Lecture 3: Q-Q plot and mathematical modeling

Statistical Methods for Data Science

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November 7, 2022

Today

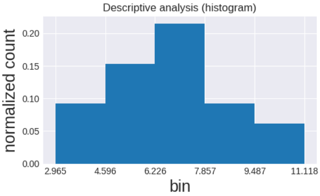
1. Compare two distributions using a Q-Q plot
   - Cumulative distribution function (CDF)
   - Quantiles of a theoretical distribution
   - Q-Q plot (quantile-quantile plot)
   - Compare two distributions
2. Mathematical modeling
3. Summary

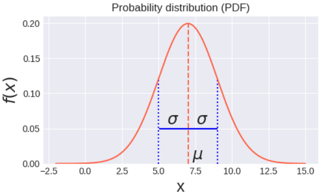
Learning outcome

- Be able to explain the following terminology: Cumulative distribution function (CDF), Q-Q plot, one-sample/two-sample tests
- Be able to compute quantiles in Python for a given theoretical probability distribution
- Understand the relation between quantile and CDF
- Be able to construct a Q-Q plot
- Be able to explain different components in a mathematical model $y = g(x; \theta \mid h)$

Recap: three questions from lecture 2

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





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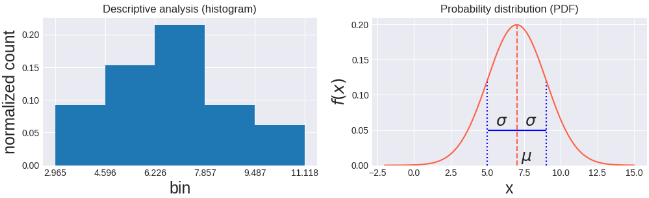

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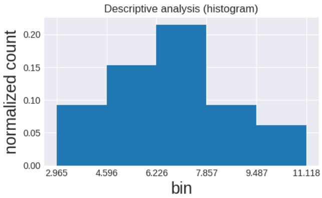

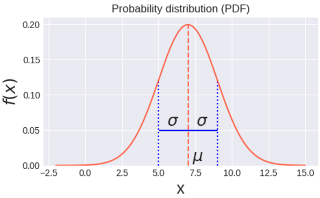

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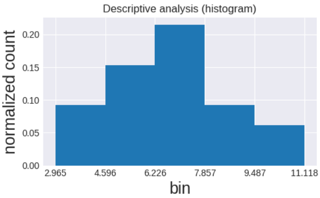

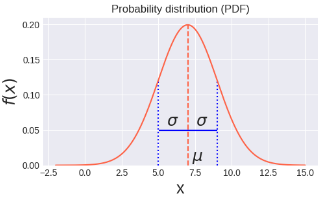

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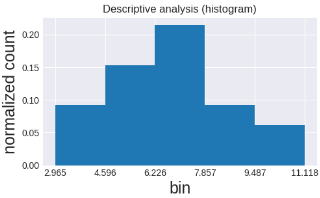

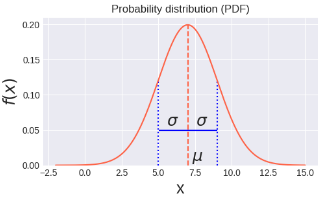

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In today's lecture, we are going to address question 2.

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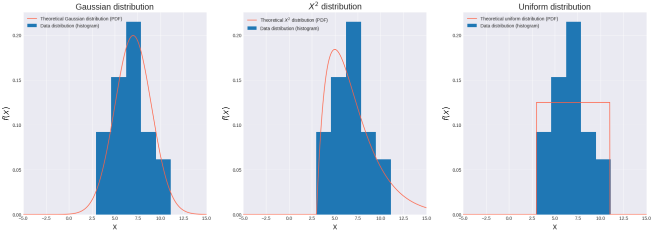
What you will learn from this section

Given a data set, you will learn how to use the Q-Q plot to choose which probability distribution best fits the data.



Which one of these three theoretical distributions seems to be the best fit?

Cumulative distribution function (CDF)

🚨 Terminology alert 🚨

For a random variable X, the **cumulative distribution function (CDF)** F_X is defined as

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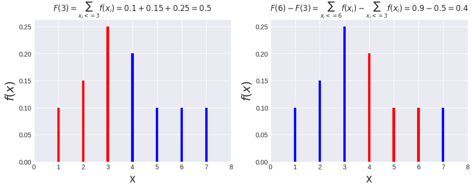
- X discrete random variable:
  - **Definition**: given the PMF f_X,

    $$F_X(\mathbf{x}) = P(X \leq \mathbf{x}) = \sum_{x_i \leq \mathbf{x}} f_X(x_i)$$

    where x_i are all the values X can take.
  - Implication:

    $$F_X(b) - F_X(a) = P(a < X \leq b) = \sum_{x_i \leq b} f_X(x_i) - \sum_{x_i \leq a} f_X(x_i)$$



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For a random variable X, the **cumulative distribution function (CDF)** F_X is defined as

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- X continuous random variable:
  - **Definition**: given the PDF f_X,

$$F_X(\mathbf{x}) = P(X \leq \mathbf{x}) = \int_{-\infty}^{\mathbf{x}} f_X(t)dt$$

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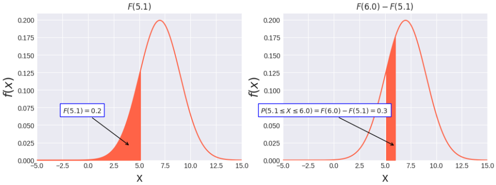
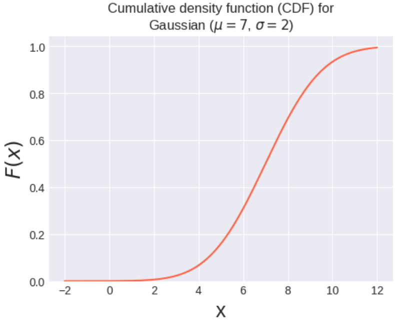
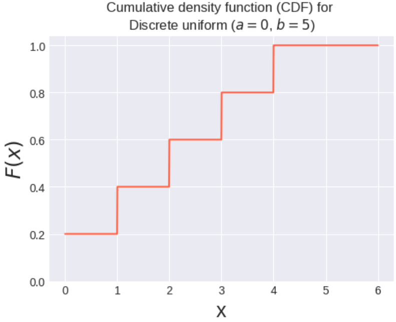


CDF example plot

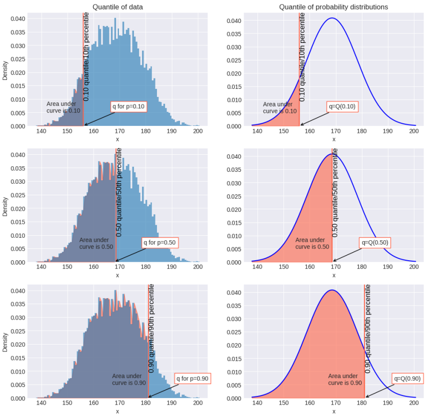




Quantiles of a theoretical distribution

Data vs probability distribution

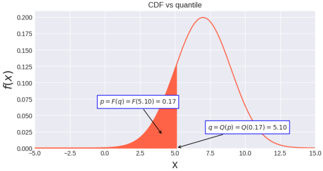
- Recall data quantile: given $p \in (0, 1)$, q is a p-quantile if $p \times 100\%$ of the data are below q
- "The area under the curve is the probability of data falling into that interval"



Quantile and CDF

- Quantile function Q is the (generalized) inverse CDF, i.e.

$$F_X(Q(p)) = p \text{ and } Q(F_X(q)) = q$$



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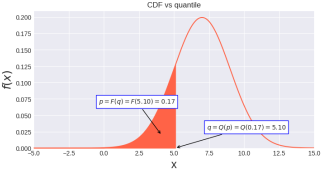

- More precisely, given $p \in (0, 1)$, let $Q(p)$ be the quantile function. Then we have

$$Q(p) = \inf\{x : F_X(x) \geq p\}$$

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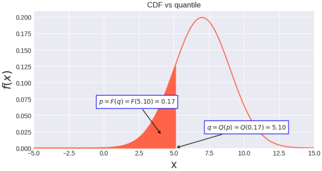

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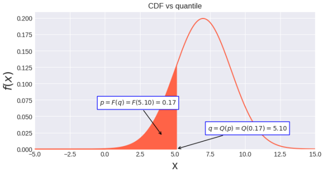

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  Given a probability p (the area under the curve), we are looking for a threshold $x = q$, where $F_X(q)$ is at least p
- In Python (scipy.stats): ppf and cdf
  e.g. `https://docs.scipy.org/doc/scipy/reference/generated/scipy.stats.norm.html`

Q-Q plot (quantile-quantile plot)

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  - Compare two data sets to see if they are from the same distribution (**two-sample tests**)
  - Compare two theoretical probability distributions (less common)

How to make the Q-Q plot

Steps: given two distributions

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  - Compute the quantile q_i^2 of the second distribution at p_i
  - Make a scatter plot of the pair (q_i^1, q_i^2)

Compare two distributions

Example

To answer the question "how do you know if my data follows a Gaussian distribution?" Let us look at your ducks

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

and make the Q-Q plots by calculating the quantiles from your data distribution and a Gaussian distribution with given $\mu = 7$ and $\sigma = 2$.

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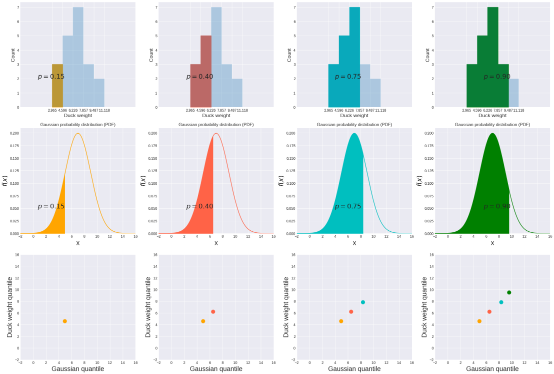
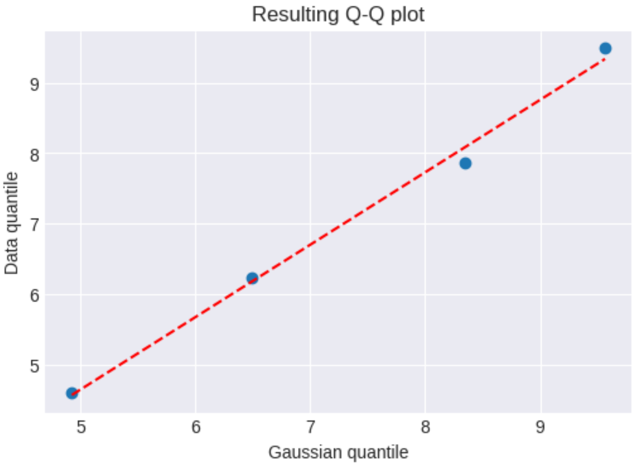
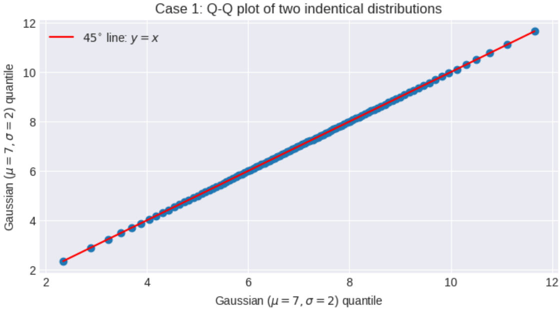


Fit a line to the Q-Q plot



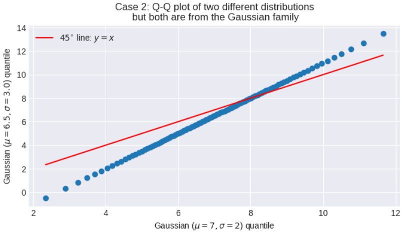
Q-Q plot interpretation: case 1

- Case 1: if the two distributions are identical, the points in the Q-Q plot should follow a 45° straight line $y = x$



Q-Q plot interpretation: case 2

- Case 2: if the two distributions are linearly related, the points in the Q-Q plot follow a straight line that is not necessarily $y = x$



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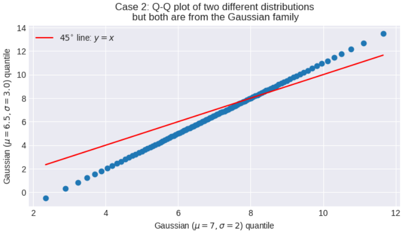

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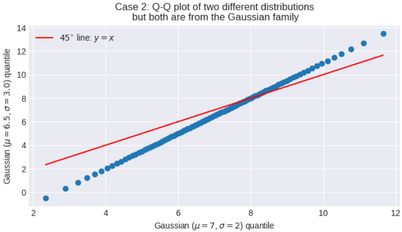
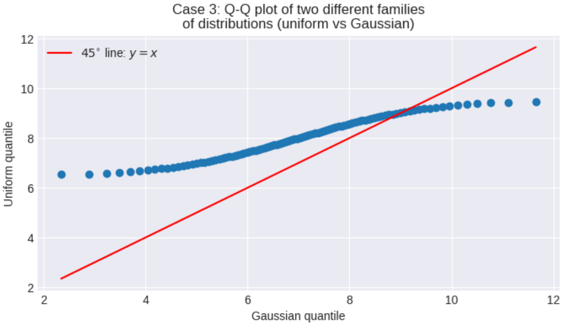


- Note: if one of the two distributions is a theoretical distribution from a **location-scale family** (e.g. Gaussian distributions), it is very likely that the other distribution is from the same family of distributions.
- Example: if the two distributions are 1) a theoretical Gaussian distribution with parameters (μ_1, σ_1) and 2) a data distribution; if the points in the Q-Q plot follow a straight line that is not $y = x$, it is very likely that the data follows a Gaussian distribution with a different set of parameters (μ_2, σ_2).

Q-Q plot interpretation: case 3

- Case 3: if the two distributions are from different families of distributions, the points in the Q-Q plot are not lying on a straight line.



Use the Q-Q plot to find a theoretical probability distribution

Steps:

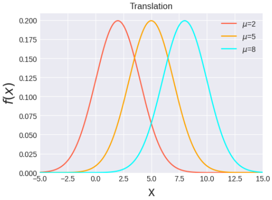
- Given a data set $\mathcal{X} = \{x_1, \cdots, x_N\}$
- Choose several candidate theoretical distributions $D_1, D_2, \cdots$
- Make the Q-Q plot for $\mathcal{X}$ vs D_i for all D_i
- Investigate the resulting Q-Q plots (case 1-3)

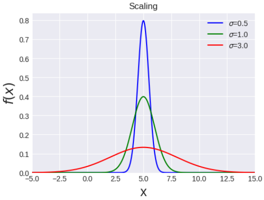
Q-Q plot: additional notes ♫ ♫ for interested readers

- The location-scale family of distributions:
  - You will recognize this when you use the **scipy.stats** library!
  - **A family of distributions**: a set of probability distributions, whose PDF/PMF have the **same functional form** with **different parameters**
  - **Definition**: a location-scale family is a family of distributions formed by translation and scaling of a standard family member, where the CDF G can be written as

$$G(x \mid location, scale) = F\left(\frac{x - location}{scale}\right)$$

    where $location \in (-\infty, \infty)$, $scale > 0$, F is the CDF of a standard family member
  - If a distribution family is a location-scale family, we know that they have nice properties we can use; for instance, the family members are linearly related
  - Gaussian distribution (PDF: $f(x) = \frac{1}{\sqrt{2\pi\sigma^2}} e^{-\frac{1}{2}\left(\frac{x-\mu}{\sigma}\right)^2}$) is a location-scale family





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  - **Example transformations**: power transformation (e.g. Box-Cox transformation, Yeo-Johnson transformation), square root transformation, reciprocal transformation, etc.

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  You can try it out in your project if you want! Does it work as expected? If not, what seems to be the problem?

A note on statistical tests for interested readers

- The Q-Q plot is essentially a visualization technique to check similarities between distributions
- There are more analytical testing techniques for the same purpose, for instance, **z-test**, **t-test**, Kolmogorov-Smirnov test, Wilcoxon's signed-rank test, Mann-Whiteney U test, $\mathcal{X}^2$-test, etc

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- How do you know which test to choose? One can ask the following questions to find an appropriate statistical test to use
  - What are the data types? Categorical? Numerical? Discrete? Continuous?
  - How many variables you have? One? Two? Many?
  - Parametric test or nonparametric test?
  - Are variables independent?
  - Do you want to compare two data distributions or a data distribution against a theoretical probability distribution?
  - If you want to compare two data distributions, are they paired?
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  - ...
- We will revisit this topic soon

Summary

- We used a Q-Q plot to visually verify the hypothesis that the data follows a Gaussian distribution by showing that points in the Q-Q plot follow a straight line
- We learned how to use a Q-Q plot to compare different probability distribution candidates for describing a data set
- Some useful concepts: cumulative distribution function (CDF), quantiles of a theoretical distribution, location-scale family of distributions
- Statistical tests as analytical alternatives to the Q-Q plot

Today

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. This is also known as mathematical modeling.

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.

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  - 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?

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You will get a new duck tomorrow and you will measure its weight when it arrives (exciting!). Can you **predict the probability** of this new duck **weighing between 5 kg and 7 kg** before measuring it?

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  Answer: define two variables $x = (x_1, x_2)$ so that we can pose the question $P(5 \leq \text{weight} \leq 7)$ in a more generic form $P(x_1 \leq \text{weight} \leq x_2)$ and solve the problem **using probabilistic models**
- 3) What is the mathematical function g that relates variables x to the target y? This comes from your (hopefully reasonable) **assumption** - hint: write down your assumption first and then try to construct g
  Answer:
  - Assumption (15 secs): the weight is generated from a theoretical probability distribution - here we assume a Gaussian distribution

    $$\text{weight} \sim \mathcal{N}(\mu, \sigma^2) \text{ , with PDF } f_{\text{weight}}(t) = \frac{1}{\sqrt{2\pi\sigma^2}} e^{-\frac{(t-\mu)^2}{2\sigma^2}} \tag{1}$$

  - Expression (15 secs): given the assumption in Eq. (1), we can write g as

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- 4) Are there any hyperparameters h in the function g? How do we choose them? (5 secs)
  Answer: By looking at Eq. (2), we don't seem to have any hyperparameter here
- 5) What are the unknown parameters θ in g? (10 secs)

Example - modeling walkthrough it's like a video game walkthrough but twice the fun!

You will get a new duck tomorrow and you will measure its weight when it arrives (exciting!). Can you **predict the probability** of this new duck **weighing between 5 kg and 7 kg** before measuring it? Let's answer the five questions!

- 1) What do we want to predict, i.e. what is the target y? (15 secs)
  Answer: $y = P(5 \leq \text{weight} \leq 7)$
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  Answer: By looking at Eq. (2), we don't seem to have any hyperparameter here
- 5) What are the unknown parameters θ in g? (10 secs)
  Answer: From Eq. (2), we see two **unknown** parameters $\theta = (\mu, \sigma)$

Example - modeling walkthrough

- Put everything together, we get our model:

$$y = P(x_1 \leq weight \leq x_2) = g(x_1, x_2; \mu, \sigma) = \int_{x_1}^{x_2} \frac{1}{\sqrt{2\pi\sigma^2}} e^{-\frac{(t-\mu)^2}{2\sigma^2}} dt \tag{3}$$

- As soon as we find the values for μ and σ, we can answer the question by plugging $x_1 = 5$ and $x_2 = 7$ into Eq. (3):

$$y = \int_{5}^{7} \frac{1}{\sqrt{2\pi\sigma^2}} e^{-\frac{(t-\mu)^2}{2\sigma^2}} dt$$

Example - Python implementation

- How do we implement this model in Python?

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- Recall the cumulative distribution function (CDF) function F on page 9

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```
from scipy.stats import norm # Gaussian (normal) distribution
mean = ... # \mu: unknown for now
std = ...  # \sigma: unknown for now
F_x1 = norm.cdf(x=5, loc=mean, scale=std) # CDF at 5
F_x2 = norm.cdf(x=7, loc=mean, scale=std) # CDF at 7
y = F_x2 - F_x1
```

There are many available probability distributions in the scipy.stats library:
https://docs.scipy.org/doc/scipy/reference/stats.html

A nonrigorous note on functions and variables

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

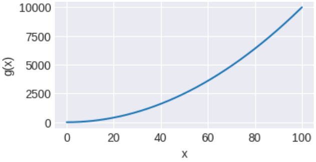
$$y = g(x)$$

- 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:

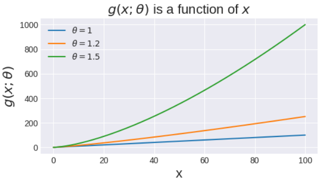
```
# Assume x can take any value between 0 and 100
xmin, xmax = 0, 100
N = 10000 # ideally, N should be infinity. But sadly, computers are discrete
          # so N has to be finite.
x = np.linspace(xmin, xmax, num=N) # all possible values for x
# Plot a function
def g(t):
    return np.power(t, 2)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



A nonrigorous note on functions and variables (cont.)

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

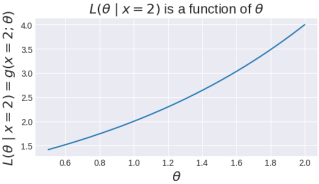
```
def g_theta(t, theta):
    return np.power(t, theta)
xmin, xmax = 0, 100 # assume x can take any value between 0 and 100
N = 10000
x = np.linspace(xmin, xmax, num=N) # all possible values for x
y = g_theta(x, 1)
plt.plot(x, y)
y = g_theta(x, 1.2)
plt.plot(x, y)
y = g_theta(x, 1.5)
plt.plot(x, y)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



A nonrigorous note on functions and variables (cont.)

- Make sure you are comfortable with this
- This is important for understanding the (¡spoiler alert!) **likelihood function**

Summary

- Mathematical modeling is to describe a system with a mathematical expression $y = g(x; \theta \mid h)$ in order to solve a range of problems.
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Practice makes perfect! Try to formulate a problem at hand using these steps to see if you understand them completely! If you have any questions, do not hesitate to ask me!

Today

So far:

- Data types, data containers, descriptive statistics (e.g. sample mean, sample variance, data quantile), visualization (e.g. histogram)
- Probability distributions, sample space, events, random variables, PMF, PDF, parameters
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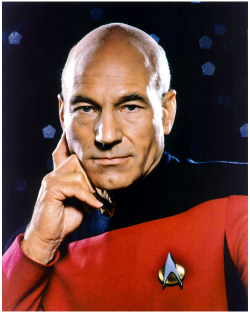
Before next lecture:

- PMF and PDF
- Independent events
- Bayes' rule



Pretty confident