Print to PDF

# Lecture 1 - Frequentist and Bayesian Overview, Probabilistic Generative Models, and Stan

## Contents



## High-Level Goals of this Course

- Use Bayesian reasoning when modeling data.
- Apply Bayesian statistics to regression models.
- Compare and contrast Bayesian and frequentist methods, and evaluate their relative strengths.
- Use appropriate statistical libraries and packages for performing Bayesian inference.

# Course Overview

- **Non-project MDS course:** eight lectures and four labs.
- Our focus is **model-building**, **computation**, and **interpretation of results**.
- We will build models in `Stan` along with `rstan`.
- Knowing how and when to use different statistical distributions is a **great asset**.
- `R` + `Stan` for lectures and labs.

# Textbook

We will use a textbook in this course. Its name is **Bayes Rules! An Introduction to Applied Bayesian Modeling**). **We will be posting suggested and optional readings of this book before our lecture time.**

# Today's Learning Objectives

1. Review statistical inference (frequentist so far!).
2. Pave the way to Bayesian statistics.
3. Introduce probabilistic generative models.
4. Illustrate the basic use of `Stan` and `rstan` via Monte Carlo simulations.
5. Differentiate probability and likelihood in Statistics.

# Loading Libraries

```r
library(tidyverse)
library(infer)
library(tidyverse)
library(cowplot)
library(datateachr)
library(bayesrules)
```

# 1. Review of Frequentist Statistical Inference

In the frequentist courses, we have used **observed data** (coming from a random sample) to **estimate** and **characterize uncertainty** in **unknown** (or **latent**) **population** quantities of interest. For instance:

- An **unknown** population mean $\mu$.
- An **unknown** population variance $\sigma^2$.
- An **unknown** population median $\mathrm{M}$.

However, what do we mean when we say **latent population** quantities? Let us find it out.

## 1.1. Latent Variables

These latent quantities may be real **but not directly observable**. Hence, they are linked to other observable variables. For example:

- Using online ad click data to estimate the total lifetime revenue.
- Using genome sequencing to infer the origin of a virus during an outbreak.
- Using robotic Light Detection and Ranging (LiDAR) sensors to estimate the robot's position.

Or **completely hypothetical**:

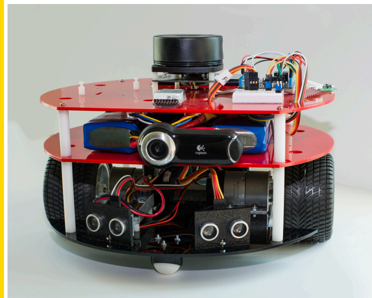
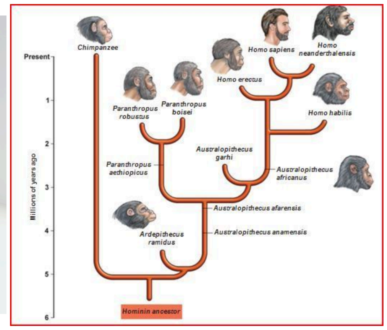
- Using tennis game win/loss data to infer a ranking of players.
- Using text data to learn the underlying hierarchy of topics.

> **Important**
>
> For these inquiries, the frequentist statistician's usual hammers are **point estimates** and **confidence intervals**.

## 1.2. Why Care About Uncertainty?

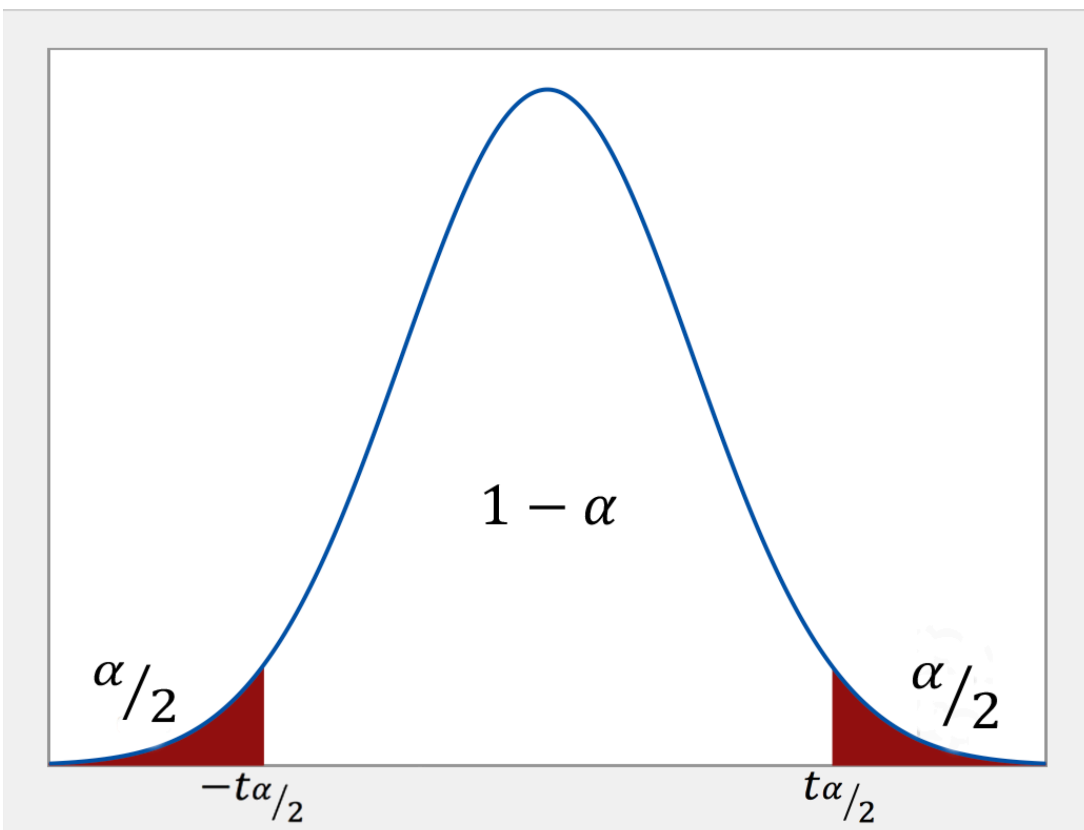
> *Cannot we just collect more data?*

Not if it is **expensive** (e.g., rocket telemetry), **fundamentally limited** (e.g., robot odometry), or **outright impossible** (e.g., ancestral species).


## 1.3. What is a Confidence Interval (CI)?

If we care about uncertainty in a **frequentist** inferential approach, what is a confidence interval?




Let us start with the first **in-class question**.

### Exercise 1

**Answer TRUE or FALSE:**

**Assuming a random sample of size $n$ composed of the random variables** $X_1, X_2, \ldots, X_n$ (not observed sampled values!), a frequentist 90%-confidence interval (CI) is a random interval that contains an unknown fixed population parameter of interest with probability 90% before observing the random data.

**A.** TRUE

**B.** FALSE

**Solution to Exercise 1**

It is **TRUE**. The above statement **theoretically** defines the frequentist random CI in the general context of a random sample composed of $n$ random variables $X_1, X_2, \dots, X_n$. Then in practice, once we **observe** the sampled data, the 90%-CI will either contain or not the unknown **fixed** population parameter of interest, which we aim to infer.

Then, suppose you have a large enough sampling budget to draw a considerable amount of $m$ random samples (i.e., **we rely on a large frequency of events!**) to make inference on your population parameter of interest and compute their corresponding frequentist 90%-CIs. Under the frequentist paradigm, approximately 90% of these $m$ CIs will contain the true **fixed** population parameter of interest (**which is unknown, and we aim to estimate!**).

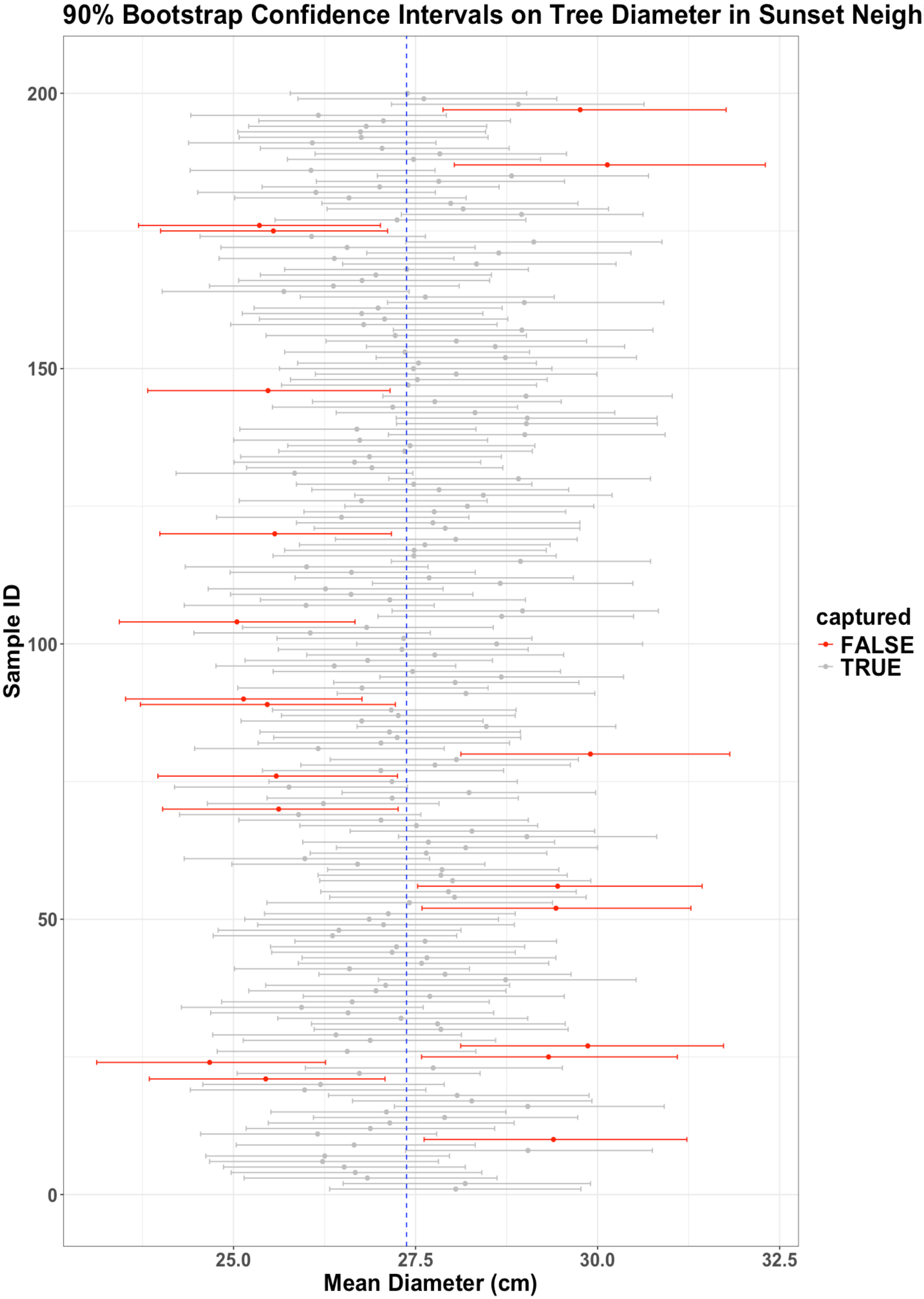
To exemplify this, I will retake **Exercise 4** from **DSCI 552**. For the sake of this review, suppose we want to make inference on the population tree diameter in the `SUNSET` neighbourhood in Vancouver. The dataset `vancouver_trees`, from package `datateachr`, has all population data for this neighbourhood. We can quickly obtain the population tree diameter in `SUNSET` which is $27.38 \text{ cm}$. Again, for the sake of this exercise, let us assume we do not know this population diameter in practice. Hence, we draw $m = 200$ random samples from this population (each with size $n = 400$) and compute the corresponding bootstrap 90%-CIs. The below table and plot indicate the following:

- The plot shows the real population diameter of $27.38 \text{ cm}$ as a blue vertical dashed line. The $m = 200$ 90%-CIs (from random samples of size $n = 400$ each) are plotted as horizontal lines. I highlighted in red those CIs that do not contain the true population mean diameter.
- Using the table, we can see that 90.5% of this $m = 200$ CIs actually captured the true population mean diameter. **That is the concept of the frequentist CI in action!**

▶ Show code cell source

A tibble: 2 × 3

| captured | samples | proportion |
|---|---|---|
| <chr> | <int> | <dbl> |
| FALSE | 19 | 0.095 |
| TRUE | 181 | 0.905 |



90% Bootstrap Confidence Intervals on Tree Diameter in Sunset Neigh
Sample ID
200
150
100
50
0
Mean Diameter (cm)
25.0
27.5
30.0
32.5
captured
FALSE
TRUE

### Exercise 2

**A CI Example with Heights**

Suppose I measure the height $X_i$ $(i = 1, 2, \dots, n)$ of a **simple randomly selected** (i.e., all subjects have the same probability of being selected) subset of students in this room. My **population of interest** is the current MDS cohort.

Assume I know our true population standard deviation $\sigma$, and I want to estimate our unknown mean $\mu$ with the sample mean

$$\bar{X} = \frac{1}{n} \sum_{i=1}^{n} X_i.$$

I design my 95% confidence interval using the Central Limit Theorem (CLT) formula:

$$\bar{X} - 1.96 \frac{\sigma}{\sqrt{n}} \leq \mu \leq \bar{X} + 1.96 \frac{\sigma}{\sqrt{n}},$$

where $1.96$ is the $0.975$-quantile of the Standard Normal distribution.

**Is this a valid confidence interval for $\mu$?**

**A.** Yes.

**B.** No.

### Solution to Exercise 2

No! This is an **asymptotic** CI assuming we have enough data that the sample mean is roughly normal by CLT.

Moreover, our height distribution is probably not unimodal!

Now, let us proceed with an open-ended question.

## Exercise 3

### A Financial CI Example

Say you collect some yearly **log returns** $X_1, \dots, X_n$ for a financial asset, and use $\bar{X} = \frac{1}{n} \sum_{i=1}^{n} X_i$ to estimate the population mean.

But real **log returns** exhibit "very large/small values" much more frequently than a Normal distribution would predict. Your boss knows this and says:

> "I know what we'll do! We'll model each $X_i$ with a Cauchy distribution."

Therefore, you **might** (*well…*) be able to compute a more suitable CI.

Nevertheless, you realize that Cauchy distributions have an undefined variance!

**How do you compute a confidence interval?**

## Solution to Exercise 3

Here, we cannot even use our usual fallback of asymptotic intervals. We could use bootstrapping, but we can do better than that with an alternative inferential tool!

**Important**

As a final thought now, before getting into our Bayesian introduction:

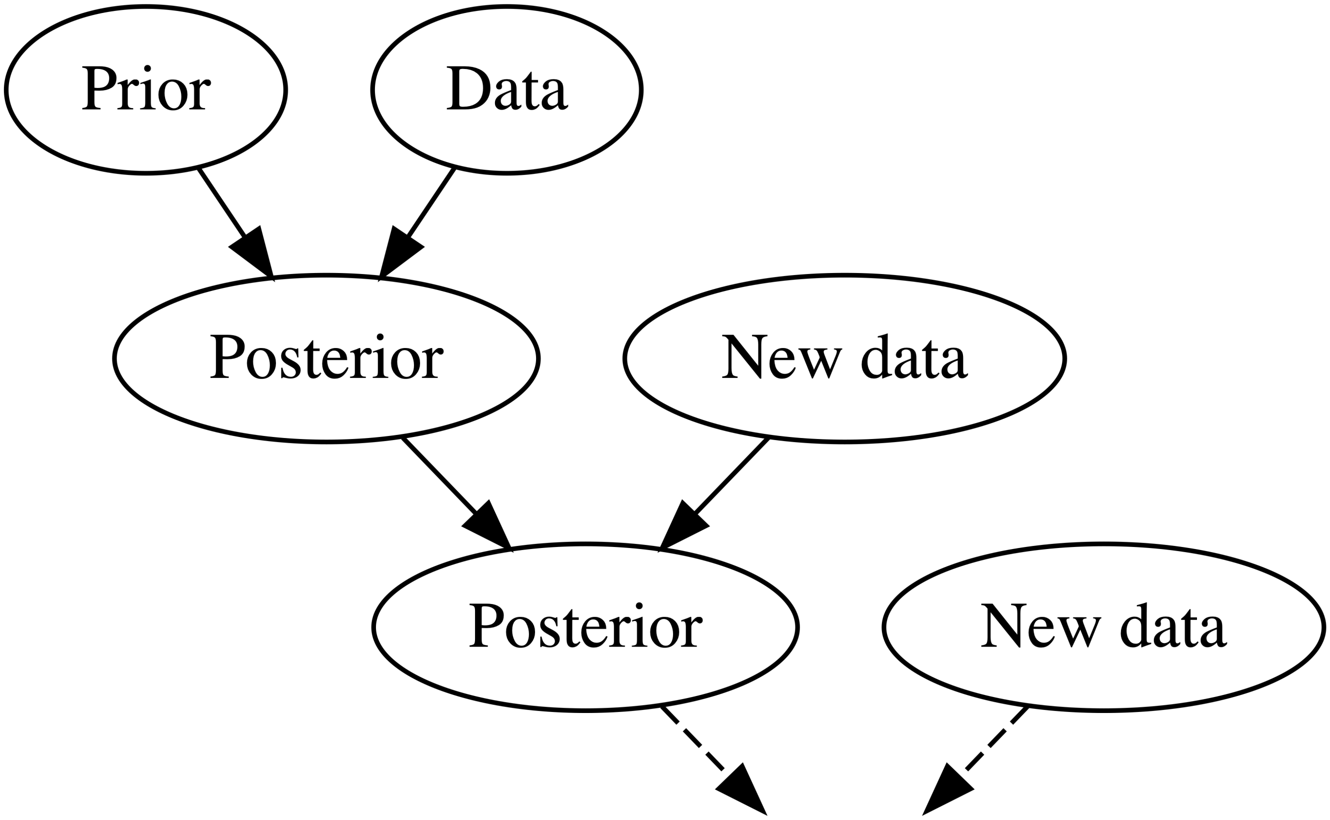
> **Even a minor change to a simple problem makes things significantly harder for frequentist methods!!!!!**

# 2. Bayesian Statistics

The **Bayesian statistical approach** addresses these challenges.

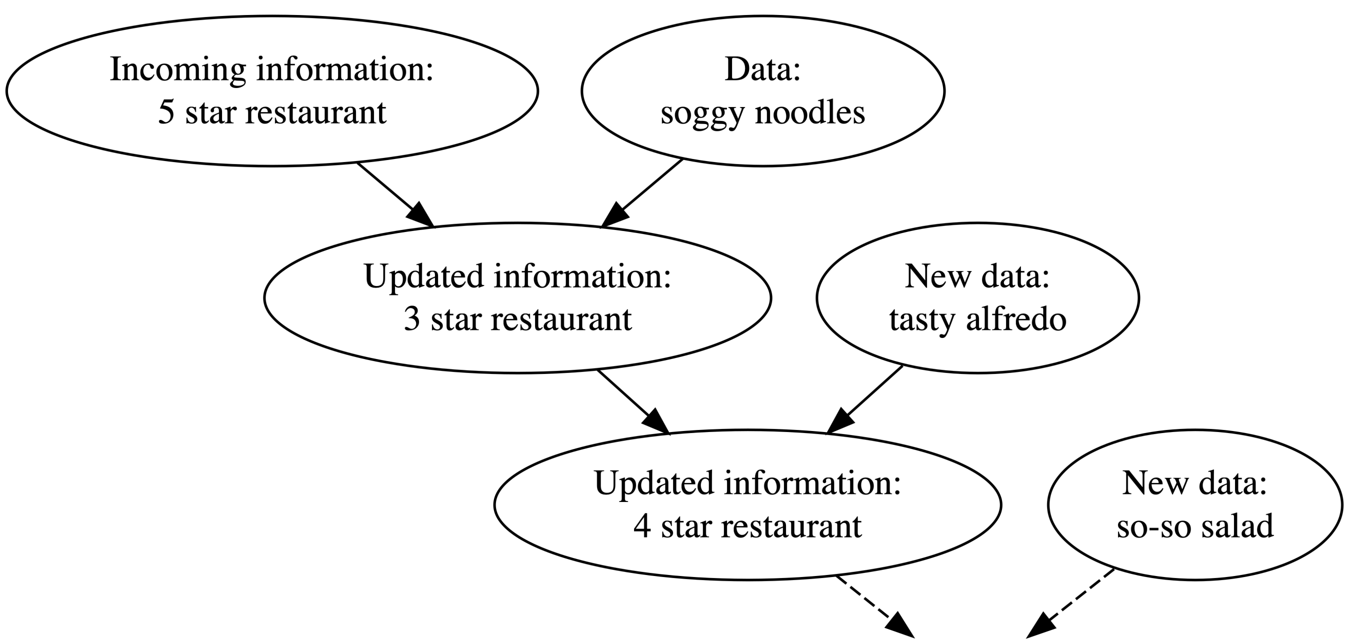
- Very flexible, handles most analysis settings.
    - Missing data, non-standard data types, non-iid, weird loss functions, adding expert knowledge.
    - *Every problem is the same, but your computer might disagree…*
- Valid inference for any (finite) amount of data.
- **Now the population parameters of interest are random variables!** They have prior and posterior distributions.
- Easy to interpret uncertainty for the population parameters.
- Posterior distribution is a "one-stop-shop" for **prediction**, **inference**, **decision-making**, etc.
- Recursive updating.

**What is recursive updating?**




*Source: [Johnson et al. (2021)]*

Let us put this concept with an example of an Italian restaurant:



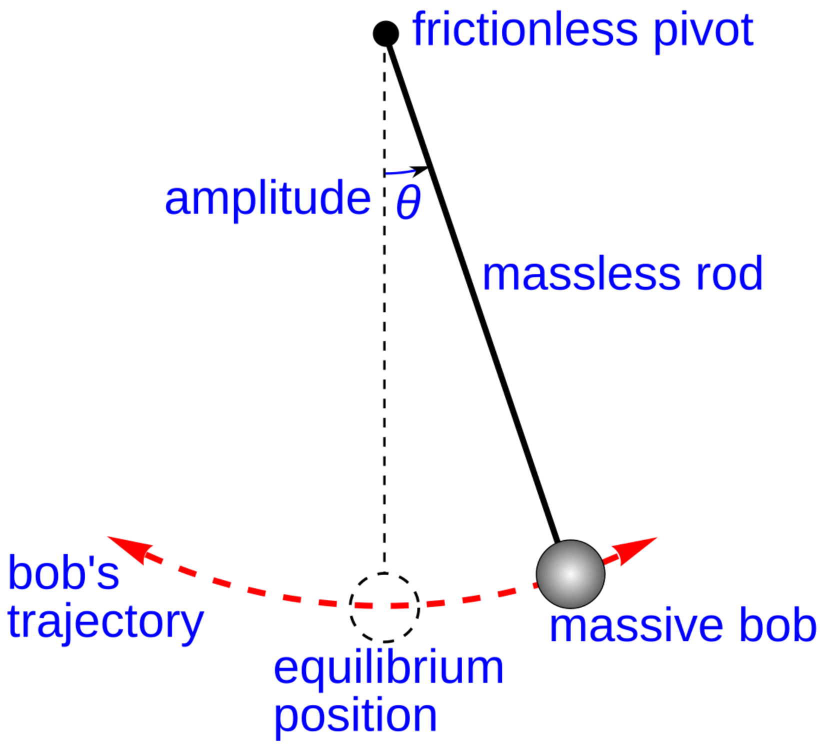
*Source: Johnson et al. (2021)*

> **Attention**
>
> **Nonetheless, there is no free lunch...**
>
> - We would often need to be much more careful about computation.
> - It requires slightly more model design work (prior).
> - Less widely used in some areas of practice, e.g., medicine.
>   - This is changing over time!

# 3. Generative Models

- **For both frequentist and Bayesian statistics**, a generative model is a simplified mathematical model for some reality: a "story about how your data were created."
- The term **generative** means the model can be used to make *synthetic* data (i.e., running computational simulations!)

## 3.1. First Example




Newton's laws of dynamics $F = m \times a$ can be used to simulate position versus time given forces.

- **What if I had noisy measurements of $F$, $m$, *and* $a$ and wanted to infer their true values?**

## 3.2. Second Example

We can model $f(\cdot)$ for whether it will rain today given a vector of **conditions/features** $\mathbf{X}$, $f(\mathbf{X}) \rightarrow \{\text{yes}, \text{no}\}$. What class of response is $f(\mathbf{X})$?

$f(\mathbf{X})$ is Bernoulli type!

Nonetheless, we cannot account for **everything**. Maybe only temperature, pressure, cloud cover, etc. Then, how do we deal with uncertainty in rain even under same measured conditions?

**We can incorporate randomness into this model!** This is analogous to $\varepsilon$ on the right-hand side of a Ordinary Least-Squares (OLS) regression equation.

# 3.3. Probabilistic Generative Models

These models incorporate randomness into the system of interest. We design them using **probability theory** to add **wiggle room** to everything:

- We can incorporate **noise in measurements** (e.g., outputs coming from the $F = m \times a$ model).
- They can be **overly simplified models with incomplete measurements** (e.g., rainy day model).
- They can even incorporate **unobservable latent variables** (e.g., hypothetical tennis rankings).

# 3.4. A Probabilistic Generative Model with a Bottle Cap Flip

You have arrived early to a movie with a friend, and have great seats. However, both of you need to use the washroom. Initially, you decide to flip a coin to see who gets to go first and who will watch the seats.

**But it is 2025 and nobody carries coins any more!** All you have is a bottle cap from your drink:

**Let us start with a FREQUENTIST inferential problem:**

What is the probability $\pi$ the bottle cap will land right side up? We can use $n$ trial tosses as data.

> **Attention**
>
> Let us reflect about the implications of using $n$ trial tosses as data. We will obtain an estimate $\hat{\pi}$ as a relative **frequency** coming from this data. Hence, the name **frequentist**.

**The Math of Generative Model for a Bottle Cap Flip**

Any probabilistic generative model involves setting up your **random variable** of interest along with your assumed distribution.

Thus, we have the following:

$$X_i \sim \text{Bernoulli}(\pi) \quad \text{for} \quad i = 1, \ldots, n.$$

- $\pi \in [0, 1]$ is the **unknown parameter** we want to estimate: **the probability the bottle cap will land right side up**.
- $X_i$ are the results of each bottle cap toss ($1 = \text{right side up}$ or $0 = \text{upside down}$).
- $X_i = 1$ is the success with probability $\pi$.

The **Bernoulli approach** is a **basic model** for this case; we could design another more complex probabilistic model that considers initial conditions, wind, and collisions!

# 4. `Stan` and `rstan` Basics

The bottle cap example was set up as a **FREQUENTIST** inferential problem (*an unknown **FIXED** parameter $\pi$ we aim to estimate*). This probabilistic generative model is a Bernoulli trial.

Since the frequentist approach relies on repeating this bottle cap toss many times to estimate $\pi$, i.e., $n \to \infty$ (**not feasible to do it during our lecture time!**), we will computationally simulate this system with a Monte Carlo simulation in a worksheet (not for marks) during `lab1`.

By definition, a Monte Carlo simulation will computationally repeat the event of interest $n$ times with random inputs to obtain our $n$ outputs of interest (a binary outcome in this case).

We can easily do this via the base `R` function `rbernoulli()` from `purrr`. But we will use this example to introduce `Stan` and `rstan`.

`Stan` is a probabilistic `C++`-based programming language for Bayesian statistical inference (**but it can also perform simple Monte Carlo simulations**). The `R` package `rstan` will allow pulling the simulation outputs from `Stan`.

## 4.1. Coding the Model and Running your Simulation

In general, we will follow these steps:

1. Code up our generative model in `Stan`.
2. Specify observed values of data to estimate using `rstan` (**not necessary for Monte Carlo simulations**).
3. Generate **synthetic data**.
4. Perform inference with your simulation outputs.

**The generative model is all you need (and all you get!)**

- Once you have a generative model, you can derive **everything**: tests, inference, etc.
- If your model **can** generate it, it will be handled in inference:
  - missing data, dependence, complex data types, etc.
- If your model **cannot** generate it, it **will not be handled**.

# 4.2. Can We Theoretically Estimate $\pi$?

Yes, we can! **Maximum likelihood estimation** (MLE) is the standard frequentist approach. Recall the procedure from **DSCI 551's `lecture7`**.

How do we find the maximum likelihood estimate for $\pi$ between 0 and 1?

- We set up the Bernoulli trial for one toss:

$$\ell(\pi \mid x_i) = P(X_i = x_i \mid \pi) = \pi^{x_i}(1-\pi)^{1-x_i} \quad \text{for} \quad x_i = 0, 1.$$

- We obtain the joint likelihood function with $n$ iid tosses:

$$\begin{aligned} \ell(\pi \mid x_1, \ldots, x_n) &= \prod_{i=1}^{n} \pi^{x_i}(1-\pi)^{1-x_i} \\ &= \pi^{\sum_{i=1}^{n} x_i}(1-\pi)^{n-\sum_{i=1}^{n} x_i}. \end{aligned}$$

- Then, the log-likelihood function:

$$\log \ell(\pi \mid x_1, \ldots, x_n) = \sum_{i=1}^{n} x_i \log(\pi) + \left(n - \sum_{i=1}^{n} x_i\right) \log(1-\pi).$$

- We take the first partial derivative of the log-likelihood function with respect to $\pi$, set it to 0, and solve for $\pi$:

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

# 4.3. Uncertainty in $\pi$

**How can we characterize the uncertainty in $\pi$ (without doing boatloads of math)?**

A bootstrap CI might be the answer, but what if we only have $n = 10$ replicates?

```r
options(repr.matrix.max.rows = 10)
library(purrr)
library(tidyverse)
library(infer)

# Obtaining sample of size n = 10
set.seed(553)
sample_n10 <- tibble(flip = as.character(rbernoulli(n = 10, p = 0.7)))
sample_n10
```

```
Warning message:
“`rbernoulli()` was deprecated in purrr 1.0.0.”
```

A tibble:

10 × 1

| flip |
|---|
| <chr> |
| TRUE |
| TRUE |
| TRUE |
| TRUE |
| TRUE |
| TRUE |
| TRUE |
| TRUE |
| FALSE |
| TRUE |

```
# Obtaining bootstrap distribution via infer
set.seed(553)
bootstrap_distribution <- sample_n10 |>
  specify(response = flip, success = "TRUE") |>
  generate(reps = 1000, type = "bootstrap") |>
  calculate(stat = "prop")
mean_stat <- mean(bootstrap_distribution$stat)
mean_stat

# Obtainig percentile 95% CI
percentile_CI <- bootstrap_distribution |>
  get_confidence_interval(level = 0.95, type = "percentile")
percentile_CI
```

0.8967

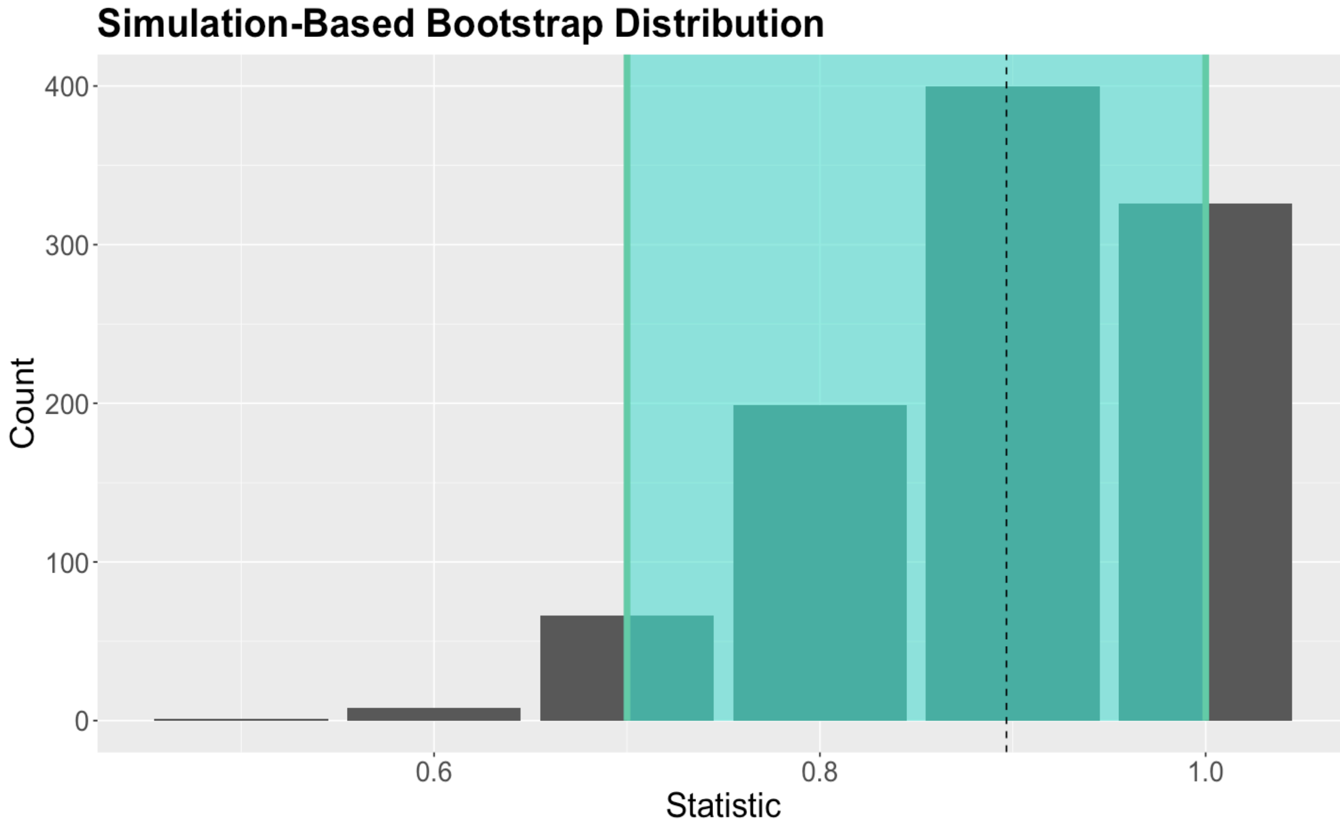
A tibble: 1 × 2

| lower_ci | upper_ci |
|---|---|
| <dbl> | <dbl> |
| 0.7 | 1 |

```
options(repr.plot.height = 7, repr.plot.width = 12)

bootstrap_plot <- bootstrap_distribution |>
  visualize(bins = 6) +
  shade_confidence_interval(endpoints = percentile_CI) +
  geom_vline(xintercept = mean_stat, linetype = "dashed") +
  theme(
    plot.title = element_text(size = 24, face = "bold"),
    axis.text = element_text(size = 17),
    axis.title = element_text(size = 21)
  ) +
  labs(x = "Statistic", y = "Count")

bootstrap_plot
```




> **Important**
>
> Our 95% bootstrap CI shows **biased results**; the lower bound is 0.7! This is not good from an inferential perspective. An easy solution would be increasing the sample size $n$, but what if this is not possible?
>
> **Bayesian inference will open up our set of possible solutions to this matter.**

# 5. Difference between Probability and Likelihood

It is important to emphasize that in Statistics, **probability** and **likelihood** are **NOT** the same. In general, **probability** refers to the chance that some outcome of interest will happen for a particular random variable. Note a probability is always bounded between $0$ and $1$. Conversely, **given some observed data**, a **likelihood** refers to how **plausible** a given **distributional parameter** is. Furthermore, a likelihood is not bounded between $0$ and $1$.

Let us explore this concept via the Binomial distribution. Let $X$ be the number of succcesses after $n$ independent Bernoulli trials with probability of success $0 \leq \pi \leq 1$. Then, $X$ is said to have a Binomial distribution:

$$X \sim \text{Binomial}(n, \pi).$$

A Binomial distribution is characterized by the probability mass function (PMF)

$$P(X = x \mid n, \pi) = \binom{n}{x} \pi^x (1 - \pi)^{n-x} \quad \text{for} \quad x = 0, 1, \dots, n. \tag{1}$$

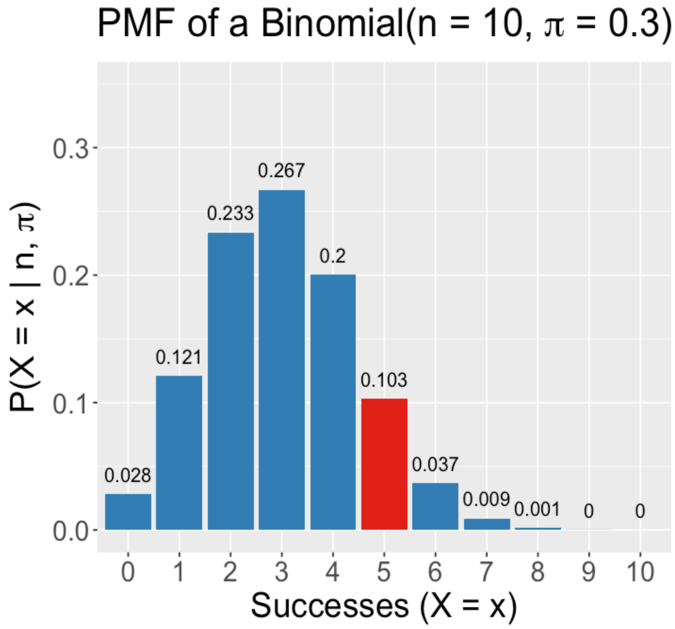
Term $\binom{n}{x}$ indicates the total number of combinations for $x$ successes out of $n$ trials:

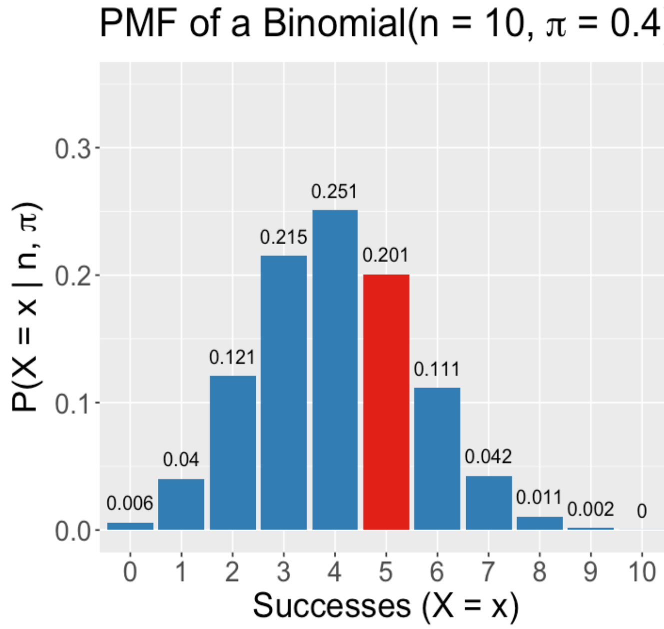
$$\binom{n}{x} = \frac{n!}{x!(n-x)!}.$$

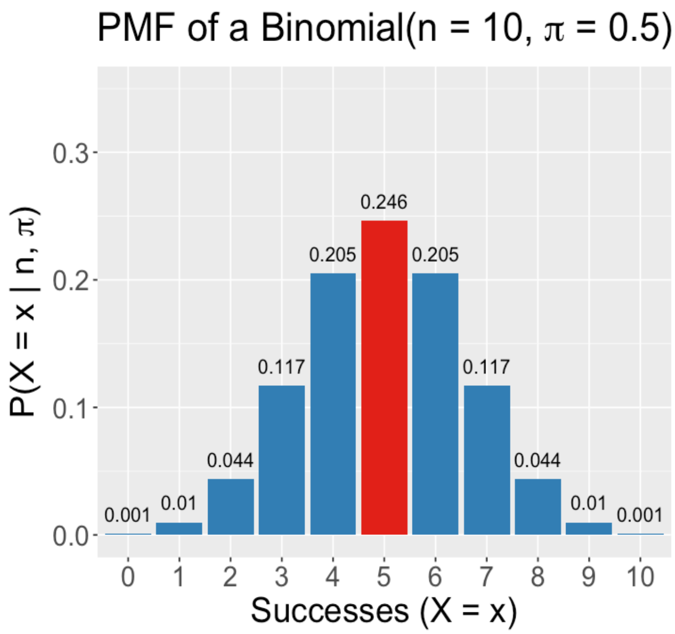
Let us plot the PMFs of six Binomial random variables. Note these plots indicate a **probability** $P(X = x \mid n, \pi)$ on their $y$-axes and they have the same number of trials $n = 10$:

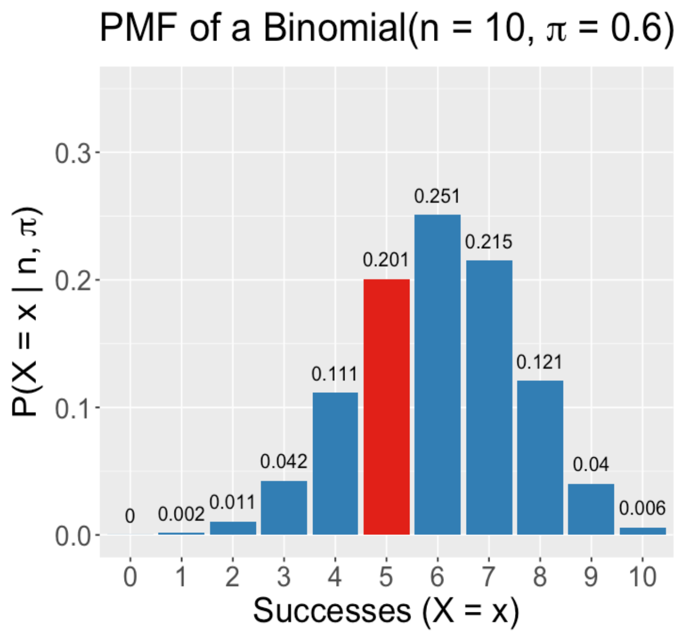
- $n = 10$ and $\pi = 0.3$.
- $n = 10$ and $\pi = 0.4$.
- $n = 10$ and $\pi = 0.5$.
- $n = 10$ and $\pi = 0.6$.
- $n = 10$ and $\pi = 0.7$.
- $n = 10$ and $\pi = 0.8$.

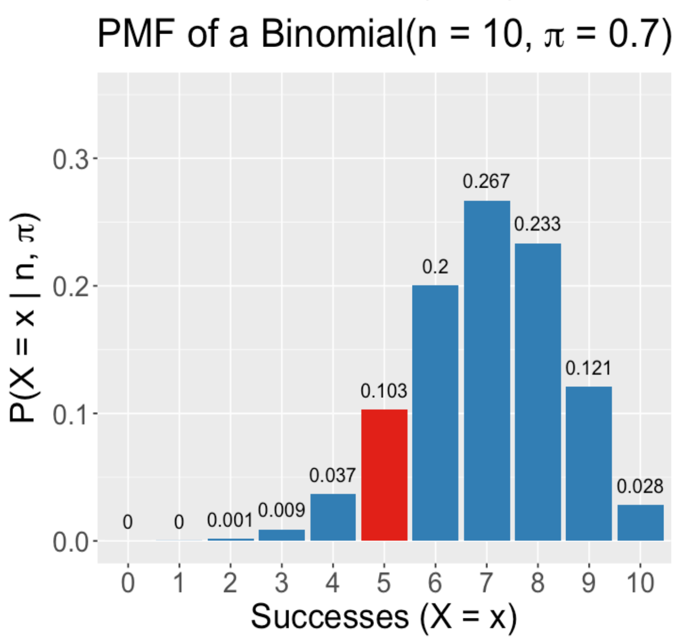
Suppose we are specifically interested in the outcome $Y = 5$, highlighted as a red bar in the six PMFs. We also indicate the **probabilities** associated to each outcome on top of each bar.

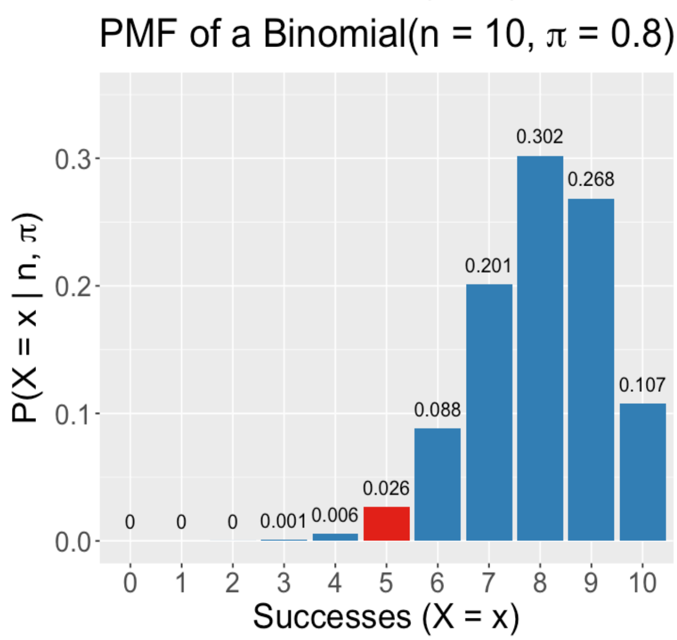

PMF of a Binomial(n = 10, π = 0.3)
P(X = x | n, π)
Successes (X = x)
0.028 0.121 0.233 0.267 0.2 0.103 0.037 0.009 0.001 0 0


PMF of a Binomial(n = 10, π = 0.4)
P(X = x | n, π)
Successes (X = x)
0.006 0.04 0.121 0.215 0.251 0.201 0.111 0.042 0.011 0.002 0


PMF of a Binomial(n = 10, π = 0.5)
P(X = x | n, π)
Successes (X = x)
0.001 0.01 0.044 0.117 0.205 0.246 0.205 0.117 0.044 0.01 0.001


PMF of a Binomial(n = 10, π = 0.6)
P(X = x | n, π)
Successes (X = x)
0 0.002 0.011 0.042 0.111 0.201 0.251 0.215 0.121 0.04 0.006


PMF of a Binomial(n = 10, π = 0.7)
P(X = x | n, π)
Successes (X = x)
0 0 0.001 0.009 0.037 0.103 0.2 0.267 0.233 0.121 0.028


PMF of a Binomial(n = 10, π = 0.8)
P(X = x | n, π)
Successes (X = x)
0 0 0 0.001 0.006 0.026 0.088 0.201 0.302 0.268 0.107

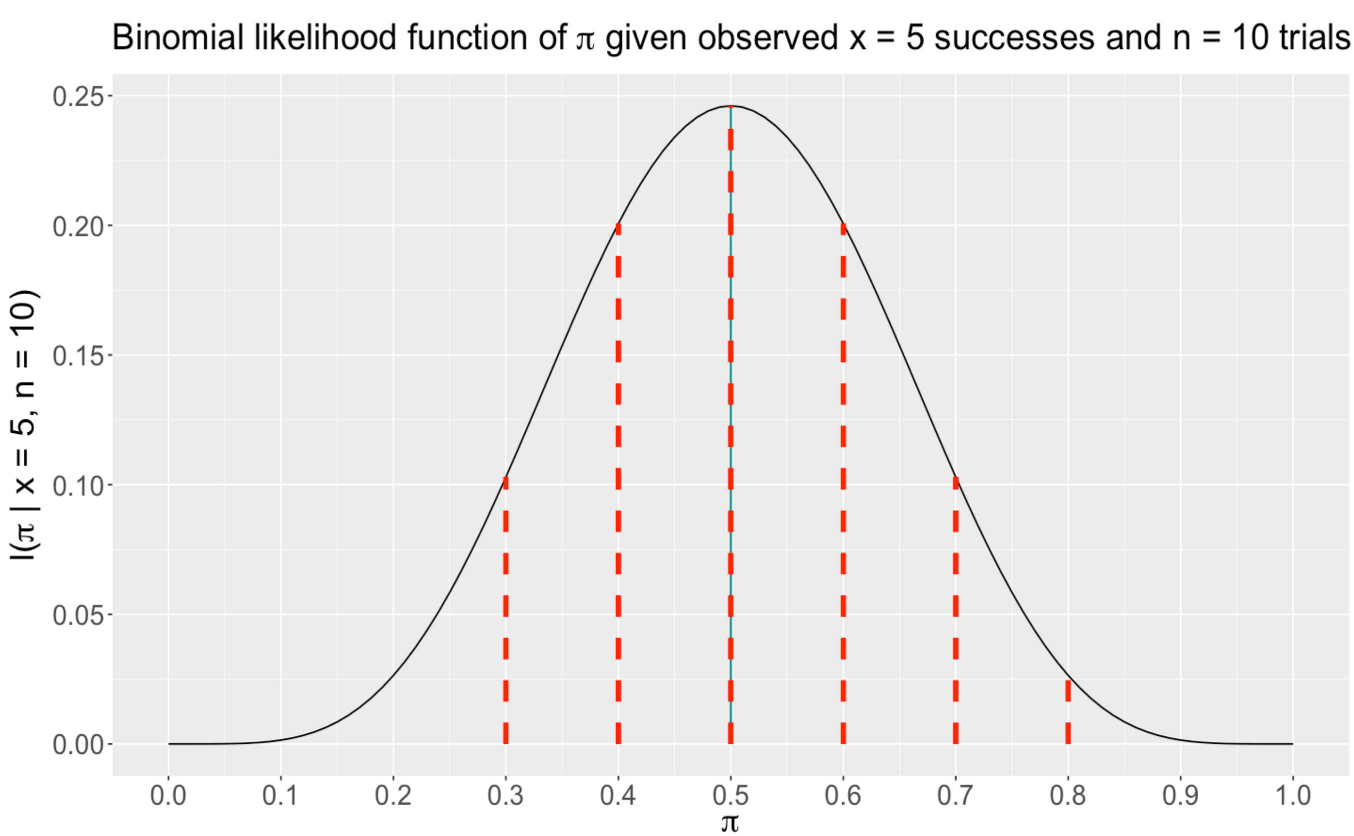
Suppose we sample data from a given Binomial population of interest, and this sample is composed of $n = 10$ trials and $x = 5$ successes. Under a frequentist paradigm, we are interested in inferring that value of $\pi$, which is the **most likely** for these values of $n$ and $x$. Then, this is what we can do:

- Our PMF (1) will become a likelihood function **given** $n = 10$ and **our observed** $x = 5$ successes (note the lowercase $x$):

$$\begin{aligned} \ell(\pi \mid x = 5, n = 10) &= P\left(X = 5 \mid n = 10, \pi\right) \\ &= \binom{10}{5} \pi^5 (1 - \pi)^{10-5}. \end{aligned} \tag{2}$$

> **Attention**
>
> The likelihood (2) is **mathematically** equal to the Binomial PMF with $n = 10$ and $X = 5$. Nevertheless, this likelihood is now **in function** of the parameter $\pi$.

- That said, the below plot shows the likelihood function (2) with the plausible range of $\pi$ on the $x$-axis (which is bounded between $0$ and $1$ since it is the probability of success in the Binomial distribution). Moreover, the likelihood values are indicated in the $y$-axis.



In the above likelihood plot, we highlighted as red vertical dashed lines those values corresponding to the red bars in the previous six Binomial PMFs (**since a probability is MATHEMATICALLY equal to a likelihood, but not STATISTICALLY**).

The plot shows that the likelihood function (2) gets maximized when $\pi = 0.5$. That said, given our observed collected sample with $x = 5$ successes with $n = 10$, a value of $\pi = 0.5$ is **the most plausible (or likely!)** in this Binomial population.

# 6. Wrapping Up with Frequentist Drawbacks

- We cannot incorporate our “expert” intuition, probabilistically speaking.
- How do we use side information, e.g., results of flips from other bottle caps?
- Asymptotic tools tend not to work well with small amounts of data.