Estimation Theory

Hebrew University of Jerusalem

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האוניברסיטה העברית בירושלים
THE HEBREW UNIVERSITY OF JERUSALEM

1. Estimators
2. Estimator Properties
3. Maximum Likelihood
4. Estimation Quality - Measure of Concentration
5. Multivariate Distributions
6. Summary

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- We can ask someone but will the answer be correct/accurate?
- We can ask multiple individuals and *estimate* the actual time as the average of their answers.

Basic Terminology

- The answers are referred to as *observations* and are denoted by $x_1, \ldots, x_m$. Our estimated time is then:

$$\overline{x} = \frac{1}{m} \sum_i x_i$$

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- We consider $x_1, \ldots, x_m$ as the *realizations* of the random variables $X_1, \ldots, X_m$.
- We assume the samples $x_1, \ldots, x_m$ follow some underlying probability distribution $\mathcal{P}$.

Definition

We say that samples $x_1, \ldots, x_m$ are *identically distributed* if they are all the realizations of random variables over the sample probability distribution

$$X_1, \ldots, X_m \sim \mathcal{P}, \quad \forall i \; X_i = x_i$$

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Definition

We say that samples $x_1, \ldots, x_m$ are *independently identically distributed* (i.i.d) if they are identically distributed and are independent

$$X_1, \ldots, X_m \overset{i.i.d}{\sim} \mathcal{P}, \quad \forall i \; X_i = x_i$$

Basic Definitions

- Assume $\mathcal{P}$ is some *parametric* distribution characterized by a set of parameters $\boldsymbol{\theta} \in \Theta$.
  - $\boldsymbol{\theta}$ a vector of parameters
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- For $\mathcal{P} := Poisson(\lambda)$ then $\boldsymbol{\theta} := \{\lambda\}$ and $\Theta := \mathbb{R}_+$
- For $\mathcal{P} := \mathcal{N}(\mu, \sigma^2)$ then $\boldsymbol{\theta} := \{\mu, \sigma^2\}$ and $\Theta := \mathbb{R} \times \mathbb{R}_+$

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- Given a sample $x_1, \ldots, x_m$, drawn i.i.d according to $\mathcal{P}(\boldsymbol{\theta})$, where we **do not know** $\boldsymbol{\theta}$, we wish to choose $\boldsymbol{\theta}^*$ that "best" fits the true $\boldsymbol{\theta}$

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- Denote $\Delta := \{\delta : \mathbb{R}^m \to \Theta\}$ the set of possible decision functions (referred to as *hypothesis class*. Also denoted as $\mathcal{H}$)
- We wish to choose the *optimal* $\delta \in \Delta$: $\delta \in \Delta$ such that $\boldsymbol{\theta}^* := \delta(x_1, \ldots, x_m)$ best describes $\boldsymbol{\theta}$.

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Definition

Let $\delta \in \Delta$ be a decision function. Then $\delta(X_1, \dots, X_m)$ is called a point statistical estimator of a parameter $\boldsymbol{\theta}$, or simply an estimator.

Estimators of Gaussians

Suppose we have obtained a sample $x_1, \ldots, x_m \overset{i.i.d}{\sim} \mathcal{P}$ for $\mathcal{N}(\mu, \sigma^2)$, and we wish to estimate μ, σ^2. How should we do so? Which estimators should we define for μ, σ^2?

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- The *sample mean* estimator is defined as:

$$\hat{\mu}_X := \frac{1}{m} \sum x_i$$

- The *sample variance* estimator is defined as:

$$\hat{\sigma}^2_X := \frac{1}{m-1} \sum (x_i - \hat{\mu}_X)^2$$

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Estimator Properties

Defining the sample mean and -variance estimators, we could have considered many other functions

$$\hat{\sigma}_1^2 := \frac{1}{m-1}\sum\left(x_i-\hat{\mu}\right)^2, \quad \hat{\sigma}_2^2 := \frac{1}{m}\sum\left(x_i-\hat{\mu}\right)^2, \quad \hat{\sigma}_3^2 := \frac{1}{m}\sum\left|x_i-\hat{\mu}\right|$$

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- What does “right”/“best” even mean?

We answer the above questions in two steps:

- Defining/deriving properties of estimators
- We need to define some criterion by which we define what “best” means

Biasness of Estimators

Observation: An estimator δ as a function of random variables $X_1, \ldots, X_m$, it itself is a *random variable*. We can therefore ask what is the *expectation* of the estimator, its variance *variance* or its distribution

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Definition

Let δ be an estimator for a parameter θ. The difference $d := \delta(X_1, \dots, X_m) - \theta$ is called the *error* of δ.

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Let δ be an estimator for a parameter θ. The quantity

$$\begin{aligned}\text{Bias}_\theta\left[\delta(X_1,\ldots,X_m)\right] &:= \mathbb{E}_{X_1,\ldots,X_m|\theta}\left[d\right]\\ &= \mathbb{E}_{X_1,\ldots,X_m|\theta}\left[\delta(X_1,\ldots,X_m)-\theta\right]\end{aligned}$$

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Definition

Let δ be an estimator for a parameter θ. δ is said to be *unbiased* iff

$$\forall\theta\in\Theta \quad \text{Bias}_{\theta}\left[\delta(X_1,\ldots,X_m)\right]=0$$

Biasness of sample mean and -variance

The sample mean is an unbiased estimator:

$$\mathbb{E}_{x_1,\ldots,x_m|\mu}\left[\hat{\mu}(x_1,\ldots,x_m)\right] = \mathbb{E}_{x_1,\ldots,x_m|\mu}\left[\frac{1}{m}\sum x_i\right]$$

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&= \tfrac{1}{m-1}\left(\sum_i \mathbb{E}\left[x_i^2\right] - \tfrac{2}{m}\sum_{i,j}\mathbb{E}\left[x_i x_j\right] + \tfrac{1}{m}\sum_{j,k}\mathbb{E}\left[x_j x_k\right]\right)
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&= \tfrac{1}{m-1}\left(\left(1-\tfrac{1}{m}\right)\sum_i \mathbb{E}\left[x_i^2\right] - \tfrac{1}{m}\sum_{i\neq j}\mathbb{E}\left[x_i x_j\right]\right)
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\end{aligned}
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Since the samples are i.i.d then:

- For any i: $\mathbb{E}\left[x_i\right]=\mathbb{E}\left[X\right], \mathbb{E}\left[x_i^2\right]=\mathbb{E}\left[X^2\right]$
- For any $i\neq j$: $\mathbb{E}\left[x_ix_j\right]=\mathbb{E}\left[x_i\right]\mathbb{E}\left[x_j\right]=\mathbb{E}^2\left[X\right]$

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&= \tfrac{1}{m-1}\left((m-1)\,\mathbb{E}\left[X^2\right] - \tfrac{m(m-1)}{m}\mathbb{E}^2\left[X\right]\right) \\
&= \mathbb{E}\left[X^2\right] - \mathbb{E}^2\left[X\right]
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&= \tfrac{1}{m-1}\left((m-1)\,\mathbb{E}\left[X^2\right] - \tfrac{m(m-1)}{m}\mathbb{E}^2\left[X\right]\right) \\
&= \mathbb{E}\left[X^2\right] - \mathbb{E}^2\left[X\right] \\
&= Var\left(X\right) \\
&= \sigma^2
\end{aligned}$$

Variance of Estimators

Definition

Let δ be an estimator for a parameter θ. The *variance* of δ is

$$Var(\delta) := \mathbb{E}_{X_1,\dots,X_m|\theta}\left[\left(\delta(X_1,\dots,X_m) - \mathbb{E}_{X_1,\dots,X_m|\theta}\left[\delta(X_1,\dots,X_m)\right]\right)^2$$

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$$\begin{array}{rcl} Var(\hat{\mu}) & = & Var\left(\frac{1}{m}\sum x_i\right) \\ & = & \frac{1}{m^2} Var\left(\sum x_i\right) \\ & = & \frac{1}{m^2}\sum Var\left(x_i\right) \end{array}$$

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The variance of an estimator provides us with an indication of how well is the estimator performing.

1. Estimators
2. Estimator Properties
3. Maximum Likelihood
4. Estimation Quality - Measure of Concentration
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6. Summary

Maximum Likelihood

Recall, given the set of possible estimators, the hypothesis class, we wanted to answer the following questions:

- Which is the “right”/“best” estimator?
- What does “right”/“best” even mean?

The properties defined above, though interesting in themselves and provide us with tools to assess our estimators, can also be used to define optimality criteria. We can decide for example that the “optimal” estimator is $\delta \in \Delta$ which is *unbiased* and with the *minimial variance* out of all unbiased estimators.

Maximum Likelihood

Another approach is by looking for the *Maximum Likelihood Estimator*, that is, the estimator under which the observed data is *most likely*.

Definition

Let $X \sim \mathcal{P}\left(\boldsymbol{\theta}\right)$ and f be the probability density function of $\mathcal{P}$. The *likelihood* function is:

$$\mathcal{L}\left(\boldsymbol{\theta}|x\right) \coloneqq f_{\boldsymbol{\theta}}\left(x\right)$$

for x the realization of X.

Maximum Likelihood of Gaussian

Consider the case of a univariate Gaussian distribution with $x_1, \ldots, x_m \overset{i.i.d}{\sim} \mathcal{N}\left(\mu, \sigma^2\right)$ and denote $\boldsymbol{\theta} = \{\mu, \sigma^2\}$.

The likelihood function is:

$$\mathcal{L}\left(\boldsymbol{\theta}|x_i\right) = f_{\boldsymbol{\theta}}(x_i) = \frac{1}{\sqrt{2\pi\sigma^2}} \exp\left(-\frac{(x_i-\mu)^2}{2\sigma^2}\right), \quad i \in [m]$$

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Since $x_1, \dots, x_m$ are i.i.d then:

$$\mathcal{L}\left(\boldsymbol{\theta}|x_1, \dots, x_m\right) \quad = \quad f_{\boldsymbol{\theta}}(x_1, \dots, x_m)$$

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Since $x_1, \ldots, x_m$ are i.i.d then:

$$\begin{array}{rcl} \mathcal{L}\left(\boldsymbol{\theta}|x_1, \ldots, x_m\right) & = & f_{\boldsymbol{\theta}}(x_1, \ldots, x_m) \\ & = & \prod_{i=1}^{m} f_{\boldsymbol{\theta}}(x_i) \end{array}$$

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Maximum Likelihood of Gaussian

Using the likelihood function we can now provide each $\boldsymbol{\theta}$ with a quantity (the likelihood) of how likely is it to have generated the observed data.
Let $x_1, x_2, x_3, x_4 \overset{i.i.d}{\sim} \mathcal{N}(\mu, \sigma^2)$ where $x_1 = -1$, $x_2 = 0$, $x_3 = 0$, $x_4 = 1$ and $\sigma^2 = 1$.

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- The likelihood of $\mu = 0$ is:

$$\begin{aligned} \mathcal{L}(\mu = 0, \sigma^2 = 1 | x_1, x_2, x_3, x_4) &= \frac{1}{(2\pi)^2} \exp(-\frac{1}{2} \sum_{i=1}^{4} x_i^2) \\ &= \frac{1}{4\pi^2} \exp(-\frac{2}{2}) \\ &\approx 0.00931 \end{aligned}$$

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- The likelihood of $\mu = 1$ is:

$$\begin{aligned} \mathcal{L}(\mu = 1, \sigma^2 = 1 | x_1, x_2, x_3, x_4) &= \frac{1}{(2\pi)^2} \exp(-\tfrac{1}{2} \textstyle\sum_{i=1}^4 (x_i - 1)^2) \\ &= \frac{1}{4\pi^2} \exp(-\tfrac{2^2+1+1}{2}) \\ &\approx 0.00126 \end{aligned}$$

Maximum Likelihood Estimator

Definition

Let $\mathcal{L}$ be the likelihood function of some probability distribution $\mathcal{P}$ characterized by $\boldsymbol{\theta} \in \Theta$. Let $X \sim \mathcal{P}(\boldsymbol{\theta})$ be a random variable and x its realization. The *Maximum Likelihood Estimator* (MLE) for $\boldsymbol{\theta}$ is

$$\hat{\boldsymbol{\theta}}^{MLE} := \underset{\boldsymbol{\theta} \in \Theta}{\operatorname{argmax}} \ \mathcal{L}\left(\boldsymbol{\theta} | x\right)$$

Let us derive the MLE of a univariate Gaussian distribution's mean $\hat{\mu}^{MLE}$, when σ^2 is known. Let $x_1, \ldots, x_m \overset{i.i.d}{\sim} \mathcal{N}(\mu, \sigma^2)$. We wish to find

$$\hat{\mu}^{MLE} = \underset{\mu \in \mathbb{R}}{\operatorname{argmax}} \ \mathcal{L}(\mu | x_1, \ldots, x_m, \sigma^2)$$

Maximum Likelihood Estimator

$$\begin{aligned}\hat{\mu}^{MLE} &= \operatorname*{argmax}_{\mu\in\mathbb{R}} \mathcal{L}(\mu|x_1,\ldots,x_m,\sigma^2) \\ &= \operatorname*{argmax}_{\mu\in\mathbb{R}} \textstyle\prod_i \frac{1}{\sqrt{2\pi\sigma^2}} \exp\left(-\frac{(x_i-\mu)^2}{2\sigma^2}\right)\end{aligned}$$

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\end{aligned}$$

Notice that the maximizer of the likelihood is also the maximizer of the *log-likelihood* as the logarithm is a monotonous increasing transformation. Thus:

Maximum Likelihood Estimator

$$\begin{aligned}\hat{\mu}^{MLE} &= \underset{\mu\in\mathbb{R}}{\operatorname{argmax}}\ \log\left(\exp\left(-\tfrac{1}{2\sigma^2}\textstyle\sum_i(x_i-\mu)^2\right)\right)\\ &= \underset{\mu\in\mathbb{R}}{\operatorname{argmax}}\ -\tfrac{1}{2\sigma^2}\textstyle\sum_i(x_i-\mu)^2\end{aligned}$$

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To find the maximizer, we derive (with respect to μ) and equate to zero:

$$\frac{\partial}{\partial\mu}\left(-\textstyle\sum_{i=1}^m (x_i-\mu)^2\right) = -\textstyle\sum_{i=1}^m \frac{\partial(x_i-\mu)^2}{\partial\mu} = \textstyle\sum_{i=1}^m 2\left(x_i-\mu\right) = 0$$

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We therefore also conclude that the sample mean minimizes the sum of squared distances

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The Distribution of An Estimator

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- In the case of the sample mean estimator, We have shown that for $x_1, \ldots, x_m \overset{i.i.d}{\sim} \mathcal{N}(\mu, \sigma^2)$ it holds that:

$$\mathbb{E}\left[\hat{\mu}\right] = \mu, \quad Var\left(\hat{\mu}\right) = \frac{\sigma^2}{m}$$

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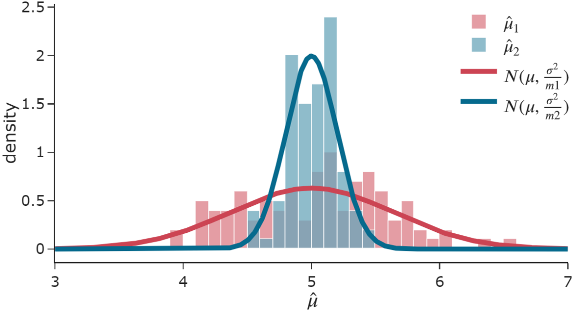
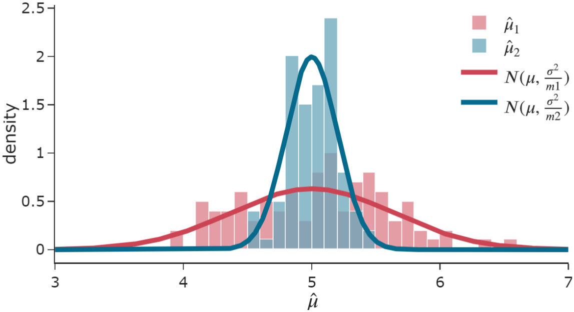
It can further be shown that: $\hat{\mu} \sim \mathcal{N}\left(\mu, \frac{\sigma^2}{m}\right)$

- Namely, this estimator follows a Gaussian distribution centered at the true value μ (unbiased) and with a variance proportional to the variance of the data, and that decays linearly in the number of samples.

The Distribution of An Estimator



The Distribution of An Estimator



We can therefore ask questions such as:

- What is the probability of estimating a certain value?
- How certain are we in our prediction? (variance? confidence-interval?)
- What is the probability of deviating from the true value, and how does it depend on the number of samples?

Coin Prediction

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- Formally, we think of (i.e *model*) a single coin flip as a Bernoulli random variable:

$$\mathcal{D}_p\left(X\right) := \begin{cases} p & X=1 \\ 1-p & X=0 \end{cases}, \quad p \in [0,1]$$

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- Given a sample of m coin tosses $S := \{x_1, \ldots, x_m\}$ we denote the probability distribution of m coin tosses by $\mathcal{D}_p^m$ and the probability of obtaining S by $\mathcal{D}_p^m(S)$.

Coin Prediction

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- The coin prediction learning algorithm takes S as input, drawn i.i.d according to $\mathcal{D}^m$ and outputs an estimation of p. We denote this by $\mathcal{A}(S)$ or $\hat{p}(S)$ or simply $\hat{p}$.

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- The coin prediction learning algorithm takes S as input, drawn i.i.d according to $\mathcal{D}^m$ and outputs an estimation of p. We denote this by $\mathcal{A}(S)$ or $\hat{p}(S)$ or simply $\hat{p}$.
- The learning algorithm we will use is to simply calculate the *empirical* proportion of heads, i.e the sample mean:

$$\hat{p}(S) = \frac{1}{m} \sum_i x_i$$

Coin Prediction

- We already know that this algorithm (estimator) is unbiased. Namely, if we sample many sets $S_j = \{x_1^{(j)}, \ldots, x_m^{(j)}\}$ and for each obtain $\hat{p}_j$, their average will be p. Formally $\mathbb{E}_S\left[\hat{p}\right] = p$.

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- **Problem:** Finite sample sets and usually only one set. Our estimation is not likely to be exactly p. We therefore settle for $\mathcal{A}$ to be accurate enough: $|\hat{p} - p| \leq \varepsilon$ for some $\varepsilon \in (0, 1)$.

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- **Problem:** Even then, unless p equals exactly to 0 or 1, there is always *some* chance to obtain S that is highly non-representative. We will therefore ask how often is $\mathcal{A}$ accurate enough, that is calculate $\mathbb{P}\left(|\hat{p} - p| \leq \varepsilon\right)$.

Coin Prediction - Markov Bounding

Recall Markov's Inequality which states that for a non-negative random variable X, with a finite expectation, for any $a > 0$ then:

$$\mathbb{P}\left(X \geq a\right) \leq \frac{\mathbb{E}\left[X\right]}{a}$$

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As $|\hat{p} - p|$ is a non-negative random variable, for any accuracy level $\varepsilon \in (0, 1)$ we can bound the probability of deviating from p by more than ε by:

$$\mathcal{D}^m\left[|\hat{p} - p| \geq \varepsilon\right] \leq \frac{\mathbb{E}\left[|\hat{p} - p|\right]}{\varepsilon}$$

Coin Prediction - Markov Bounding

We bound the expectation from above as follows. Since $Var(A) = \mathbb{E}\left[A^2\right] - \mathbb{E}^2\left[A\right]$ then:

$$Var\left(|\hat{p} - p|\right) = \mathbb{E}\left[|\hat{p} - p|^2\right] - \mathbb{E}^2\left[|\hat{p} - p|\right]$$

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$$\mathbb{E}^2\left[\left|\hat{p}-p\right|\right] \leq \mathbb{E}\left[\left|\hat{p}-p\right|^2\right]$$

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Next:

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Next:

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 & = & \mathbb{E}\left[(\hat{p}-\mathbb{E}\left[\hat{p}\right])^2\right] & = & Var\left(\hat{p}\right) \\
 & = & Var\left(\frac{1}{m}\sum x_i\right) & = & \frac{1}{m^2}Var\left(\sum x_i\right) \\
 & = & \frac{p(1-p)}{m} & \leq & \frac{1}{4m}
\end{array}$$

Coin Prediction - Markov Bounding

Therefore:

$$\mathbb{E}^2\left[|\hat{p} - p|\right] \leq \frac{1}{4m} \quad \Rightarrow \quad \mathbb{E}\left[|\hat{p} - p|\right] \leq \frac{1}{\sqrt{4m}}$$

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Put all together then:

$$\mathcal{D}^m\left[|\hat{p}-p| \geq \varepsilon\right] \leq \frac{\mathbb{E}[|\hat{p}-p|]}{\varepsilon} \leq \frac{1}{\sqrt{4m\varepsilon^2}}$$

$$\Updownarrow$$

$$\mathcal{D}^m\left[|\hat{p}-p| \leq \varepsilon\right] \geq 1-\frac{1}{\sqrt{4m\varepsilon^2}}$$

Coin Prediction - Markov Bounding

As a last step, denote $\delta = \frac{1}{\sqrt{4m\varepsilon^2}}$. Solving for m then: $m = \frac{1}{4\varepsilon^2\delta^2}$

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This means that for any $\varepsilon, \delta \in (0,1)$, if we use a sample of size at least $m = \lceil \frac{1}{4\varepsilon^2\delta^2} \rceil$ then

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Namely, by providing *enough* samples, we can guarantee with *confidence* of $1 - \delta$ that our estimation is *accurate* (ε) enough.

Coin Prediction - Chebyshev Bounding

We can improve the upper bound achieved using Markov's Inequality by including the estimator's second moment (i.e its variance).

- That is, achieve a tighter bound on the needed number of samples to achieve a given accuracy and confidence levels.

Definition

Let X be a random variable with a finite mean and variance. Then, for every $\varepsilon \geq 0$:

$$\mathbb{P}\left(|X - \mathbb{E}\left[X\right] \geq \varepsilon|\right) \leq \frac{Var(X)}{\varepsilon^2}$$

Coin Prediction - Chebyshev Bounding

So, given a sample $x_1 \dots, x_m \overset{i.i.d}{\sim} Ber(p)$ we bound the deviance of $\hat{p}$ from its expected value as follows:

$$\mathbb{P}\left[|\hat{p} - \mathbb{E}\left[\hat{p}\right]| \geq \varepsilon\right] \overset{unbiased}{=} \mathbb{P}\left[|\hat{p} - p| \geq \varepsilon\right] \overset{Cheb.}{\leq} \frac{Var(\hat{p})}{\varepsilon^2}$$

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&= \quad \frac{1}{\varepsilon^2} Var\left(\frac{1}{m}\sum x_i\right) \quad \overset{i.i.d}{=} \quad \frac{1}{m^2\varepsilon^2}\sum Var\left(x_i\right)
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We conclude that for any $\varepsilon, \delta \in (0,1)$, if we provide $m \geq \lceil \frac{1}{4\delta\varepsilon^2} \rceil$ samples then:

$$\mathcal{D}^m\left[|\hat{p} - p| \leq \varepsilon\right] \geq 1 - \delta$$

1. Estimators
2. Estimator Properties
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Multivariate Distributions

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Consider for example describing human weight and height.

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Consider for example describing human weight and height.

- It is possible to model (i.e describe how the data behaves) each push property independently. For example:

$$w_1, \ldots, w_m \overset{i.i.d}{\sim} \mathcal{N}\left(75, 3\right)$$

$$h_1, \ldots, h_m \overset{i.i.d}{\sim} \mathcal{N}\left(170, 5\right)$$

Multivariate Distributions

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- To model such connection we must first define *multivarite* probabilities.

Definition

Let $X_1, \ldots, X_d$ be a finite set of random variables defined over the same probability space. Then $X := (X_1, \ldots, X_d)^\top$ is called a *random vector*

That is, a random vector is a map from the probability space to $\mathbb{R}^d$.

Multivariate Distributions

Definition

Let $X := (X_1, \ldots, X_d)^\top$ be a random vector. The *joint probability distribution distribution* of $X_1, \ldots, X_d$ is the corresponding probability distribution on all possible outputs of $X_1, \ldots, X_d$.

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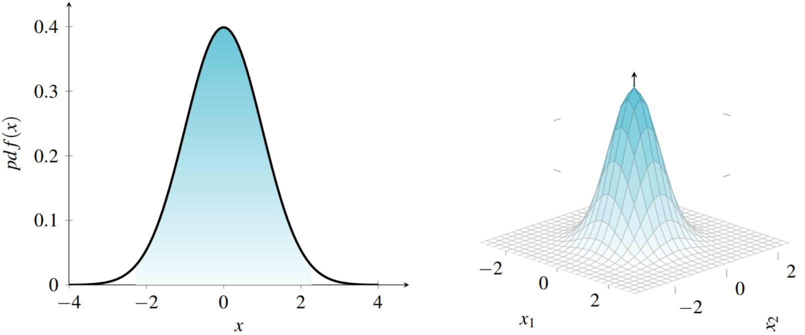
Definition

Let $X := (X_1, \ldots, X_d)^\top$ be a random vector. The *covariance matrix* Σ is a $d \times d$ matrix whose (i, j) entry is the covariance

$$\Sigma_{ij} := COV(X_i, X_j) = \mathbb{E}\left[(X_i - \mathbb{E}[X_i])(X_j - \mathbb{E}[X_j])\right]$$

Multivariate Gaussian Distribution

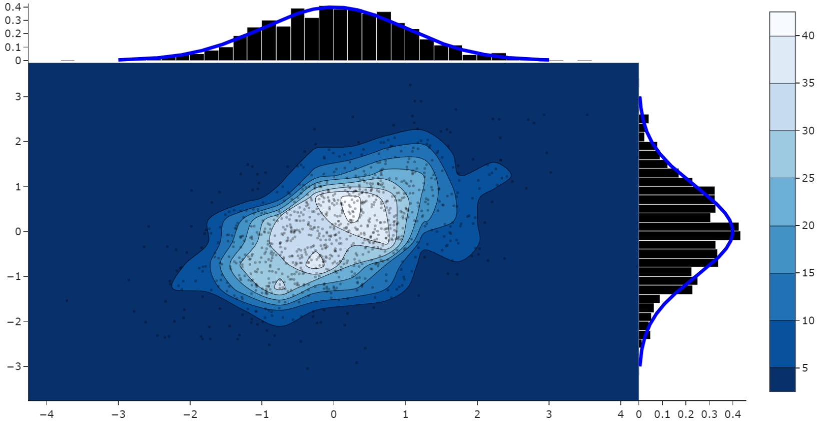


***(a)** Univariate Gaussian* $\mathcal{N}(0,1)$

***(b)** Bivariate Gaussian* $\mathcal{N}(0,I_2)$

Note: the contour lines of a Gaussian distribution as ellipsoids.

Multivariate Gaussian Distribution - Empirical



Note: the contour lines simply capture the *empirical* density of the data.

Multivariate Gaussian Distribution

Definition

A random vector $X := (X_1, \ldots, X_d)^\top$ follows a *multivariate normal distribution* with expectation $\mu \in \mathbb{R}^d$ and covariance matrix $\Sigma \in \mathbb{R}^{d \times d}$ if it has a joint probability density function of the form:

$$f\left(X\right) = \frac{1}{\sqrt{\left(2\pi\right)^d \left|\Sigma\right|}} \exp\left\{-\frac{1}{2}(X - \mu)^\top \Sigma^{-1} \left(X - \mu\right)\right\}$$

In this case we write $X \sim \mathcal{N}\left(\mu, \Sigma\right)$

Definition

Let $X := (X_1, \ldots, X_d)^\top$ be a random vector with a joint probability distribution function. The *marginal distribution* of a subset of coordinates $A \in [d]$ and $B = [d] \backslash A$, is the probability distribution of the coordinates in the set:

$$f(X_A) := \int_{X_B} f(X_A, X_B)\, dX_B$$

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In the case of the Gaussian distribution, the marginal distributions (of any coordinate subset size) is also a Gaussian distribution

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Claim: Let $X \sim \mathcal{N}(\mu, \Sigma)$ be a bivariate Gaussian, i.e $X = (X_1, X_2)^\top$, with a diagonal covariance matrix:

$$X \sim \mathcal{N}\left(\begin{bmatrix} \mu_1 \\ \mu_2 \end{bmatrix}, \begin{bmatrix} \sigma_1^2 & 0 \\ 0 & \sigma_2^2 \end{bmatrix}\right)$$

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In the case of the Gaussian distribution, the marginal distributions (of any coordinate subset size) is also a Gaussian distribution

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The marginal distribution of coordinate i is

$$f(X_i) = \frac{1}{\sqrt{2\pi\sigma_i^2}} \exp\left(-\frac{1}{2}\left(\frac{X_i - \mu_i}{\sigma_i}\right)^2\right)$$

Estimators of Multivariate Gaussian Distribution

Returning to the task of describing human weight and height, we can now model each observation as a *vector* $\mathbf{x} \in \mathbb{R}^d$, being the realization of a *random vector* $X := (X_{weight}, X_{height})^\top$.

- Therefore a sample is $S := \{\mathbf{x}_1, \ldots, \mathbf{x}_m\}$, where each $\mathbf{x}_i$ is the realization of X_i.

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- The j'th property $\mathbf{x}_i(j)$ is the realization of the j'th coordinate of X_i: $X_i^{(j)}$.

Estimators of Multivariate Gaussian Distribution

Now, given a sample of m i.i.d observations we wish to estimate the distribution parameters

$$\mathbf{x}_1, \ldots, \mathbf{x}_m \overset{i.i.d}{\sim} \mathcal{N}\left(\begin{bmatrix} 75 \\ 170 \end{bmatrix}, \begin{bmatrix} 3 & 1 \\ 1 & 5 \end{bmatrix} \right)$$

- The multivariate *sample mean* estimator is simply the univariate estimator of each variable:

$$\hat{\mu} := \begin{bmatrix} \vdots \\ \hat{\mu}_j \\ \vdots \end{bmatrix} = \begin{bmatrix} \vdots \\ \frac{1}{m} \sum_i x_{i,j} \\ \vdots \end{bmatrix}$$

Estimators of Multivariate Gaussian Distribution

- To define an estimator for the covariance matrix we first define an estimator of the sample covariance between two random variables. The *unbised* sample covariance estimator between X_i, X_j is given by

$$\hat{\sigma}\left(X_i, X_j\right) := \frac{1}{m-1}\sum_k \left(x_{ki} - \hat{\mu}_i\right)\left(x_{kj} - \hat{\mu}_j\right)$$

- Then, the *sample covariance matrix* estimator is a $d \times d$ matrix $\hat{\Sigma}$ such that

$$\hat{\Sigma}_{ij} := \hat{\sigma}\left(X_i, X_j\right), \quad i, j \in [d]$$

Estimators of Multivariate Gaussian Distribution

In matrix notation, for $\mathbf{X} \in \mathbb{R}^{m \times d}$ whose rows are the samples $\mathbf{x}_1, \ldots, \mathbf{x}_m$ the:

- biased sample covariance matrix is given by

$$\hat{\Sigma} := \frac{1}{m} \sum_{i=1}^{m} \left(\mathbf{x}_i - \hat{\mu}\right) \left(\mathbf{x}_i - \hat{\mu}\right)^\top = \frac{1}{m} \widetilde{\mathbf{X}}^\top \widetilde{\mathbf{X}}$$

for $\widetilde{\mathbf{X}}$ being the centered matrix: $\widetilde{\mathbf{X}}_{\cdot,i} := \mathbf{X}_{\cdot,i} - \hat{\mu}$.

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- We have seen how to **estimate univariate and multivariate Gaussian** distributions