# Lecture 3: Q-Q plot and mathematical modeling

## Statistical Methods for Data Science

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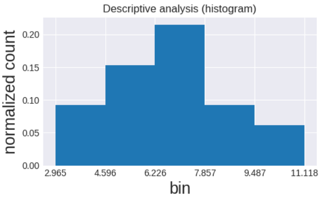
# Today

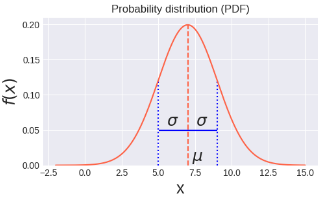
# Learning outcome

- 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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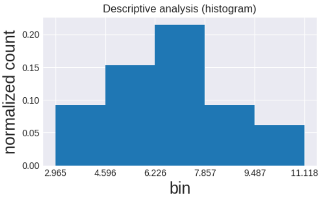


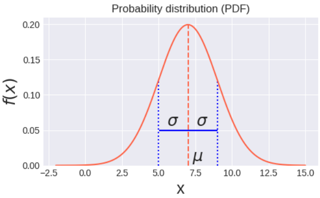


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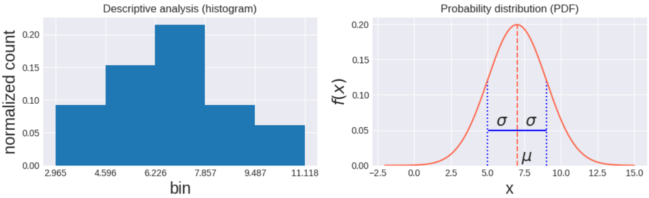


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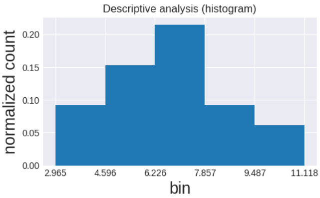


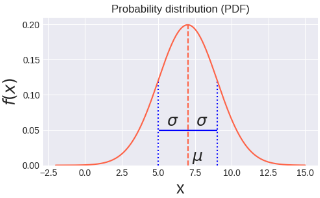


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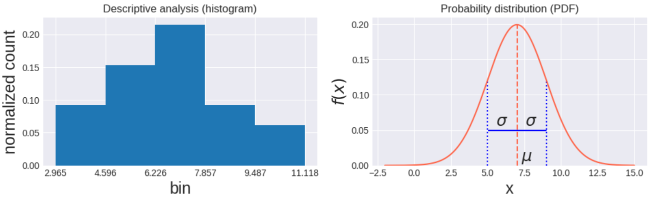


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- ? Question 3: How do I find the unknown parameters?

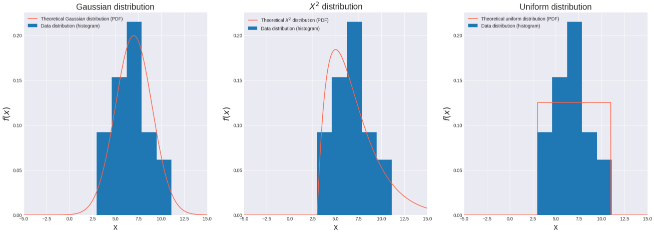
In today's lecture, we are going to address question 2.

# 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

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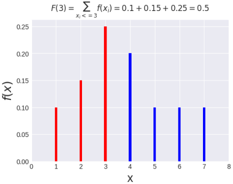
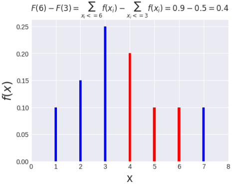
- $X$ discrete random variable:
  - **Definition**: given the PMF $f_X$,

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

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

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



# Terminology alert

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

$$F_X(x) = P(X \leq x)$$

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

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

  - Implication:

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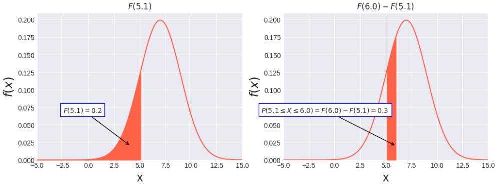
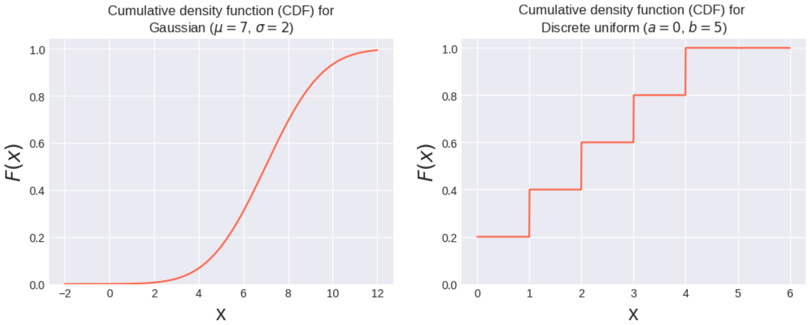


# CDF example plot

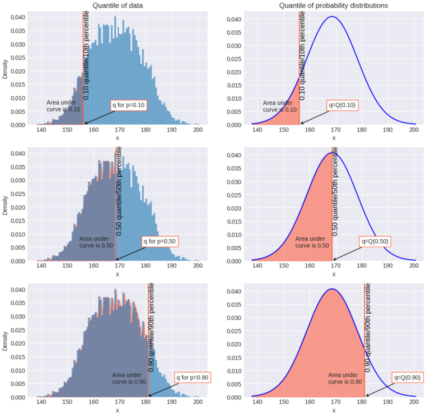


# Quantiles of a theoretical distribution

# 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 $q$
- Theoretical distribution quantile: given $p \in (0, 1)$, $q = Q(p)$ is a $p$-quantile if
  1) $P(X \leq q) \geq p$
  
  and
  
  2) $P(X \geq q) \geq 1 - p$

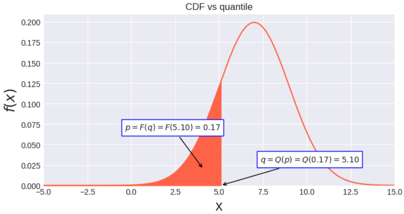
  where $Q$ is called the quantile function.



# Quantile and CDF

- Quantile function $Q$ is the inverse CDF, i.e.

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



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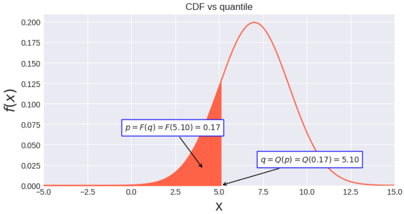


- More precisely, given $p \in (0, 1)$, let $Q(p)$ be the quantile function. Then we have

$$Q(p) = F_X^{-1}(p) = \inf\{x : F_X(x) \geq p\}$$

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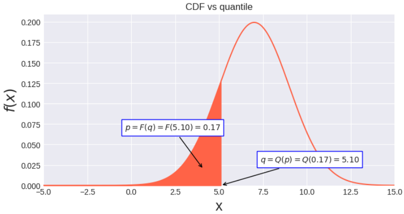


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- In Python (scipy.stats): ppf and cdf
  e.g. `https://docs.scipy.org/doc/scipy/reference/generated/scipy.stats.norm.html`

# 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

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

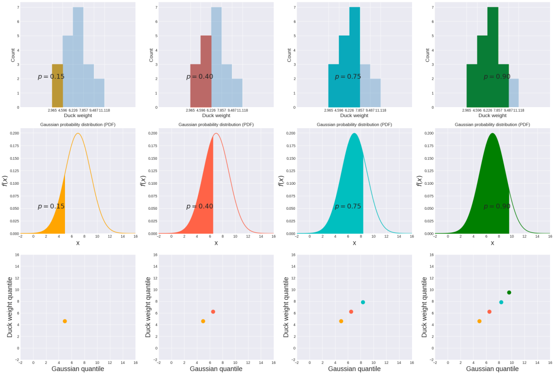
# Compare two distributions

# Example

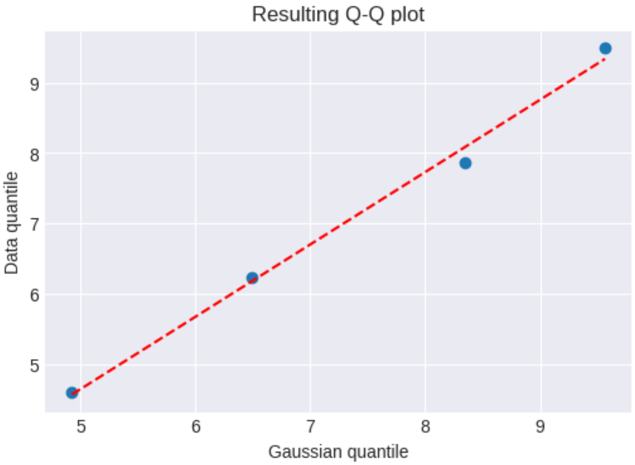
To answer the question "how do you know if my data follows a Gaussian distribution?" Let us look at your ducks

| 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 $\sigma = 2$. Three steps (cf. 16): choose $p = [0.15, 0.40, 0.75, 0.90]$

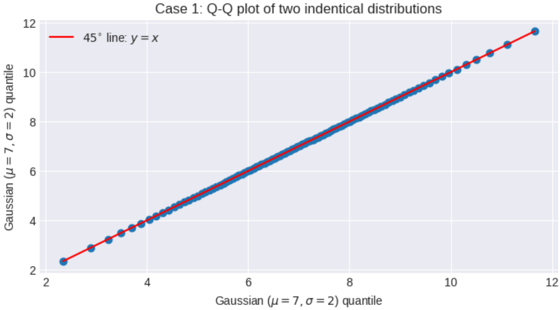


# Fit a line to the Q-Q plot



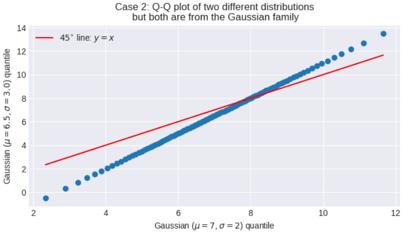
# Q-Q plot interpretation: case 1

- 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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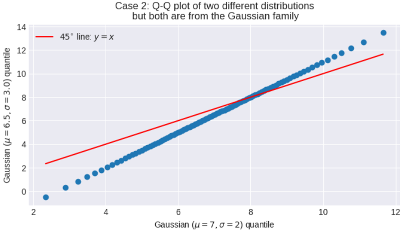


  - Note: if one of the two distributions is a theoretical distribution from a **location-scale family** (e.g. Gaussian distributions), it is very likely that the other distribution is from the same family of distributions.

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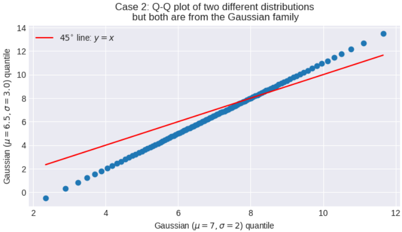
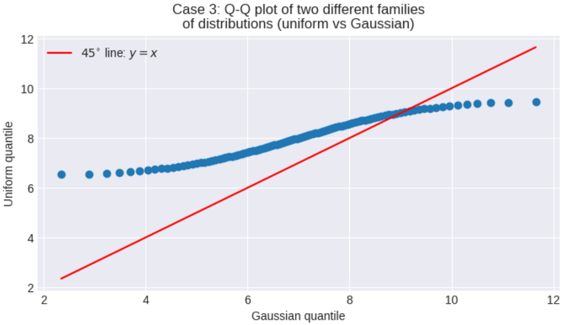



- Note: if one of the two distributions is a theoretical distribution from a **location-scale family** (e.g. Gaussian distributions), it is very likely that the other distribution is from the same family of distributions.
- Example: if the two distributions are 1) a theoretical Gaussian distribution with parameters $(\mu_1, \sigma_1)$ 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 $(\mu_2, \sigma_2)$.

# 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:

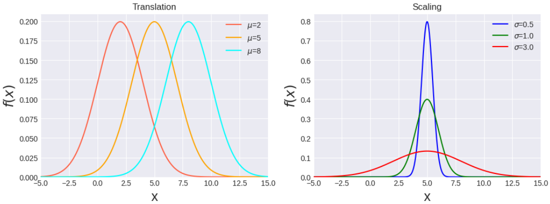
- Given a data set $\mathcal{X} = \{x_1, \cdots, x_N\}$
- Choose several candidate theoretical distributions $D_1, D_2, \cdots$
- Make the Q-Q plot for $\mathcal{X}$ vs $D_i$ for all $D_i$
- Investigate the resulting Q-Q plots (case 1-3)

# 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 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.

    **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?
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    - ...
- We will revisit this topic soon

# Summary

- In this session, we used a Q-Q plot to visually verify the hypothesis that the data follows a Gaussian distribution because the 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: $x$, $y$, $\theta$ 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 $x$?
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  **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 $\mu$ and $\sigma$, we can answer the question by plugging $x_1 = 5$ and $x_2 = 7$ into Eq. (3):

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Note: think about why "weight" is not the variable $x$ in this example?

# Example - Python implementation

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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 $y$:

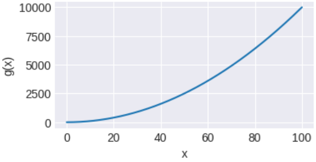
$$y = g(x)$$

- 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 $\theta$ and hyperparameters $h$ to $g$, $g(x; \theta \mid h)$ is still a function of $x$.
- In a plot, the variable should always be on the $x$-axis!
- If we are interested in the behavior of $y$ in terms of $\theta$, we can construct a different function $L$ that takes $\theta$ as the variables $y = L(\theta)$ to relate $\theta$ 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:

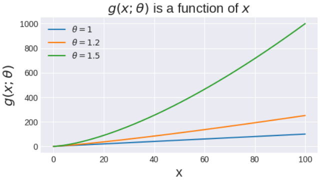
```
# Assume x can take any value between 0 and 100
xmin, xmax = 0, 100
N = 10000 # ideally, N should be infinity. But sadly, computers are discrete
          # so N has to be finite.
x = np.linspace(xmin, xmax, num=N) # all possible values for x
# Plot a function
def g(t):
    return np.power(t, 2)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



# A nonrigorous note on functions and variables (cont.)

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

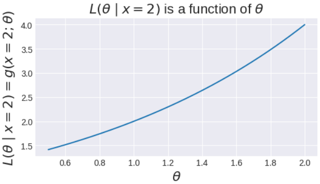
```
def g_theta(t, theta):
    return np.power(t, theta)
xmin, xmax = 0, 100 # assume x can take any value between 0 and 100
N = 10000
x = np.linspace(xmin, xmax, num=N) # all possible values for x
y = g_theta(x, 1)
plt.plot(x, y)
y = g_theta(x, 1.2)
plt.plot(x, y)
y = g_theta(x, 1.5)
plt.plot(x, y)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

1. Compare two distributions using a Q-Q plot
2. Mathematical modeling
3. Summary

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