu_{P}.$$

- Thus, $\hat{\mu} = \frac{1}{n} \sum_{i=1}^{n} w(X_i) X_i$ is an unbiased estimator of μ_P .

- On the other hand, the variance of the estimator is

$$V[\hat{\mu}] = V[\frac{1}{n} \sum_{i=1}^{n} w(X_i) X_i] = \sum_{i=1}^{n} V[\frac{1}{n} w(X_i) X_i]$$

$$= \sum_{i=1}^{n} \frac{1}{n^2} V[w(X_i) X_i] = \sum_{i=1}^{n} \frac{1}{n^2} V[w(Y) Y]$$

$$= \frac{1}{n} V[w(Y) Y].$$

- This can be upper-bounded as

$$\begin{split} &\frac{1}{n}\mathbb{V}[w(Y)Y] = \frac{1}{n}\left(\mathbb{E}[(w(Y)Y)^2] - (\mathbb{E}[w(Y)Y])^2\right) \\ &\leq \frac{1}{n}(\mathbb{E}[C^2Y^2] + \mu_P^2) = \frac{1}{n}(C^2\mathbb{E}[Y^2] - \mu_P^2) \\ &= \frac{1}{n}(C^2(\sigma_Q^2 + \mu_Q^2) - \mu_P^2). \end{split}$$

- To summarize, the MSE of the estimator is

$$\mathbb{E}[(\hat{\mu} - \mu_P)^2] = \frac{1}{n} \mathbb{V}[w(Y)Y] \leq \frac{1}{n} (C^2(\sigma_Q^2 + \mu_Q^2) - \mu_P^2).$$

- Therefore, the MSE decreases to 0 as $n \to \infty$:
 - ▶ i.e., the estimator $\hat{\mu} = \frac{1}{n} \sum_{i=1}^{n} w(X_i) X_i$ is consistent in estimating μ_P .
- The weight function w(x) is called the importance weight of a point x.
- The way of constructing an estimator by weighting each sample point X_i by $w(X_i)$ is called importance weighting.

- Importance weighting is a widely used technique, examples including:
 - Domain shift adaptation in machine learning.
 - Estimation of treatment effects in causal inference.
 - Monte Carlo for efficient simulations.
- If you are interested in the first, you can for instance look at [Sugiyama and Kawanabe, 2012].

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Variance of Unbiased Estimators may be Large

- We demonstrate here that sometimes biased estimators may be "better" than unbiased estimators.
- The key is an approach called shrinkage or regularization, which is ubiquitous in statistics and machine learning.

Variance of Unbiased Estimators may be Large

- We have seen the bias-variance decomposition of the MSE:

$$\mathbb{E}[\|\hat{\theta}_n - \theta^*\|^2] = \underbrace{\mathbb{E}[\|\hat{\theta}_n - \mathbb{E}[\hat{\theta}_n]\|^2]}_{\textit{Variance}} + \|\underbrace{\mathbb{E}[\hat{\theta}_n] - \theta^*}_{\textit{Bias}}\|^2$$

- The MSE decomposes into the bias and variance.
- For an <u>unbiased</u> estimator (i.e.,the bias is zero), the MSE is equal to the variance:

$$\mathbb{E}[\|\hat{\theta}_n - \theta^*\|^2] = \underbrace{\mathbb{E}[\|\hat{\theta}_n - \mathbb{E}[\hat{\theta}_n]\|^2]}_{\text{Variance}}.$$

- This variance may be large if, e.g.,
 - ▶ the sample size *n* is small
 - ▶ the dimensionality of $\hat{\theta}_n$ is large (in multivariate cases).
- In such a situation, a biased estimator with a lower variance may have a smaller MSE than the unbiased estimator.

Variance Reduction in Mean Estimation

- To describe this, consider the mean estimation problem.
- Let $X \sim P$, and $X_1, \ldots, X_n \sim P$ (i.i.d.).
- We saw that the empirical average

$$\hat{\mu} = \frac{1}{n} \sum_{i=1}^{n} X_i$$

is an unbiased estimator of the mean of

$$\mu_P := \mathbb{E}_{X \sim P}[X],$$

and the MSE is given by

$$\mathbb{E}[(\hat{\mu} - \mu_P)^2] = \frac{\mathbb{V}[X]}{n}.$$

- We'll show that there are biased estimators that have smaller MSE than the empirical average.

Empirical Average as a Least-Squares Solution

- We first show that the empirical average $\hat{\mu} = \frac{1}{n} \sum_{i=1}^{n} X_i$ is the solution to the following optimization problem

$$\hat{\mu} = \arg\min_{\alpha \in \mathbb{R}} \frac{1}{n} \sum_{i=1}^{n} (\alpha - X_i)^2.$$

- i.e., we consider a least-squares problem (fitting a constant α to the data X_1, \ldots, X_n).
- To solve this, set the the derivative of the objective function with respect to α to be zero:

$$\frac{d}{d\alpha}\left(\frac{1}{n}\sum_{i=1}^{n}(\alpha-X_{i})^{2}\right)=\frac{1}{n}\sum_{i=1}^{n}2(\alpha-X_{i})=2\alpha-\frac{2}{n}\sum_{i=1}^{n}X_{i}=0.$$

- Thus, the α that minimizes the objective function is

$$\alpha = \frac{1}{n} \sum_{i=1}^{n} X_i,$$

i.e., the empirical average.

Regularized Least Squares and Shrinkage Estimator

- We then consider a modified optimization problem, adding a regularization term:

$$\hat{\mu}_{\lambda} := \arg\min_{\alpha \in \mathbb{R}} \frac{1}{n} \sum_{i=1}^{n} (\alpha - X_i)^2 + \lambda \alpha^2,$$

where $\lambda \geq 0$ is a regularization constant.

- The solution is given by setting the derivative of the objective function to be 0:

$$\frac{d}{d\alpha}\left(\frac{1}{n}\sum_{i=1}^{n}(\alpha-X_i)^2+\lambda\alpha^2\right)=\frac{1}{n}\sum_{i=1}^{n}2(\alpha-X_i)+2\lambda\alpha$$
$$=2\alpha-\frac{2}{n}\sum_{i=1}^{n}X_i+2\lambda\alpha=2\alpha(1+\lambda)-\frac{2}{n}\sum_{i=1}^{n}X_i=0.$$

- Thus, the solution is given by

$$\alpha = \frac{1}{(1+\lambda)} \frac{1}{n} \sum_{i=1}^{n} X_i =: \hat{\mu}_{\lambda}$$

Regularized Least Squares and Shrinkage Estimator

$$\hat{\mu}_{\lambda} = \frac{1}{(1+\lambda)} \frac{1}{n} \sum_{i=1}^{n} X_{i}.$$

- Large λ shrinks the solution $\hat{\mu}_{\lambda}$ towards 0.
 - In this sense, this is called a shrinkage estimator.
- $\lambda = 0$ recovers the empirical average $\hat{\mu}_0 = \frac{1}{n} \sum_{i=1}^n X_i$.

- The expectation of $\hat{\mu}_{\lambda}$ is

$$\mathbb{E}[\hat{\mu}_{\lambda}] = \mathbb{E}\left[\frac{1}{(1+\lambda)}\frac{1}{n}\sum_{i=1}^{n}X_{i}\right] = \frac{1}{(1+\lambda)}\mu_{P}.$$

- Thus, the (squared) bias of $\hat{\mu}_{\lambda}$ is

$$(\mathbb{E}[\hat{\mu}_{\lambda}] - \mu_P)^2 = (\frac{1}{(1+\lambda)}\mu_P - \mu_P)^2 = \frac{\lambda^2 \mu_P^2}{(1+\lambda)^2}.$$

- Thus, the bias increases as λ increases.
- On the other hand, the variance of $\hat{\mu}_{\lambda}$ is

$$\mathbb{V}[\hat{\mu}_{\lambda}] = \mathbb{V}\left[\frac{1}{1+\lambda} \frac{1}{n} \sum_{i=1}^{n} X_{i}\right]$$

$$= \frac{1}{(1+\lambda)^{2}} \mathbb{V}\left[\frac{1}{n} \sum_{i=1}^{n} X_{i}\right] = \frac{1}{(1+\lambda)^{2}} \frac{\mathbb{V}[X]}{n}.$$

- Thus, the variance decreases as λ increases.

- Thus, the MSE of $\hat{\mu}_{\lambda}$ is

$$\mathbb{E}[(\hat{\mu}_{\lambda} - \mu_{P})^{2}] = \mathbb{V}[\hat{\mu}_{\lambda}] + (\mathbb{E}[\hat{\mu}_{\lambda}] - \mu_{P})^{2}$$
$$= \frac{1}{(1+\lambda)^{2}} \frac{\mathbb{V}[X]}{n} + \frac{\lambda^{2} \mu_{P}^{2}}{(1+\lambda)^{2}}$$

- Let's draw some observations. Assume $\mu_P \neq 0$.

- By an easy calculation, the MSE of $\hat{\mu}_{\lambda} = \frac{1}{(1+\lambda)} \frac{1}{n} \sum_{i=1}^{n} X_i$ can be shown to be smaller than that of the empirical average $\hat{\mu} = \frac{1}{n} \sum_{i=1}^{n} X_i$:

$$\mathbb{E}[(\hat{\mu}_{\lambda} - \mu_{P})^{2}] < \mathbb{E}[(\hat{\mu} - \mu_{P})^{2}]$$

if $\lambda > 0$ is chosen so that

$$\frac{\lambda}{2+\lambda} \le \frac{\mathbb{V}[X]}{n \; \mu_P^2}.$$

Some interpretations:

- When $\mathbb{V}[X]/n$ is large (e.g., when n is small), a large λ can be taken (and more shrinkage).
- When the mean μ_P^2 is small, a large λ can be taken (and more shrinkage).

Exercise: Perform numerical experiments to confirm that the shrinkage estimator can have a smaller MSE.

- For a right choice of $\lambda > 0$, we need to know $\mathbb{V}[X]$ and μ_P .
 - ▶ Therefore this estimator is not practically useful.
- However, under some assumptions (e.g., P is a Gaussian), there is a way of choosing λ without the knowledge of $\mathbb{V}[X]$ and μ_P .
 - ➤ This resulting estimator is called the James-Stein estimator; see [Efron and Hastie, 2016, Section7] [Berger, 1985, Section 5.4].

Regularization for Variance Reduction

- Anyway, this example illustrates that artificially introducing a bias is often useful to reduce the variance.
- In this spirit, regularization has been widely used in many statistical methods: e.g.,
 - $ightharpoonup L_2$ and L_1 regularization in regression and classification (supervised learning)
 - Early stopping in optimization algorithms for machine learning algorithms.
- In supervised learning problems, a good regularization constant can be chosen by, e.g., cross validation
 - See e.g. the MALIS and ASI courses.

Summary of the Lecture

- We introduced several important concepts in statistical estimation.
- When constructing statistical estimators, always pay attention to
 - what is your quantity of interest (in the population).
 - how your data were generated.
 - whether your estimator is biased or unbiased.
 - how much your estimate would have variance.



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