Exercises with Estimation

EES 4891/5891

Probability & Statistics for Geosciences

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Learning Goals

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- Understand what Bayes’s theorem means
- Understand the different terms:
  - Likelihood
  - Prior distribution
  - Evidence
  - Posterior distribution
- Understand how Bayesian methods iteratively improving estimates as you get more data.
- Understand difficulties in applying Bayesian methods
  - Choosing priors
  - Solving integrals
- Recognize the major methods for solving Bayesian integrals
  - Conjugate Priors
  - Monte-Carlo
- Understand differences between Bayesian and Maximum Likelihood estimation.
  - Bayesian *credibility interval* estimates vs. frequentist *confidence interval* estimates

Getting Started

Getting Started

- Go to the GitHub Classroom assignment at https://classroom.github.com/a/q_7M5SKb and accept the assignment

- Open RStudio and create a project using version control from the GitHub repository for your assignment.

Semester Project

- I will post the assignment later this week
- The big picture is:
  - You will pick a data set you're interested in.
  - I can meet with you or consult by email to help you
  - You will examine the variables in your data set:
    - What is the distribution like?
    - Can you estimate parameters for the distribution?
  - Use the data set to ask research questions:
  - Write a report describing your data set and what you learned from it

- Examples of Research Questions:
  - Are variables for some parts of the data set distributed differently from others?
    - e.g., was the distribution of droughts different in the Little Ice Age than in the Medieval Warm Period?
    - Use statistical tests for difference
  - Is there a relation between different variables?
    - Covariance and Correlation
    - Regression Analysis
    - Principal Components Analysis
  - Are there spatial or temporal patterns?
    - Seasonality
    - Autocorrelation

Bayesian Estimation

The Problem with Likelihood

- Likelihood $L(X|\theta) = L(x_1, x_2, \ldots, x_N|\theta)$ tells you the probability that you will observe data x_i if the parameter θ has a certain value.
- What you really want to know is the probability $P(\theta|X)$ that the parameter θ will have a certain value if you observe data $x_1, x_2, \ldots, x_N$.
- Bayes's Theorem relates this probability to the likelihood:

$$\underbrace{P(\theta|X)}_{\text{Posterior}} = \frac{\overbrace{P(X|\theta)}^{\text{Likelihood}} \; \overbrace{P(\theta)}^{\text{Prior}}}{\underbrace{P(X)}_{\text{Evidence}}}$$

- The textbook provides alternate names:
  - The likelihood $P(X|\theta)$ can also be called the *data distribution*
  - The evidence $P(X)$ can also be called the *marginal distribution*
  - *Posterior* and *prior* are short for *posterior distribution* and *prior distribution*
- This points out a big challenge: If you use *maximum likelihood estimation* to estimate the value of θ, you don't know the probability that the result θ_{MLE} is the true value of θ unless you also know the *prior* $P(\theta)$ and the *evidence* $P(X)$

Bayes's Theorem

- Bayes's Theorem:

$$\underbrace{P(\theta|X)}_{\text{Posterior}} = \frac{\overbrace{P(X|\theta)}^{\text{Likelihood}} \quad \overbrace{P(\theta)}^{\text{Prior}}}{\underbrace{P(X)}_{\text{Evidence}}}$$

  - What do the *posterior*, *likelihood*, *prior* and *evidence* mean?
    - **Likelihood:** $P(X|\theta)$ is the probability that you would observe data X if θ has a certain value.
    - **Prior:** $P(\theta)$ is the probability distribution for θ, based on everything you knew *before* you make new observations.

- What do the *posterior*, *likelihood*, *prior* and *evidence* mean?
  - **Evidence:** $P(X)$ is the probability of observing X, regardless of the value of θ. It can be written

$$P(X) = \int_{-\infty}^{\infty} P(X|\theta)P(\theta)\,\mathrm{d}\theta,$$

    The integral of the *likelihood* times the *prior*.
  - **Posterior:** $P(\theta|X)$ is an updated probability distribution for θ, incorporating the new information you learned from your observations X.

Interpreting Bayes's Theorem

- You start out with some sense of the plausible range of values for θ, and maybe that some values are more likely than others.
  - This is your *prior*.
- You make a new measurement.
  - Use the new measurement to update your *prior* into a *posterior*
- Now the *posterior* from your previous measurement becomes the *prior* for your next measurement.
  - Use the new measurement to update your current *prior* into a new *posterior*.
- Repeat:
  - Every time you make a new measurement, you use the previous *posterior* as the *prior* and combine that with the new data to create an updated *posterior*.

Example: What Fraction of the Earth is Water?

What Fraction of the Earth is Water?

- You have a globe and want to figure out what fraction of the earth's surface is water.
- Toss the globe in the air, catch it, and note whether your index finger is on water or land: outcomes are *W* and *L*.
- At every toss, use Bayes's theorem to update your estimate of the fraction that is water.

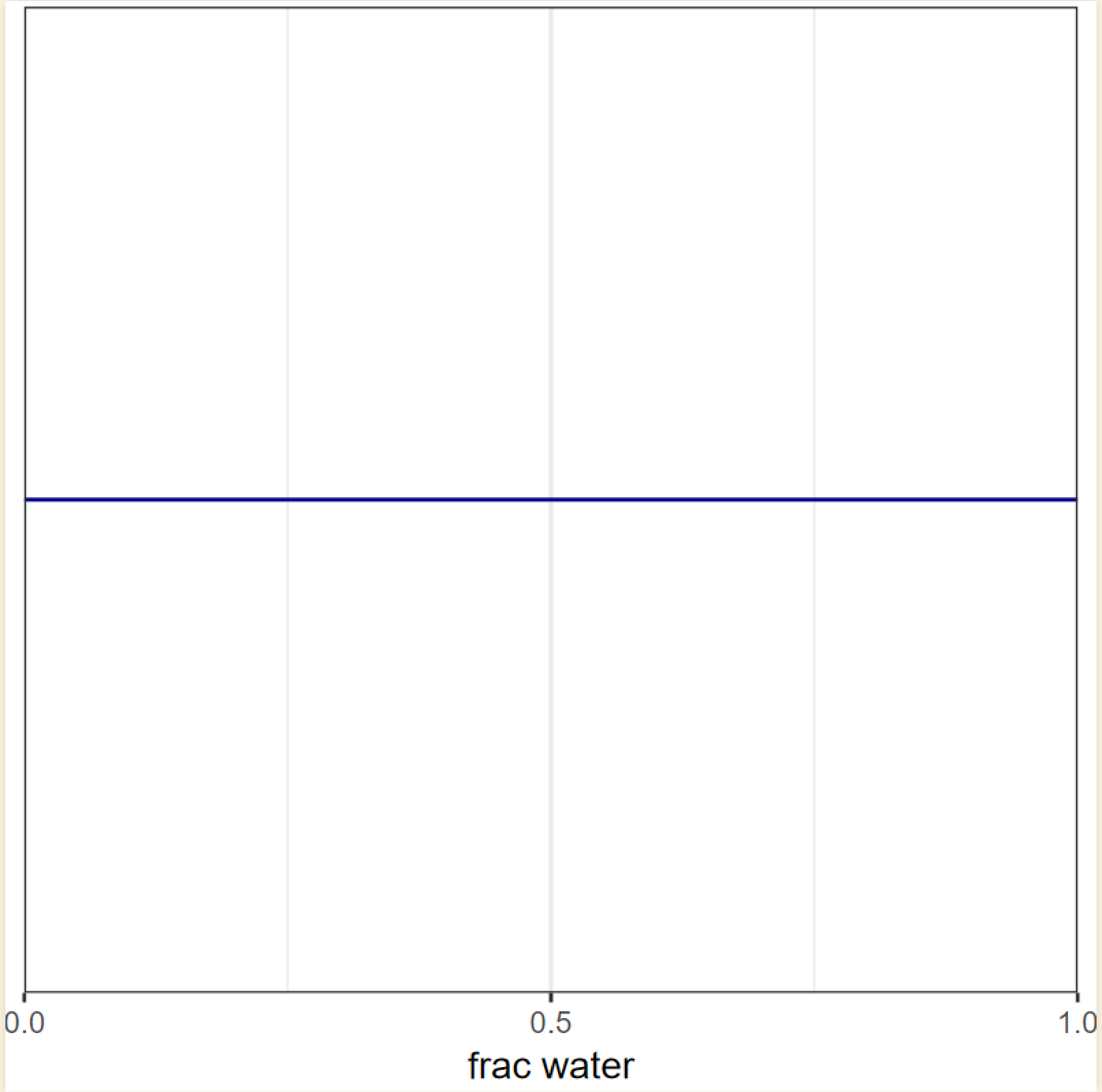
First toss

- θ is the fraction of the earth's surface covered by water
- Before the first toss, pick a prior probability distribution for the fraction that's water.
- Suppose we don't know anything.
  - Pick $\mathbb{P}(\theta) = \mathbf{Uniform}(0, 1)$, a uniform prior:
- Toss the globe and your finger lands on water.
- Update the probability:

$$P(\theta|W) = \frac{P(W|\theta)P(\theta)}{p(W)},$$

where p is the probability of water, and W is measuring water.

Prior:



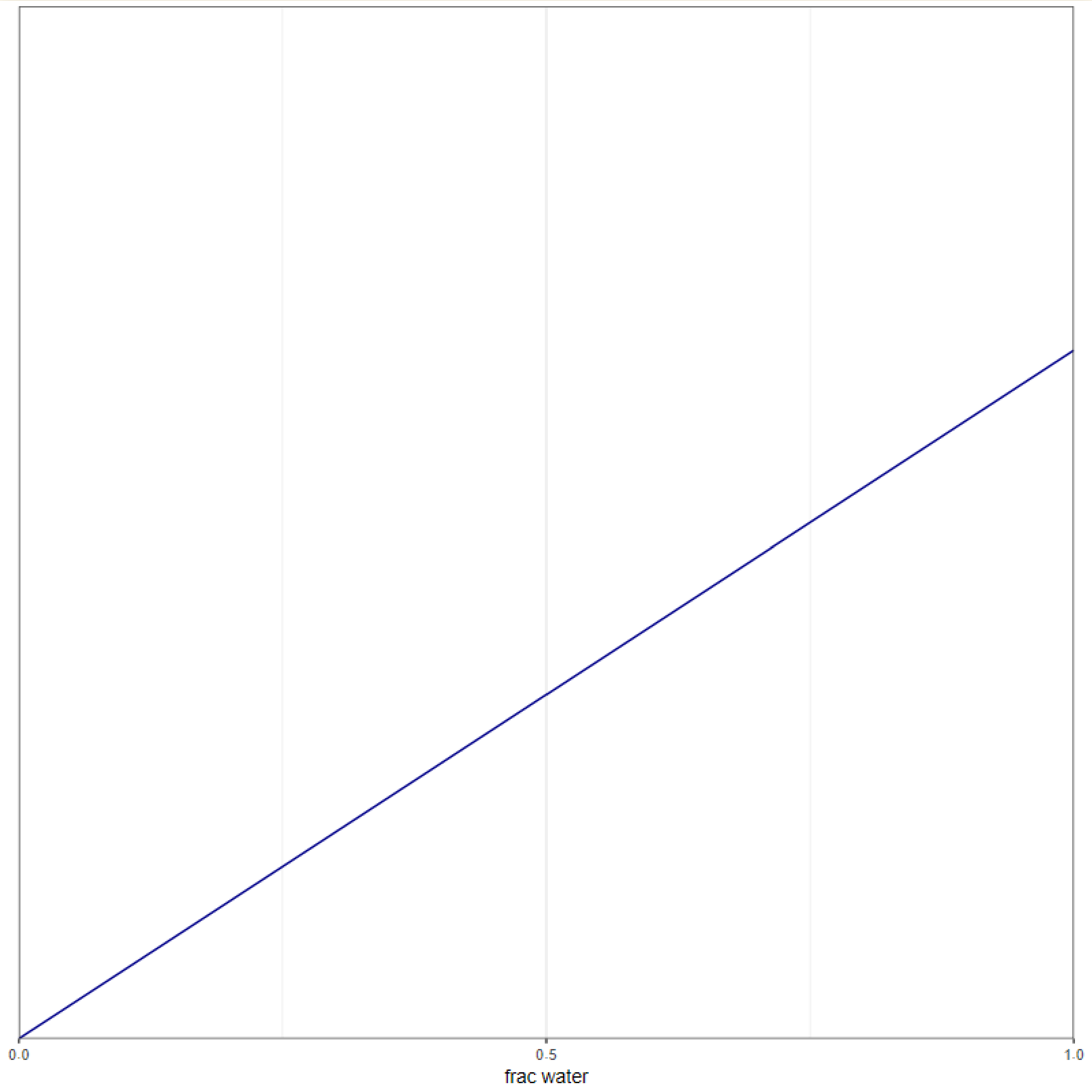
The calculation:

$$P(\theta|W) = \frac{P(W|\theta)P(\theta)}{P(W)},$$

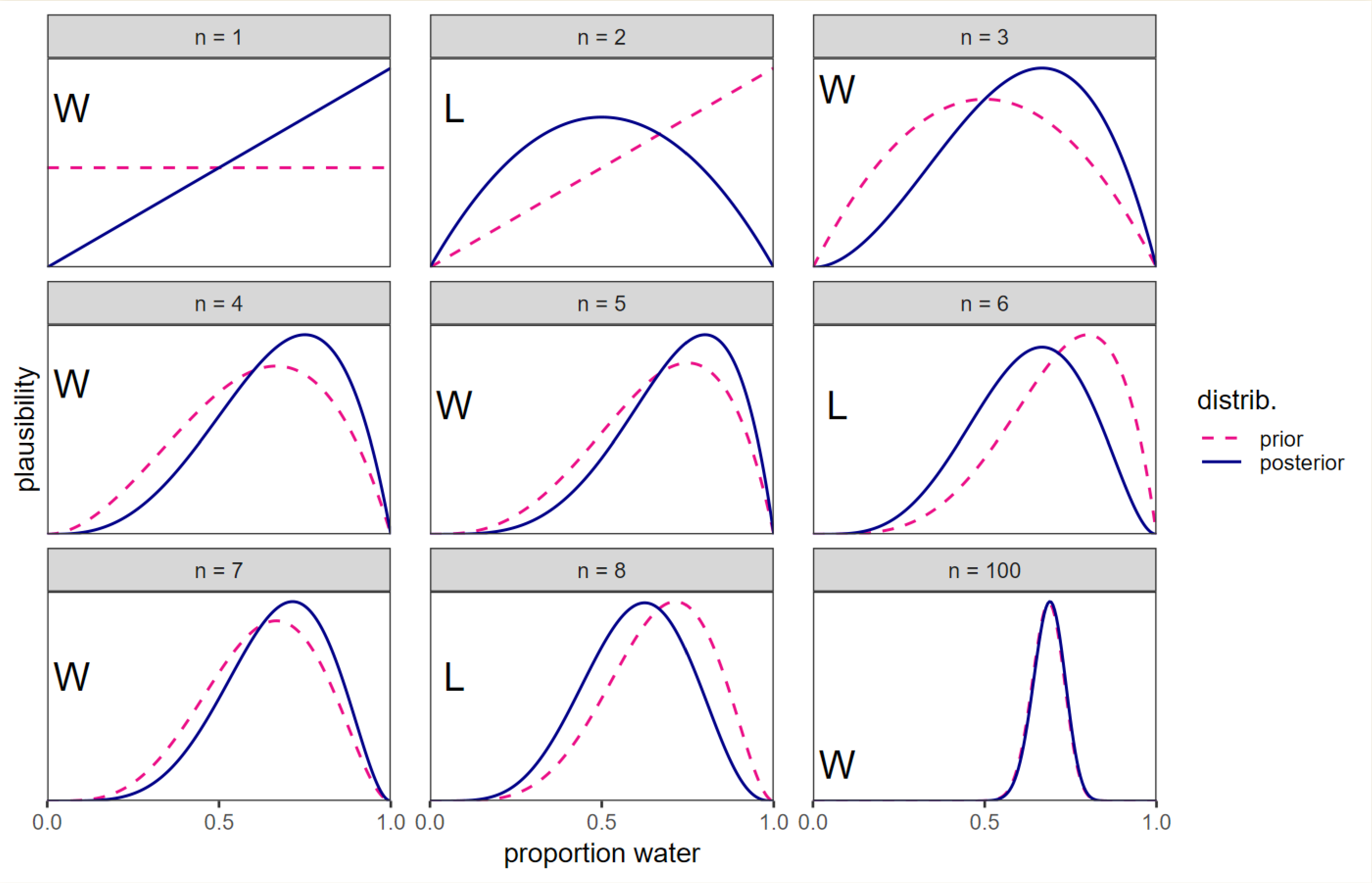
- $P(W|\theta) = \theta$
- $P(\theta) = 1$ (it's a uniform distribution

$$P(W) = \int_0^1 P(W|\theta)P(\theta)\,\mathrm{d}\theta = \int_0^1 \theta \times 1\,\mathrm{d}\theta$$
$$= \left.\frac{\theta^2}{2}\right|_0^1 = \frac{1}{2}$$

- so the posterior $P(\theta|W) = 2\theta$
- Use this posterior as the prior for the next toss...

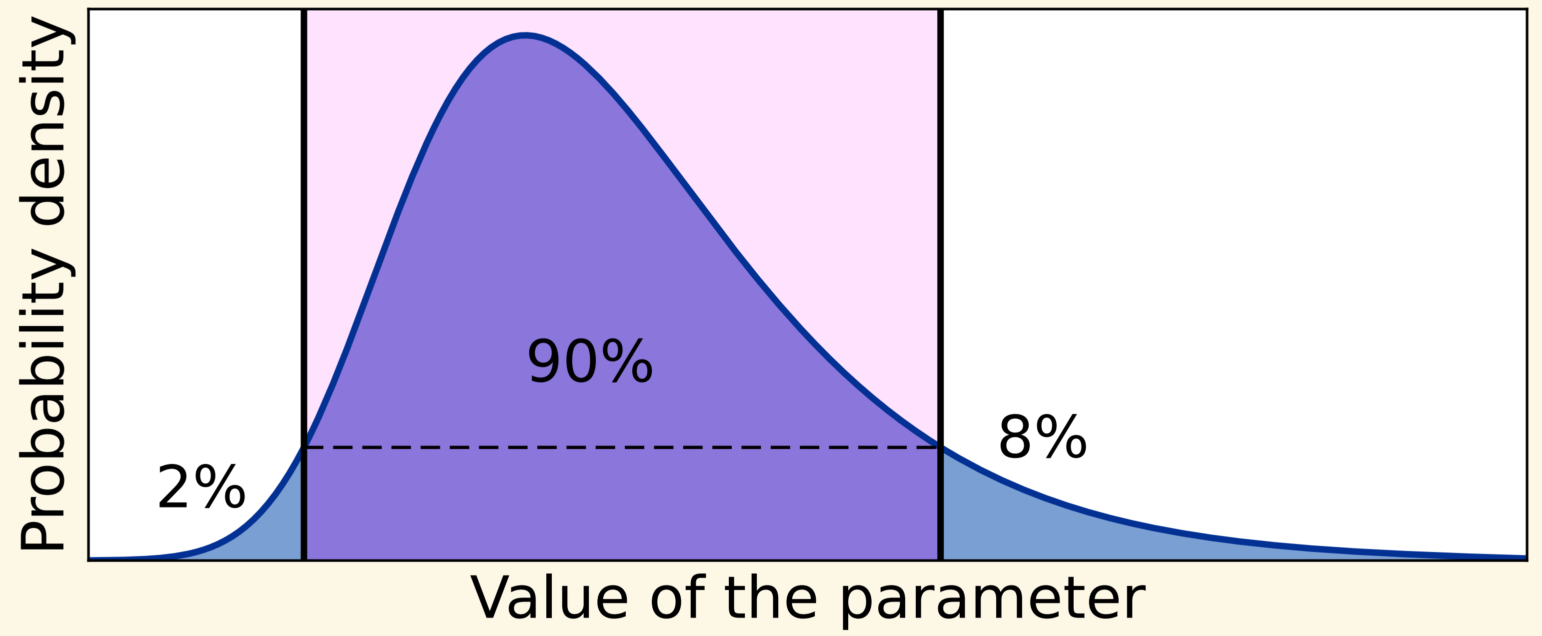


Subsequent tosses



Bayesian Estimation:

- Maximum Likelihood Estimation gives you a *point estimate* for θ.
- Bayesian Estimation gives you the whole posterior probability distribution for θ
  - **Interval Estimation:** Use the posterior to esstimate the *Credible Interval* that contains a certain fraction of the *posterior probability density*



- You could draw many possible 90% credible intervals.
  - We usually use the *Smallest Credible Interval*, also known as the *Highest Density Interval*.
- *Credible Intervals* vs. *Confidence Intervals*
  - **Bayesian:** 90% *Credible Interval* for θ means there is a 90% probability that the true value of θ is within the interval
  - **Frequentist:** 90% *Confidence Interval* means that if you repeat the experiment many times and calculate the 90% *confidence interval* for each experiment, the true value of θ will be within the *confidence interval* for 90% of the experiments.
    - It doesn't say anything about the probability that *your* experiment is in the 90% or the 10%.

Challenges for Bayesian Methods

Challenges for Bayesian Methods

- Selecting a prior:
  - Before you make your first measurement, how do you choose a prior?
  - Uniform prior?
    - Works if θ must lie within a finite range
    - Makes the fewest assumptions about θ
  - Other function?
    - Criticism of *subjectivity*:
      - You can get any result you want by choosing a suitable prior.
    - Rebuttal: You usually know something.
      - If a potential result would not be believable, your prior should exclude it
        - A rock can't be 12 billion years old.
        - Past climates can't have global temperature $> 100^\circ$C.

- Computing the *evidence*

$$P(X) = \int_{-\infty}^{\infty} P(X|\theta)P(\theta)\,\mathrm{d}\theta$$

  - Integrals can be hard to solve
  - Conjugate Priors:
    - Many *likelihood* functions $P(X|\theta)$ have *conjugate priors* $P(\theta)$ that have known evidence integrals
  - Numerical Integration:
    - Computers can approximately solve integrals that can't be solved analytically.

Conjugate Priors

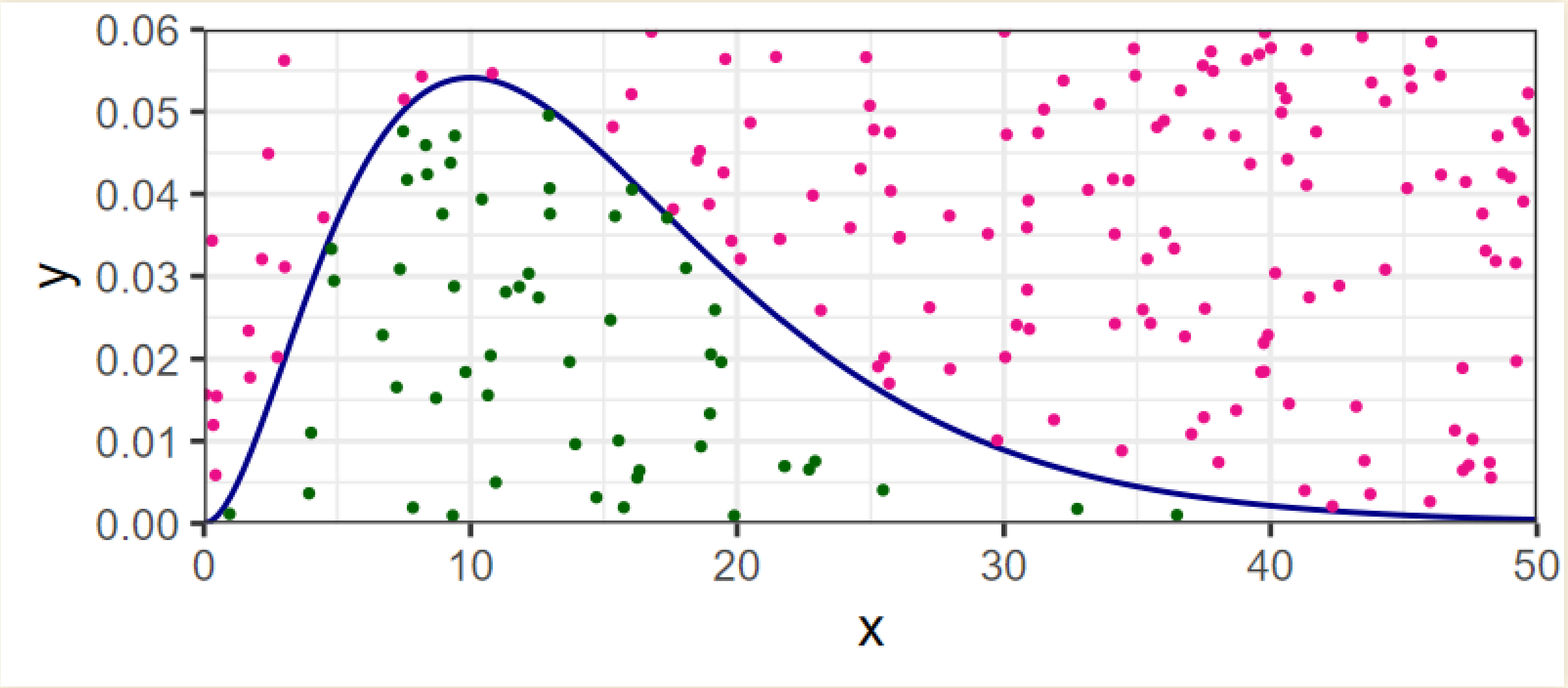
Likelihood, θ	**Conjugate Prior**	**Posterior**
Binomial, k	Beta	Beta Binomial
Poisson, λ (rate)	Gamma	Negative Binomial
Normal, μ	Normal	Normal
Normal, σ^2	Inverse Gamma	Student t
Exponential, λ (rate)	Gamma	Lomax
Gamma, θ (scale)	Inverse Gamma	Compound Gamma

- Problems:
  - Not all likelihoods have conjugate priors
  - Conjugate prior may not be a good representation of what you know about θ.

Numerical Integration

- Monte Carlo Integration
  - Invented around 1946 by Stanislaw Ulam for designing nuclear bombs
  - To solve

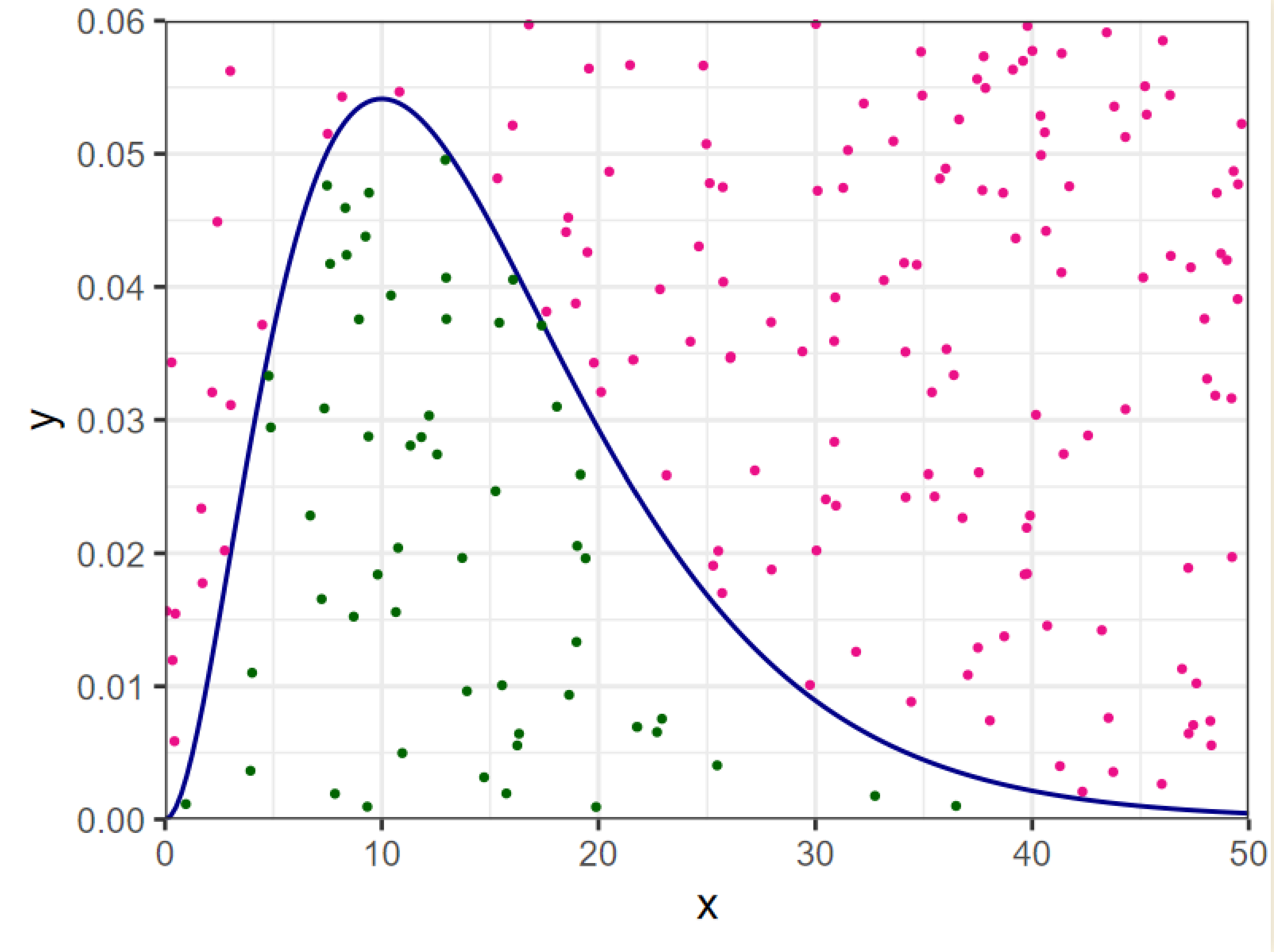
$$\int_a^b f(x)\,\mathrm{d}x$$



1. Plot $f(x)$ from a to b, and choose numbers c and d, so $f(x)$ is betwee and d
2. Pick N pairs of random numbers (x_i, y_i) where x_i is between a and b, and y_i is between c and d
3. Count the number that lie on or belo the function: $y_i \leq f(x_i)$
4. $\int_a^b f(x)\,\mathrm{d}x \approx (b-a)(d-c)\frac{N_{be}}{N}$

Example

$f(x) = \text{Gamma}(x, \text{shape} = 3, \text{scale} = 5)$



- Sample 200 points with $a = 0$, $b = 50$, $c = 0$, and $d = 0.06$.
- $N_{\text{below}} = 55$, so our estimate of the integral is

$$\frac{55}{200} \times (50 - 0)(0.06 - 0) = 0.825$$

- We can use R to figure out the actual value of the integral: `pgamma(50, shape=3, scale=5)` $= 1.000.$
- If we repeat with $N = 1000$, we get $N_{\text{below}} = 323$, and our estimte of the integral is

$$\frac{323}{1000} \times (50 - 0)(0.06 - 0) = 0.969$$

Challenges with Monte-Carlo Integration

- Monte-Carlo methods are very easy for integrating over one variable (one-dimensional integrals).
- But many statistical analyses have many parameters
  - Advanced regression analyses may have dozens or even hundreds of parameters.
  - This means doing an integral in dozens or hundreds of dimensions.
  - The *curse of dimensionality* says that it's very hard to sample efficiently in more than a few dimensions.
    - It took 1000 samples to get close to the correct value of the integral in our example
    - To achieve similar coverage in 10 dimensions would require 10^10 samples: 10 billion samples.
  - There are more efficient methods of sampling than just picking random numbers
  - But the *curse of dimensionality* is still a problem.
  - The biggest obstacle to Bayesian analysis is the computational work needed to solve the evidence integral.

Exercises with Estimation