Lecture 4: Parameter Estimation (Part I)

Statistical Methods for Data Science

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Today

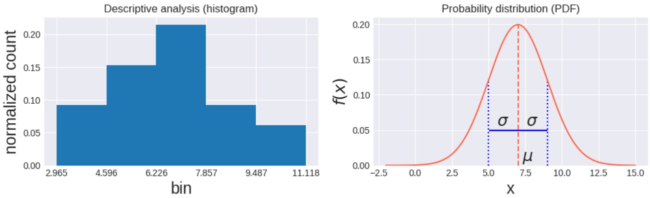
1. Mathematical modeling
2. Parameter estimation
   - Maximum likelihood estimation (MLE)
   - Likelihood and likelihood function
   - Joint probability distribution
   - Independence
3. Summary

Learning outcome

- Be able to explain different components in a mathematical model $y = g(x; \theta \mid h)$
- Understand the purpose and general steps of parameter estimation
- Be able to explain these concepts: joint probability distribution, independent and identically distributed (i.i.d.) random variables, likelihood function, maximum likelihood

Recap: three questions from lecture 2

Jack suggested to use a Gaussian distribution to model your data.



- ✅ Question 1: Why should I use probability distributions instead of histograms?
- ✅ Question 2: How do you know if my data follows a Gaussian distribution?
- ? Question 3: How do I find the unknown parameters?

In today's lecture, we are going to address question 3.

Today

1. Mathematical modeling
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What you will learn from this section

In the previous section, we have touched upon the topic of choosing a probabilistic model to describe a given data set.

Generally speaking, given a data set and a problem to be solved, you need to formulate the solution mathematically so that you can write a computer program to solve the problem. This is the main task for a data scientist.

This section aims to help you get started by providing explicit components and steps for formulating mathematical models.

Terminology

- What is mathematical modeling? - Mathematical modeling is to *describe* a system using the language of mathematics in order to solve **a range of problems**.
- What the *description* looks like in data science:

$$y = g(x; \theta \mid h)$$

- Left hand side:
  - y: target or label - what you want to predict; **a result** that answers the question at hand
- Right hand side:
  - x: variables or features - placeholder for data in order to solve *a range of* problems; **the input**
  - g: model - a mathematical function that can be used to solve a given range of problems - a model is given by domain experts or derived from your assumption; can be selected from established models; **known** except for some parameters
  - h: hyperparameters - part of the model g (given or derived from your assumption); **known** (but you might need to "guess" them first)
  - θ: parameters - part of the model g; in a data-driven paradigm θ is **unknown**; need to be estimated from data
- Symbols:
  - Semicolon (";") is used to emphasize that θ is not known for free - it needs to be estimated
  - Bar ("|" pronounced "*given*") is used to indicate that h is known to you
- Note: x, y, θ and h are not necessarily scalars; they can be multiple scalars, vectors or more complex data structures; g can be complex functions, for instance, a machine learning model or a deep neural network.

Five questions

Overwhelmed? Take it easy! Here is something that helps you get started! Answer these five questions in the language of mathematics step by step:

- 1) What do we want to predict, i.e. what is the target y?
- 2) What are the variables x?
- 3) What is the mathematical function g that relates variables x to the target y?
- 4) Are there any hyperparameters h in the function g? How do we choose them?
- 5) What are the unknown parameters θ in g? **How do we estimate them from data?**

Probabilistic modeling

Model data using probability distributions
Example:

$$y = g(x_1, x_2; \mu, \sigma) = P(x_1 \leq weight \leq x_2) = \int_{x_1}^{x_2} f_X(t)dt = \int_{x_1}^{x_2} \frac{1}{\sqrt{2\pi\sigma^2}} e^{-\frac{(t-\mu)^2}{2\sigma^2}} dt$$

- 1) What do we want to predict, i.e. what is the target y? - The probability of the event $x_1 \leq weight \leq x_2$
- 2) What are the variables x? - x_1 and x_2
- 3) What is the mathematical function g that relates variables x to the target y? - The integral of the Gaussian PDF
- 4) Are there any hyperparameters h in the function g? How do we choose them? - There is none in this case
- 5) What are the unknown parameters - μ and σ **How do we estimate them from data?**

General steps of parameter estimation for probabilistic models

- Note: the estimate of θ is denoted as $\hat{\theta}$.
- General steps for parameter estimation for a probabilistic model g
  - a) Describe the **experiments**
  - b) Describe the **data** generated from the experiments
  - c) Describe the **random variables**
  - d) Identify **parameters of interest** θ
  - e) Choose an **estimation method**, e.g. MLE/MAP
  - f) **Compute** $\hat{\theta}$ typically by solving an optimization problem
    - Closed-form solution for simple cases
    - Iterative methods for general cases
  - g) Evaluation: estimate and report the uncertainty of $\hat{\theta}$ (later)
- **Underlying assumption**: the data we use for parameter estimation is generated from the same distribution as the data we use for prediction.

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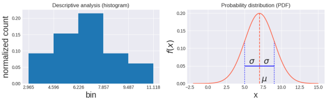
Overview

Given a dataset and a problem to be solved, now you know how to choose a probability distribution. However, the model has unknown parameters. In this section, you will learn how to estimate these parameters from data.

- There are two important parameter estimation methods: 1) the **maximum likelihood estimation (MLE)** and 2) the **maximum a posteriori estimation**.
- Concepts such as likelihood function, independent and identically distributed random variables, prior, posterior, Bayes' rule, etc are important building blocks for future machine learning models.

Overview (cont.)



- In a Gaussian distribution, what are the parameters to be estimated? mean μ and standard deviation σ
- The **maximum likelihood estimates** are the sample mean $\bar{x}$ and the sample standard deviation s for parameters μ and σ, respectively.

$$\hat{\mu} = \bar{x} = \frac{1}{N}\sum_{i=1}^{N} x_i$$

$$\hat{\sigma} = s = \sqrt{\frac{1}{N-1}\sum_{i=1}^{N}(x_i - \bar{x})^2}$$

- Straightforward for Gaussian distribution! Gaussian is great!
- However, it is not straightforward for all distributions - it is important to properly understand the MLE framework.

Maximum likelihood estimation (MLE)

Simplest case study: estimate one parameter given one observation

- **Model** g (cf. lecture 3):
  - **Assumption**: a duck's weight is drawn from a Gaussian distribution with standard deviation σ and mean μ

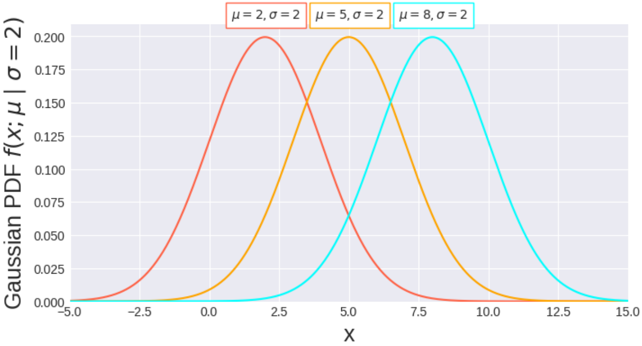
  To simplify the problem for illustration purposes, let's only look at one parameter for now:
  - We assume that σ is known to us: $\sigma = 2$
  - Unknown parameter: μ

  We want to estimate this unknown parameter by collecting some data from experiments.
- **Experiment**: we weigh a duck and observe its weight
- **Data**: the duck weighs 4 kg
- **Random variable**: $X = x$ if a duck weighs x kg
- **Parameter of interest**: μ
- **Estimation method**: the maximum likelihood estimation for μ
- **Compute** $\hat{\mu}_{MLE}$ by maximizing the **likelihood function**

Can you guess what result we are going to get? $\hat{\mu}_{MLE} = 4$

Intuition

Which Gaussian distribution is most “likely” to be the underlying model for the given data $x = 4$?

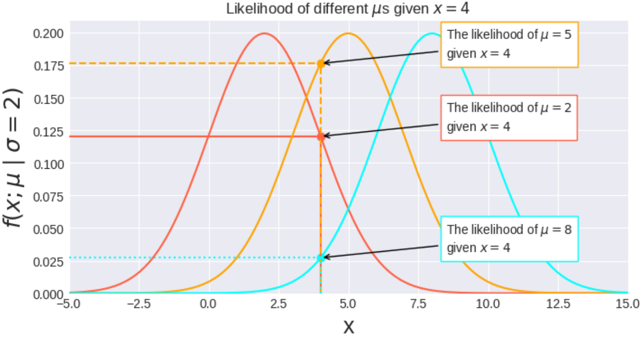


Likelihood and likelihood function

🚨 Terminology alert 🚨 - likelihood

Assumption (reminder): weights x follow a Gaussian distribution with unknown parameter μ and known $\sigma = 2$

- **Likelihood of μ** given data $x = 4$ is $f(x = 4; \mu \mid \sigma = 2)$



A nonrigorous note on functions and variables

- Let g be a function that relates input variables x to a target y:

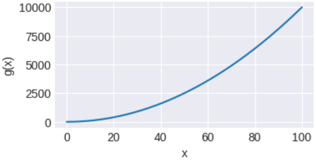
$$y = g(x)$$

- Typically, we care about the behavior of y for **all possible values for x**. This is called **generalization** in machine learning.
- Even if we add parameters θ and hyperparameters h to g, $g(x; \theta \mid h)$ is still a function of x.
- In a plot, we typically place the variable on the x-axis!
- If we are interested in the behavior of y in terms of θ, we can construct a different function L that takes θ as the variables $y = L(\theta)$ to relate θ to y.

A nonrigorous note on functions and variables (cont.)

- Example: $y = g(x) = x^2$
- In Python, **all possible values for x** means something like this:

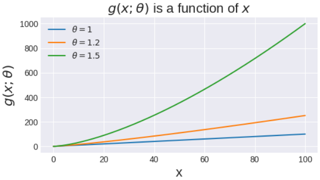
```
# Assume x can take any value between 0 and 100
xmin, xmax = 0, 100
N = 10000 # ideally, N should be infinity. But sadly, computers are discrete
          # so N has to be finite.
x = np.linspace(xmin, xmax, num=N) # all possible values for x
# Plot a function
def g(t):
    return np.power(t, 2)
y = g(x)
plt.plot(x, y)
```



A nonrigorous note on functions and variables (cont.)

- Now we add a parameter θ to g: $y = g(x; \theta) = x^{\theta}$

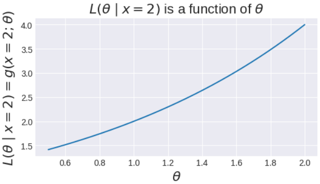
```
def g_theta(t, theta):
    return np.power(t, theta)
xmin, xmax = 0, 100 # assume x can take any value between 0 and 100
N = 10000
x = np.linspace(xmin, xmax, num=N) # all possible values for x
y = g_theta(x, 1)
plt.plot(x, y)
y = g_theta(x, 1.2)
plt.plot(x, y)
y = g_theta(x, 1.5)
plt.plot(x, y) # x is still on the x-axis
```



A nonrigorous note on functions and variables (cont.)

- Now we define a new function: $y = L(\theta \mid x = 2) = g(x = 2; \theta) = 2^\theta$

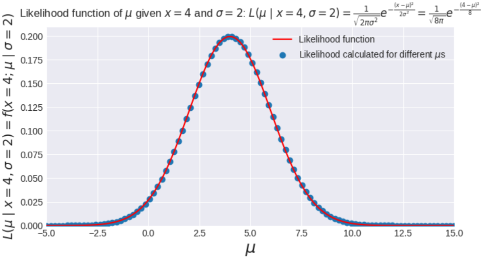
```
def L(t):
    return g_theta(2, t)
# Now theta is the variable! So we need to get all possible values for theta
# Assume theta can take any value between 0.5 and 2
theta_min, theta_max = 0.5, 2
N = 10000
thetas = np.linspace(theta_min, theta_max, num=N) # all possible values for theta
y = L(thetas)
plt.plot(thetas, y) # theta is on the x-axis now
```



Terminology alert - likelihood function

- **Likelihood function of μ** given data $x = 4$ for $-\infty \leq \mu \leq \infty$:

$$\begin{aligned} L(\mu \mid x = 4, \sigma = 2) &= f(x = 4; \mu \mid \sigma = 2) \\ &= \frac{1}{\sqrt{2\pi\sigma^2}} e^{-\frac{(x-\mu)^2}{2\sigma^2}} \\ &= \frac{1}{\sqrt{8\pi}} e^{-\frac{(4-\mu)^2}{8}} \end{aligned}$$

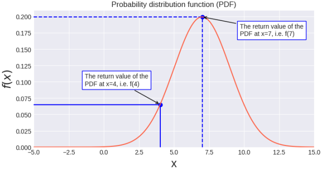


- A tiny note about symbol (most abstract), definition (less abstract) and computation (concrete - something you can implement it in Python)

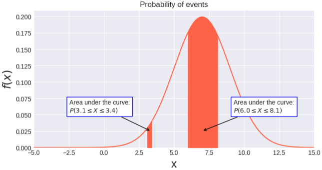
Recall: probability density function and probability of events

Gaussian distribution with $\mu = 7$, $\sigma = 2$

- Probability density function $f(x \mid \mu = 7, \sigma = 2)$:



- Probability of events $P(x_1 \leq X \leq x_2)$:



Probability of events vs likelihood function

- Probability of events given $\mu = 7$ and $\sigma = 2$:

$$\begin{aligned} g(x_1, x_2 \mid \mu = 7, \sigma = 2) &= P(x_1 \leq X \leq x_2) \\ &= \int_{x_1}^{x_2} f_X(t)dt = \int_{x_1}^{x_2} \frac{1}{\sqrt{2\pi\sigma^2}} e^{-\frac{(t-\mu)^2}{2\sigma^2}} dt \\ &= \int_{x_1}^{x_2} \frac{1}{\sqrt{8\pi}} e^{-\frac{(t-7)^2}{8}} dt \end{aligned}$$

  Here x_1 and x_2 are the **variables** - when we change x_1 and x_2, we get a different probability $g(x_1, x_2 \mid \mu = 7, \sigma = 2)$.

- Likelihood function for a given observation $x = 4$ (with known $\sigma = 2$):

$$L(\mu \mid x = 4, \sigma = 2) = \frac{1}{\sqrt{8\pi}} e^{-\frac{(4-\mu)^2}{8}}$$

  Here μ is the **variable** - when we change μ, we get a different likelihood $L(\mu \mid x = 4, \sigma = 2)$.

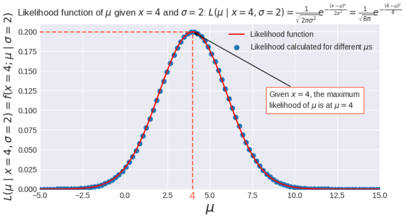
Maximum likelihood

From the likelihood function

$$L(\mu \mid x = 4, \sigma = 2) = \frac{1}{\sqrt{8\pi}} e^{-\frac{(4-\mu)^2}{8}}$$

We can now define the **maximum likelihood** of μ given $x = 4$:

$$\text{the maximum likelihood of } \mu = \max(L(\mu \mid x = 4, \sigma = 2))$$



The value of μ that maximizes the likelihood function is called the **maximum likelihood estimation** (MLE) of μ. In this case, $\hat{\mu}_{\text{MLE}} = 4$.

Note: $\hat{}$ here means that $\hat{\mu}$ is an estimate instead of the true value μ.

Comparison

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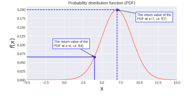
<tr><td>Probability density function</td><td>
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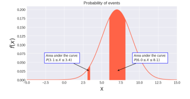
<tr><td>Probability of events</td><td>
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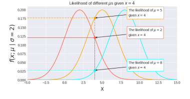
<tr><td>Likelihood of a parameter given data</td><td>
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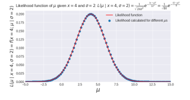
<tr><td>Likelihood function of a parameter given data</td><td>
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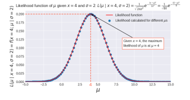
<tr><td>Maximum likelihood estimation</td><td>
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Summary: what have we done so far?

- We observe one data point $x = 4$.
- We assume that duck weights are drawn from a *Gaussian distribution* with known $\sigma = 2$ and unknown μ. We need to estimate μ.
- We write down the likelihood function: $L(\mu \mid x = 4, \sigma = 2) = \frac{1}{\sqrt{8\pi}} e^{-\frac{(4-\mu)^2}{8}}$.
- The maximum likelihood estimation of μ is defined as:

$$\hat{\mu}_{\text{MLE}} = \arg\max_{\mu} L(\mu \mid x = 4, \sigma = 2) = \arg\max_{\mu} \frac{1}{\sqrt{8\pi}} e^{-\frac{(4-\mu)^2}{8}} \quad (1)$$

Remaining questions

- We can't estimate the whole distribution from only one data point $x = 4$! What if we have more than one observation?
- How can we maximize the likelihood function and find the value of $\hat{\mu}_{MLE}$ analytically?
- What if σ is also unknown?
- What about discrete distributions?

Case study: parameter estimation given more observations

- **Model**:
  - Assumption: a duck's weight is drawn from a Gaussian distribution with known standard deviation $\sigma = 2$ and unknown mean μ
- **Experiment**: we observe 20 ducks
- **Data**:

duck id	1	2	3	4	···	19	20
weight	6.98	5.43	2.97	7.07	···	4.63	7.27

- **Parameter of interest**: μ
- **Estimation method**: maximum likelihood estimation
- **Compute** $\hat{\mu}_{MLE}$ by maximizing the likelihood function
- Recall: when we only have one observation $x = 4$, the likelihood function looks like this

$$L(\mu \mid x = 4, \sigma = 2) = f(x = 4; \mu \mid \sigma = 2) = \frac{1}{\sqrt{2\pi\sigma^2}} e^{-\frac{(x-\mu)^2}{2\sigma^2}} = \frac{1}{\sqrt{8\pi}} e^{-\frac{(4-\mu)^2}{8}}$$

- Educated guess 🤔 - now we have more observations, the likelihood function probably should look like this:

$$L(\mu \mid x_1 = 6.98, \cdots, x_{20} = 7.27, \sigma = 2) = \boxed{f(x_1 = 6.98, \cdots, x_{20} = 7.27; \mu \mid \sigma = 2)}$$

Joint probability distribution

🚨 Terminology alert 🚨 - joint probability distribution 👯

Given two random variables X and Y, we use their **joint probability distribution** to characterize their behaviors:

$$F_{X,Y}(x,y) = P(X \leq x, Y \leq y) \text{ joint CDF}$$

- X, Y discrete: joint PMF $f_{X,Y}(x,y) = P(X = x, Y = y)$
- X, Y continuous: joint PDF $f_{X,Y}(x,y)$

- Bummer: these expressions are usually quite hard to obtain...
- Solution: we impose some assumptions to make the calculation easier.

Independence

Independence 😼

- Recall independent events: two events A and B are independent if and only if

$$P(A \text{ and } B) = P(A \cap B) = P(A)P(B)$$

New! **Independent random variables**: random variables X, Y are independent if and only if

$$F_{X,Y}(x, y) = P(X \leq x, Y \leq y) = P(X \leq x)P(Y \leq y) = F_X(x)F_Y(y)$$

- X, Y discrete:

$$f_{X,Y}(x, y) = P(X = x, Y = y) = P(X = x)P(Y = y) = f_X(x)f_Y(y)$$

  where $f_{X,Y}(x, y)$ is the joint PMF
- X, Y continuous:

$$f_{X,Y}(x, y) = f_X(x)f_Y(y)$$

  where $f_{X,Y}(x, y)$ is the joint PDF

- This idea generalizes to more than two random variables

Independence 😼

Any number of random variables:

- Given n random variables $X_1, X_2, \cdots, X_n$ with CDF $F_{X_i}(x_i)$,

$$F_{X_1,\cdots,X_n}(x_1, \cdots, x_n) = \prod_{i=1}^{n} F_{X_i}(x_i)$$

  where $F_{X_1,\cdots,X_n}(x_1, \cdots, x_n)$ is the joint CDF
  - X_i discrete with PMF $f_{X_i}(x)$:

$$f_{X_1,\cdots,X_n}(x_1, \cdots, x_n) = \prod_{i=1}^{n} f_{X_i}(x_i)$$

    where $f_{X_1,\cdots,X_n}(x_1, \cdots, x_n)$ is the joint PMF
  - X_i continuous with PDF $f_{X_i}(x)$:

$$f_{X_1,\cdots,X_n}(x_1, \cdots, x_n) = \prod_{i=1}^{n} f_{X_i}(x_i)$$

    where $f_{X_1,\cdots,X_n}(x_1, \cdots, x_n)$ is the joint PDF
- Now we have turned the joint probability distribution into multiplications of things we know how to compute. Yay!

Back to the case study

The likelihood function

$$L(\mu \mid x_1 = 6.98, \cdots, x_{20} = 7.27, \sigma = 2) = \boxed{f(x_1 = 6.98, \cdots, x_{20} = 7.27; \mu \mid \sigma = 2)}$$

- **Model**:
  - Assumption: the weight is drawn from a Gaussian distribution with known standard deviation $\sigma = 2$ and unknown mean μ
- **Experiment**: we weigh 20 ducks
- **Data**:

duck id	1	2	3	4	$\cdots$	19	20
weight	6.98	5.43	2.97	7.07	$\cdots$	4.63	7.27

- **Random variable**: we define 20 random variables X_i : duck weight $\rightarrow \mathbb{R}$, where X_i are **independent and identically distributed (i.i.d)** Gaussian random variables
  - $X_1, \cdots, X_{20}$ are independent - [new!] assumption:

$$f_{X_1,\cdots,X_{20}}(x_1 = 6.98, \cdots, x_{20} = 7.27) = f_{X_1}(x = 6.98) \cdots f_{X_{20}}(x = 7.27)$$

  - $X_1, \cdots, X_{20}$ are identically distributed - they have the same PDF:

$$f_{X_1}(x; \mu \mid \sigma) = \cdots = f_{X_{20}}(x; \mu \mid \sigma) = f(x; \mu \mid \sigma)$$

  where $\sigma = \sigma_1 = \sigma_2 = \cdots = \sigma_{20} = 2$ and $\mu = \mu_1 = \mu_2 = \cdots = \mu_{20}$.
- **Parameter of interest**: μ
- **Estimation method**: maximum likelihood estimation
- **Compute** $\hat{\mu}_{MLE}$ by maximizing the likelihood function

Today

Summary

So far:

- Data types and data containers
- Descriptive data analysis: descriptive statistics, visualization
- Probability distributions, events, random variables, PMF, PDF, parameters
- CDF, Q-Q plot, how to compare two distributions (data vs theoretical, data vs data)
- Modeling
- Parameter estimation: maximum likelihood estimation (to be continued...)

Next (part II):

- Maximum a posteriori estimation

Before next lecture:

- Conditional probability, i.i.d. random variables

Until next time!