

Math for ML

Week 5.1: Basic Probability Theory, Models, and Data

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Logistics & Announcements

Lesson Overview

Probability Spaces. We'll review the basic axioms and components of probability: sample space, events, and probability measures. This allows us to ditch these notions and introduce *random variables*.

Random variables. Review of the definition of a random variable, its *distribution/law*, its PDF/PMF/CDF, and joint distributions of several RVs.

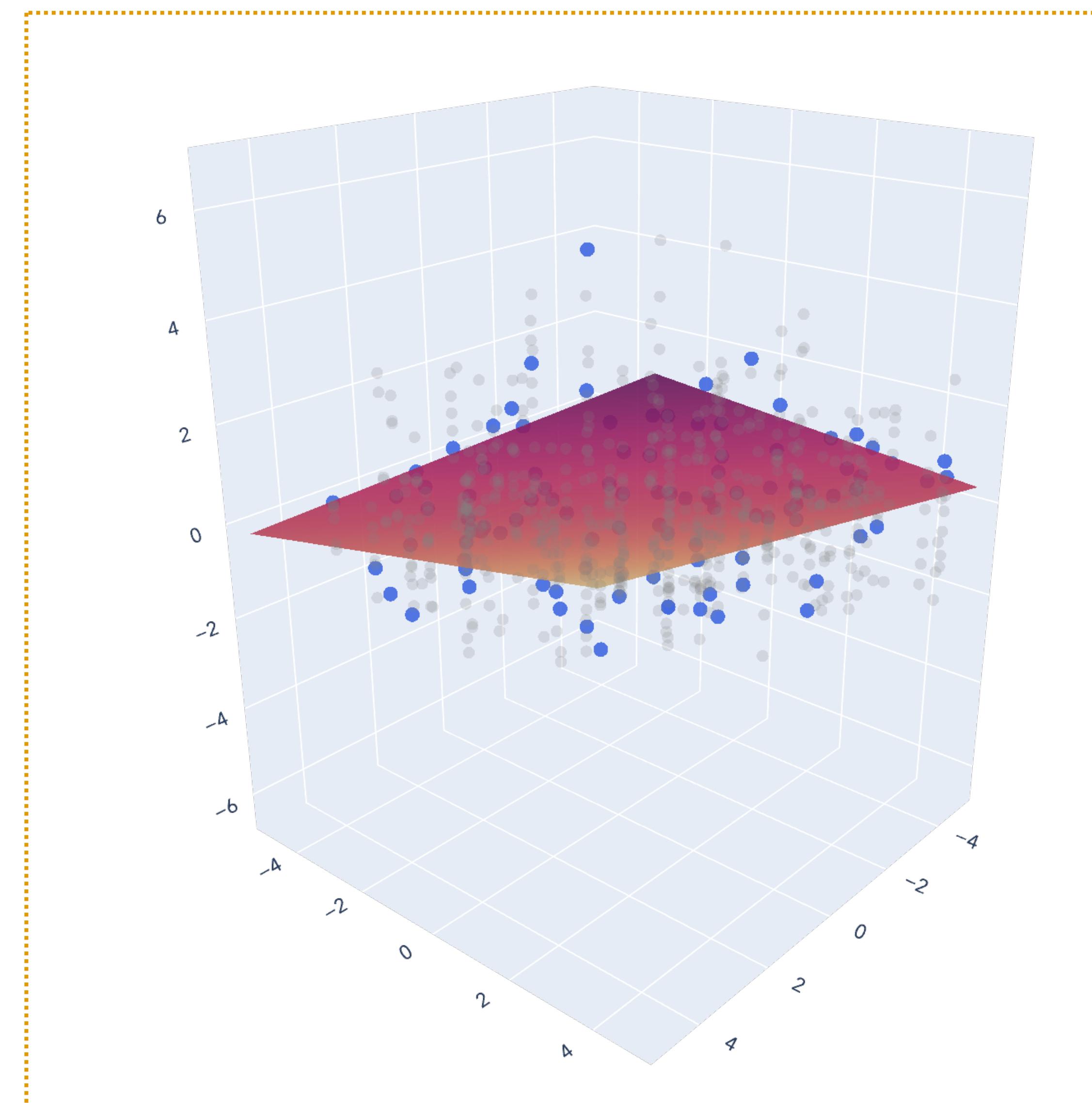
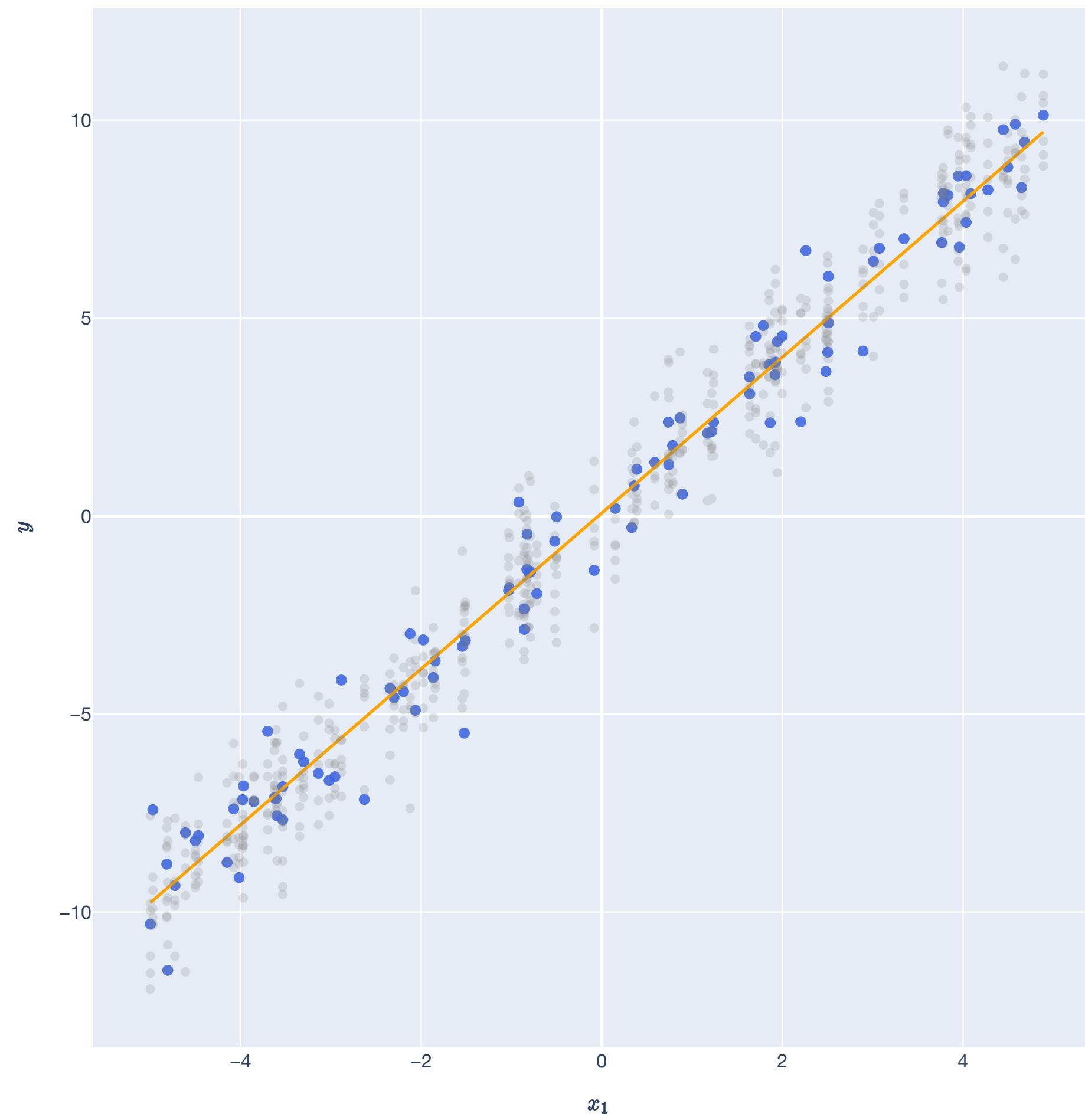
Expectation, variance, and covariance. Review of these basic summary statistics of random variables and common properties.

Random vectors. Introduce the idea of a *random vector*, which is just a list of multiple random variables. Discuss generalizations of expectation and variance to random vectors.

Data as random, statistical model of ML. Introduce a statistical model of ML and the random error model. Introduce *modeling assumptions*. State and prove basic statistical properties of the OLS estimator.

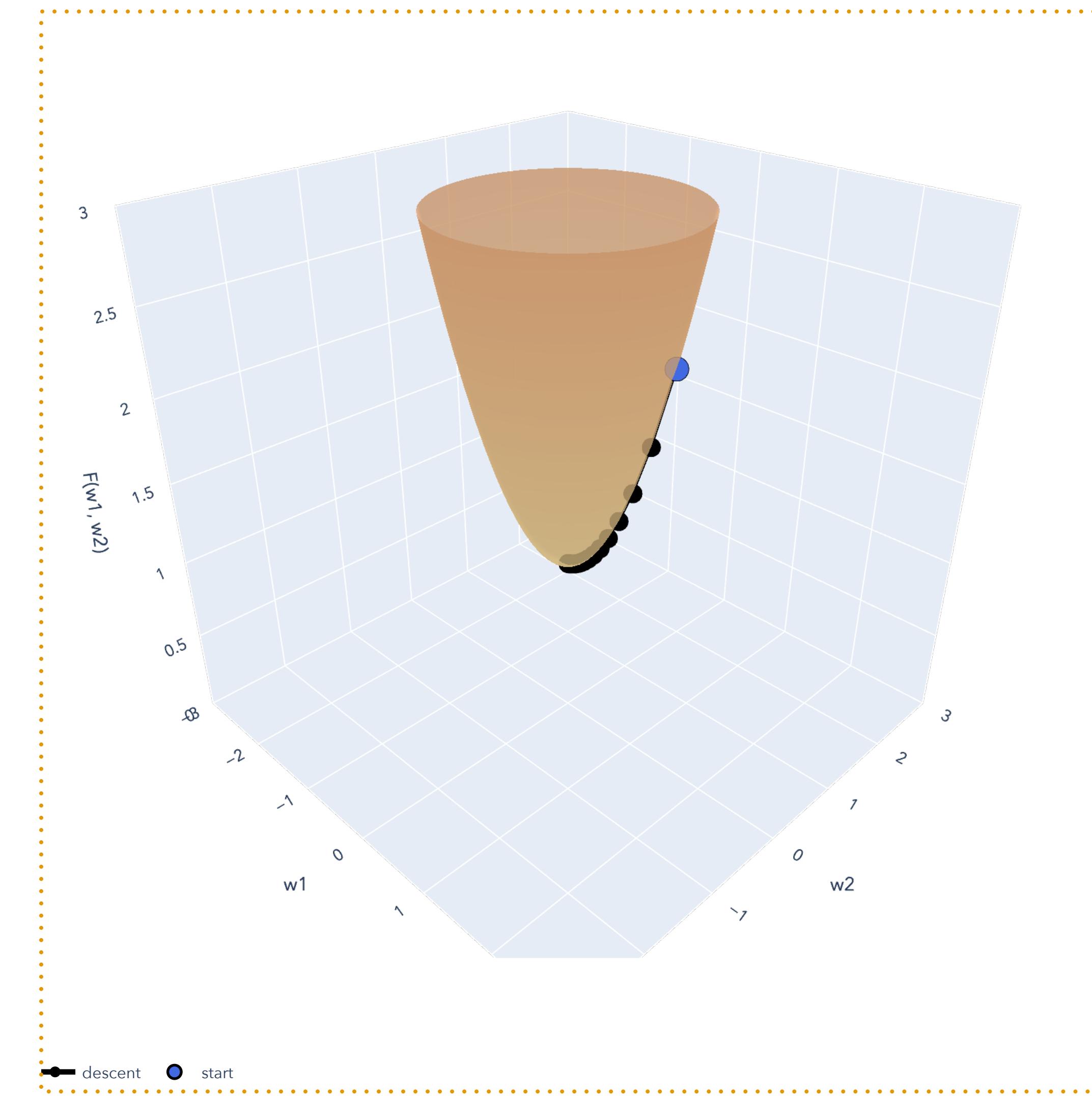
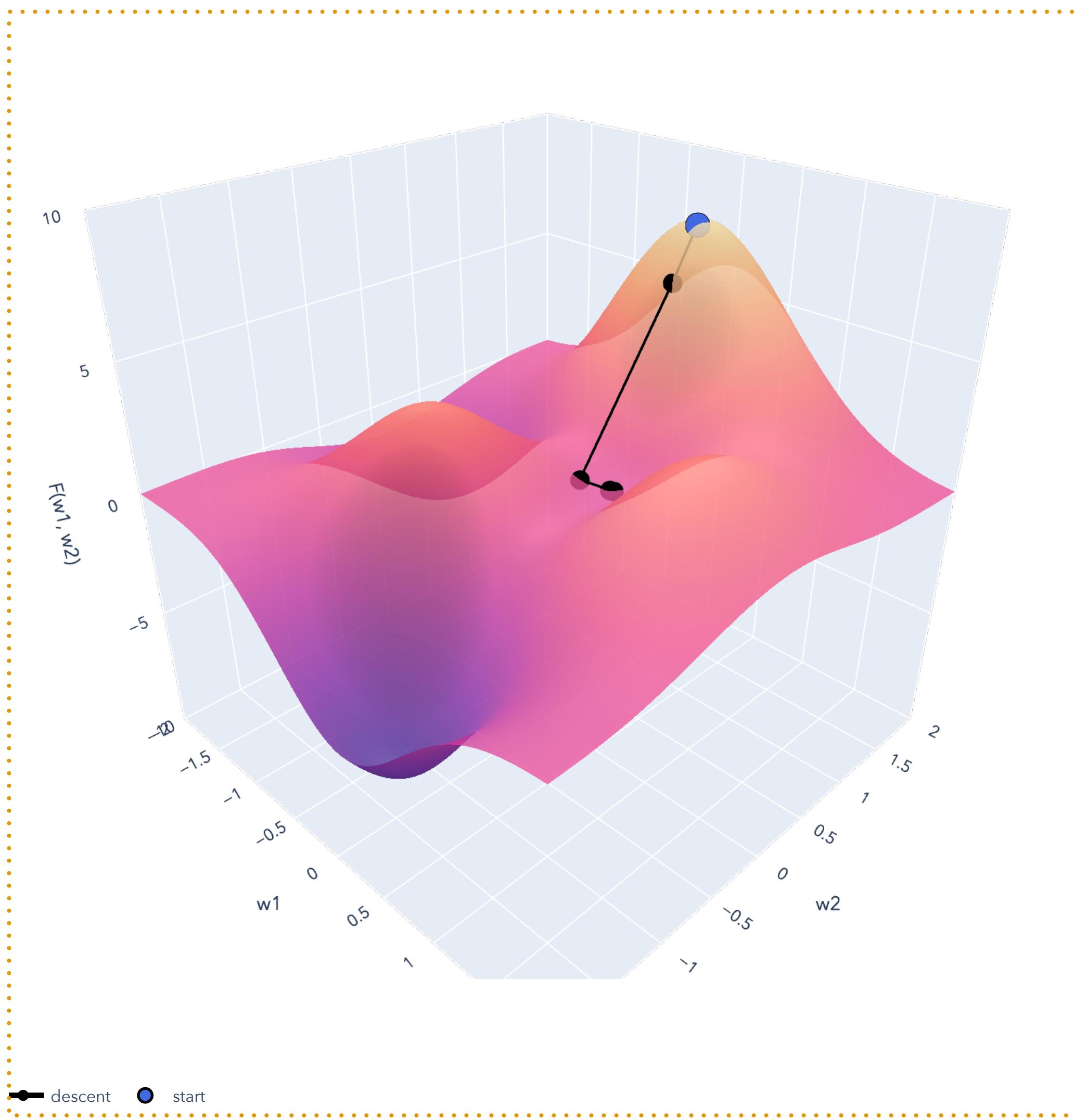
Lesson Overview

Big Picture: Least Squares



Lesson Overview

Big Picture: Gradient Descent



Motivation

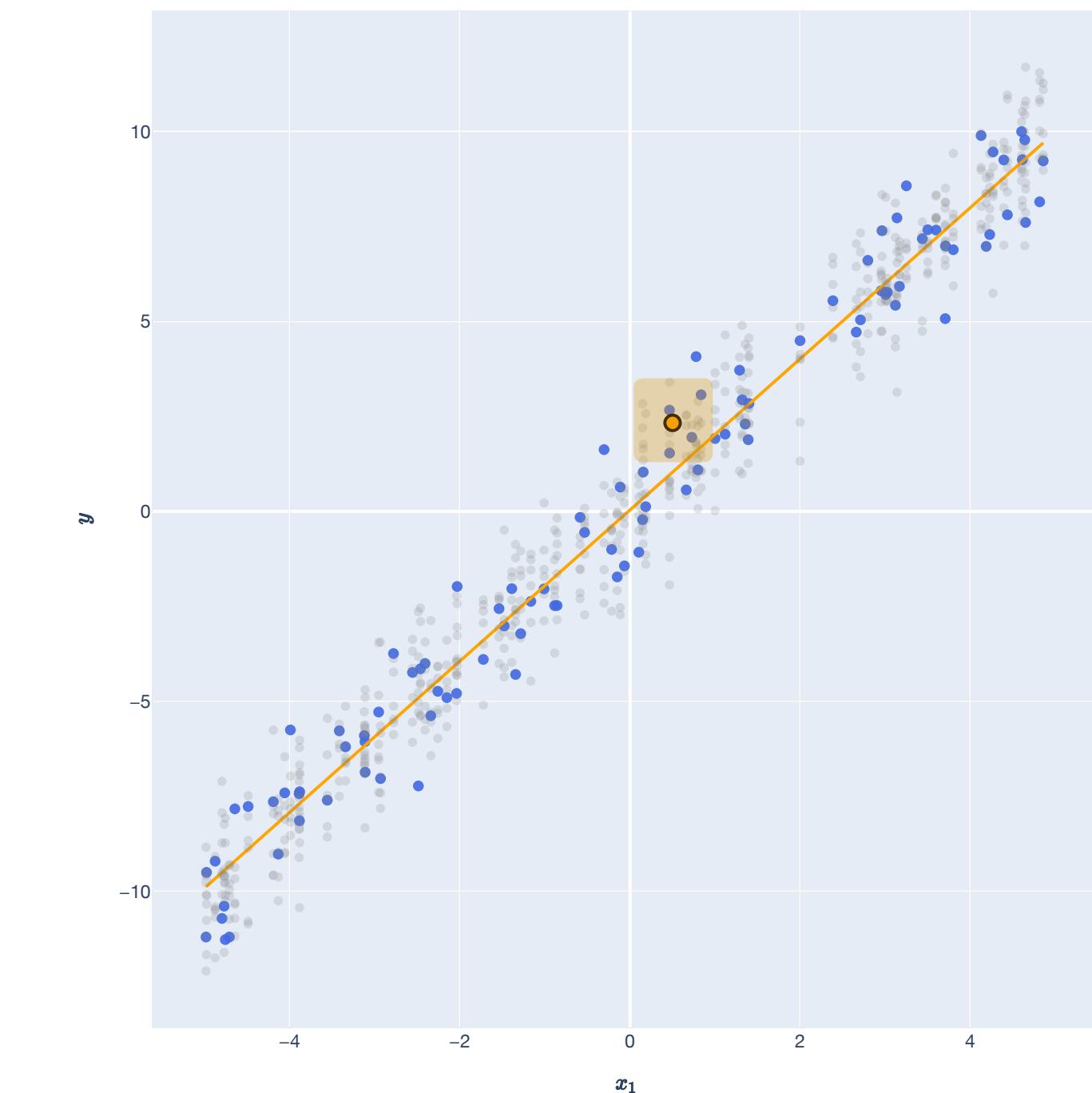
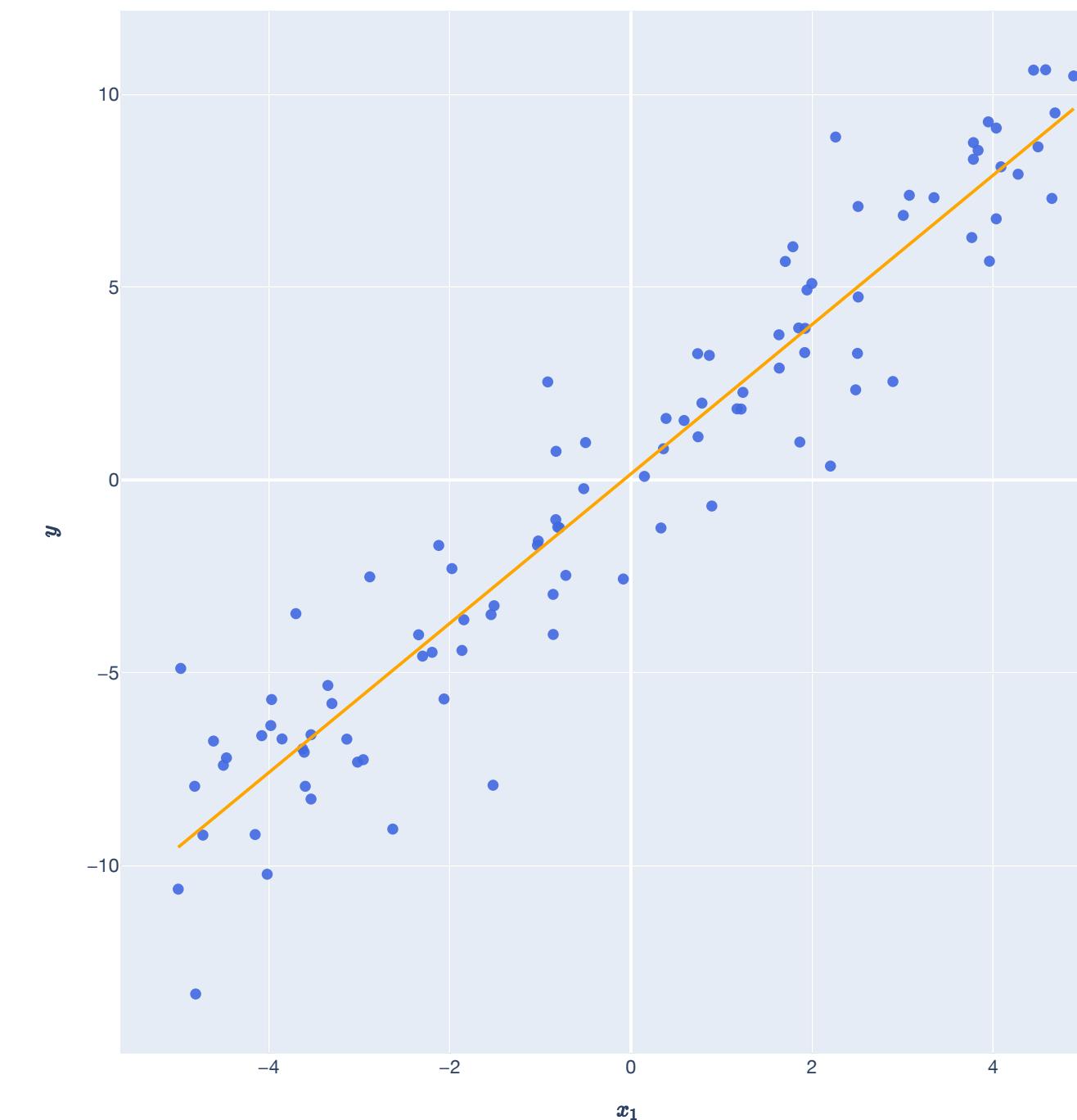
Data as randomly distributed

Regression

Setup

What we've been doing so far: Collect labeled training data \implies Fit the model \hat{w}

Hope training data looks like new data: Generalize on new x_0 .



Regression

Setup (Example View)

Observed: Matrix of *training samples* $\mathbf{X} \in \mathbb{R}^{n \times d}$ and vector of *training labels* $\mathbf{y} \in \mathbb{R}^n$.

$$\mathbf{X} = \begin{bmatrix} \leftarrow & \mathbf{x}_1^\top & \rightarrow \\ & \vdots & \\ \leftarrow & \mathbf{x}_n^\top & \rightarrow \end{bmatrix} \quad \mathbf{y} = \begin{bmatrix} y_1 \\ \vdots \\ y_n \end{bmatrix}, \text{ where } \mathbf{x}_1, \dots, \mathbf{x}_n \in \mathbb{R}^d.$$

Unknown: *Weight vector* $\mathbf{w} \in \mathbb{R}^d$ with weights w_1, \dots, w_d .

Goal: For each $i \in [n]$, we predict: $\hat{y}_i = \mathbf{w}^\top \mathbf{x}_i = w_1 x_{i1} + \dots + w_d x_{id} \in \mathbb{R}$.

Choose a weight vector that “fits the training data”: $\mathbf{w} \in \mathbb{R}^d$ such that $y_i \approx \hat{y}_i$ for $i \in [n]$, or:

$$\mathbf{X}\mathbf{w} = \hat{\mathbf{y}} \approx \mathbf{y}.$$

Regression

Setup (Feature View)

Observed: Matrix of *training samples* $\mathbf{X} \in \mathbb{R}^{n \times d}$ and vector of *training labels* $\mathbf{y} \in \mathbb{R}^n$.

$$\mathbf{X} = \begin{bmatrix} \uparrow & & \uparrow \\ \mathbf{x}_1 & \dots & \mathbf{x}_d \\ \downarrow & & \downarrow \end{bmatrix} \quad \mathbf{y} = \begin{bmatrix} y_1 \\ \vdots \\ y_n \end{bmatrix}, \text{ where } \mathbf{x}_1, \dots, \mathbf{x}_d \in \mathbb{R}^n.$$

Unknown: *Weight vector* $\mathbf{w} \in \mathbb{R}^d$ with weights w_1, \dots, w_d .

Choose a weight vector that "fits the training data": $\mathbf{w} \in \mathbb{R}^d$ such that $y_i \approx \hat{y}_i$ for $i \in [n]$, or:

$$\mathbf{X}\mathbf{w} = \hat{\mathbf{y}} \approx \mathbf{y}.$$

Regression

Setup

Ultimate Goal: Given a new, unseen $(\mathbf{x}_0, y_0) \in \mathbb{R}^d \times \mathbb{R}$, we wanted to generalize:

$$\hat{\mathbf{w}}^\top \mathbf{x}_0 \approx y_0.$$

To do this, we fit the “training data”: $\hat{\mathbf{w}} \in \mathbb{R}^d$ such that $y_i \approx \hat{y}_i$ for $i \in [n]$, or:

$$\mathbf{X}\hat{\mathbf{w}} = \hat{\mathbf{y}} \approx \mathbf{y}.$$

To find $\hat{\mathbf{w}}$, we follow the *principle of least squares*.

$$\hat{\mathbf{w}} = \arg \min_{\mathbf{w} \in \mathbb{R}^d} \|\mathbf{X}\mathbf{w} - \mathbf{y}\|^2$$

Regression

Setup

Least squares expanded is just:

$$\|\mathbf{X}\mathbf{w} - \mathbf{y}\|^2 = \sum_{i=1}^n (\mathbf{w}^\top \mathbf{x}_i - y_i)^2$$

Put a $1/n$ in front, and it looks like we're minimizing an average:

$$\frac{1}{n} \|\mathbf{X}\mathbf{w} - \mathbf{y}\|^2 = \frac{1}{n} \sum_{i=1}^n (\mathbf{w}^\top \mathbf{x}_i - y_i)^2$$

Regression

Setup, with randomness

Observed: Matrix of *training samples* $\mathbf{X} \in \mathbb{R}^{n \times d}$ and vector of *training labels* $\mathbf{y} \in \mathbb{R}^n$.

Random vector $\mathbf{x}_i \in \mathbb{R}^d$

$$\mathbf{X} = \begin{bmatrix} \mathbf{x}_1^\top & \\ \vdots & \\ \mathbf{x}_n^\top & \end{bmatrix}$$

Random variable y_i

$$\mathbf{y} = \begin{bmatrix} y_1 \\ \vdots \\ y_n \end{bmatrix}, \text{ where } \mathbf{x}_1, \dots, \mathbf{x}_n \in \mathbb{R}^d.$$

... from the joint distribution $\mathbb{P}_{\mathbf{x}, y}$ over $\mathbb{R}^d \times \mathbb{R}$!

Unknown: Weight vector $\mathbf{w} \in \mathbb{R}^d$ with weights w_1, \dots, w_d .

Goal: For each $i \in [n]$, we predict: $\hat{y}_i = \mathbf{w}^\top \mathbf{x}_i = w_1 x_{i1} + \dots + w_d x_{id} \in \mathbb{R}$.

Our "model", a function that we hope "generalizes" well to new datapoint (\mathbf{x}_0, y_0) .

Choose a weight vector that "fits the training data": $\mathbf{w} \in \mathbb{R}^d$ such that $y_i \approx \hat{y}_i$ for $i \in [n]$, or:

$$\mathbf{X}\mathbf{w} = \hat{\mathbf{y}} \approx \mathbf{y}.$$

Because we assume that $(\mathbf{x}_0, y_0) \sim \mathbb{P}_{\mathbf{x}, y}$ as well!

Regression

Setup, with randomness

To choose a model (*predictor/classifier/etc.*) $f: \mathbb{R}^d \rightarrow \mathbb{R}$, we want to minimize the expected squared loss, or the **risk**:

$$\mathbb{E}_{\mathbf{x},y}[(y - f(\mathbf{x}))^2] = \int (y - f(\mathbf{x}))^2 d\mathbb{P}(\mathbf{x}, y)$$

...but we can't know the true distribution, so as a substitute, minimize the **empirical risk**:

$$\hat{R}(f) := \frac{1}{n} \sum_{i=1}^n (y_i - f(\mathbf{x}_i))^2.$$

Regression

Setup, with randomness

Our choice of f is $f_{\mathbf{w}}(\mathbf{x}) = \mathbf{w}^\top \mathbf{x}$, a linear model, so risk:

$$\mathbb{E}_{\mathbf{x},y}[(y - \mathbf{w}^\top \mathbf{x})^2] = \int (y - \mathbf{w}^\top \mathbf{x})^2 d\mathbb{P}(\mathbf{x}, y)$$

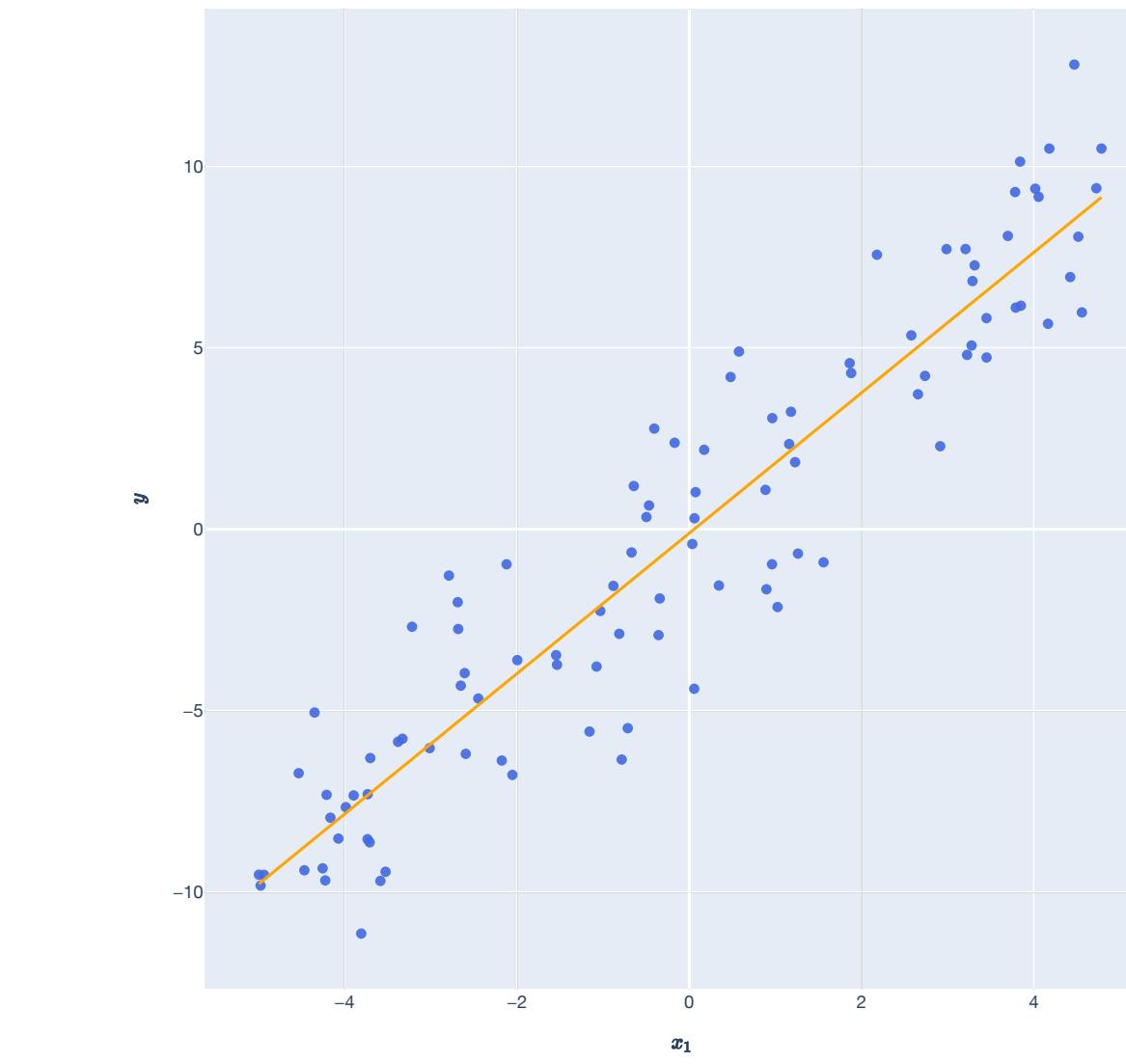
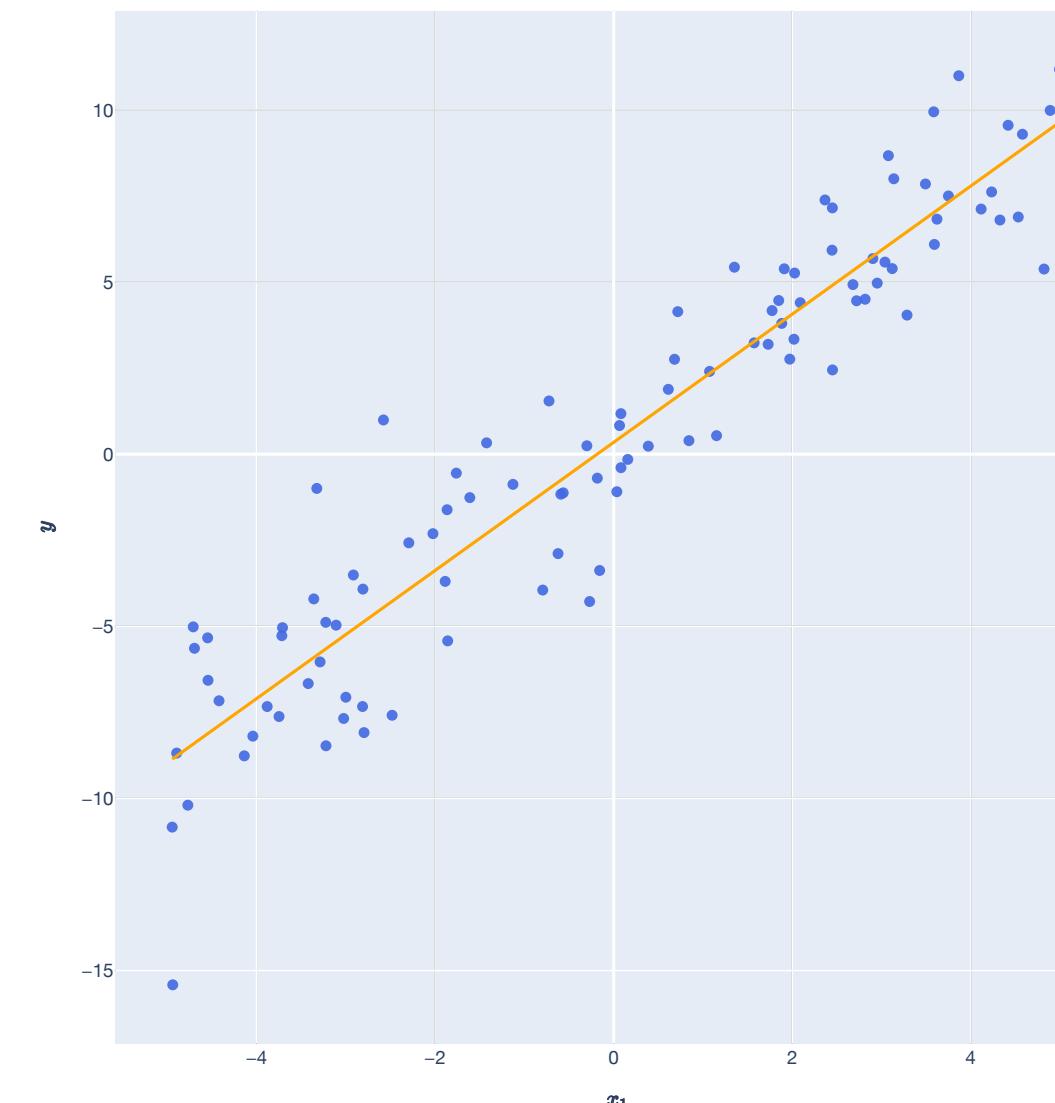
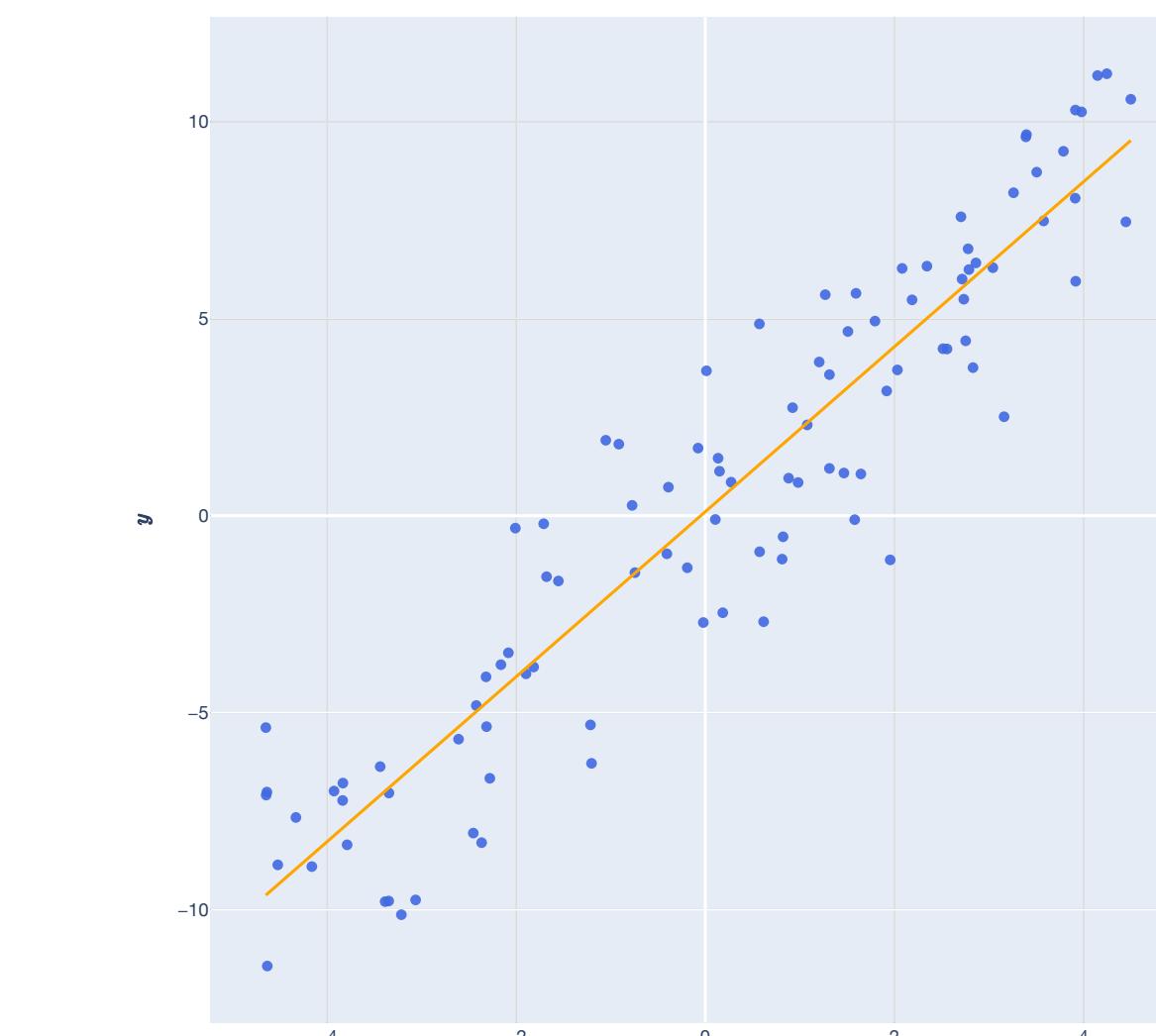
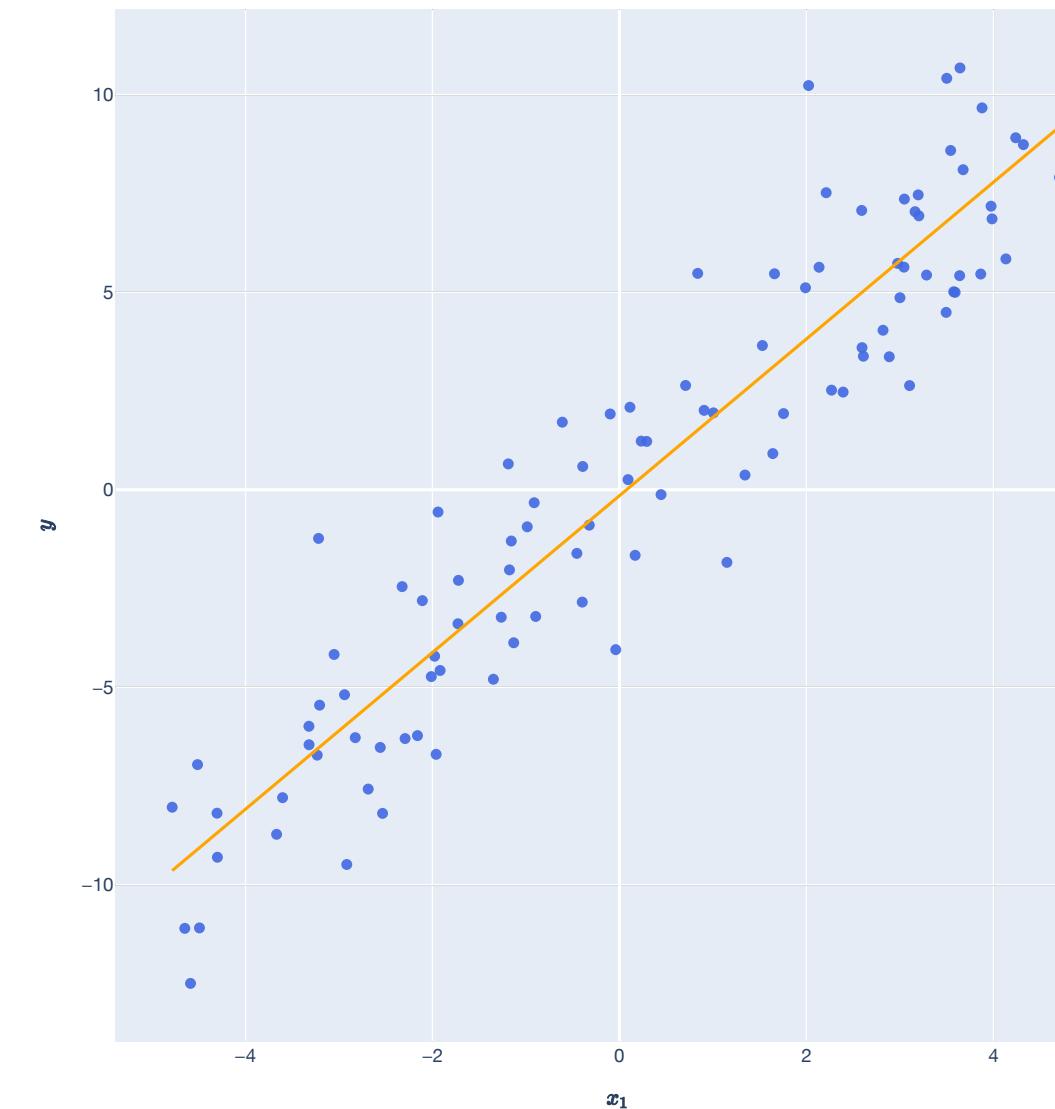
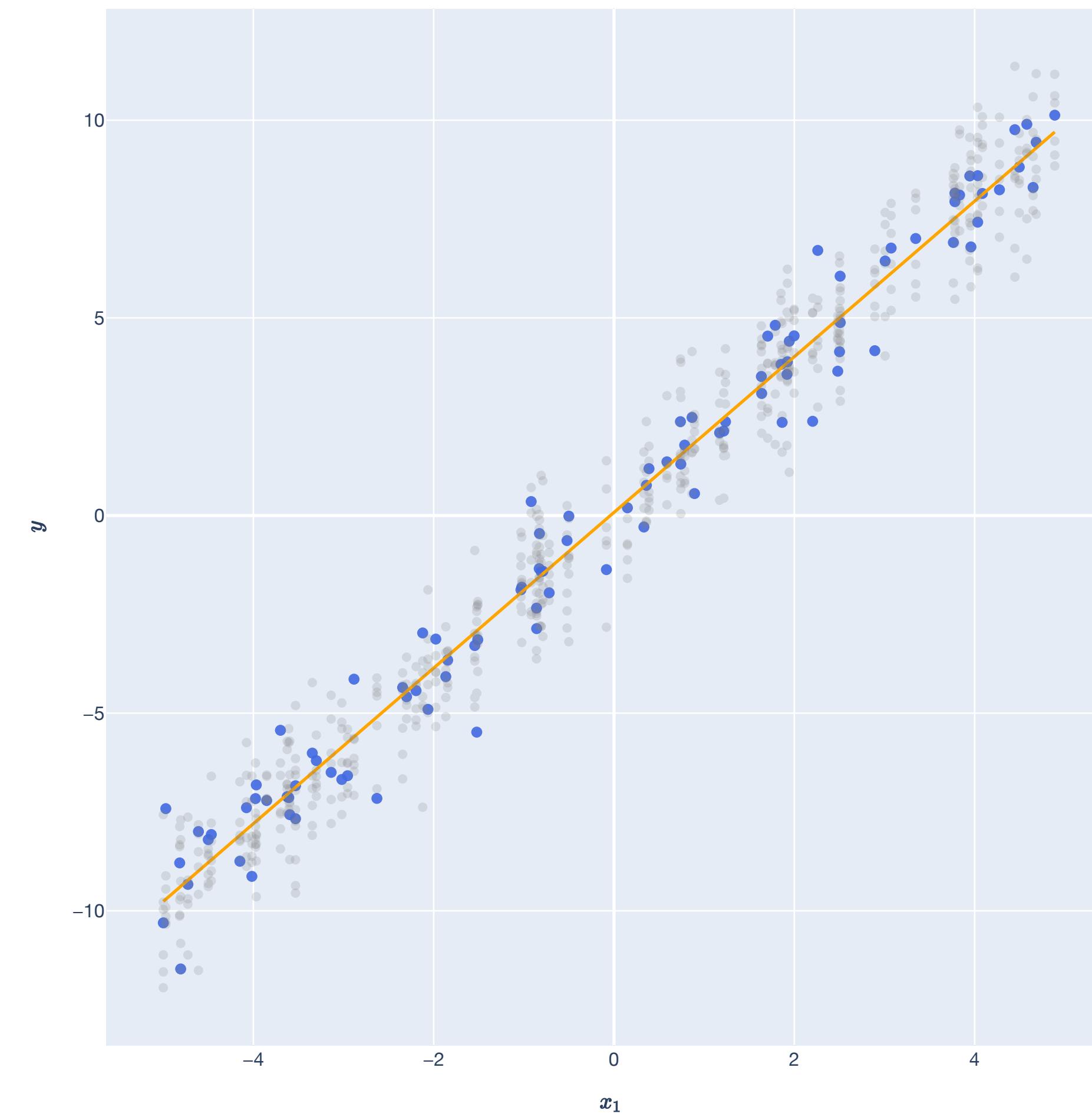
...but we can't know the true distribution, so as a substitute, minimize the empirical risk:

$$\hat{R}(f_{\mathbf{w}}) := \frac{1}{n} \sum_{i=1}^n (y_i - \mathbf{w}^\top \mathbf{x}_i)^2 = \frac{1}{n} \|\mathbf{X}\mathbf{w} - \mathbf{y}\|^2.$$

which is just our least squares error, scaled by $1/n$!

Regression

Modeling randomness

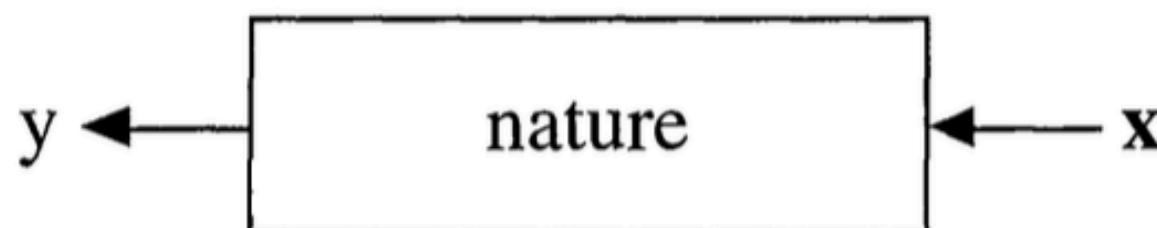


The “Story” of Probability and Statistics

Modeling randomness

1. INTRODUCTION

Statistics starts with data. Think of the data as being generated by a black box in which a vector of input variables \mathbf{x} (independent variables) go in one side, and on the other side the response variables \mathbf{y} come out. Inside the black box, nature functions to associate the predictor variables with the response variables, so the picture is like this:



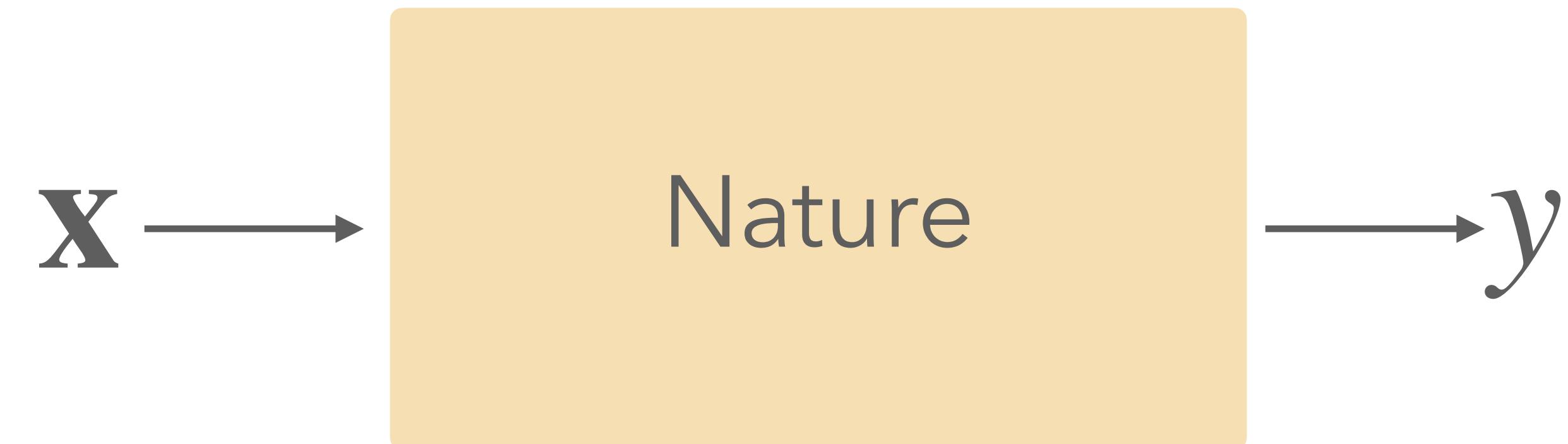
There are two goals in analyzing the data:

Prediction. To be able to predict what the responses are going to be to future input variables;

Information. To extract some information about how nature is associating the response variables to the input variables.

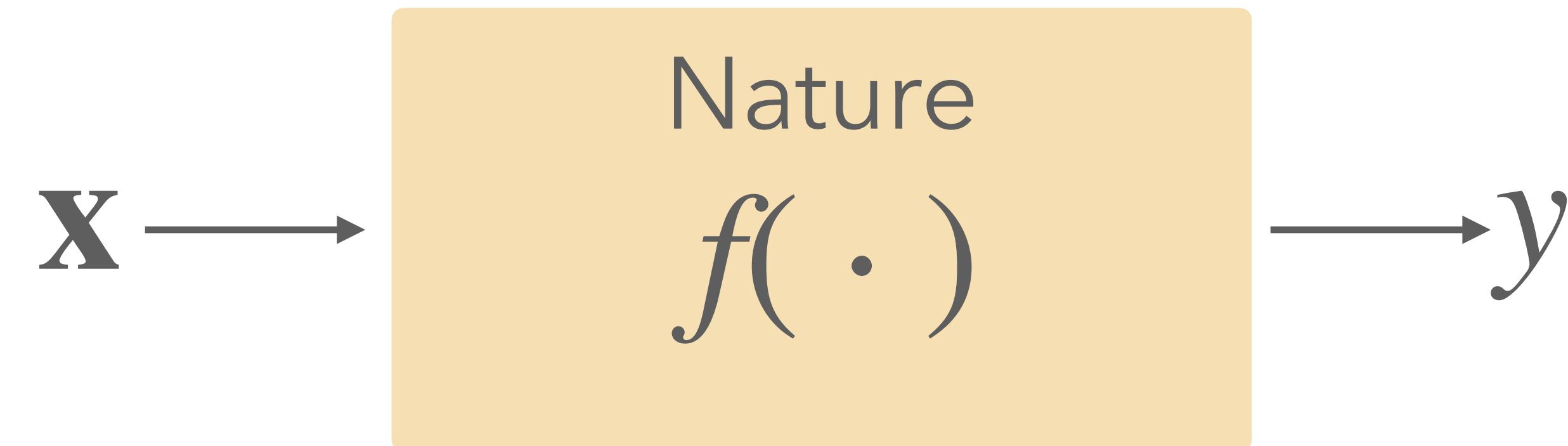
The “Story” of Probability and Statistics

Modeling randomness



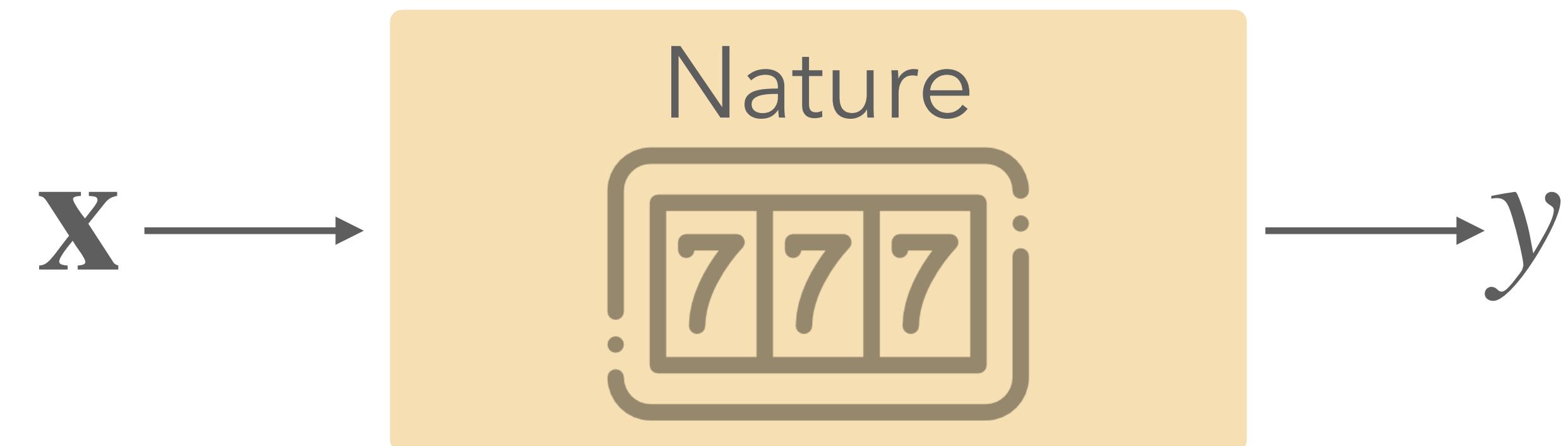
The “Story” of Probability and Statistics

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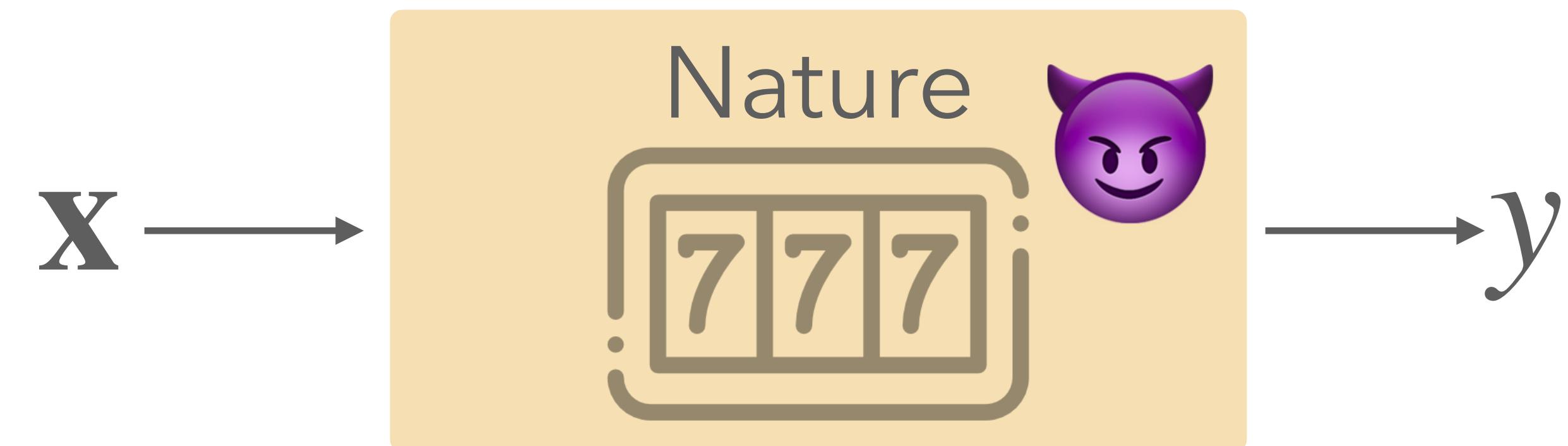
The “Story” of Probability and Statistics

Modeling randomness



The “Story” of Probability and Statistics

Modeling randomness



Probability Spaces

Sample Spaces, Events, and Random Variables

Sample Space

Example: Flipping 2 fair coins

Consider the following experiment:

Alice and Bob both have a fair coin. They each flip their coins simultaneously, and the result can be either H or T .

What are the possible outcomes of this experiment?

$H H$	$T H$
$H T$	$T T$

Ω

Sample Space

Intuition and definition

The sample space of some experiment on which we want to model probabilities is the set of all possible outcomes.

Denote this Ω .

Example:

$$\Omega = \{HH, HT, TH, TT\}.$$

HH	TH
HT	TT
Ω	

Events

Intuition and definition

Given a sample space Ω , an **event** is a subset $A \subseteq \Omega$ of outcomes.

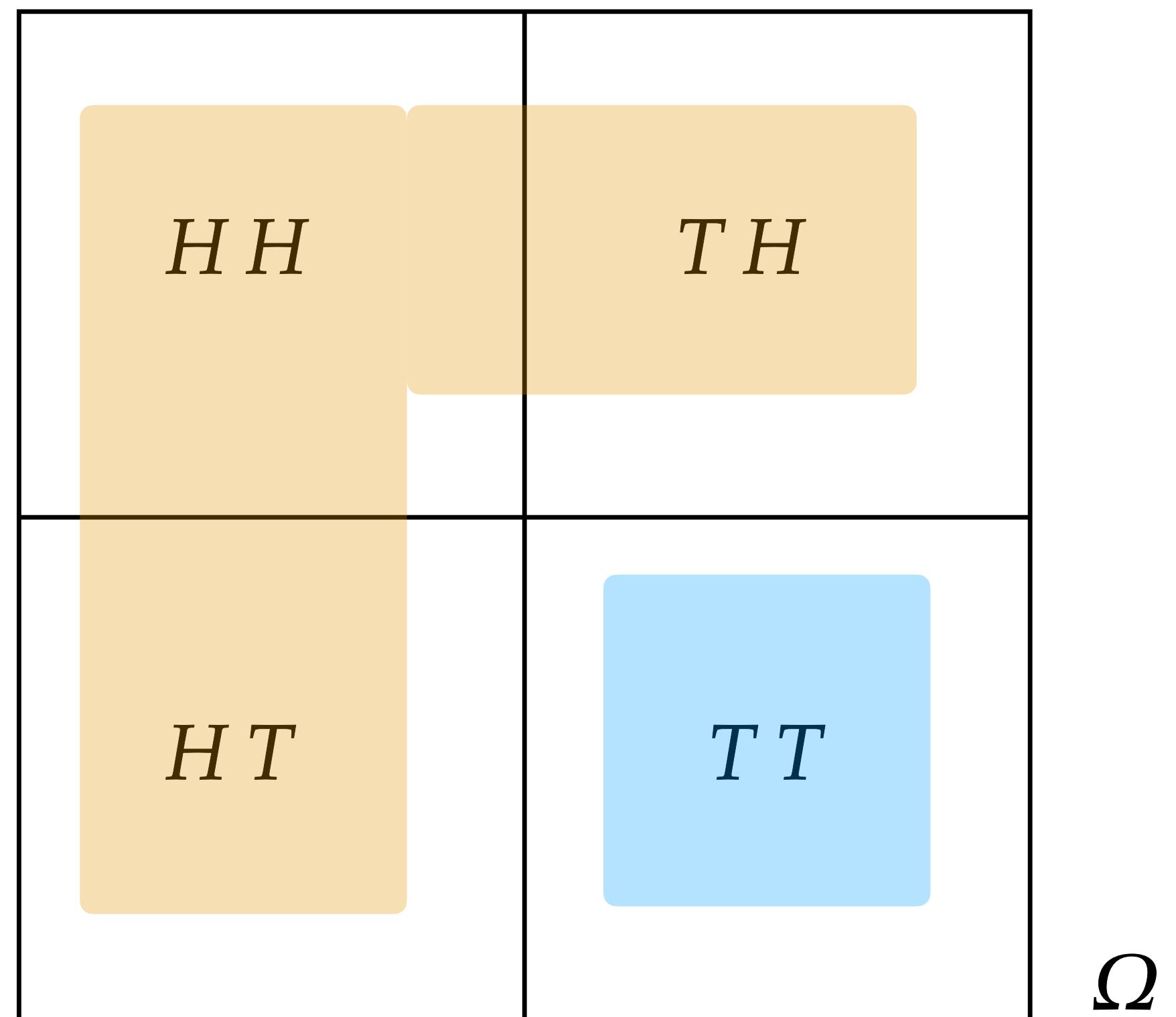
Denote a collection of events \mathcal{A} .

Example:

$A = \{HT, TH, HH\} = \{"\text{at least 1 head"}\}$

$B = \{TT\} = \{"\text{no heads"}\}$

$\mathcal{A} = \{\emptyset, \{HH\}, \{HT\}, \dots, \{HH, HT, TH, TT\}\}$



Events

Intuition and definition

Events are subsets, so they obey the usual rules and definitions of set logic.

$A \cup B$ (union)

$A \cap B$ (intersection)

A^C (complement)

Example:

$A = \{HT, TH\} = \{"\text{exactly 1 head"}\}$

$A^C = \{HH, TT\}$

HH	TH
HT	TT

Ω

Probability Measure

Intuition and definition

A probability measure is a set function

$$\mathbb{P} : \mathcal{A} \rightarrow [0,1]$$

mapping from sets to a number in $[0,1]$.

For event $A \in \mathcal{A}$, we call $\mathbb{P}(A)$ the probability of A.

“degree of belief” or “long-run frequency.”

Or just the “mass” of a particular subset!

$\mathbb{P}(\{HH\}) = 0.2$	HH	TH	Ω
	HT	TT	Ω

Probability Measure

Axiomatic Properties

A *valid* probability measure \mathbb{P} satisfies:

1. The measure of the entire sample space:

$$\mathbb{P}(\Omega) = 1.$$

2. For disjoint events A_1, A_2, A_3, \dots

$$\mathbb{P}(A_1 \cup A_2 \cup A_3 \cup \dots) = \mathbb{P}(A_1) + \mathbb{P}(A_2) + \mathbb{P}(A_3) + \dots$$

also known as countable additivity.

$$\mathbb{P}(\{HH, TH, HT, TT\}) = 1$$

HH	TH
HT	TT
	Ω

Probability Measure

Properties of probability measures

1. **Complements.** For any event $A \in \mathcal{A}$, the probability of the complement is:
 $\mathbb{P}(A^C) = 1 - \mathbb{P}(A)$.
2. **Subsets of events.** For two events $A, B \in \mathcal{A}$, if $A \subseteq B$, then: $\mathbb{P}(B) \leq \mathbb{P}(A)$.
3. **Unions of events.** For any two events $A, B \in \mathcal{A}$, $\mathbb{P}(A \cup B) = \mathbb{P}(A) + \mathbb{P}(B) - \mathbb{P}(A \cap B)$.
4. **Union bound.** For any finite collection of events A_1, \dots, A_n ,

$$\mathbb{P}(A_1 \cup \dots \cup A_n) \leq \sum_{i=1}^n \mathbb{P}(A_i).$$

Probability Measure

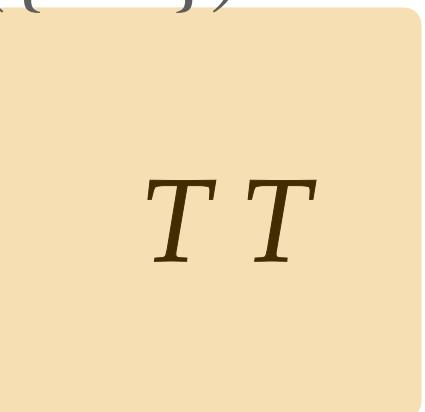
Example Measures

For discrete outcome spaces, a common way to measure probabilities is to weigh outcomes equally probable:

$$\mathbb{P}(\{\omega\}) = 1/\Omega \text{ for } \omega \in \Omega.$$

This isn't the only valid measure, e.g.

$$\mathbb{P}(\{HH\}) = 1$$

$\mathbb{P}(\{HH\}) = 1/4$ 	$\mathbb{P}(\{TH\}) = 1/4$ 
$\mathbb{P}(\{HT\}) = 1/4$ 	$\mathbb{P}(\{TT\}) = 1/4$ 

Ω

Conditional Probabilities

Intuition and definition

For events A, B , the **conditional probability** of B given A is:

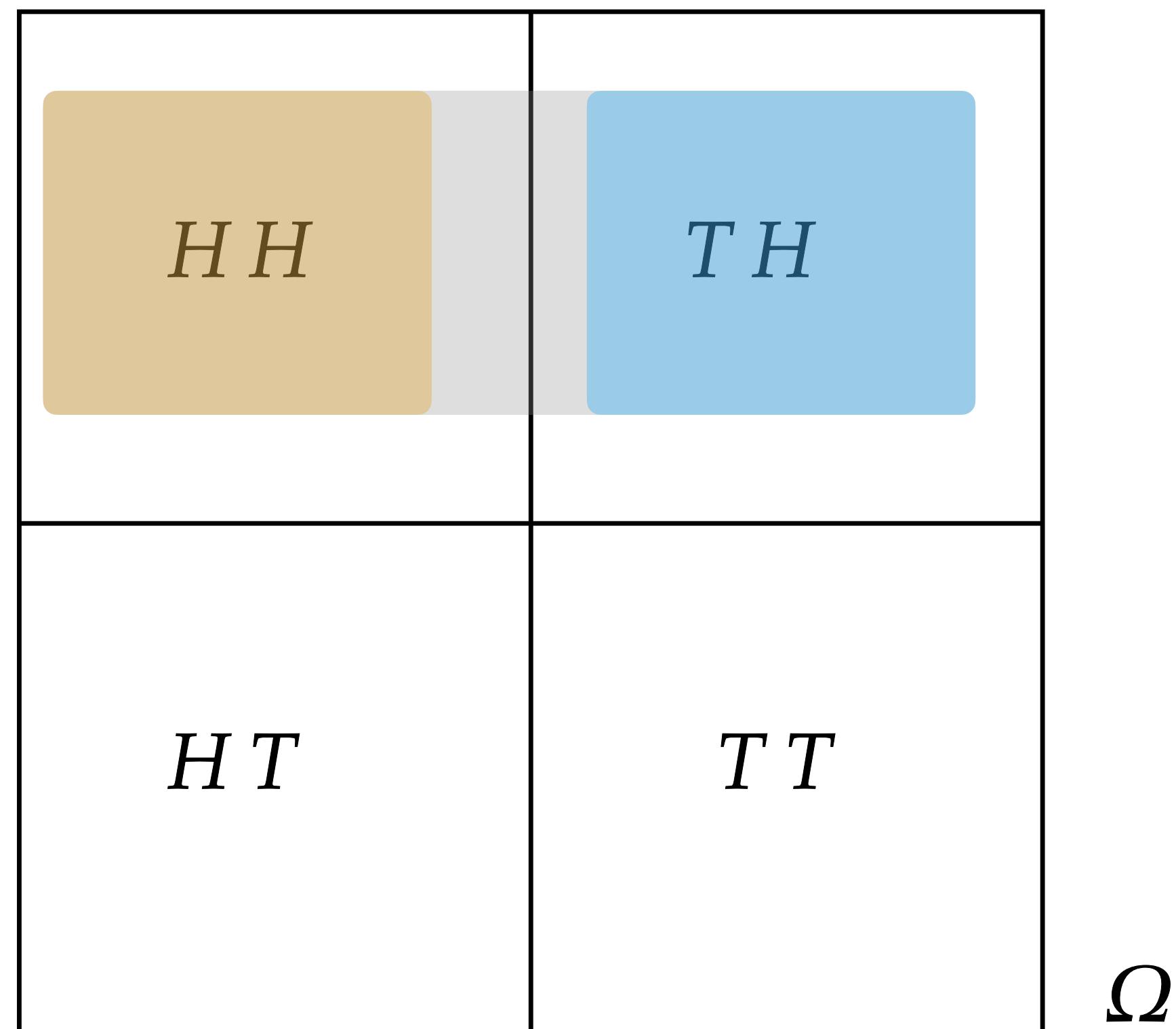
$$\mathbb{P}(B | A) = \frac{\mathbb{P}(A \cap B)}{\mathbb{P}(A)}.$$

Example:

$A = \{\text{Bob's coin is } H\}$

$B = \{\text{Alice's coin is } T\}$

$C = \{\text{Alice's coin is } H\}$



Conditional Probabilities

Chain Rule and Bayes' Rule

The chain rule of conditional probability is:

$$\mathbb{P}(A \cap B) = \mathbb{P}(A | B)\mathbb{P}(B) = \mathbb{P}(B | A)\mathbb{P}(A).$$

This easily gives us Bayes' rule:

$$\mathbb{P}(A | B) = \frac{\mathbb{P}(B | A)\mathbb{P}(A)}{\mathbb{P}(B)}.$$

Bayes' rule can be thought of as how we "update our beliefs."

Conditional Probabilities

Law of Total Probability

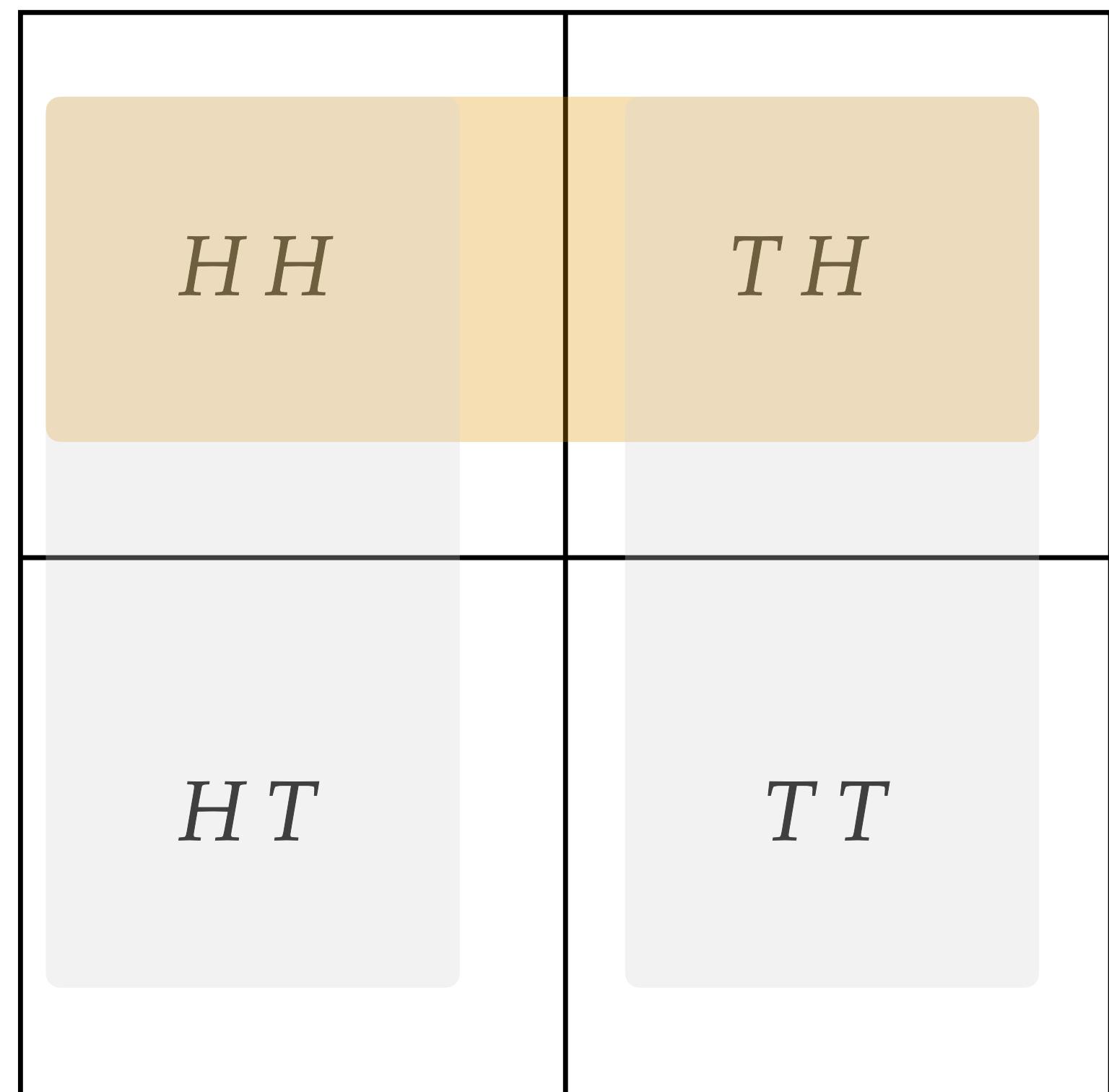
The [law of total probability](#) allows us to chop up probabilities into an exact sum of distinct events.

If B_1, B_2, B_3, \dots is a *countable* collection of events, then, for any event A :

$$\mathbb{P}(A) = \sum_i \mathbb{P}(A \cap B_i)$$

$$\mathbb{P}(A) = \sum_i \mathbb{P}(A | B_i) \mathbb{P}(B_i)$$

Super useful: commit this to memory!



Probability Space

Intuition and definition

A *sample space*, *event space* (σ -algebra), and *probability measure* ($\Omega, \mathcal{A}, \mathbb{P}$) is called a probability space.

Example:

$$\Omega = \{HH, HT, TH, TT\}$$

$$\mathcal{A} = \{\emptyset, \{HH\}, \{HT\}, \dots, \{HH, HT, TH, TT\}\}$$

$$\mathbb{P}(\{\omega\}) = 1/4 \text{ for all } \omega \in \Omega.$$

HH	TH
HT	TT
	Ω

Probability Space

Intuition and definition

A sample space, event space (σ -algebra), and probability measure($\Omega, \mathcal{A}, \mathbb{P}$) is called a probability space.

We avoid dealing with these directly! Instead, we use random variables as an “interface.”

$H H$	$T H$
$H T$	$T T$
Ω	

Random Variables

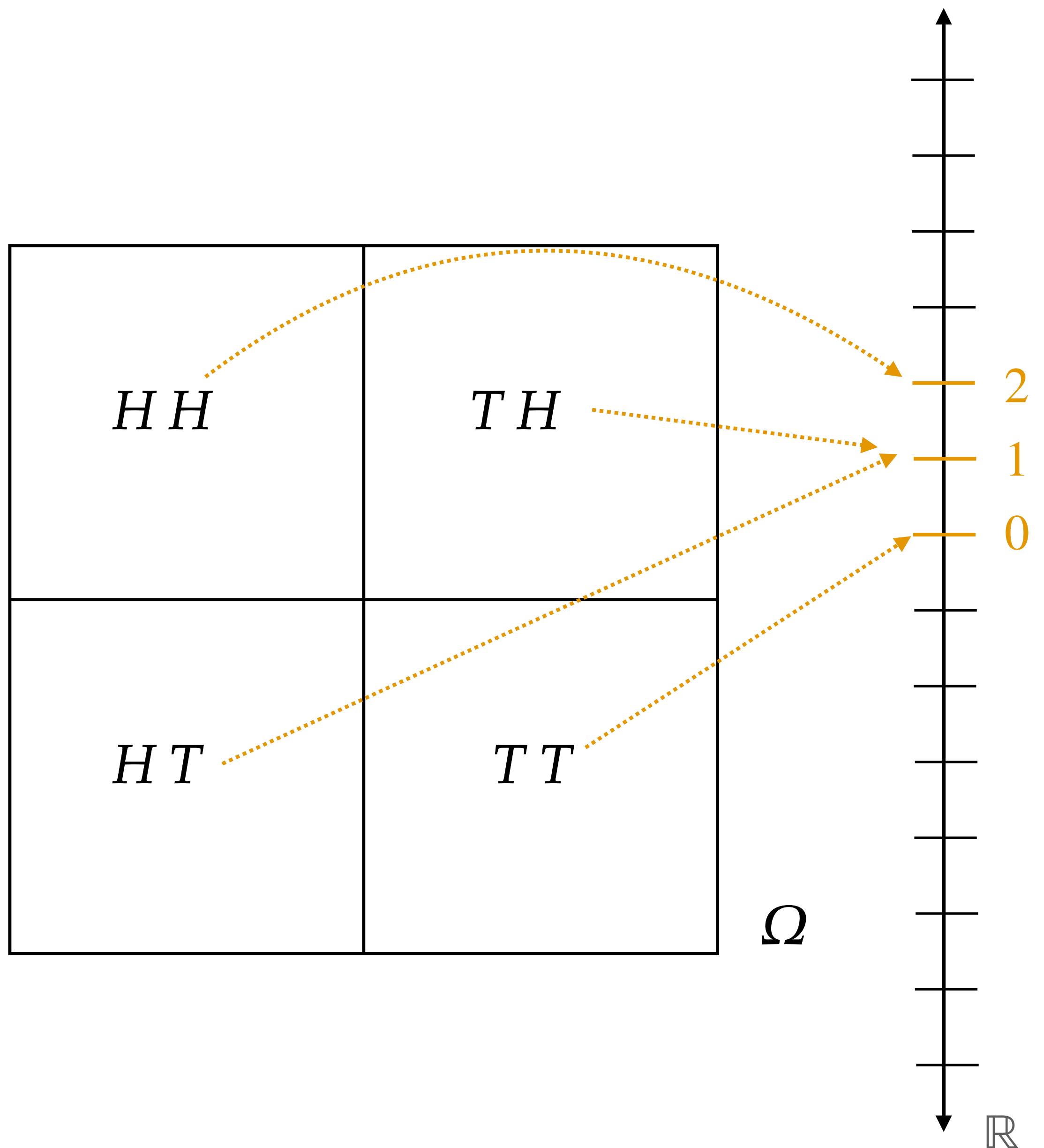
Example: Flipping 2 fair coins

Consider the following function:

$$X : \Omega \rightarrow \mathbb{R}$$

where $X(\omega) = \text{number of heads, } H.$

Random variables are *functions* that assign a number to every outcome in the sample space.



Random Variables

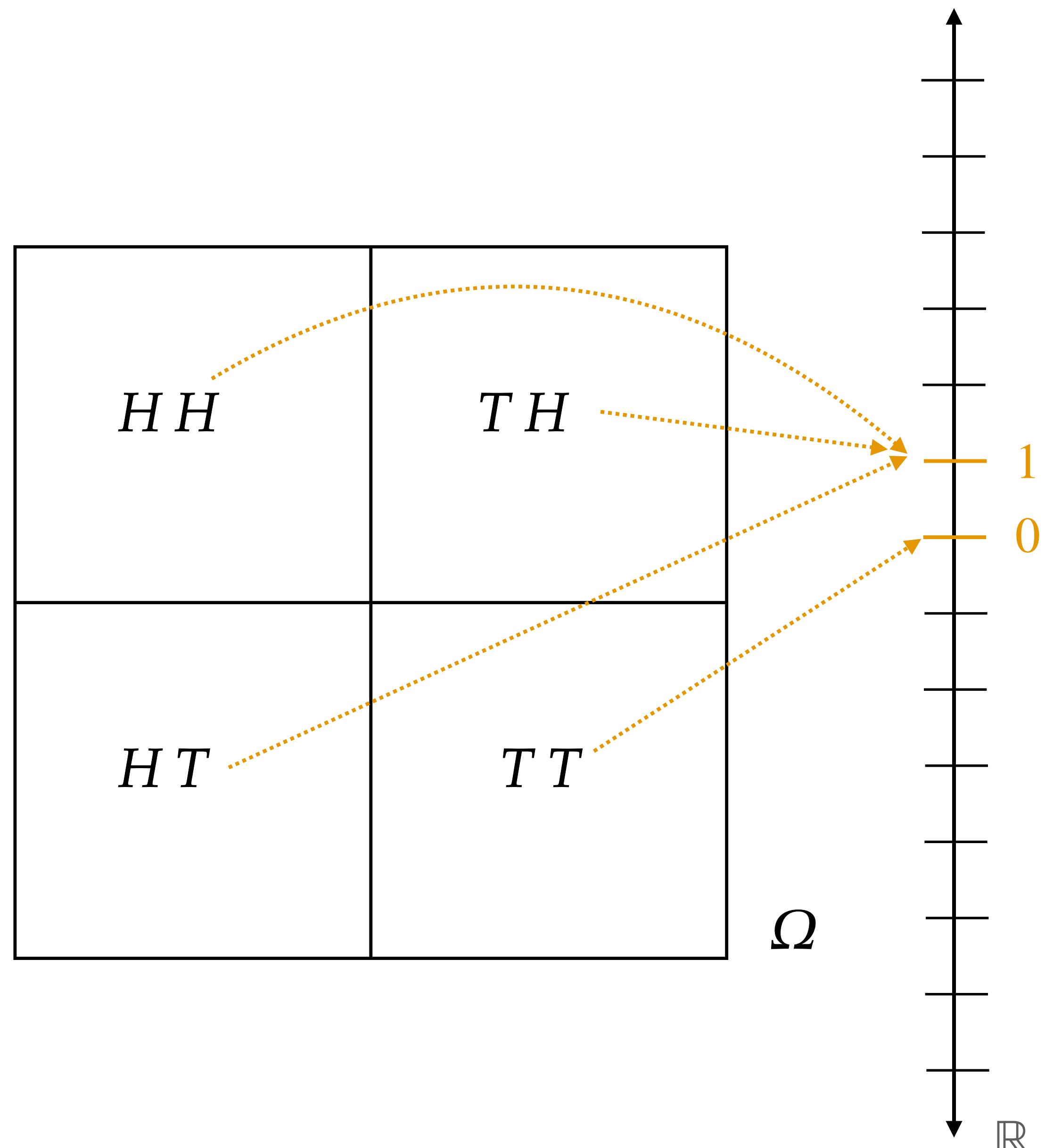
Example: Flipping 2 fair coins

Consider the following function:

$$X : \Omega \rightarrow \mathbb{R}$$

where $X(\omega) = 1$ if at least one H , and 0 otherwise.

Random variables are *functions* that assign a number to every outcome in the sample space.



Random Variables

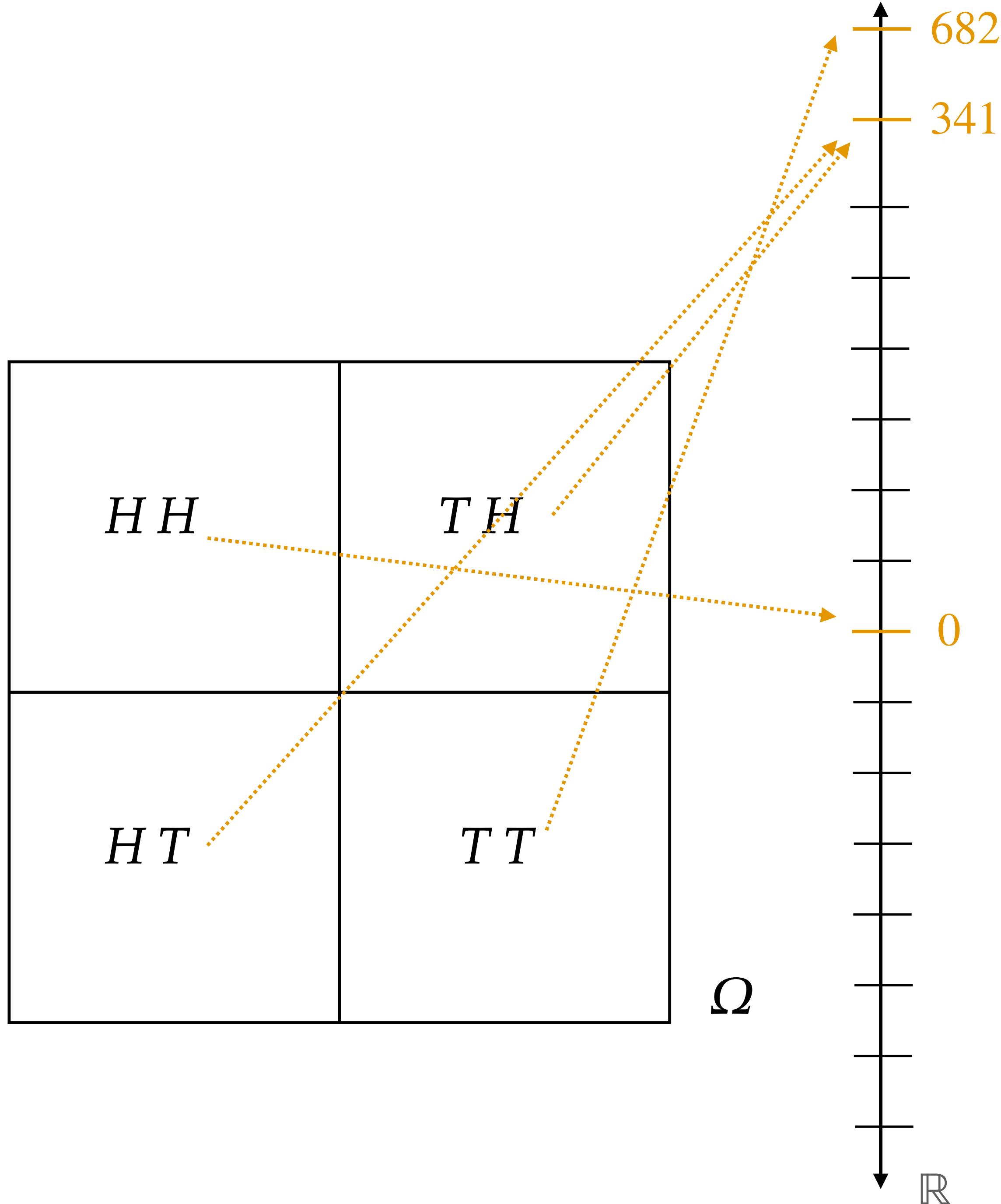
Example: Flipping 2 fair coins

Consider the following function:

$$X : \Omega \rightarrow \mathbb{R}$$

where $X(\omega) = 341x$ where x is the number of T .

Random variables are *functions* that assign a number to every outcome in the sample space.

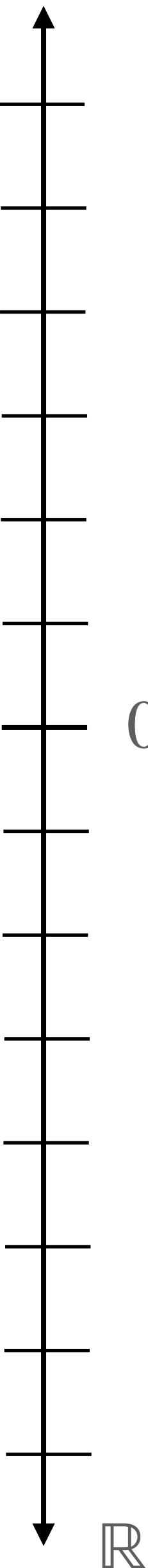
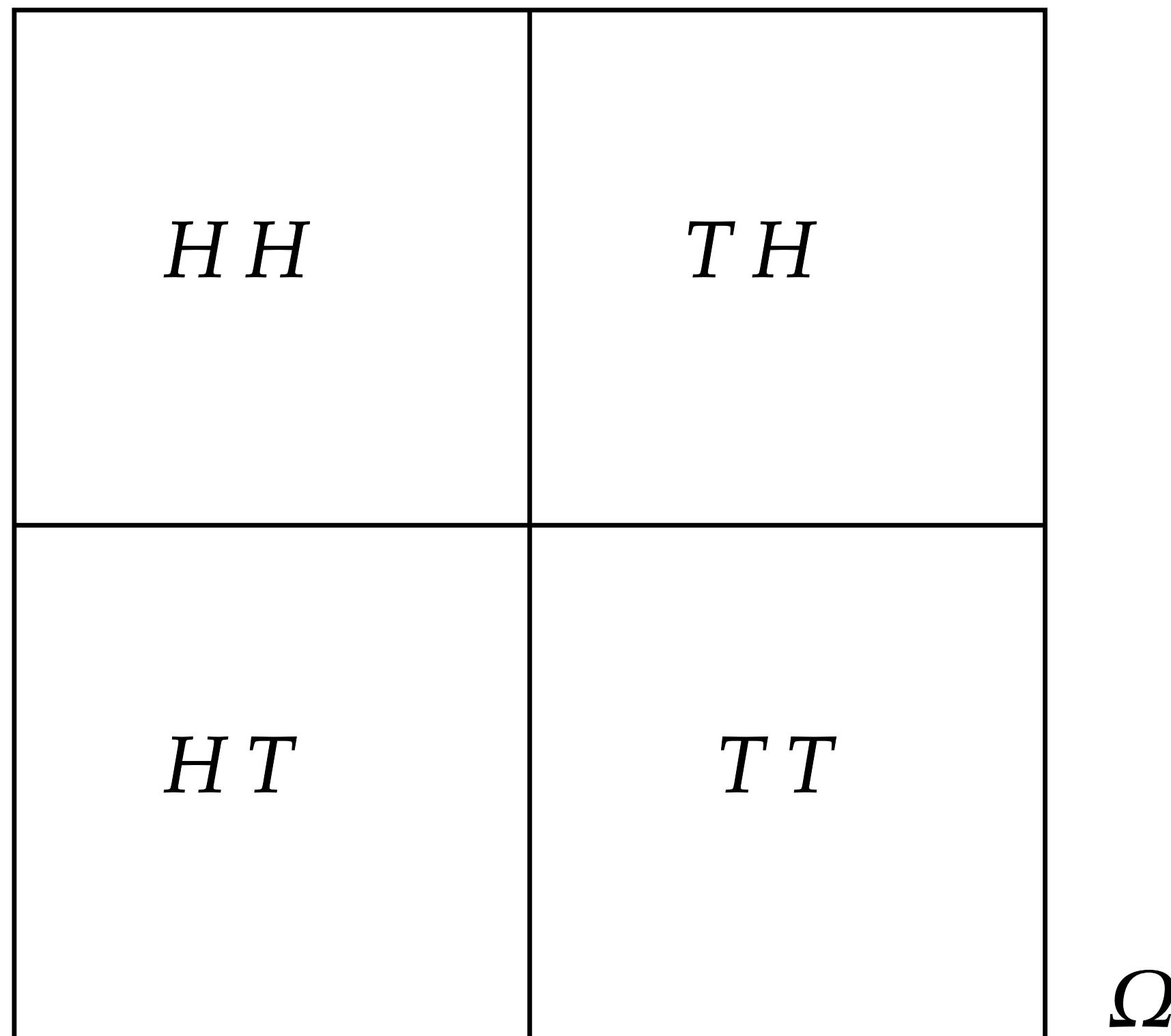


Random Variable

Intuition and definition

A random variable is a function $X : \Omega \rightarrow \mathbb{R}$ that takes outcomes $\omega \in \Omega$ of the sample space and maps them to real values.

We use random variables to talk about events without referencing the underlying sample space.



Random Variable

Intuition and definition

Let $X : \Omega \rightarrow \mathbb{R}$ be defined as

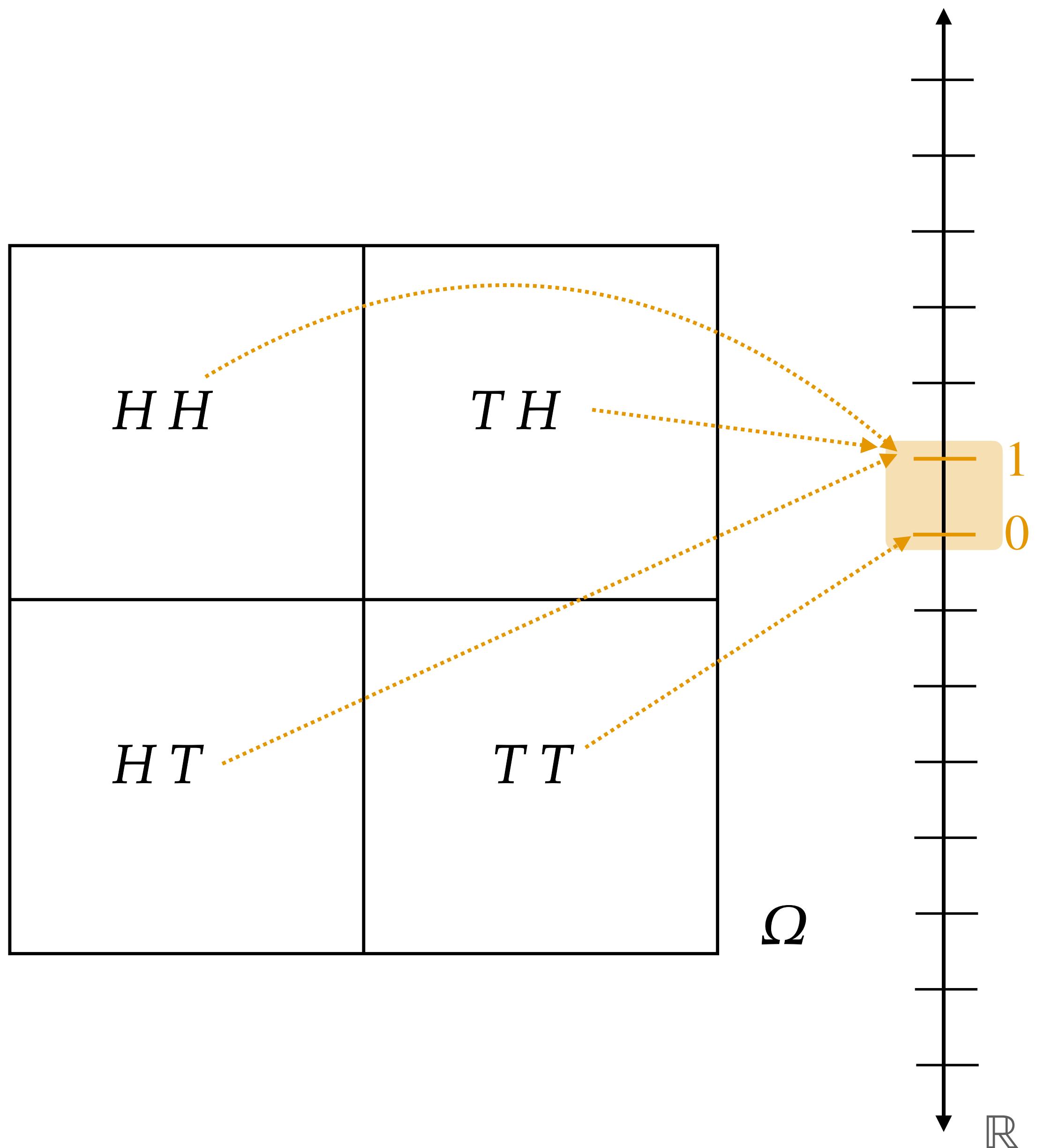
$$X(\omega) = \# \text{ of heads, } H.$$

Let the underlying probability measure assign outcomes to be equally likely:

$$\mathbb{P}(\{\omega\}) = 1/4$$

Then, for any $S \subseteq \mathbb{R}$,

$$\mathbb{P}_X(S) = \mathbb{P}(X \in S).$$



Random Variable

Intuition and definition

Let $X : \Omega \rightarrow \mathbb{R}$ be defined as

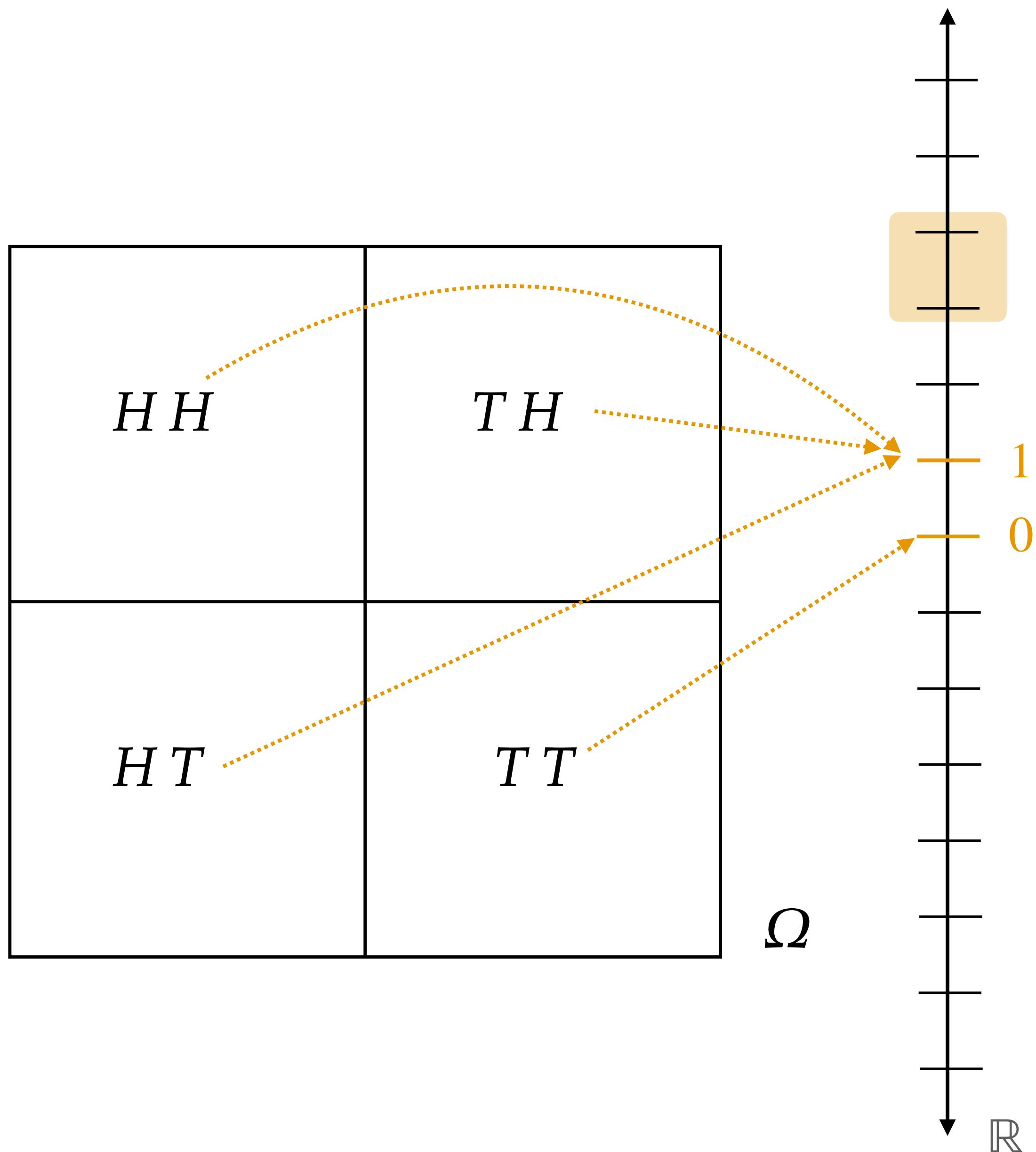
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Random Variable

Intuition and definition

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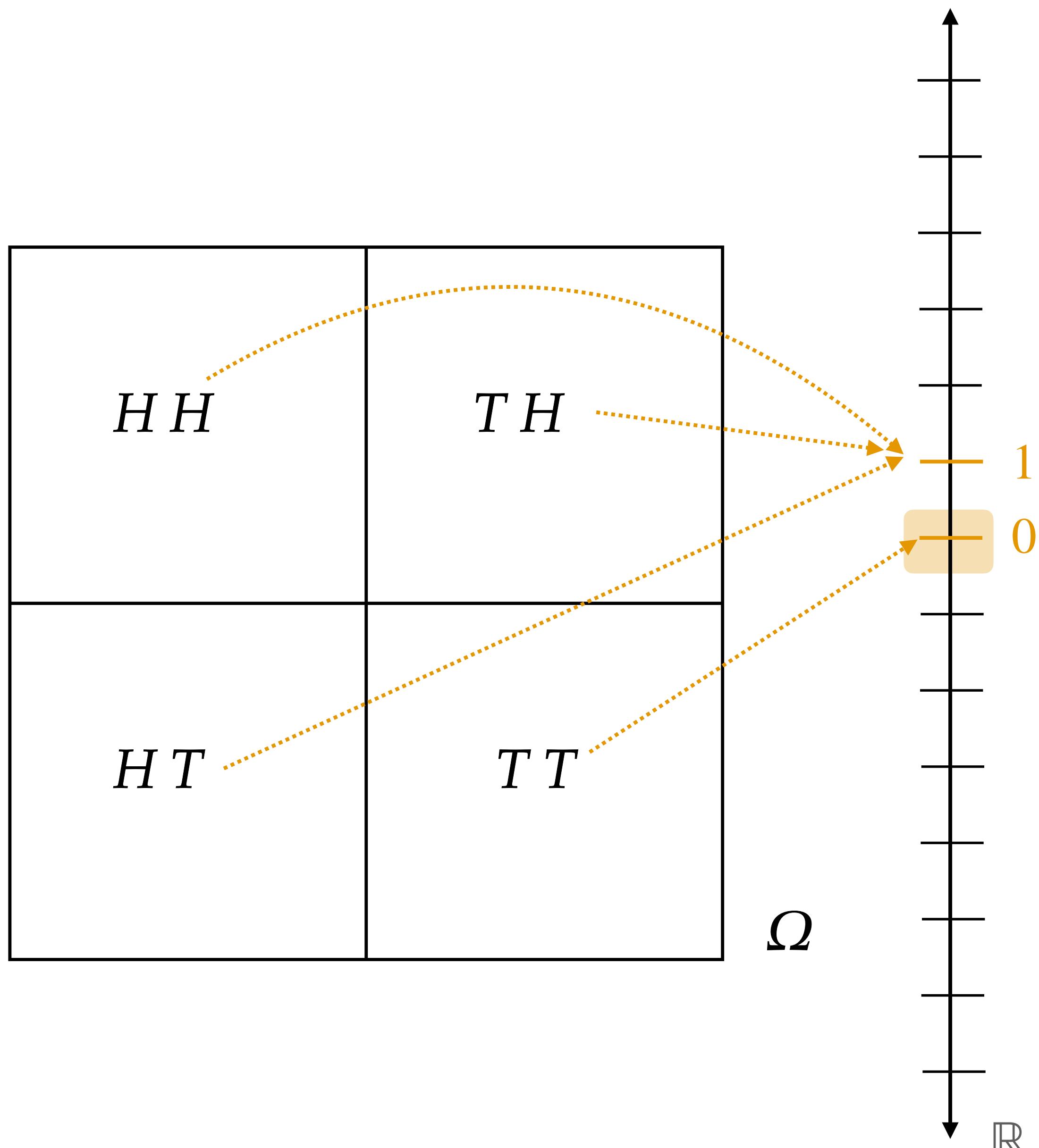
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Random Variable

Intuition and definition

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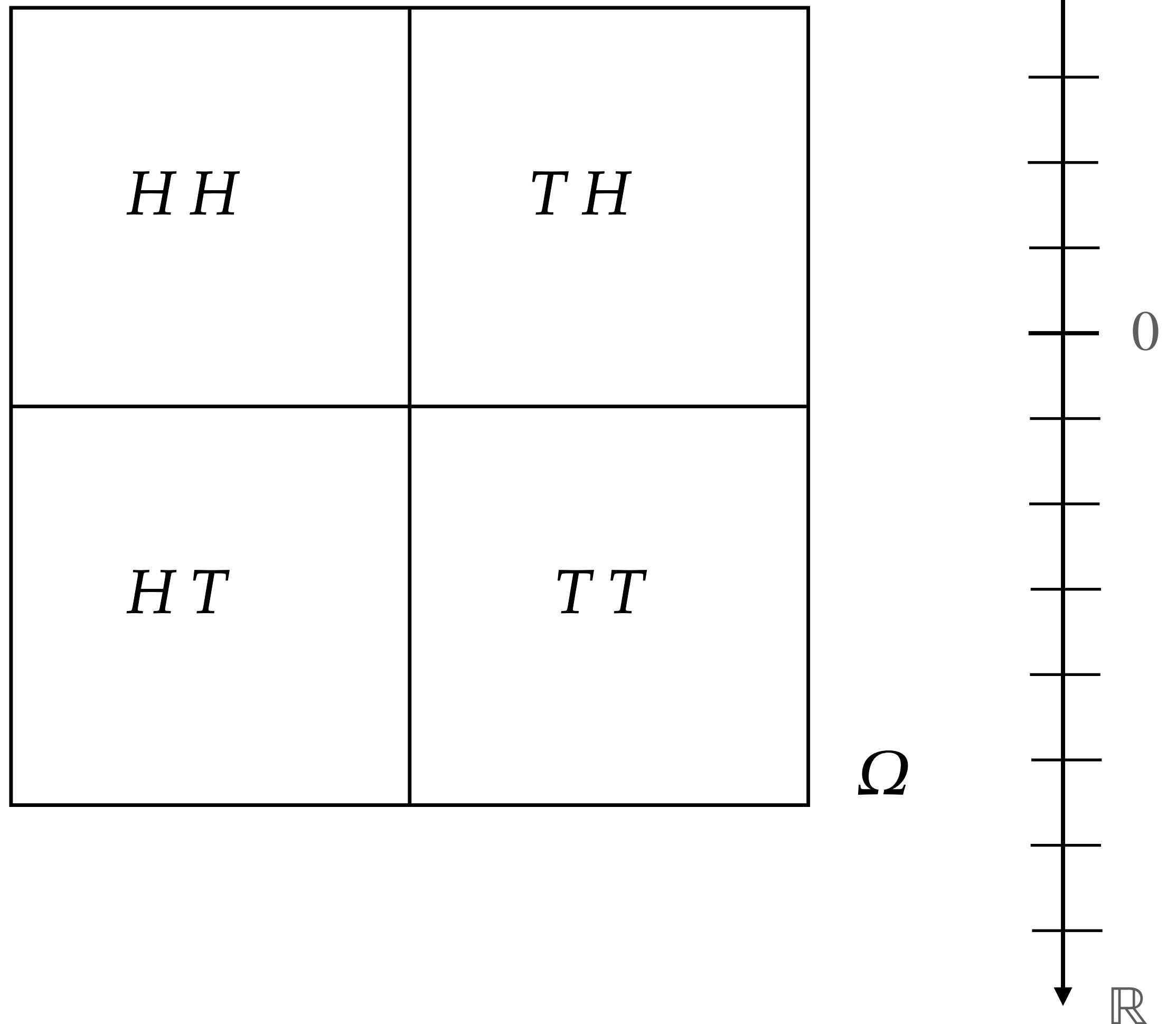
For any $S \subseteq \mathbb{R}$,

$$\mathbb{P}_X(S) = \mathbb{P}(X \in S) = \mathbb{P}(\{\omega \in \Omega : X(\omega) \in S\})$$

Example.

What's $\mathbb{P}_X(1)$?

What's $\mathbb{P}_X(20)$?



Random Variable

The distribution of a random variable

Let $(\Omega, \mathcal{A}, \mathbb{P})$ be some underlying probability space.

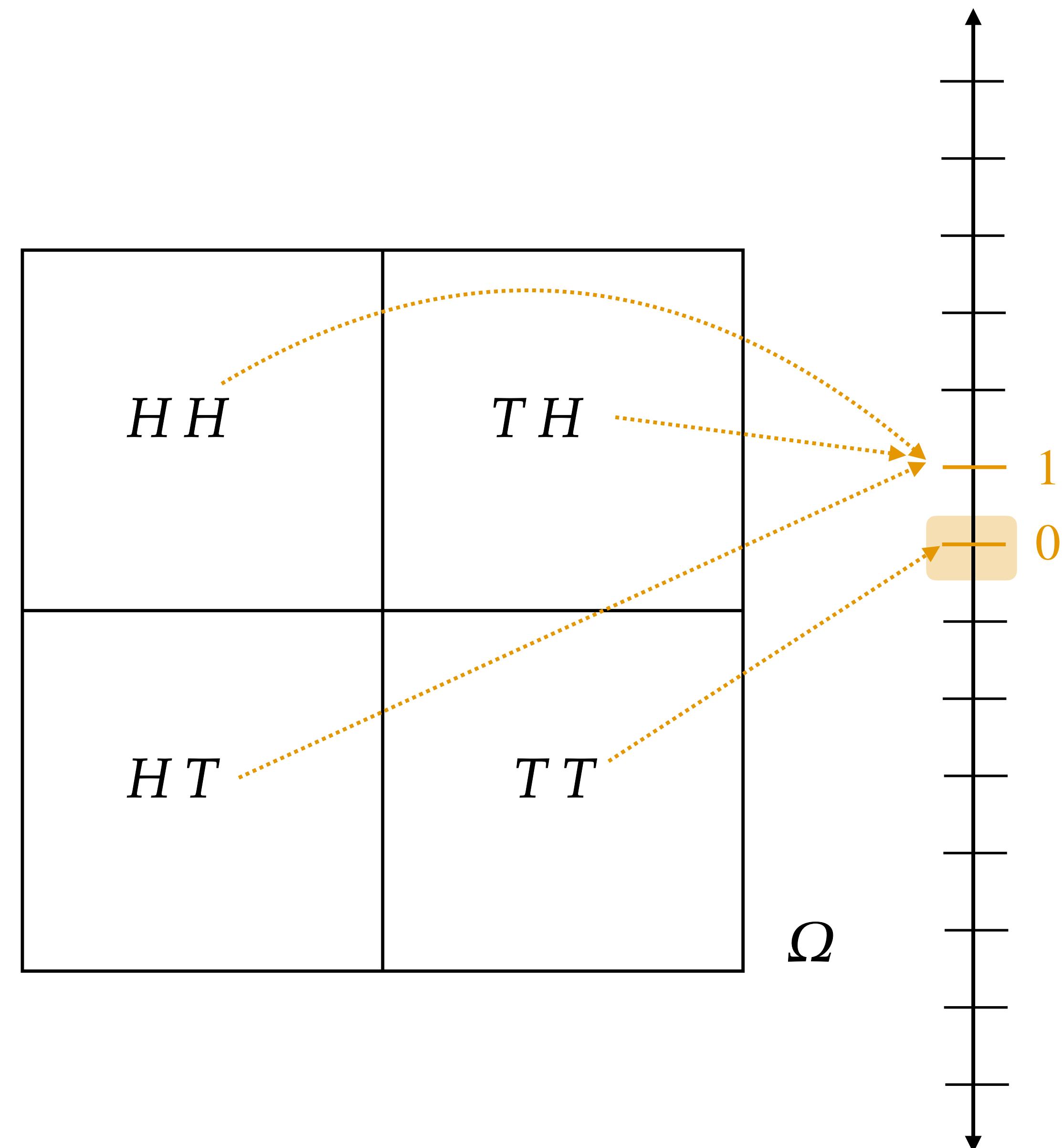
Random variables $X : \Omega \rightarrow \mathbb{R}$ come with a distribution/
law, \mathbb{P}_X . This implicitly defines a measure on \mathbb{R} .

For $S \subseteq \mathbb{R}$,

$$\mathbb{P}_X(S) = \mathbb{P}(X \in S) = \mathbb{P}(X^{-1}(S)) = \mathbb{P}(\{\omega \in \Omega : X(\omega) \in S\})$$

.

This allows us to just talk about the numbers in \mathbb{R} !



Probability Spaces

Putting everything together

The sample space is the set of all possible outcomes:

$$\Omega = \{HH, TH, HT, TT\}.$$

The event space (σ -algebra) is some collection of events:

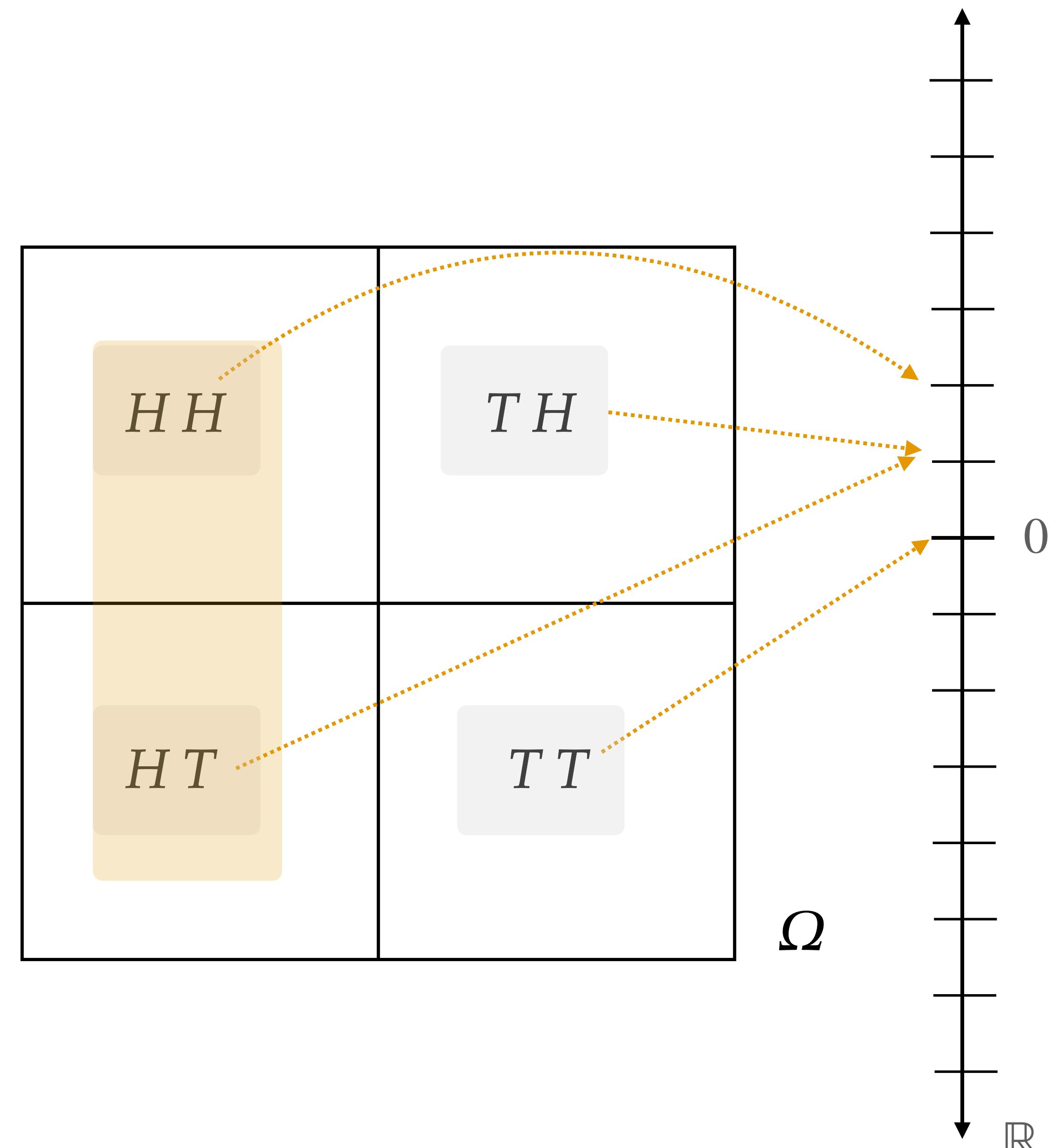
$$\mathcal{A} = \{\emptyset, \{HH\}, \{TT\}, \dots, \{HH, HT, TH, TT\}\}$$

The probability measure is how we measure the “mass” of events:

$$\mathbb{P}(\omega) = 1/4 \text{ for } \omega \in \Omega.$$

A random variable on $(\Omega, \mathcal{A}, \mathbb{P})$ is a function $X : \Omega \rightarrow \mathbb{R}$ associating outcomes $\omega \in \Omega$ to numbers in \mathbb{R} :

$$X(\omega) = \# \text{ of heads in } \omega$$



Probability Spaces

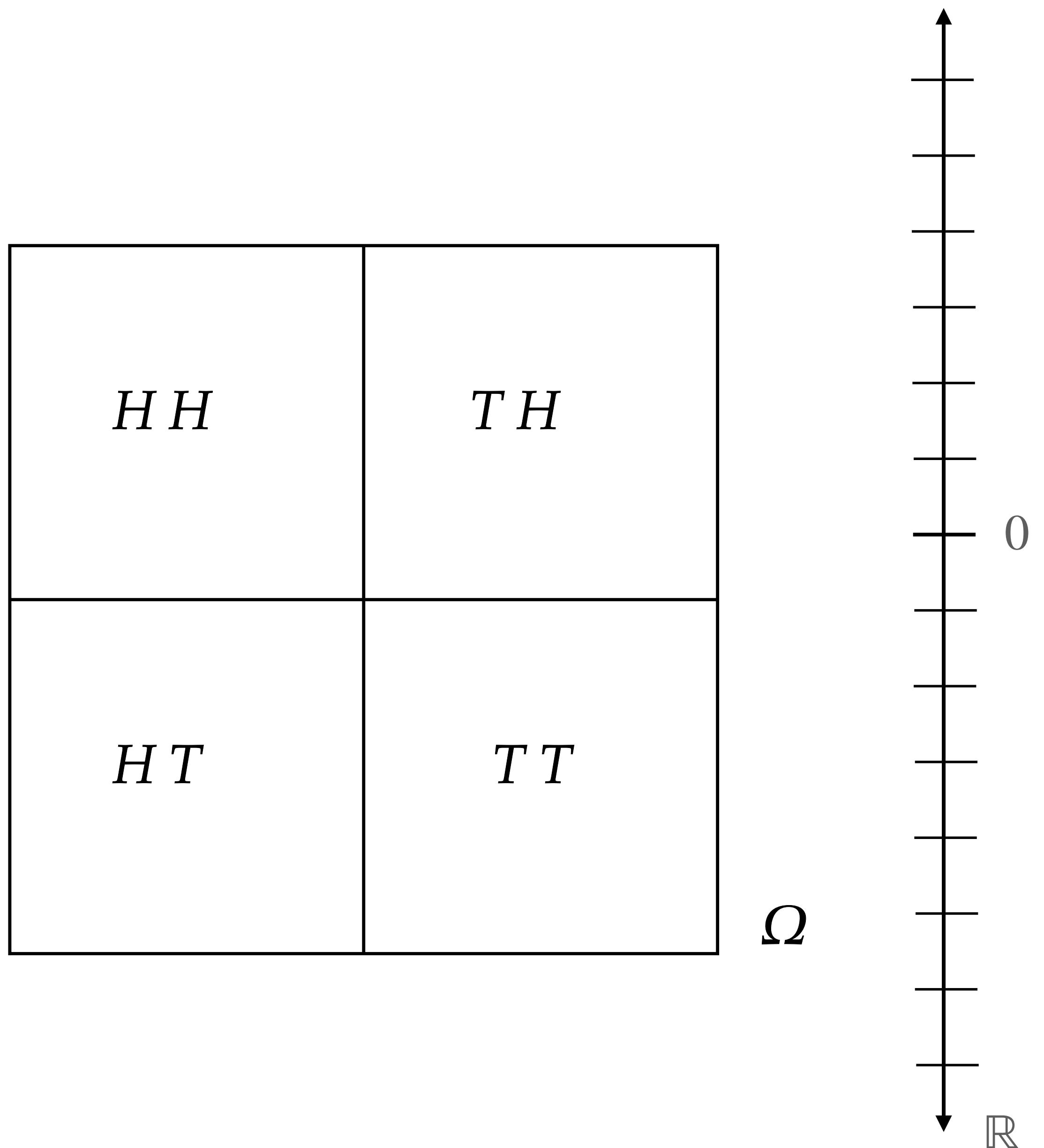
Putting everything together

Example:

Compute $\mathbb{P}(X = 0)$:

Compute $\mathbb{P}(X = 1)$:

Compute $\mathbb{P}(X = 2)$:



Random Variables

Distributions of random variables

Cumulative Distribution Function

Intuition and definition

Let $X : \Omega \rightarrow \mathbb{R}$ be some random variable (*on an underlying probability space $(\Omega, \mathcal{A}, \mathbb{P})$*).

The cumulative distribution function (CDF) of X is the function $F_X : \mathbb{R} \rightarrow [0,1]$ defined as:

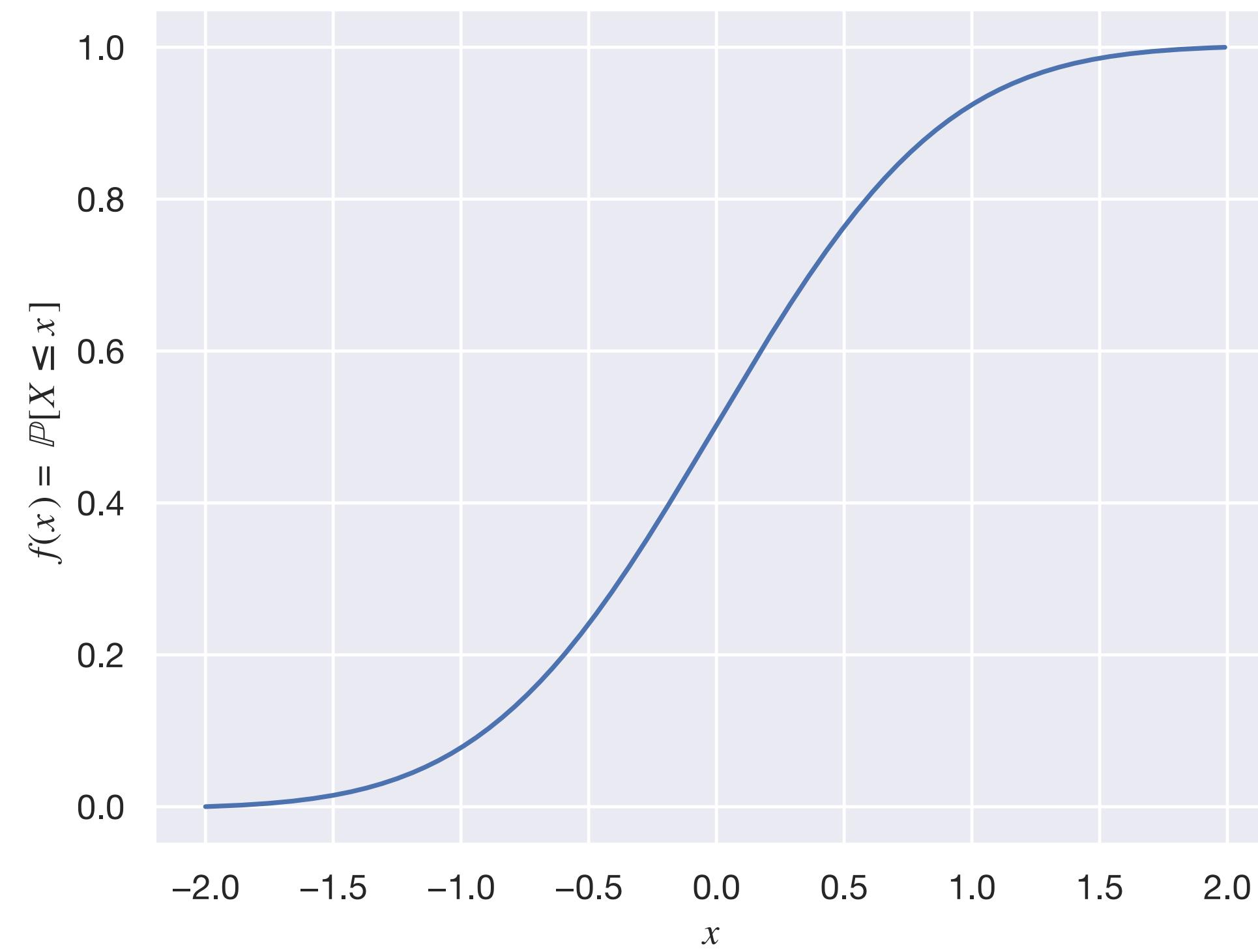
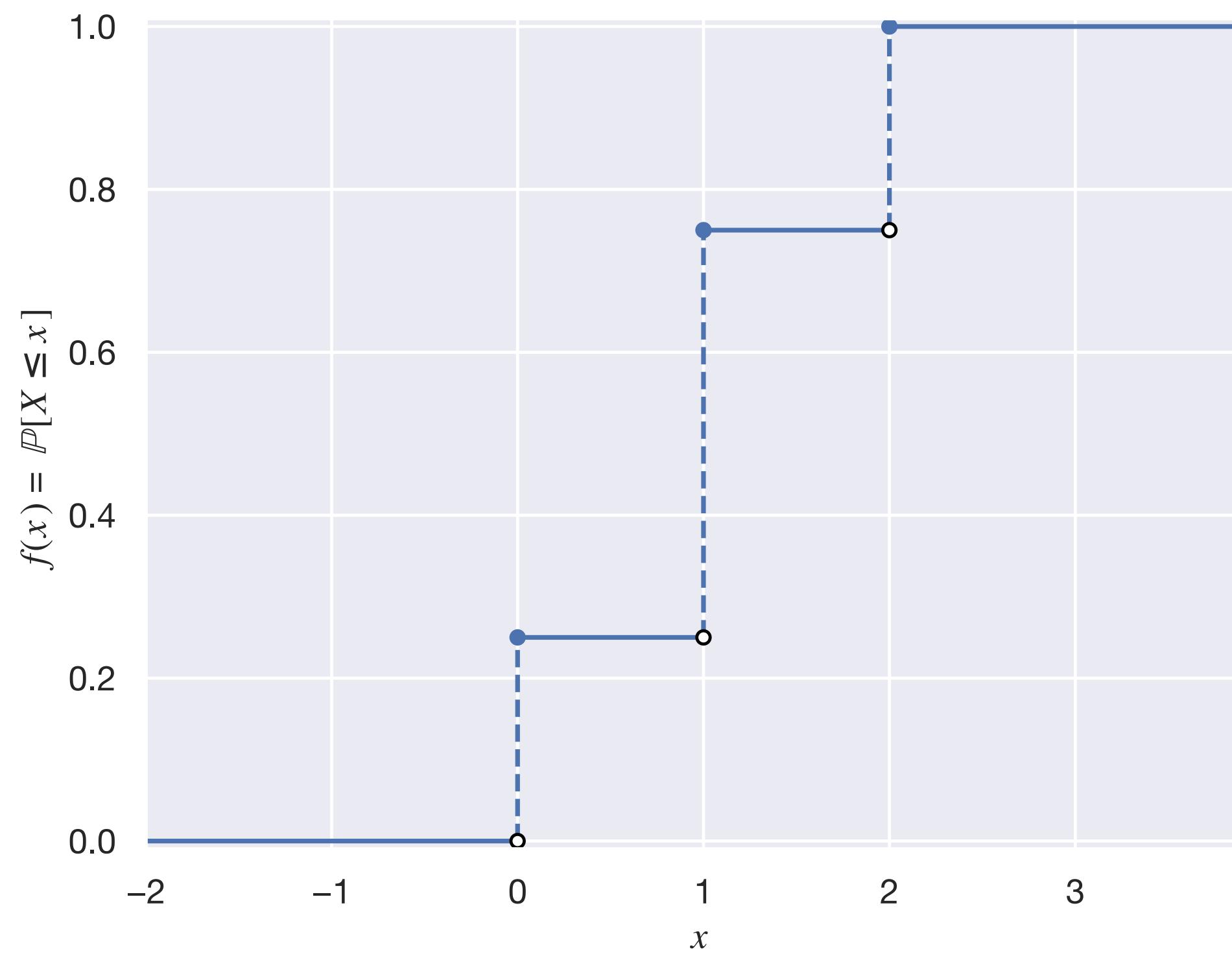
$$F_X(x) = \mathbb{P}(X \leq x)$$

This function allows us to get probabilities in an interval:

$$\mathbb{P}(a \leq X \leq b) = F(b) - F(a)$$

Cumulative Distribution Function

Examples



Cumulative Distribution Function

Properties

Right-continuous. For any $a \in \mathbb{R}$, CDF satisfies:

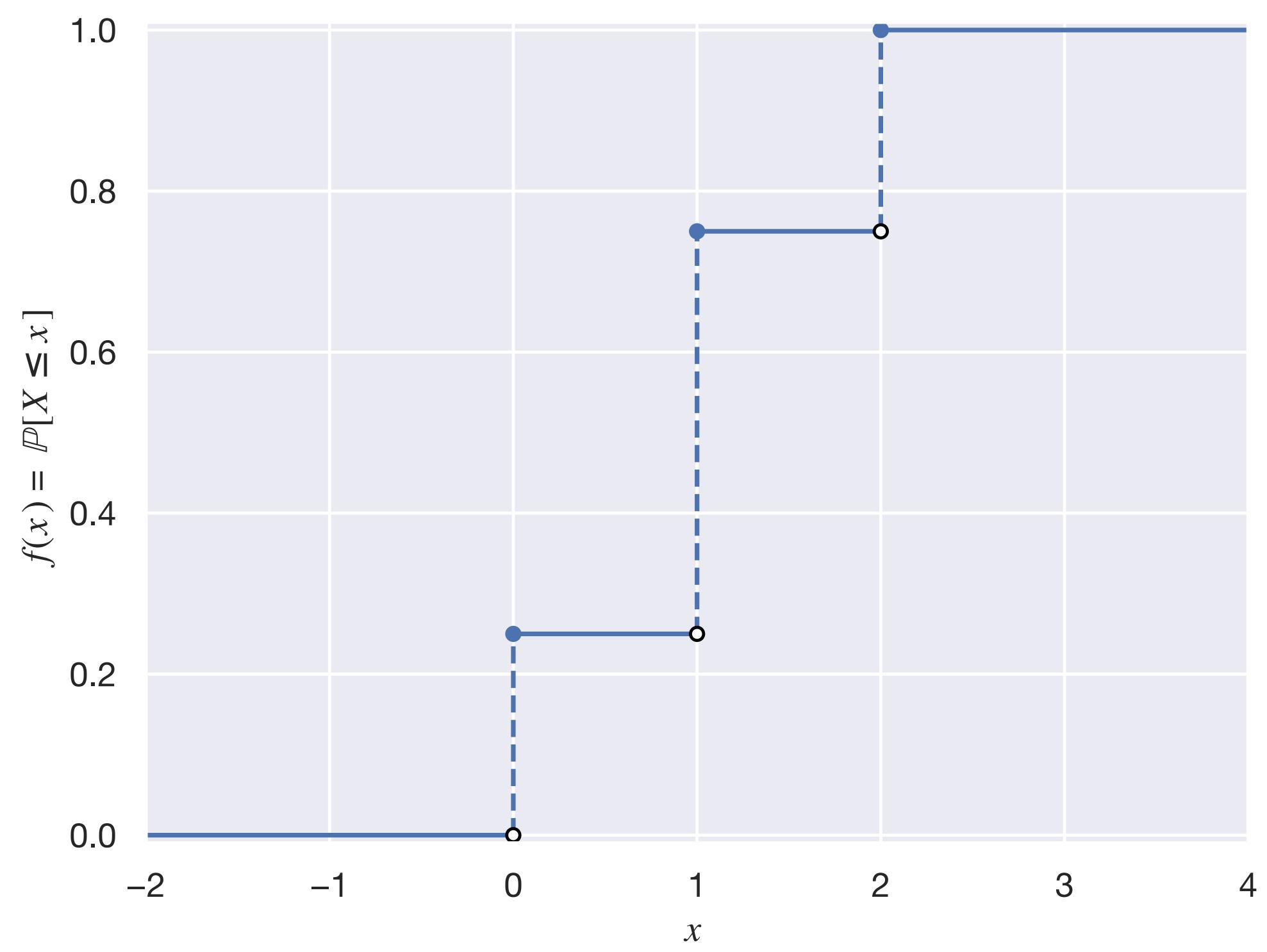
$$\lim_{x \rightarrow a^+} f(x) = f(a).$$

Monotonically nondecreasing. For every $x \leq y$,

$$F_X(x) \leq F_X(y).$$

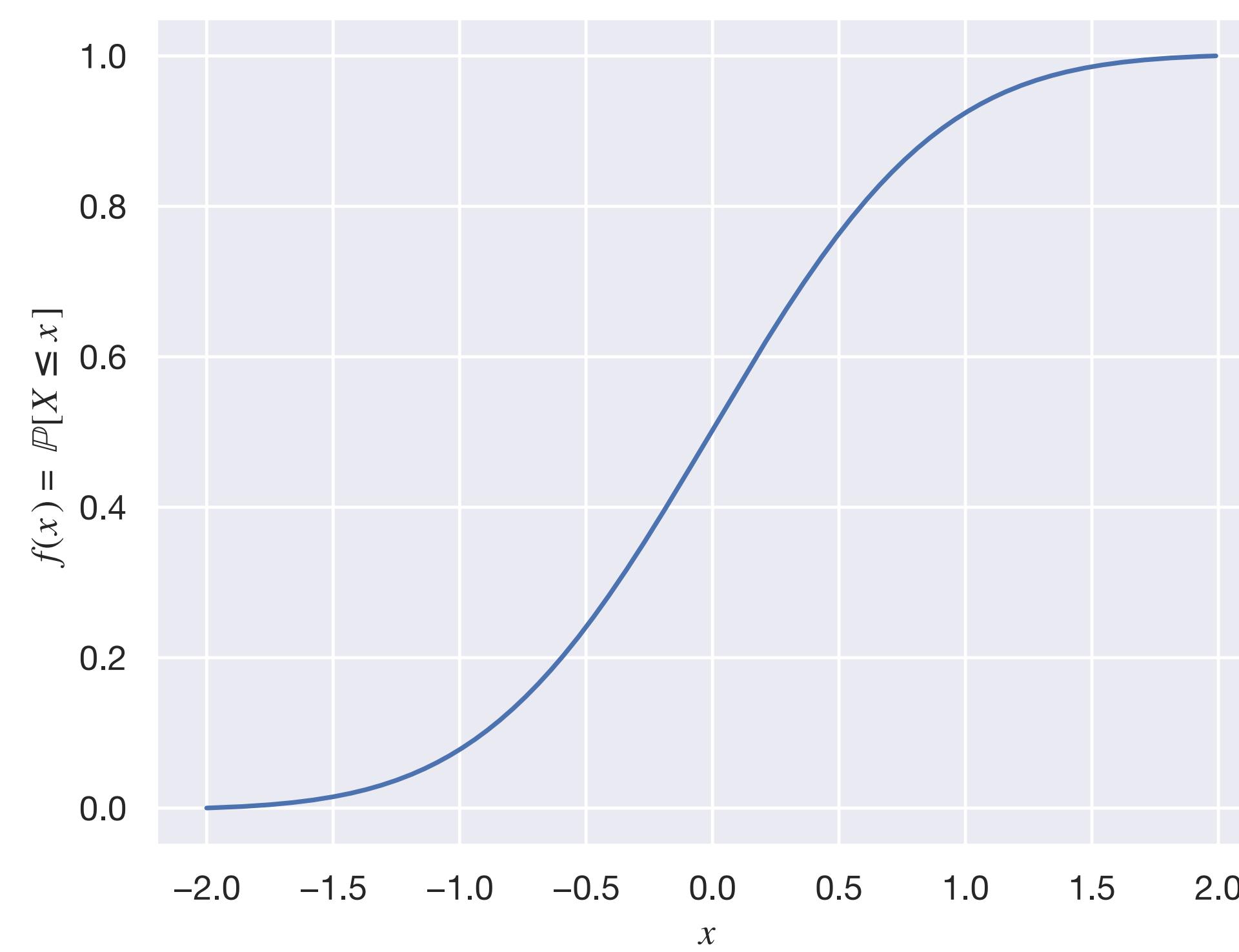
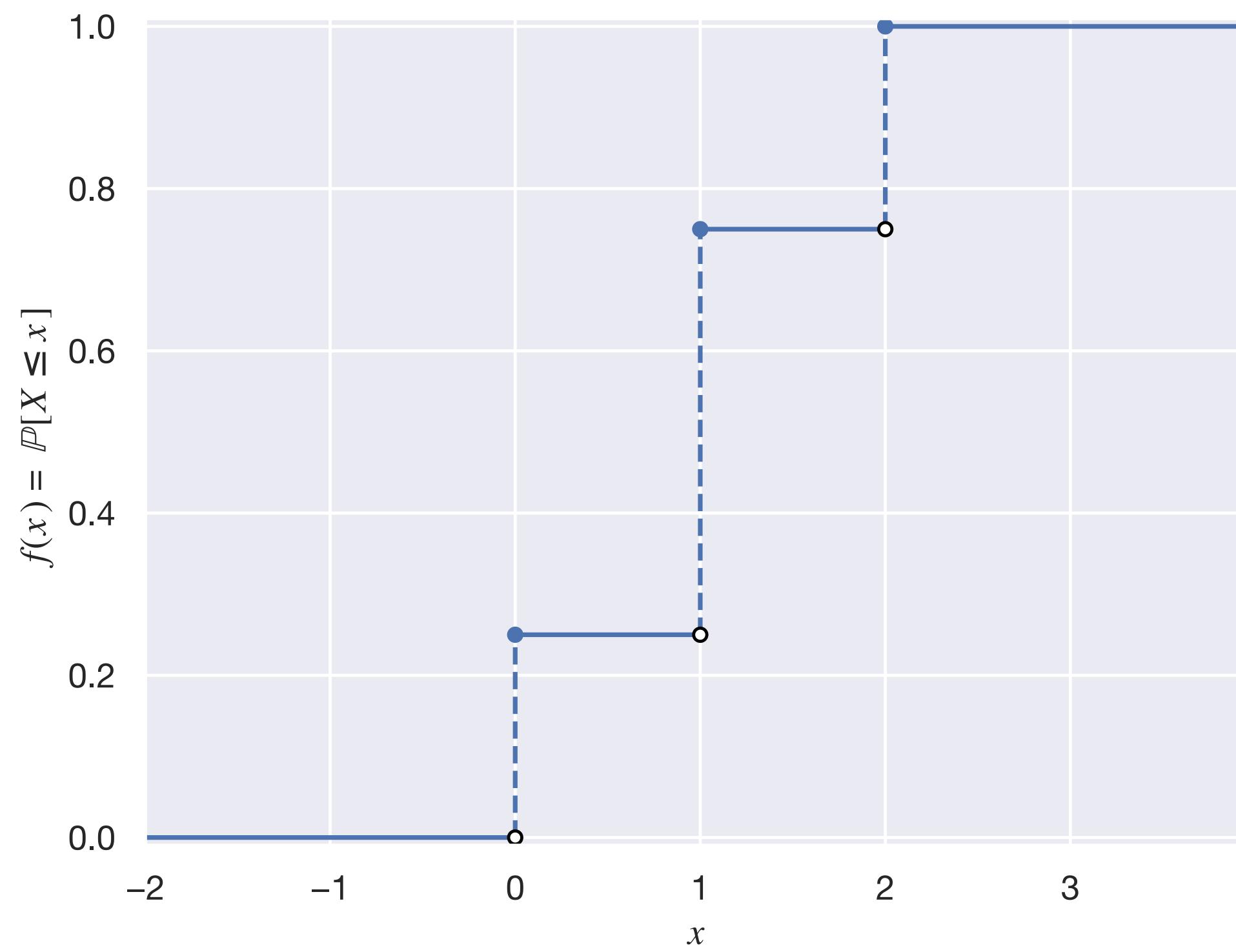
Limits at infinities. The limits at infinity are:

$$\lim_{x \rightarrow -\infty} F_X(x) = 0 \text{ and } \lim_{x \rightarrow \infty} F_X(x) = 1.$$



Discrete vs. Continuous RVs

Difference in CDF



Discrete Random Variables

Intuition and definition

A discrete random variable is a random variable whose range

$$X(\Omega) = \{x \in \mathbb{R} : X(\omega) = x \text{ for some } \omega \in \Omega\}$$

is *countable* or *finite*.

Example.

$X : \{HH, HT, TH, TT\} \rightarrow \mathbb{R}$ with $X(\omega)$ counting the number of heads.

$X : [0,1] \rightarrow \mathbb{R}$ defined by $X(\omega) = 0$ if $\omega < 0.5$ and $X(\omega) = 1$ otherwise.

Discrete Random Variables

Probability mass function

A discrete random variable X has a probability mass function (PMF) $p_X : \mathbb{R} \rightarrow [0,1]$ defined by:

$$p_X(x) = \mathbb{P}[X = x].$$

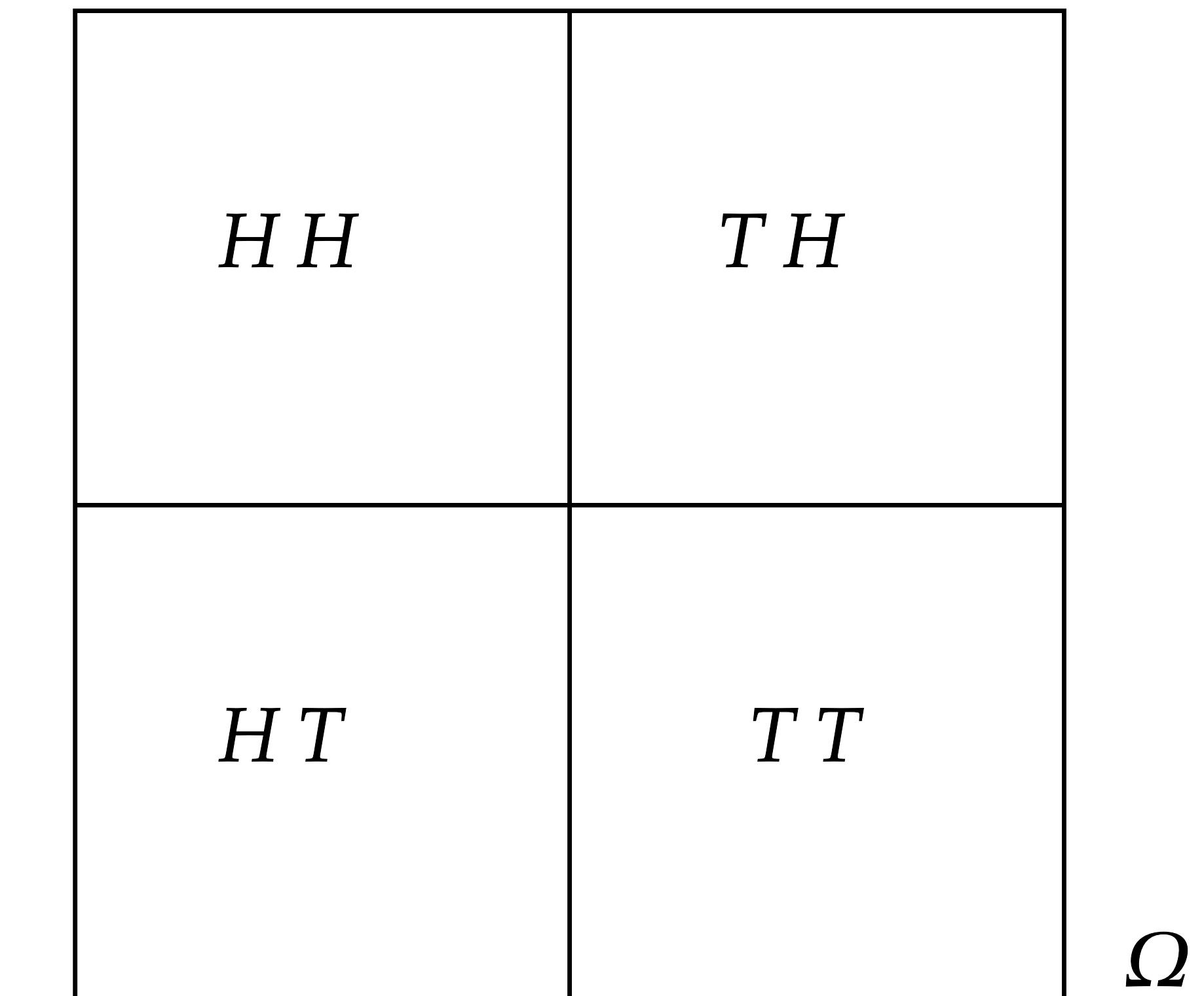
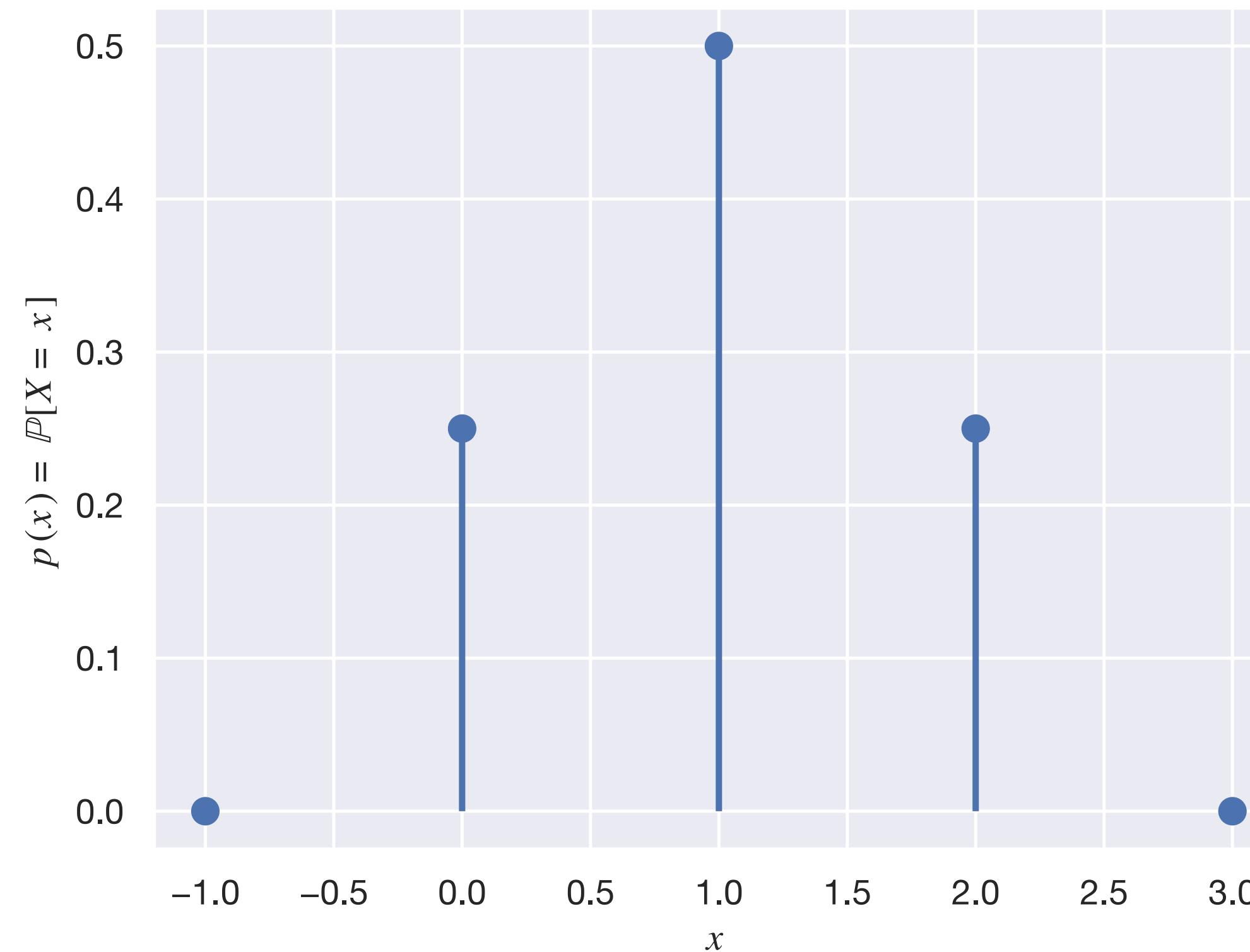
Example. What's the PMF of the RV $X : \Omega \rightarrow \mathbb{R}$ with $X(\omega)$ counting the number of heads?

$H H$	$T H$
$H T$	$T T$
	Ω

Discrete Random Variables

Example: Flipping 2 fair coins

Example. What's the PMF of the RV $X : \Omega \rightarrow \mathbb{R}$ with $X(\omega)$ counting the number of heads?



Continuous Random Variables

Intuition and definition

A continuous random variable is a random variable whose range

$$X(\Omega) = \{x \in \mathbb{R} : X(\omega) = x \text{ for some } \omega \in \Omega\}$$

is *uncountably infinite*.

For continuous random variables, the probability at any point $x \in \mathbb{R}$ is zero!

$$\mathbb{P}[X = x] = 0.$$

So there is no “probability mass function,” but there is a probability density function.

Continuous Random Variables

Probability density functions

A continuous random variable X has a probability density function (PDF) $p_X : \mathbb{R} \rightarrow \mathbb{R}$

For all $x \in \mathbb{R}$, $p_X(x) \geq 0$ and $\int_{\mathbb{R}} p_X(z)dz = 1$.

To get probabilities from the PDF:

$$\mathbb{P}(a \leq X \leq b) = \int_a^b p_X(z)dz.$$

We can also obtain the CDF by the fundamental theorem of calculus:

$$p_X(x) = F'(x).$$

Continuous Random Variables

Intuition for the PDF

PDFs do NOT immediately give probabilities (unlike PMFs).

Think of them in analogy to the physical notion of *density*:

$$\text{density} = \frac{\text{mass}}{\text{volume}}.$$

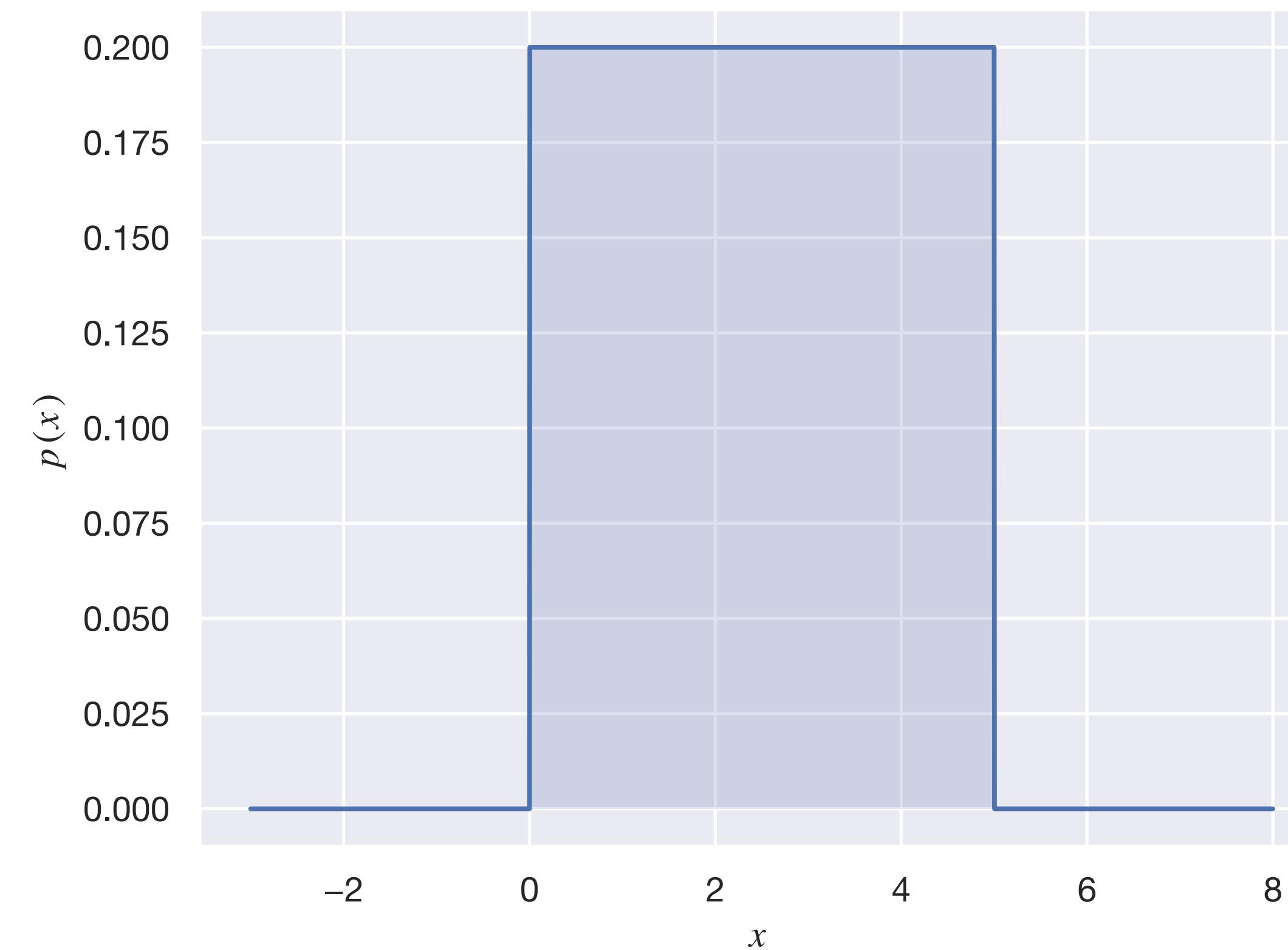
In an infinitesimally small interval, we can get a probability:

$$\mathbb{P}(x - \epsilon \leq X \leq x + \epsilon) = \int_{x-\epsilon}^{x+\epsilon} p_X(z) dz \approx 2\epsilon p_X(x).$$

Continuous Random Variables

Example: Picking uniformly in the interval

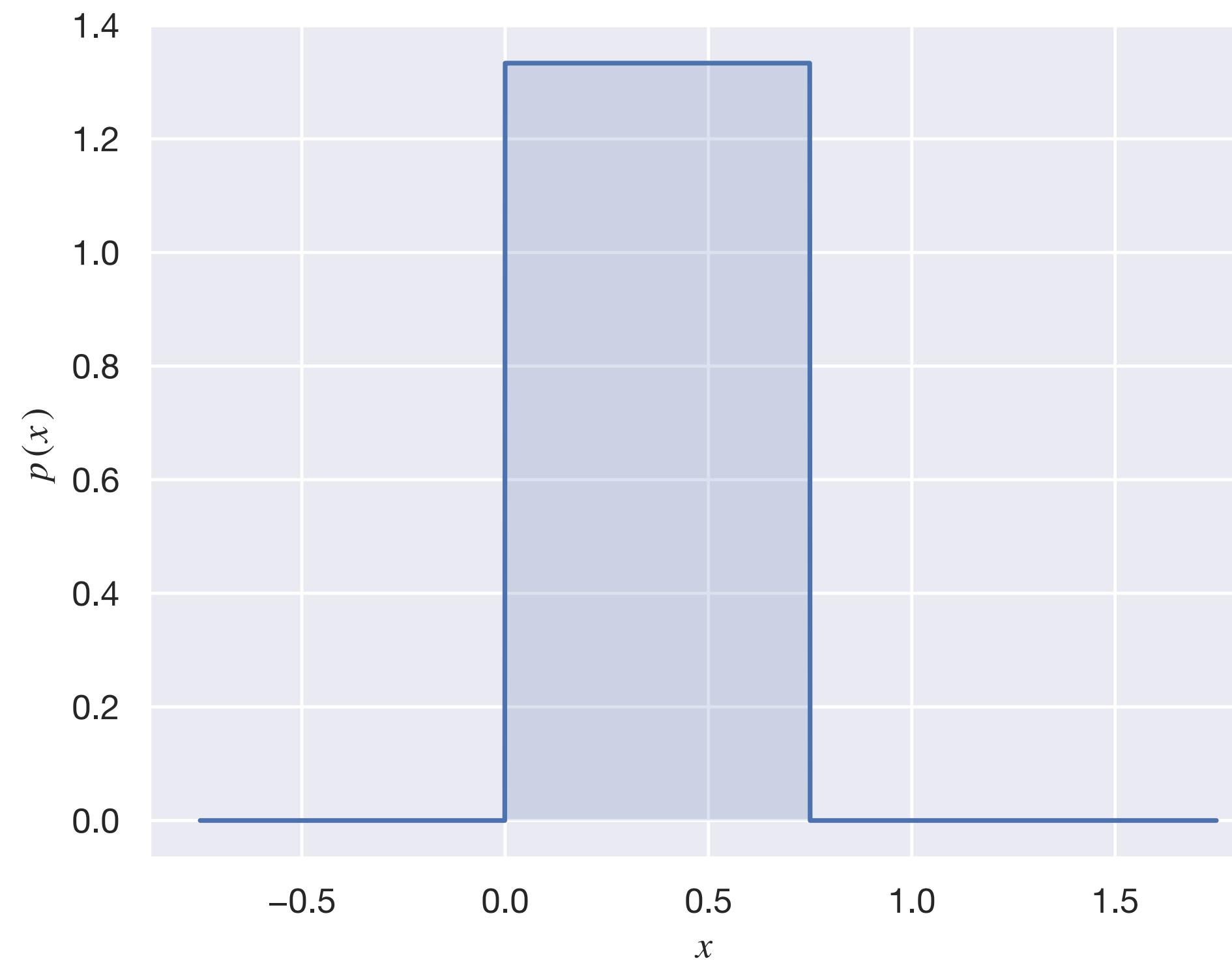
Example. What's the PDF of the RV $X : \Omega \rightarrow \mathbb{R}$ with the uniform random variable on $[0,5]$?



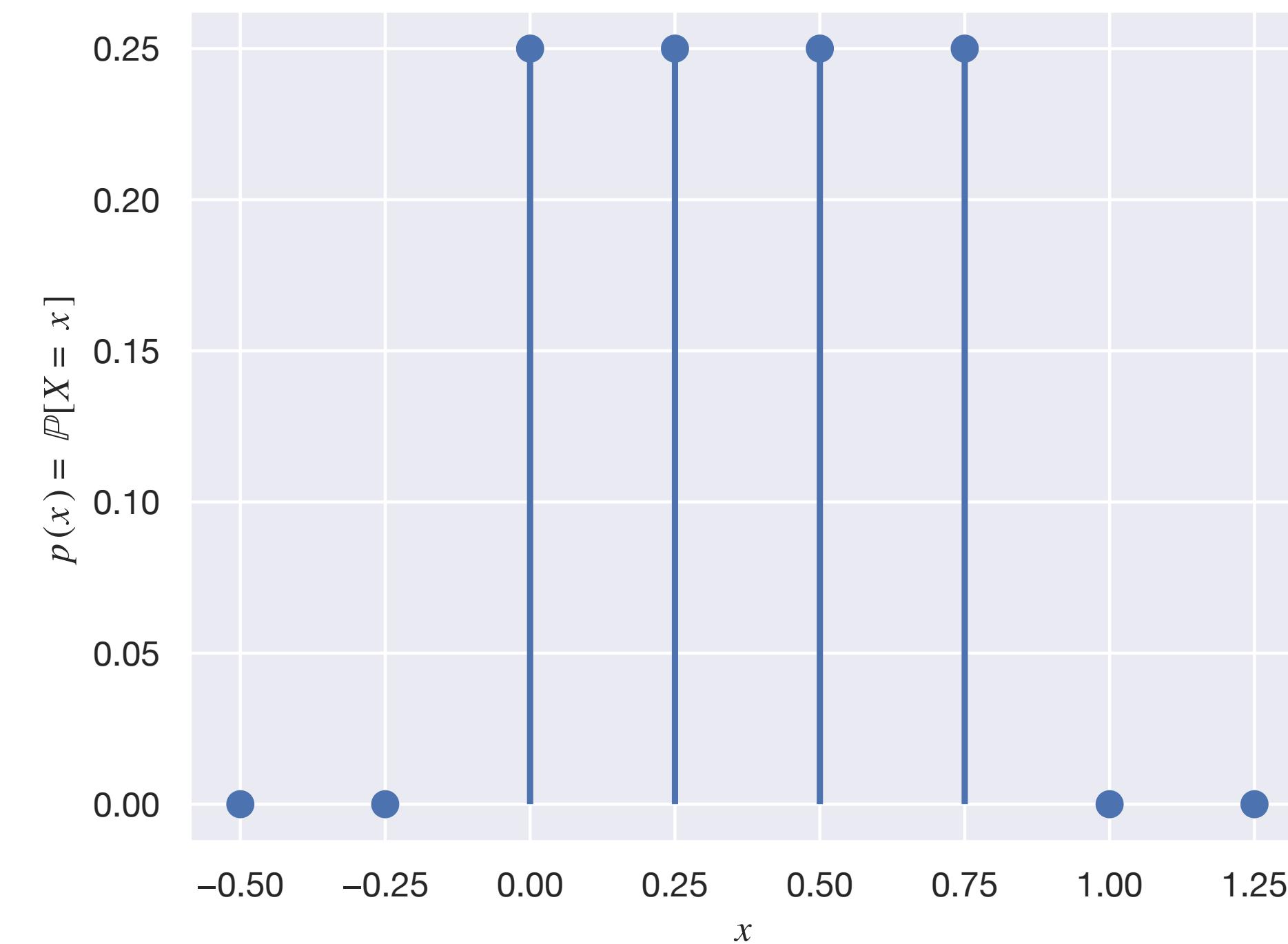
Continuous vs. Discrete RVs

Example: Uniform Discrete and Uniform Continuous PDFs

Continuous RV uniform on $[0,0.75]$.



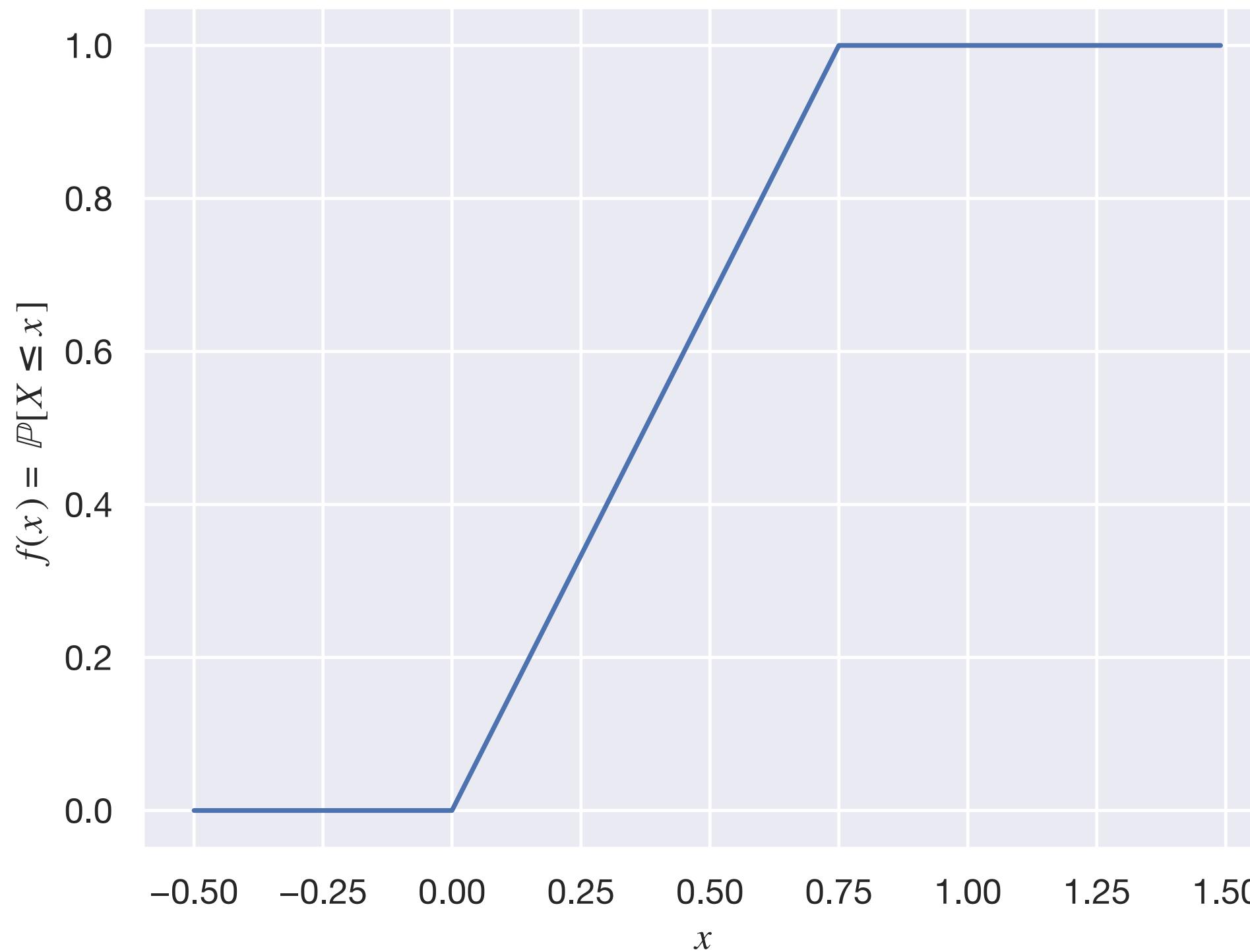
Discrete RV uniform on $\{0,0.25,0.5,0.75\}$.



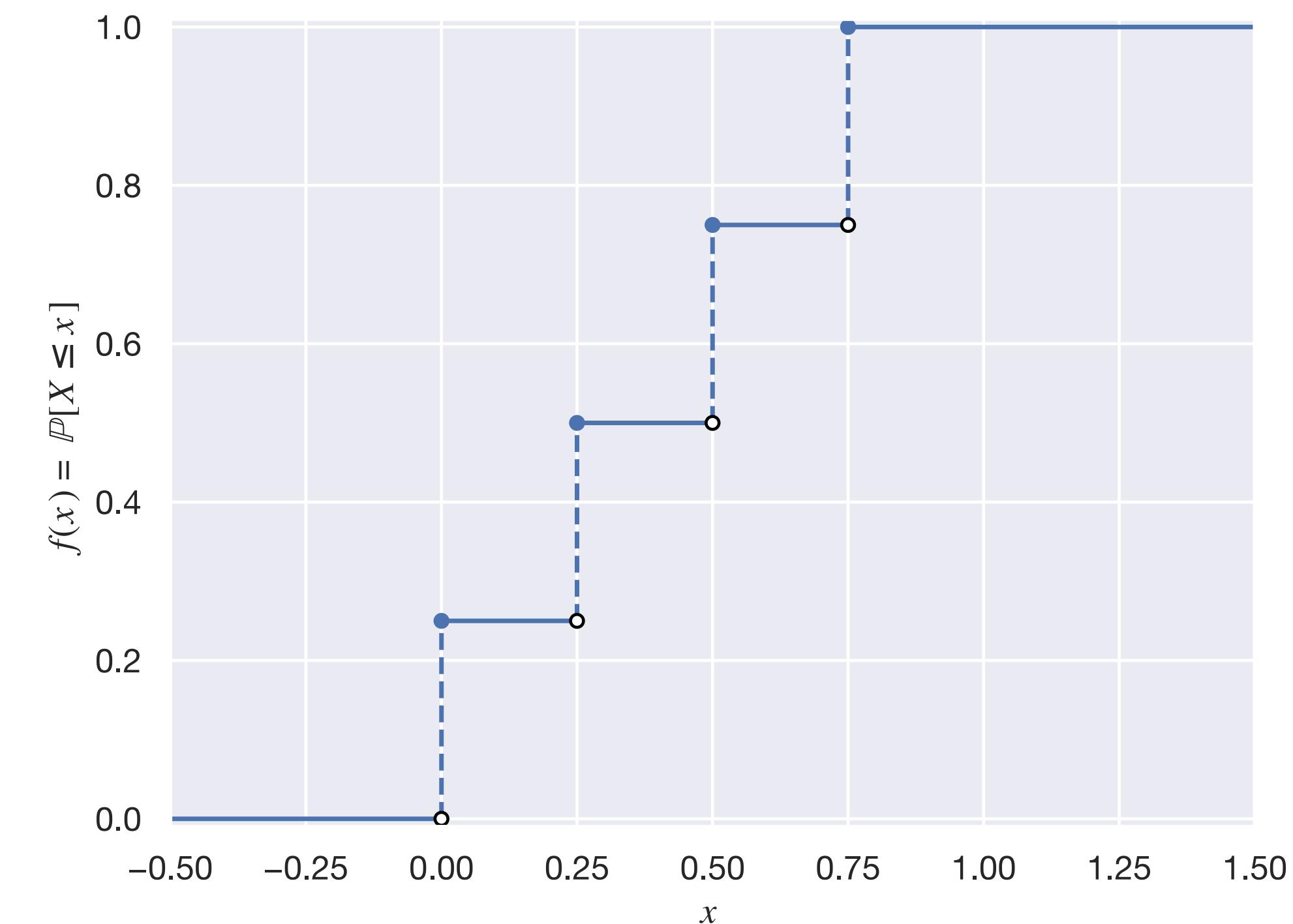
Continuous vs. Discrete RVs

Example: Uniform Discrete and Uniform Continuous CDFs

Continuous RV uniform on $[0,0.75]$.



Discrete RV uniform on $\{0,0.25,0.5,0.75\}$.



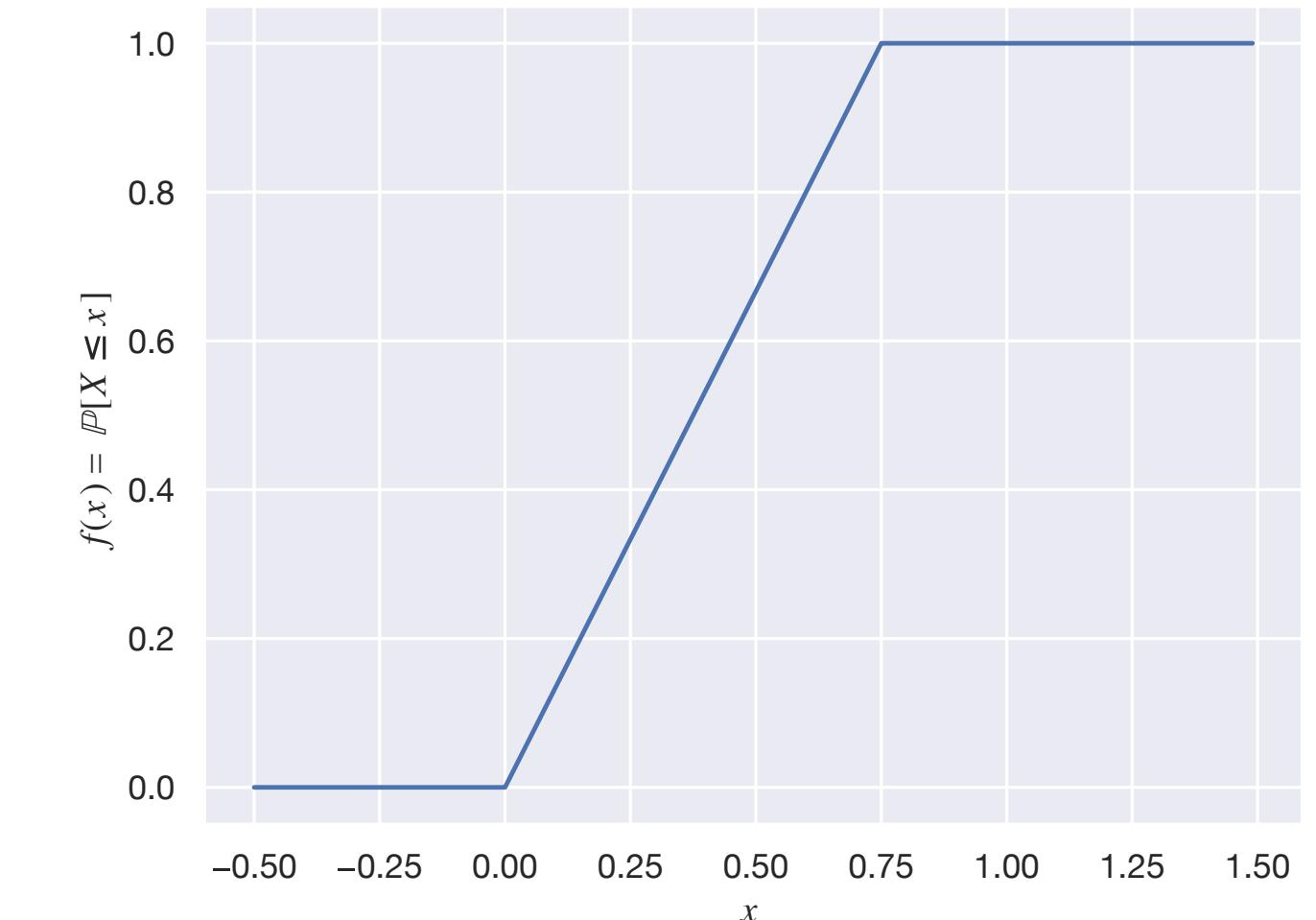
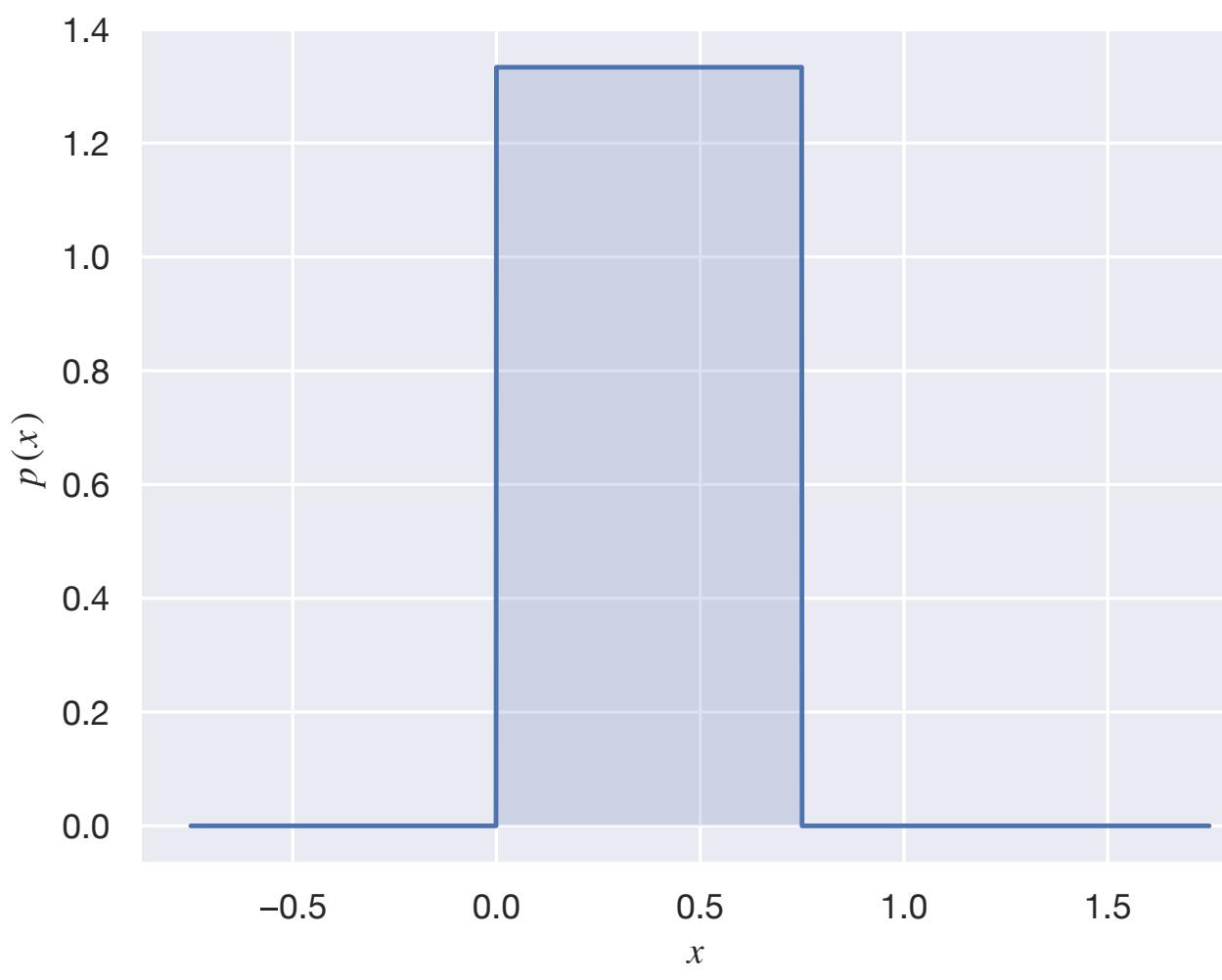
Continuous vs. Discrete RVs

Summary

For continuous RVs,

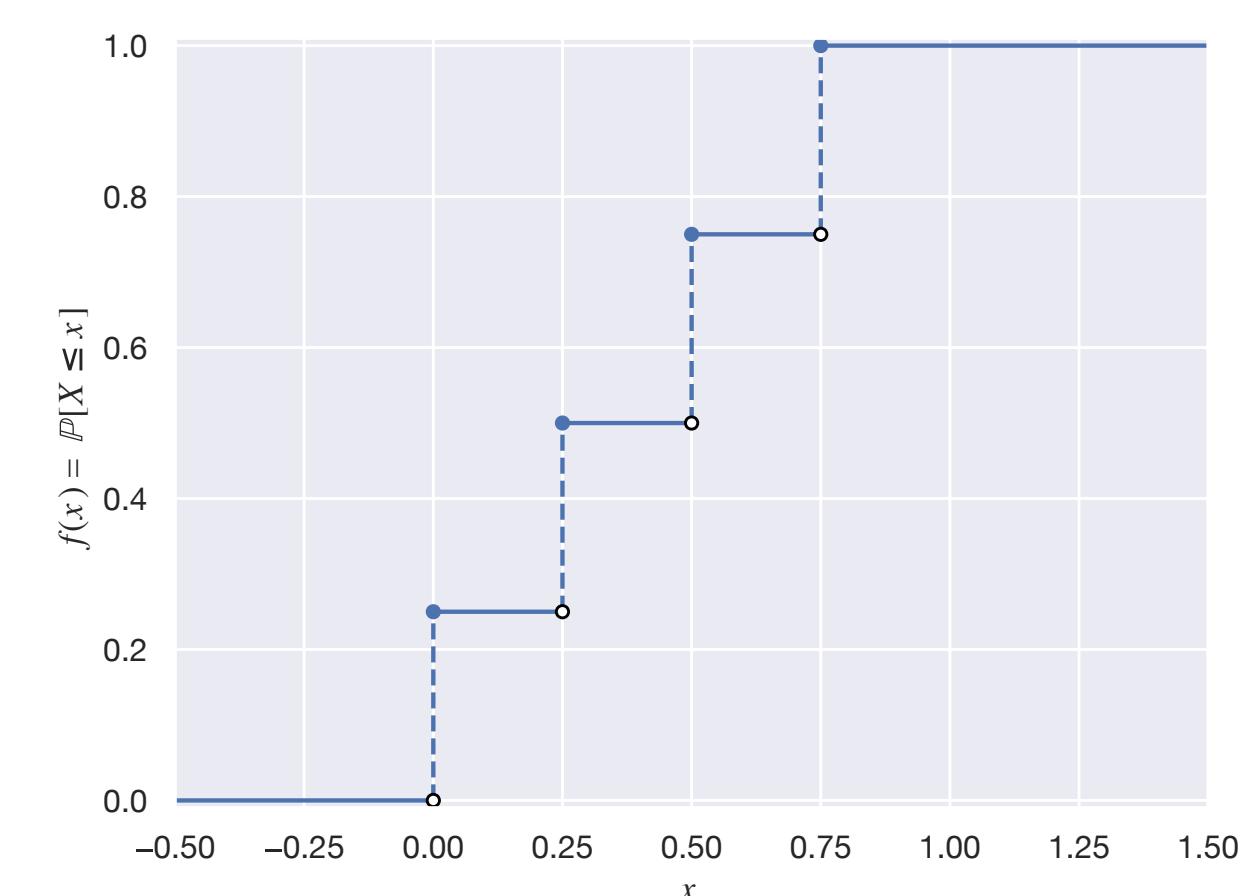
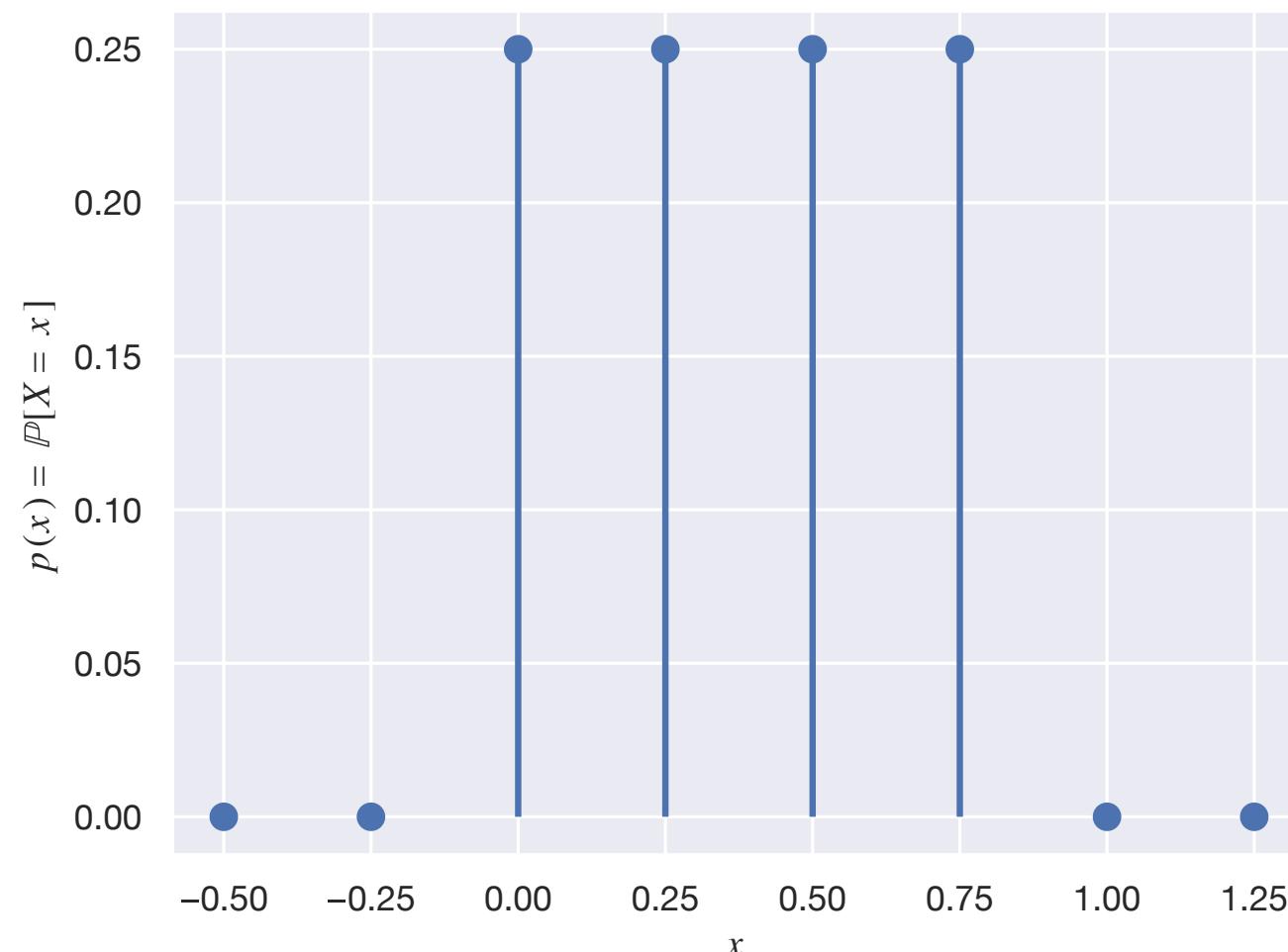
$$\mathbb{P}(X = x) = 0$$

$$\mathbb{P}(b \leq X \leq b) = \int_a^b p_X(x)dx$$



For discrete RVs,

$$\mathbb{P}(X = x) \in [0,1].$$



Random Variables

Multiple random variables

Joint Distribution

Example: Tossing coins and rolling die

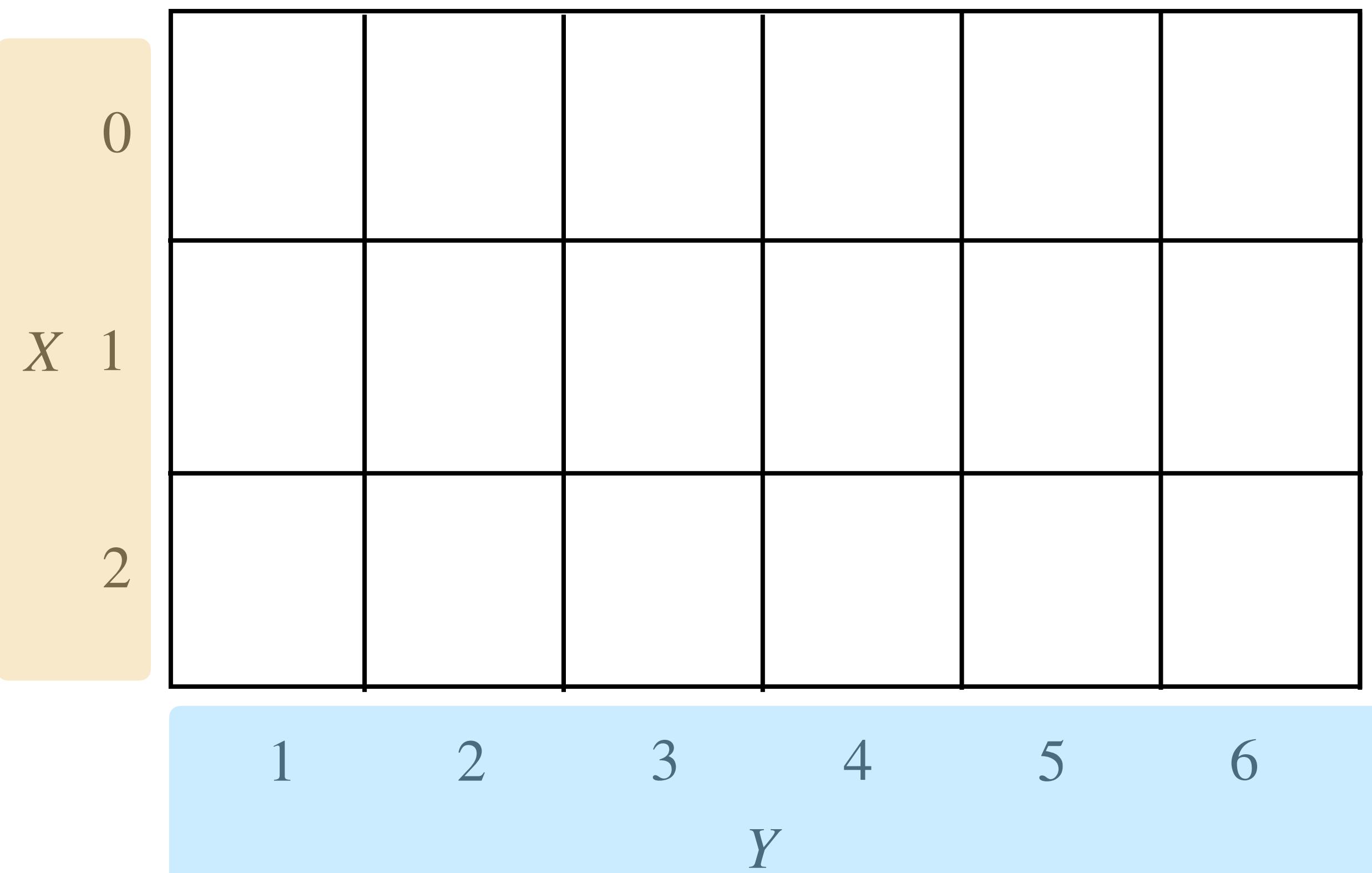
Consider two experiments:

Alice tosses a fair coin, Bob tosses a fair coin.

Charlie rolls a fair six-sided die.

Let X count the # of heads for Alice and Bob.

Let Y be the # on the face of Charlie's die.



Joint Distribution

Definition

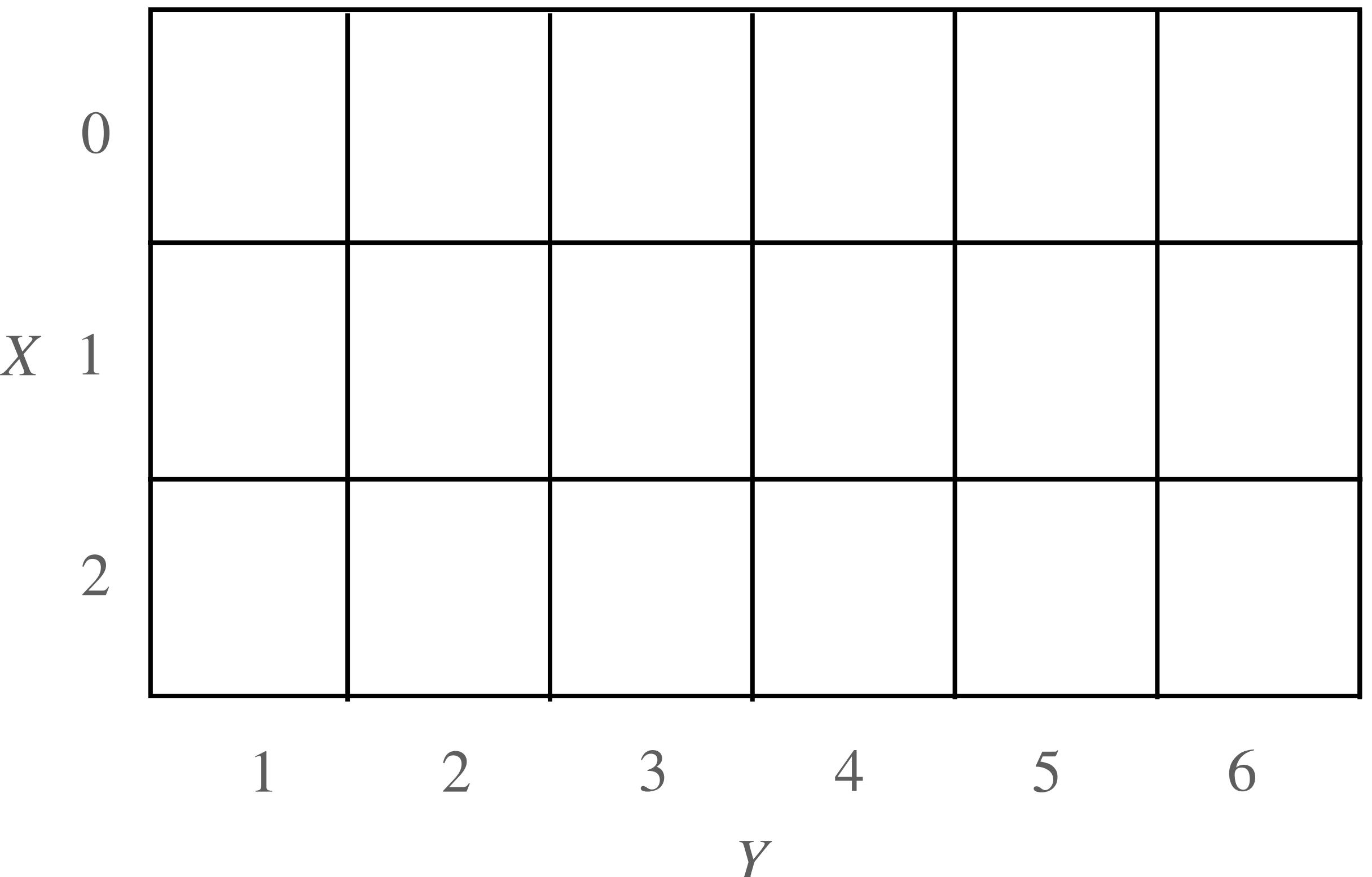
Let X_1, \dots, X_n be random variables.

The **joint distribution** of X_1, \dots, X_n is the probability distribution $\mathbb{P}_{X_1, \dots, X_n}$ with corresponding PMF/PDF:

$$p_{X_1, \dots, X_n}(x_1, \dots, x_n).$$

For discrete random variables,

$$p_{X_1, \dots, X_n}(x_1, \dots, x_n) = \mathbb{P}(X_1 = x_1, \dots, X_n = x_n).$$



Joint Distribution

Definition

$$p_{X,Y}(x,y) = \mathbb{P}(X = x, Y = y) = \mathbb{P}(\text{the number of heads is } x \text{ and the die is } y)$$

Let X_1, \dots, X_n be random variables.

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For discrete random variables,

$$p_{X_1, \dots, X_n}(x_1, \dots, x_n) = \mathbb{P}(X_1 = x_1, \dots, X_n = x_n).$$

	0	1/24	1/24	1/24	1/24	1/24	1/24
X	1	1/12	1/12	1/12	1/12	1/12	1/12
	2	1/24	1/24	1/24	1/24	1/24	1/24
	1	2	3	4	5	6	Y

Joint Distribution

Definition

$$p_{X,Y}(x,y) = \mathbb{P}(X = x, Y = y) = \mathbb{P}(\text{the number of heads is } x \text{ and the die is } y)$$

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The **joint distribution** of X_1, \dots, X_n is the probability distribution $\mathbb{P}_{X_1, \dots, X_n}$ with corresponding PMF/PDF:

$$p_{X_1, \dots, X_n}(x_1, \dots, x_n).$$

Joint distribution of example: $p_{X,Y}(x, y)$.

$$p_{X,Y}(1,1) = 1/12$$

	0	1/24	1/24	1/24	1/24	1/24	1/24
X	1	1/12	1/12	1/12	1/12	1/12	1/12
	2	1/24	1/24	1/24	1/24	1/24	1/24
	1	2	3	4	5	6	Y

Marginal Distribution

Definition

For two random variables X, Y with joint distribution $p_{X,Y}(x, y) \dots$

The marginal distribution of X is obtained by “summing out”/“integrating out” the variable we don’t care about:

$$p_X(x) = \sum_y p_{X,Y}(x,y)$$

$$p_X(x) = \int_{-\infty}^{\infty} p_{X,Y}(x,y)dy$$

0	$1/24$	$1/24$	$1/24$	$1/24$	$1/24$	$1/24$	$1/4$
$X = 1$	$1/12$	$1/12$	$1/12$	$1/12$	$1/12$	$1/12$	$1/2$
2	$1/24$	$1/24$	$1/24$	$1/24$	$1/24$	$1/24$	$1/4$
	1	2	3	4	5	6	
				Y			

Marginal Distribution

Definition

For two random variables X, Y with joint distribution $p_{X,Y}(x, y) \dots$

The marginal distribution of X is obtained by "summing out"/"integrating out" the variable we don't care about:

$$p_X(x) = \sum_y p_{X,Y}(x, y)$$

$$p_X(x) = \int_{-\infty}^{\infty} p_{X,Y}(x, y) dy$$

		1/6	1/6	1/6	1/6	1/6	1/6
0		1/24	1/24	1/24	1/24	1/24	1/24
	X	1/12	1/12	1/12	1/12	1/12	1/12
2		1/24	1/24	1/24	1/24	1/24	1/24
	1						
	2						
	3						
	4						
	5						
	6						
							Y

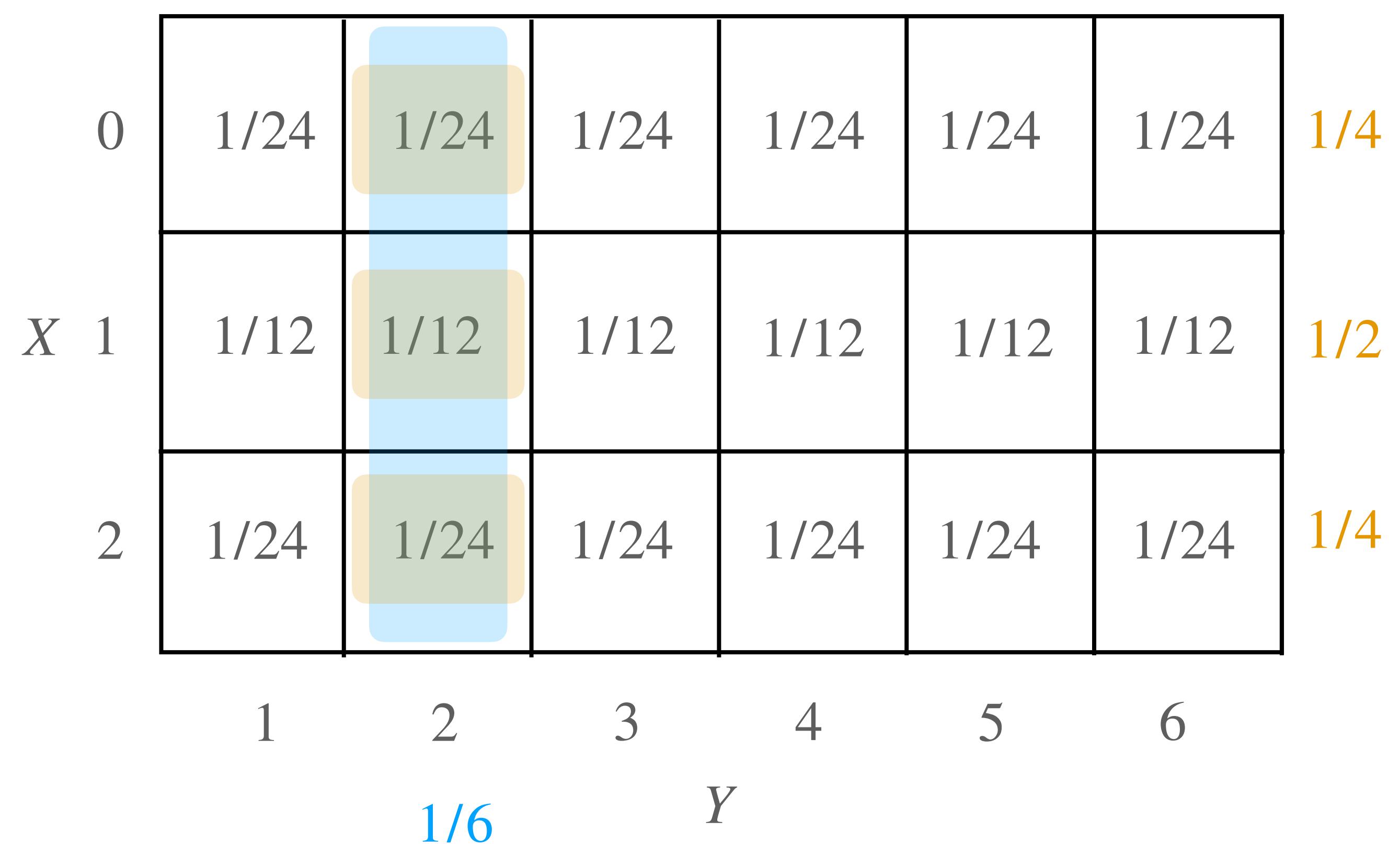
Conditional Distribution

Definition

For two random variables X, Y with joint distribution $p_{X,Y}(x, y) \dots$

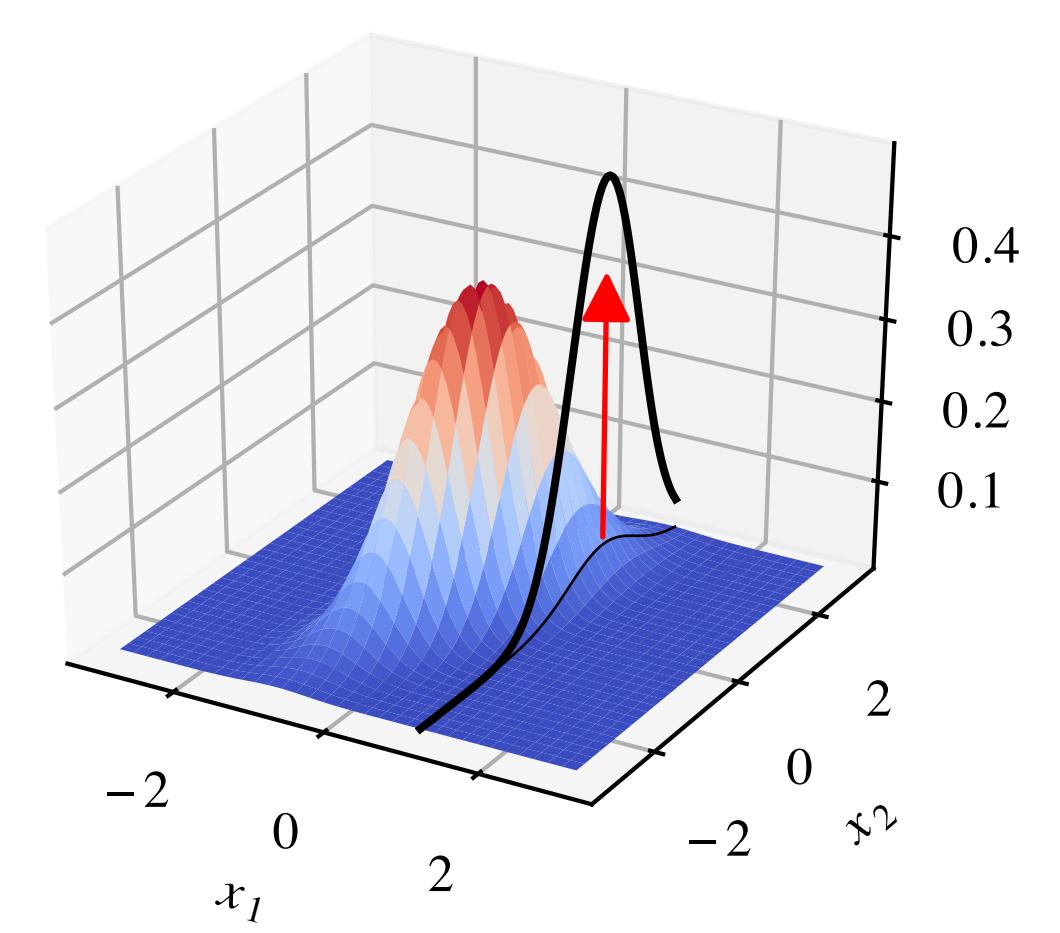
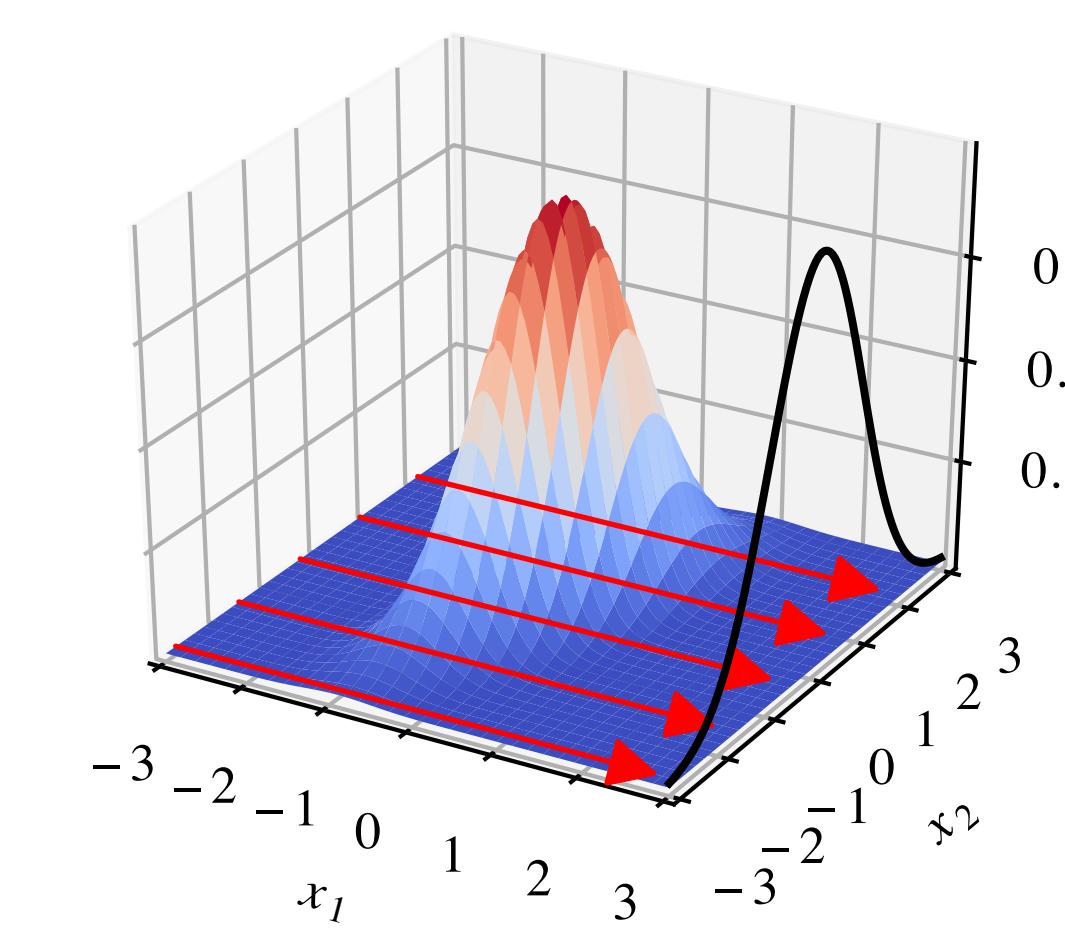
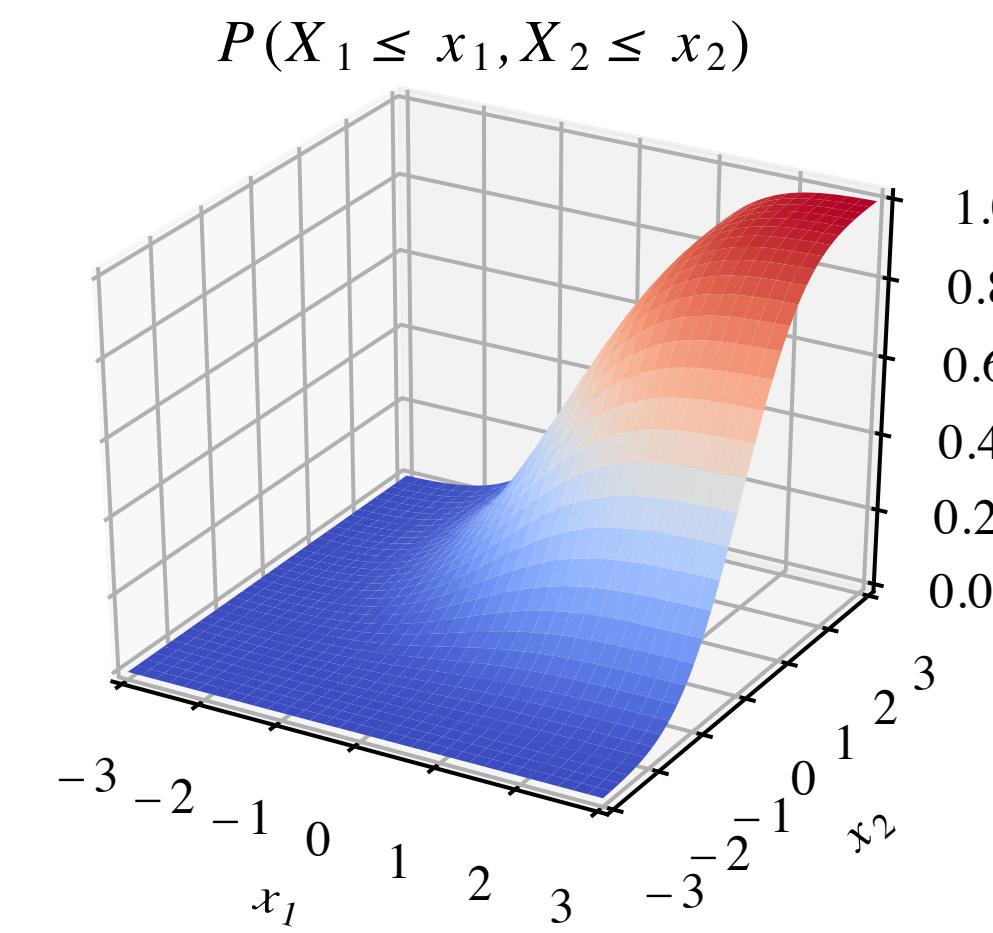
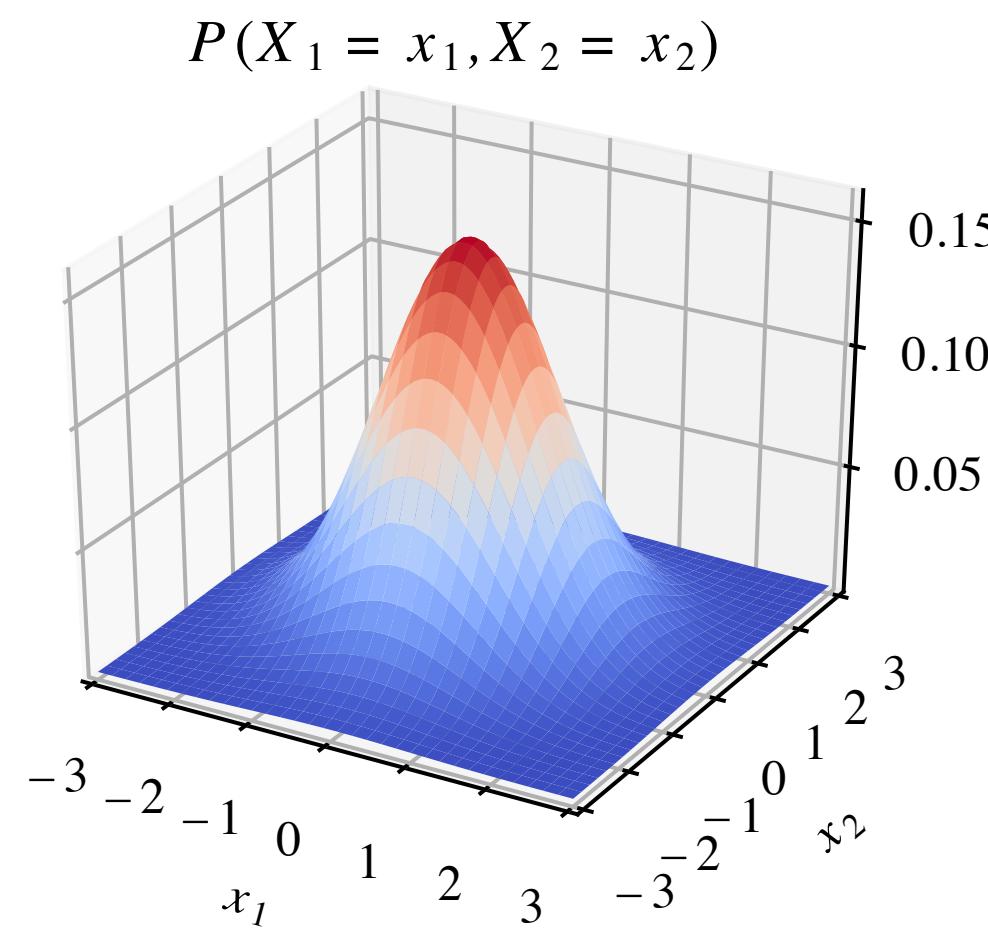
The conditional distribution of X given $Y = y$ is given by *only* considering the events where $Y = y$.

$$p_{X|Y}(x | y) = \frac{p_{X,Y}(x, y)}{p_Y(y)}$$



Joint Continuous Distributions

Joint, marginal, and conditional



Joint Distributions

Summary

Let $p_{X,Y}(x, y)$ be a joint distribution.

The sum rule/marginalization allows us to get from a joint to a marginal distribution.

$$p_X(x) = \begin{cases} \sum_y p_{X,Y}(x, y) & Y \text{ is discrete} \\ \int_{-\infty}^{\infty} p_{X,Y}(x, y) & Y \text{ is continuous} \end{cases}$$

The product rule/factorization “factors” the joint distribution into marginal and conditional.

$$p_{X,Y}(x, y) = p_{Y|X}(y | x)p_X(x) = p_{X|Y}(x | y)p_Y(y).$$

Independence

Intuition and definition

Two RVs X, Y are **independent** if their joint distribution factors into their respective distributions:

$$p_{X,Y}(x,y) = p_X(x)p_Y(y).$$

Another definition: the conditional distribution is the marginal.

$$p_{X|Y}(x \mid y) = p_X(x) \text{ and } p_{Y|X}(y \mid x) = p_Y(y).$$

Let $\{X_i\}_{i \in I}$ be a collection of RVs indexed by I . $\{X_i\}$ are **independent** if

$$p_{X_{i_1}, \dots, X_{i_k}}(X_{i_1}, \dots, X_{i_k}) = \prod_{j=1}^k p_{X_{i_j}}(x_{i_j}) \text{ for any subset of indices } \{i_1, \dots, i_k\} \in I,$$

Independence

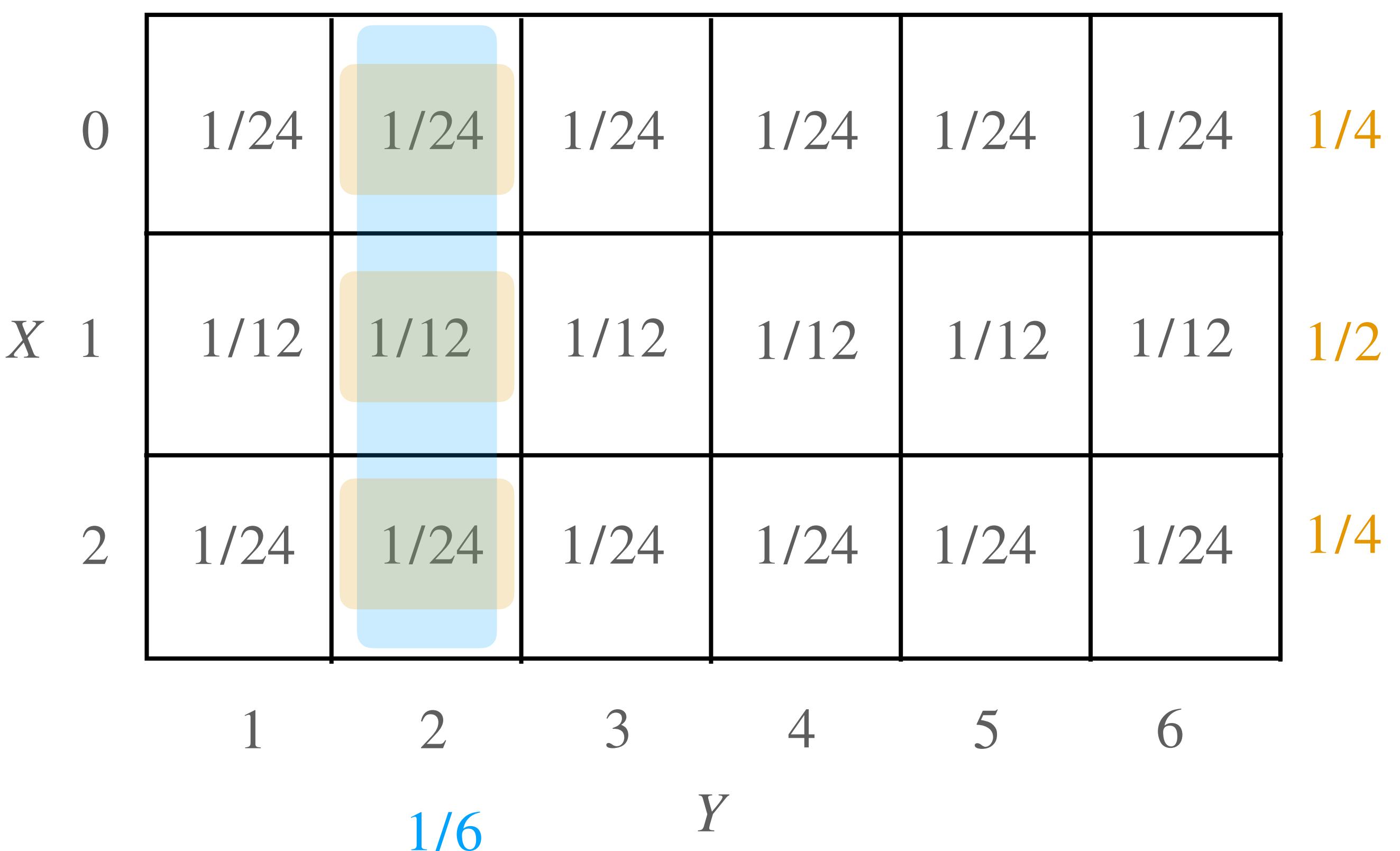
Intuition and definition

Two RVs X, Y are independent if their joint distribution factors into their respective distributions:

$$p_{X,Y}(x,y) = p_X(x)p_Y(y).$$

Another definition: the conditional distribution is the marginal.

$$p_{X|Y}(x | y) = p_X(x) \text{ and } p_{Y|X}(y | x) = p_Y(y).$$



Independence

Independent and identically distributed (i.i.d.)

A collection of random variables X_1, \dots, X_n are independent and identically distributed (i.i.d.) if their joint distribution can be factored entirely:

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

and all the X_i have the same distribution.

Very common assumption in ML!

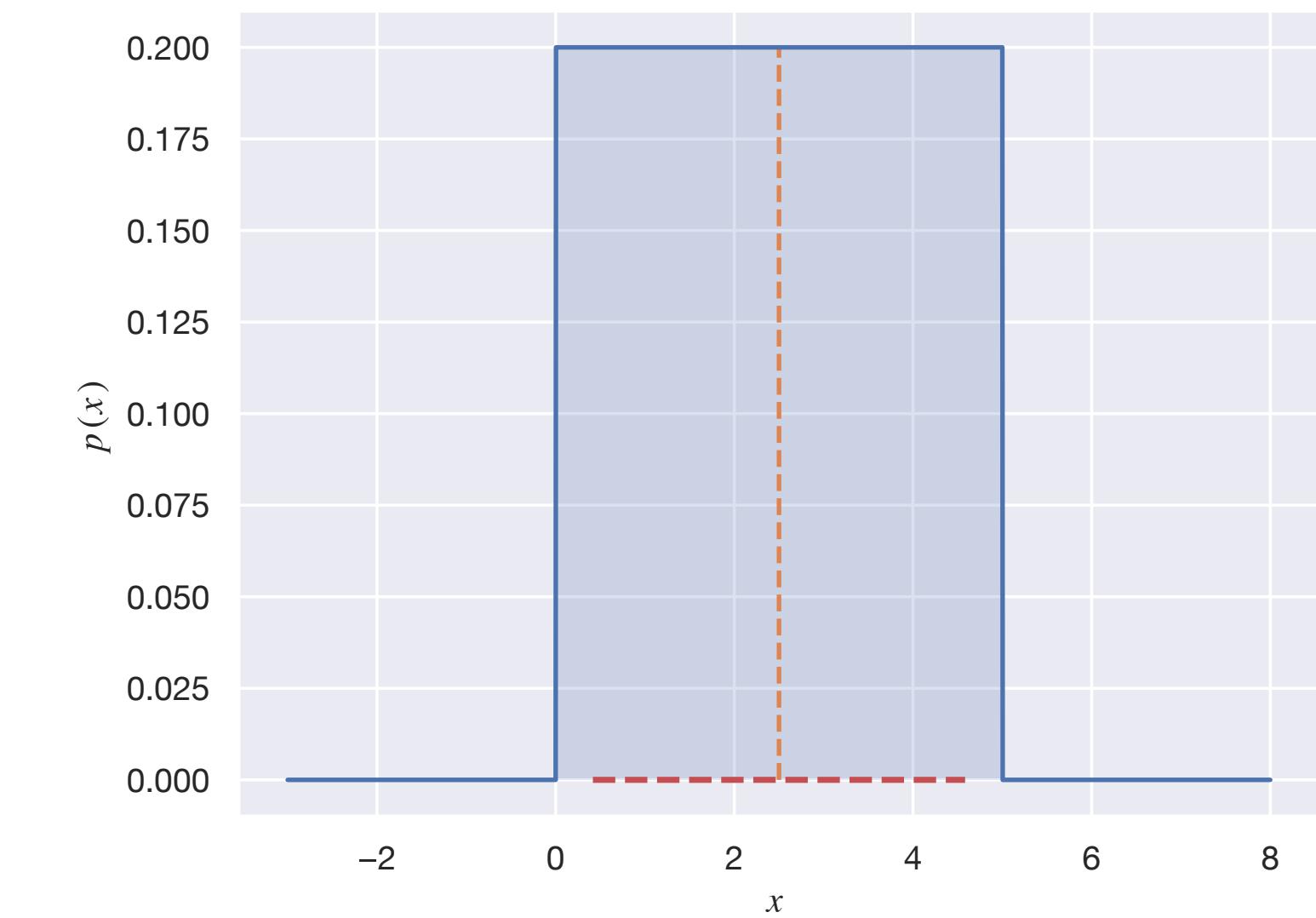
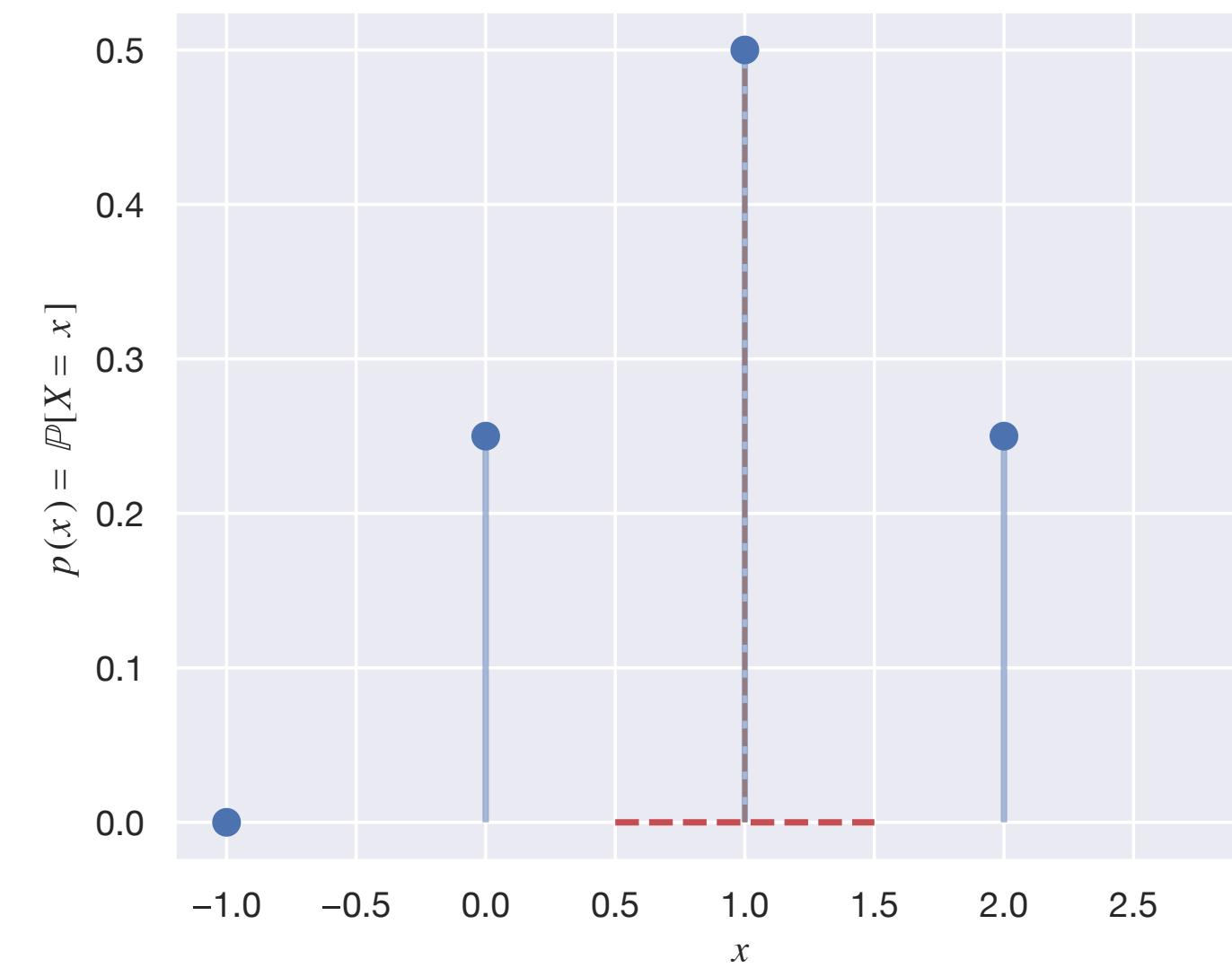
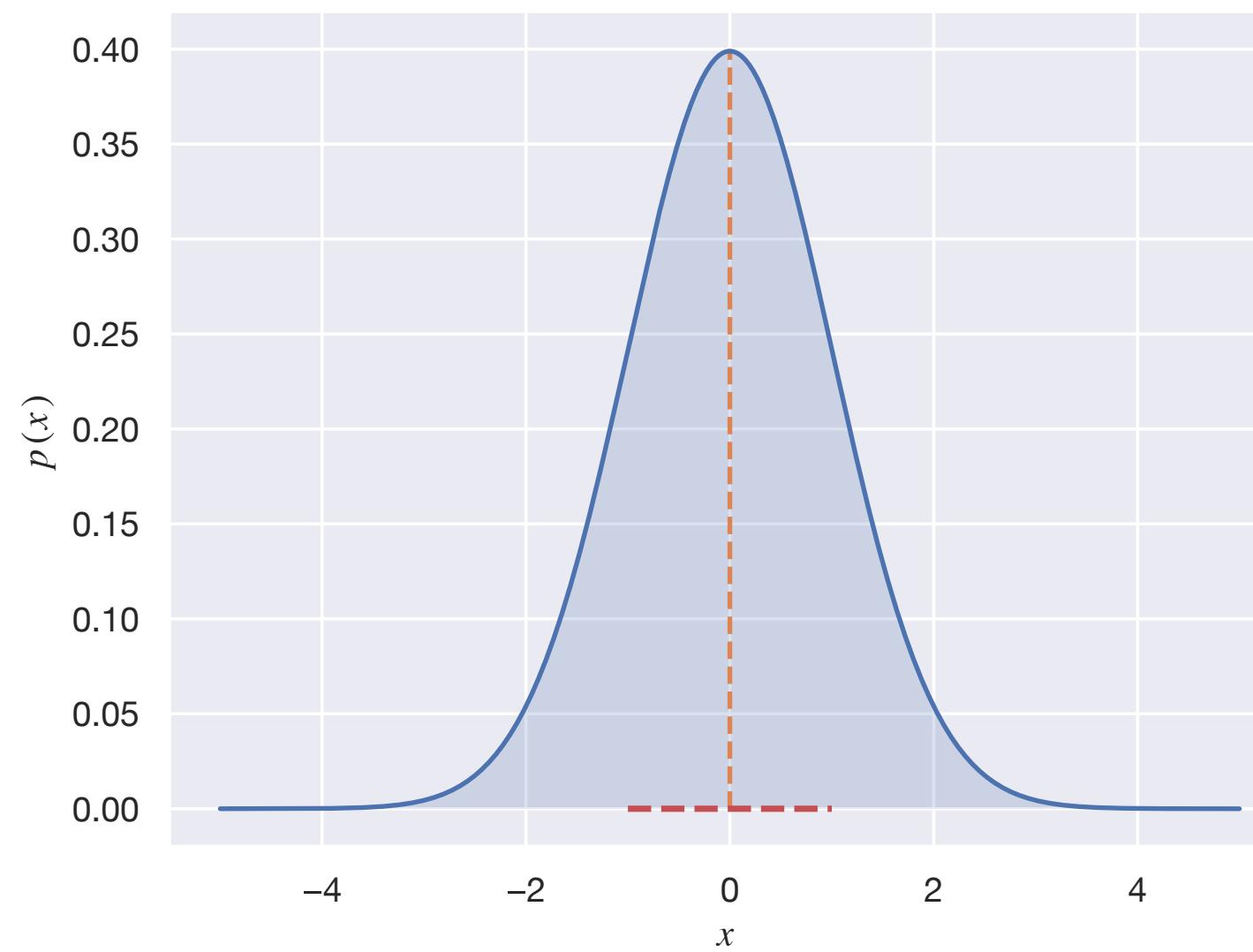
Expectation

Definition and Properties

Expected Value

Intuition

The expectation/expected value or mean of a random variable is its “center of mass.”



Expected Value

Definition

The expectation/expected value or mean of a random variable X is

$$\mathbb{E}[X] = \sum_x xp_X(x) \text{ for discrete } X$$

$$\mathbb{E}[X] = \int_{-\infty}^{\infty} xp_X(x)dx \text{ for continuous } X$$

A function of a random variable is a random variable!

Functions of RVs are RVs

Very important fact!

A function of a random variable is a random variable!

Expected Value

Properties of the expected value

Linearity. The expectation is a linear operator:

$$\mathbb{E}[\alpha X] = \alpha \mathbb{E}[X] \text{ and } \mathbb{E}[X + Y] = \mathbb{E}[X] + \mathbb{E}[Y], \text{ for any random variables } X \text{ and } Y$$

Product (for independent RVs). For *independent* random variables X, Y

$$\mathbb{E}[XY] = \mathbb{E}[X]\mathbb{E}[Y].$$

More generally, for independent X_1, \dots, X_n :

$$\mathbb{E} \left[\prod_{i=1}^n X_i \right] = \prod_{i=1}^n \mathbb{E}[X_i].$$

Conditional Expectation

Intuition

The conditional expectation is the “best guess” of a RV’s expectation, given an event.

Depending on context, this is a *random variable* or a *function*.

$\mathbb{E}[X | Y = y]$ is a function $g(y) = \mathbb{E}[X | Y = y]$.

$\mathbb{E}[X | Y]$ is a random variable $g(Y)$.

Conditional Expectation

Intuition

Consider the roll of a six-sided fair die.

Let $X = 1$ if the roll is even, $X = 0$ otherwise.

Let $Y = 1$ if the roll is prime, $Y = 0$ otherwise.

What is $\mathbb{E}[X]$?

What is $\mathbb{E}[X | Y = 1]$?

What is $\mathbb{E}[X | Y = 0]$?

What is $\mathbb{E}[X | Y = y]$ and $\mathbb{E}[X | Y]$?

	1	2	3	4	5	6
X	0	1	0	1	0	1
Y	0	1	1	0	1	0

Conditional Expectation

Definition (given events)

If A is an event and X is a discrete random variable, the conditional expectation of X given A is:

$$\mathbb{E}[X | A] = \sum_x \mathbb{P}_X[X = x | A].$$

If X, Y are discrete random variables, the conditional expectation of X given $Y = y$ is:

$$\mathbb{E}[X | Y = y] = \sum_x x p_{X|Y}(x | y) = \sum_x x \mathbb{P}[X = x | Y = y].$$

If X, Y are continuous random variables with joint density $p_{X,Y}(x, y)$, Y 's marginal $p_Y(y)$ and conditional density $p_{X|Y}(x | y) = \frac{p_{X,Y}(x, y)}{p_Y(y)}$, the conditional expectation of X given $Y = y$ is:

$$\mathbb{E}[X | Y = y] = \int_{-\infty}^{\infty} x p_{X|Y}(x | y) dx.$$

Conditional Expectation

Definition (given a random variable)

For two RVs X and Y , think of the conditional expectation of Y given X as the “best guess” of Y only using the information from X :

$\mathbb{E}[Y | X]$ is a *random variable* (a function $g(X)$ of the RV X).

We can obtain this random variable by figuring out the function $g(x)$ for $\mathbb{E}[Y | X = x]$ and then “plugging back in” the random variable $g(X)$.

Conditional Expectation

Definition (given a random variable)

Example. A stick of length 1 is broken at a point X chosen uniformly at random. Given that $X = x$, choose another breakpoint Y uniformly on the interval $[0,x]$.

What is the random variable $\mathbb{E}[Y | X]$?

What is its mean?

Conditional Expectation

Properties of conditional expectation

Independence. If X is independent of Y ,

$$\mathbb{E}[X | Y] = \mathbb{E}[X].$$

Pulling out what's known. For any function h ,

$$\mathbb{E}[h(X)Y | X] = h(X)\mathbb{E}[Y | X].$$

Linearity. For any random variables X, Y, Z and scalar $\alpha \in \mathbb{R}$,

$$\mathbb{E}[X + Y | Z] = \mathbb{E}[X | Z] + \mathbb{E}[Y | Z] \text{ and } \mathbb{E}[\alpha X | Z] = \alpha\mathbb{E}[X | Z].$$

Law of total expectation/tower rule. For any random variables X, Y ,

$$\mathbb{E}[\mathbb{E}[Y | X]] = \mathbb{E}[Y].$$

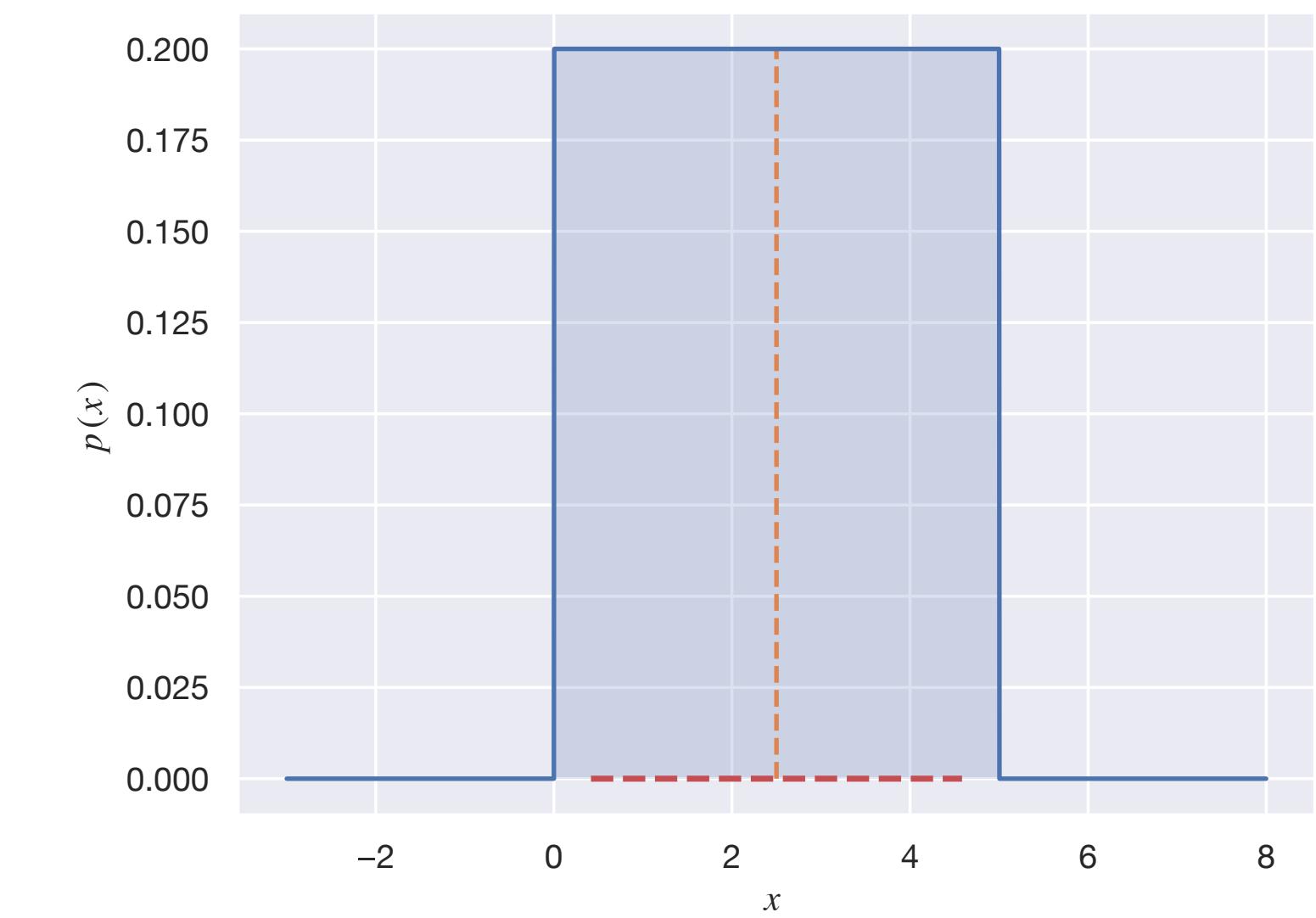
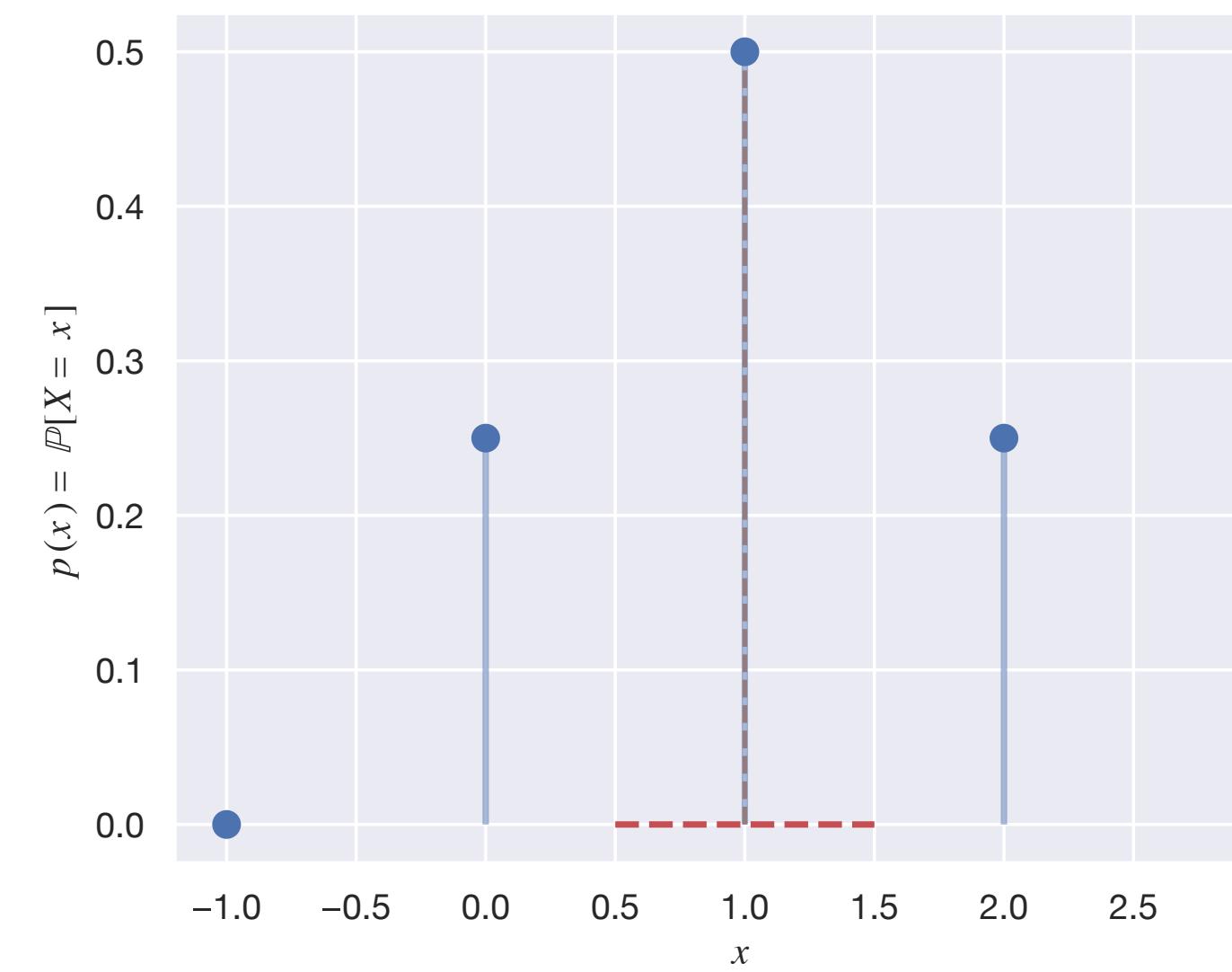
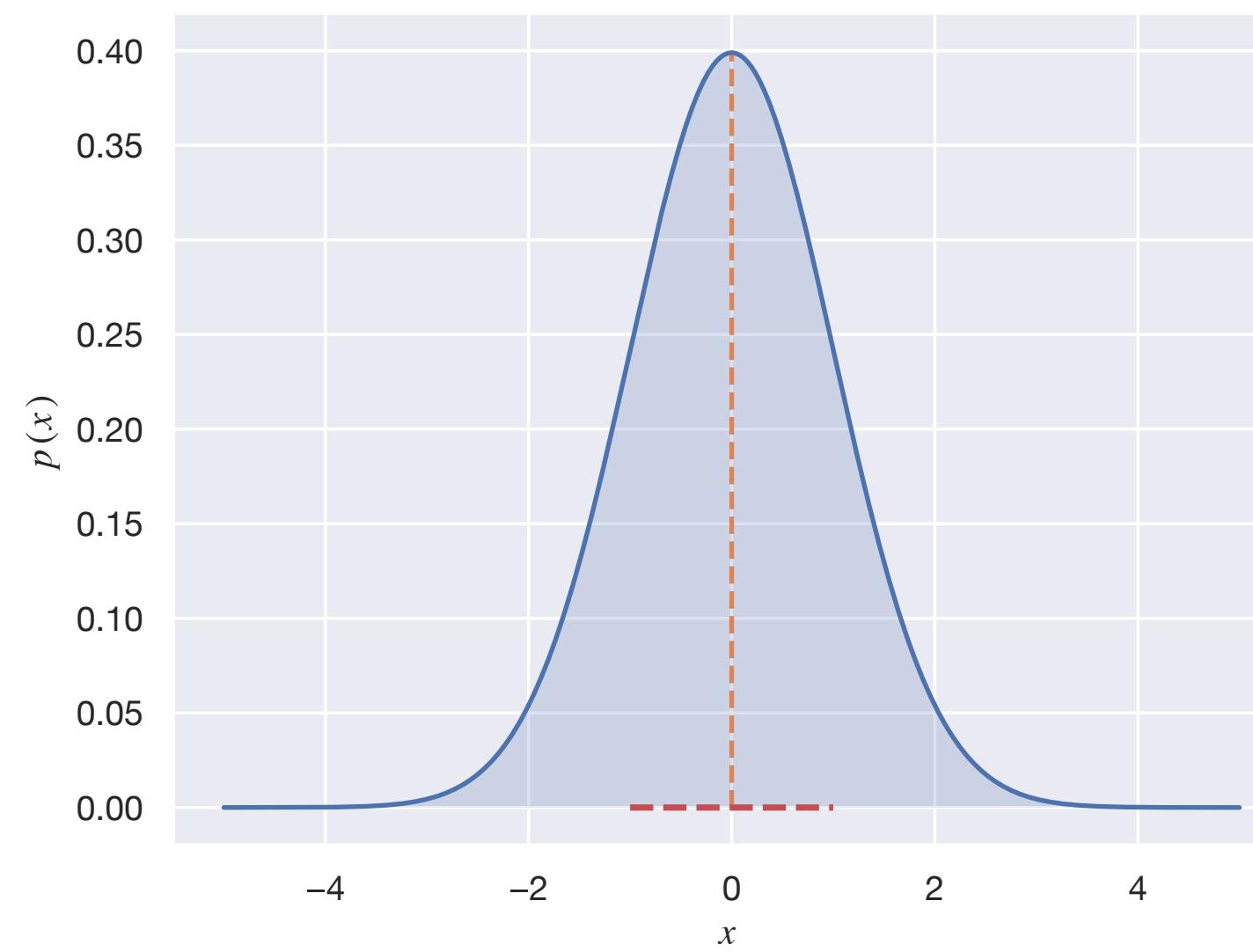
Variance

Definition and Covariance

Variance

Intuition

The variance of a random variable is how “spread” around its expectation it is.



Variance

Definition

The variance of a random variable $\text{Var}(X)$ is:

$$\text{Var}(X) = \mathbb{E}[(X - \mathbb{E}[X])^2].$$

This can also be written (using linearity of expectation):

$$\text{Var}(X) = \mathbb{E}[X^2] - \mathbb{E}[X]^2.$$

The standard deviation is $\sqrt{\text{Var}(X)}$.

Variance

Properties of variance

The variance is *NOT* linear, but we do have, for $\alpha, \beta \in \mathbb{R}$,

$$\text{Var}(\alpha X + \beta) = \alpha^2 \text{Var}(X).$$

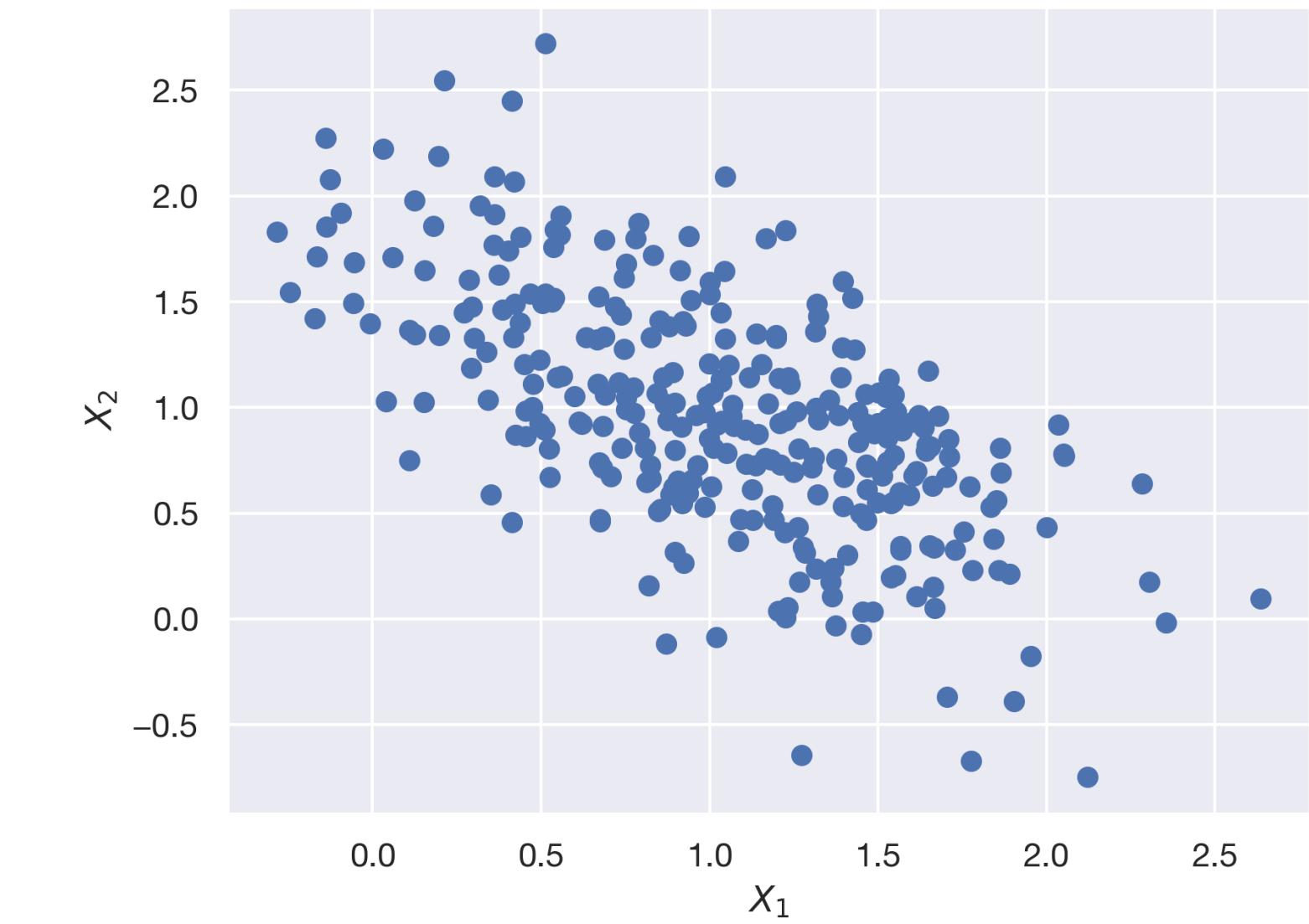
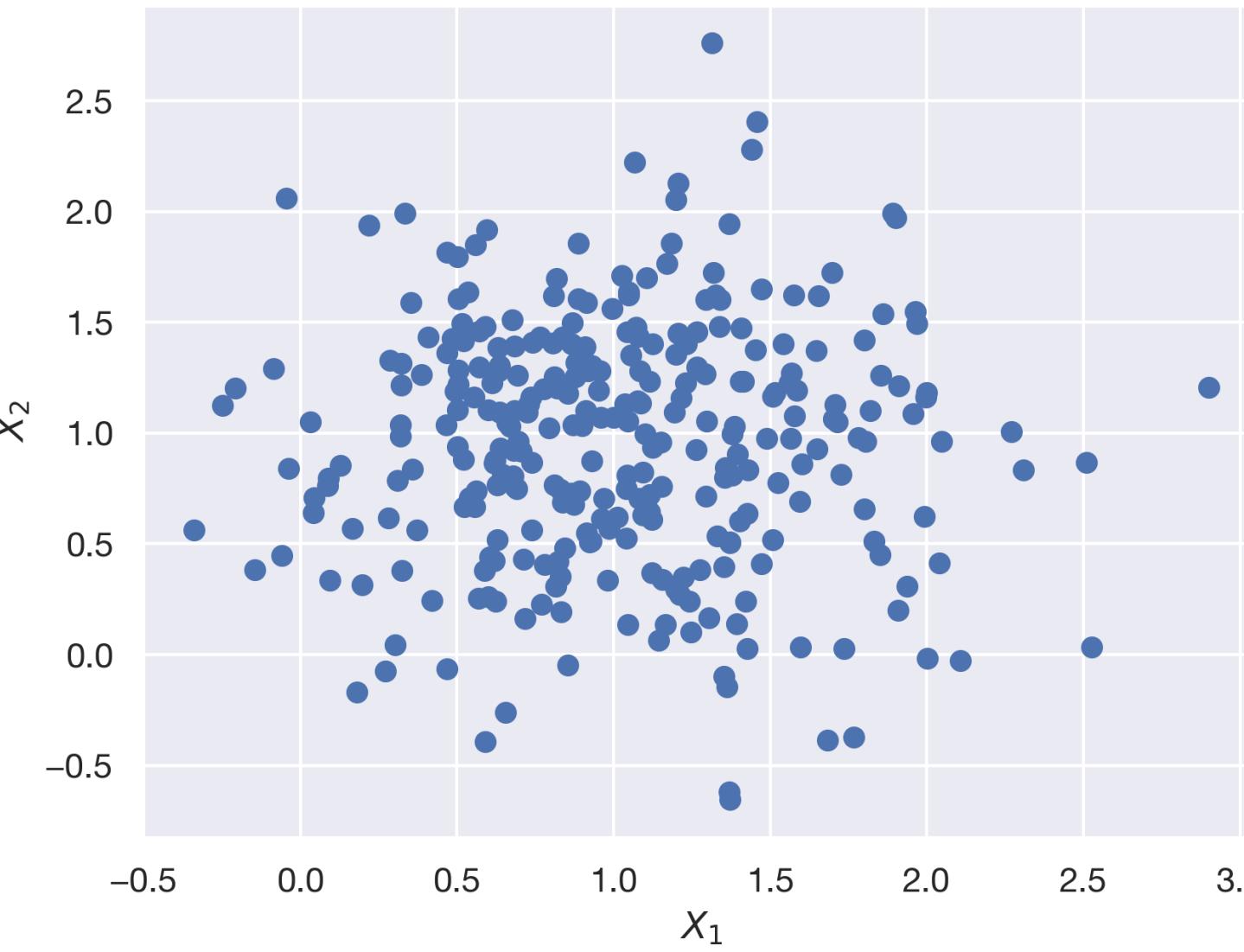
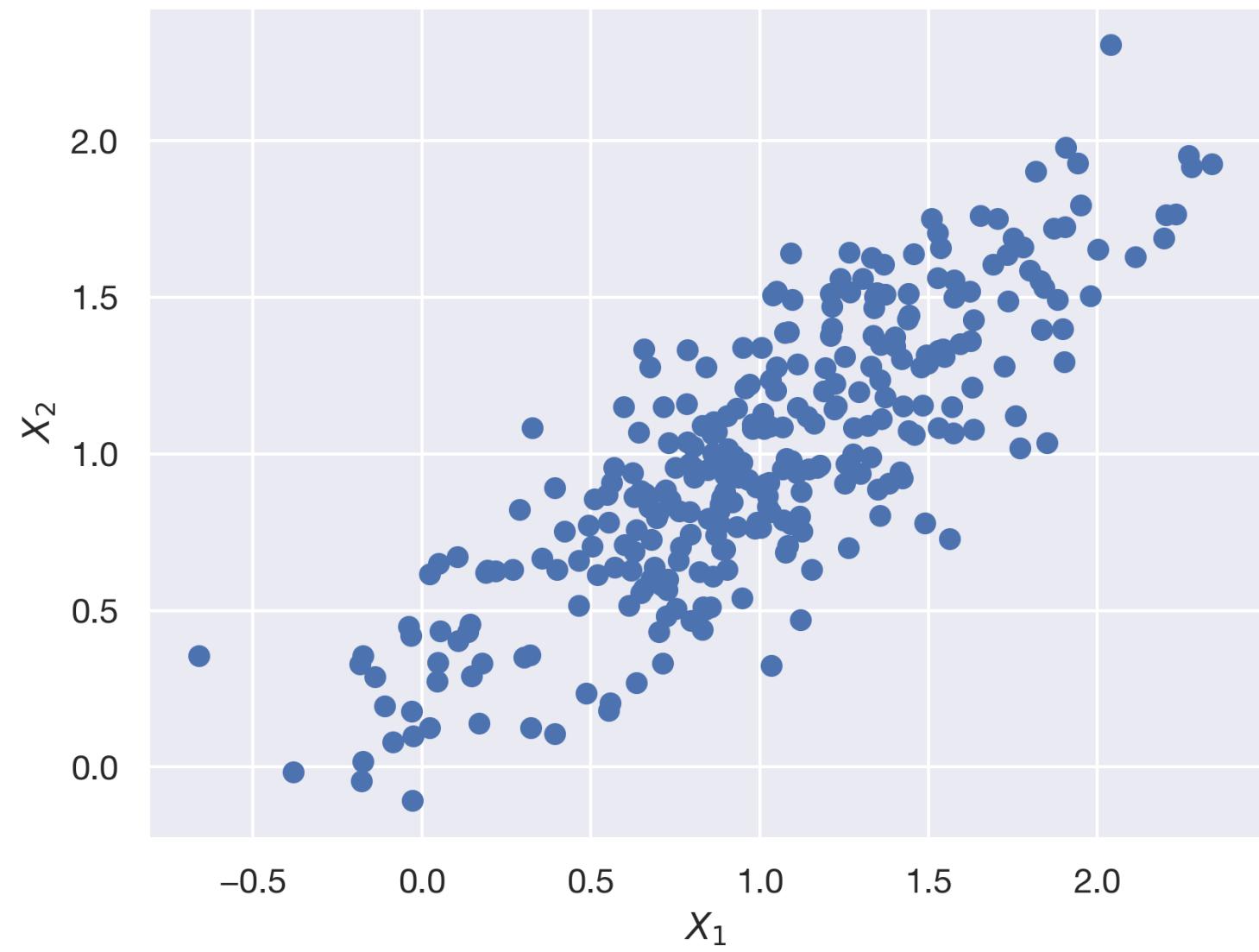
If X_1, \dots, X_n are independent (more generally, *uncorrelated*),

$$\text{Var}(X_1 + \dots + X_n) = \text{Var}(X_1) + \dots + \text{Var}(X_n).$$

Covariance

Intuition

The covariance measures the linear relationship between two random variables.



Covariance

Definition

The covariance of X, Y is

$$\text{Cov}(X, Y) = \mathbb{E}[(X - \mathbb{E}[X])(Y - \mathbb{E}[Y])].$$

The outer expectation is over both X and Y (their joint distribution). Equivalently:

$$\text{Cov}(X, Y) = \mathbb{E}[XY] - \mathbb{E}[X]\mathbb{E}[Y].$$

The correlation is what we get from normalizing the covariance:

$$\rho(X, Y) = \frac{\text{Cov}(X, Y)}{\sqrt{\text{Var}(X)\text{Var}(Y)}}$$

Covariance

Properties of covariance

Covariance follows the “symmetry” property:

$$\text{Cov}(X, Y) = \text{Cov}(Y, X).$$

Covariance follows the “bilinearity” property:

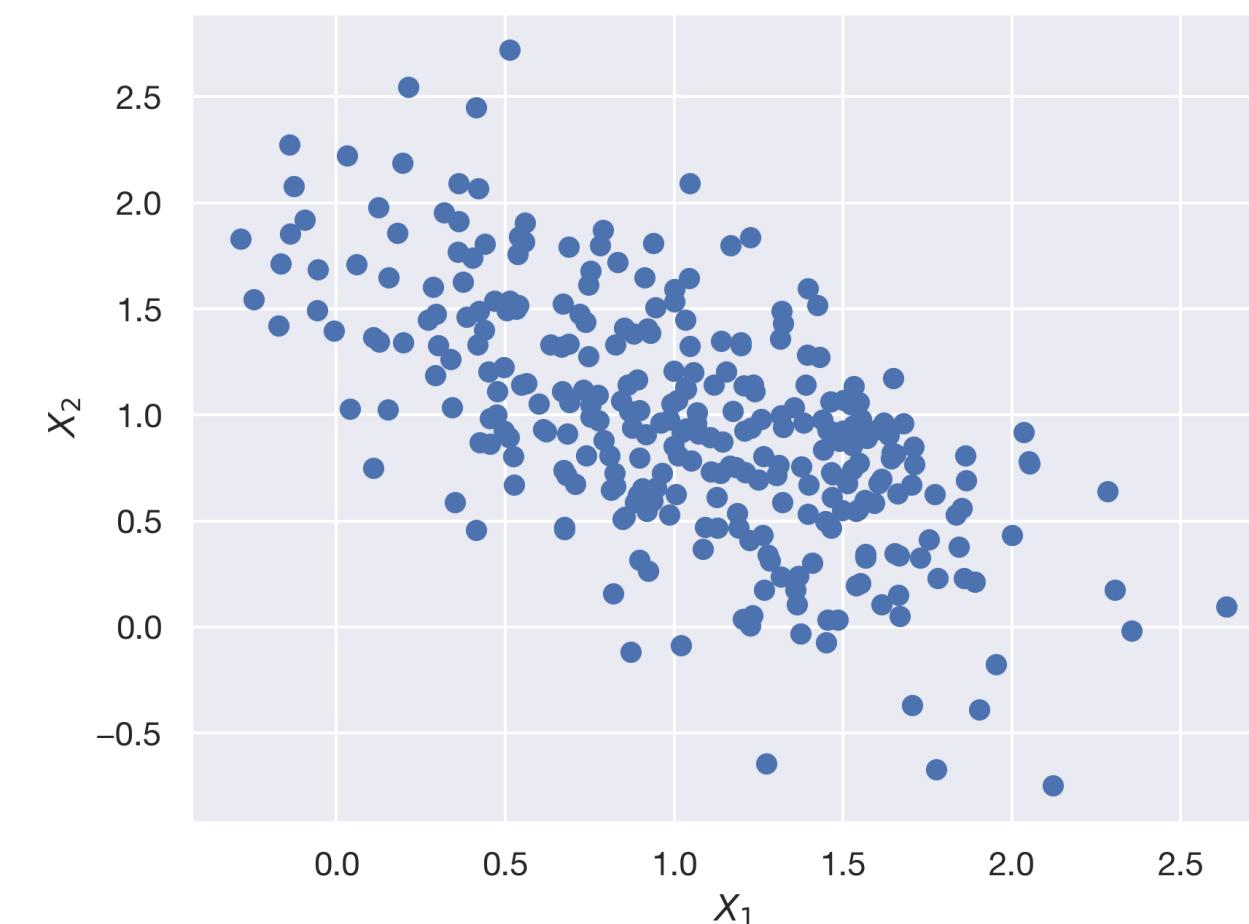
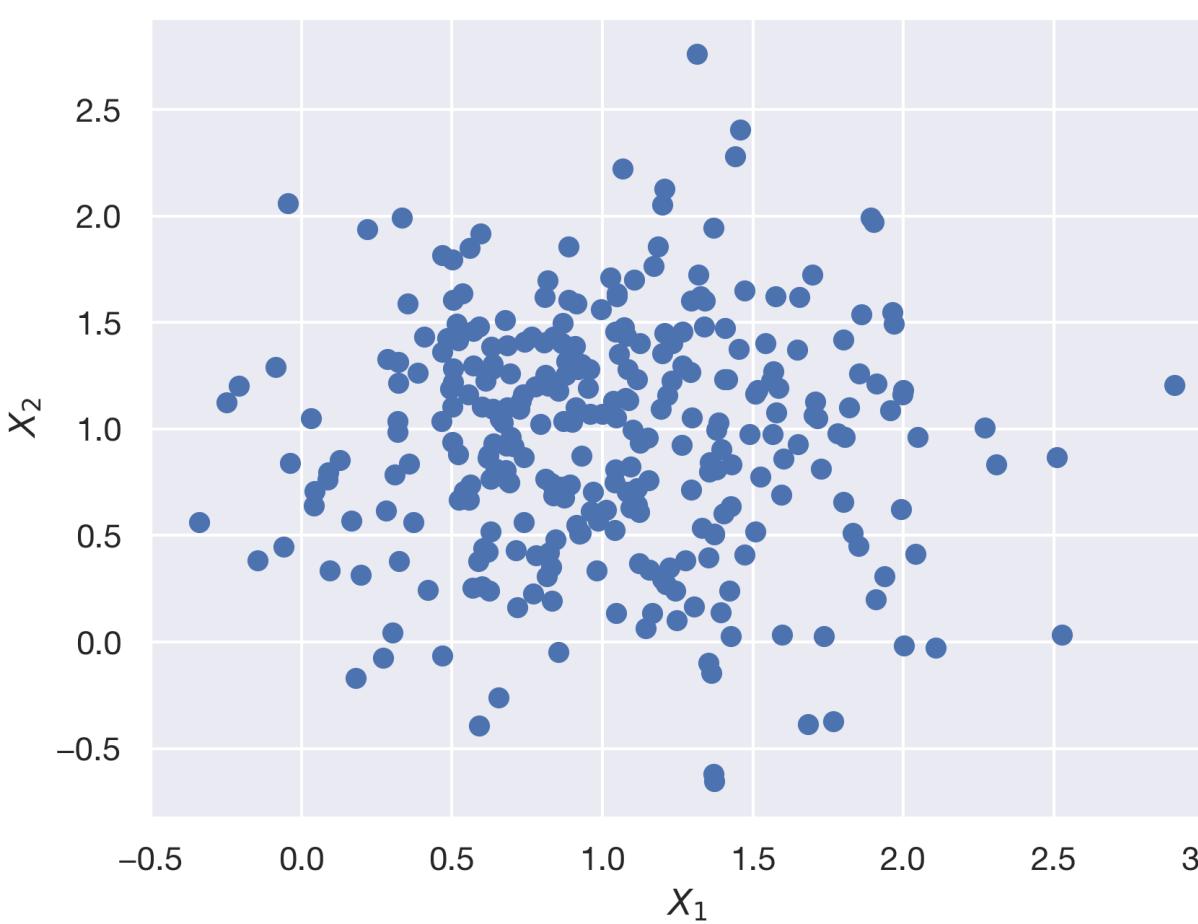
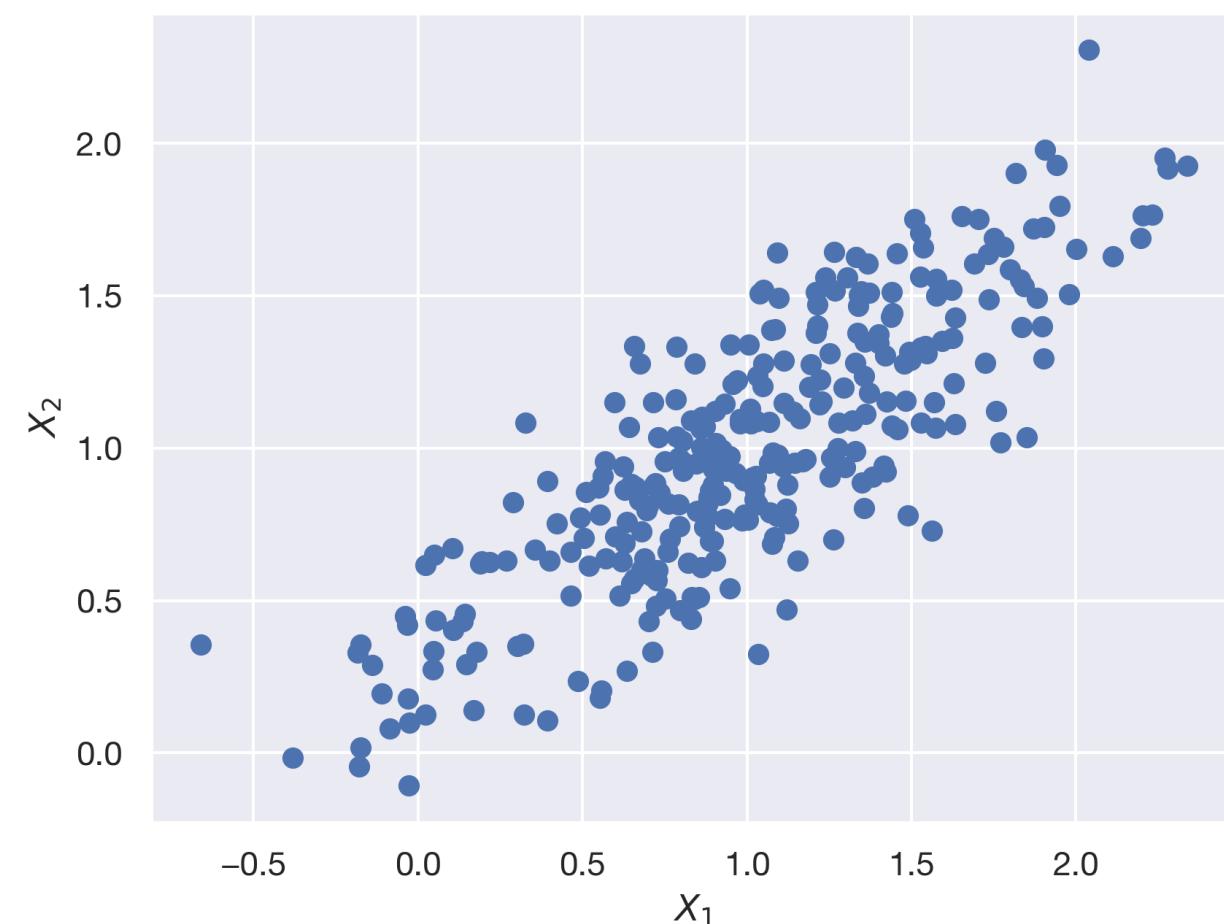
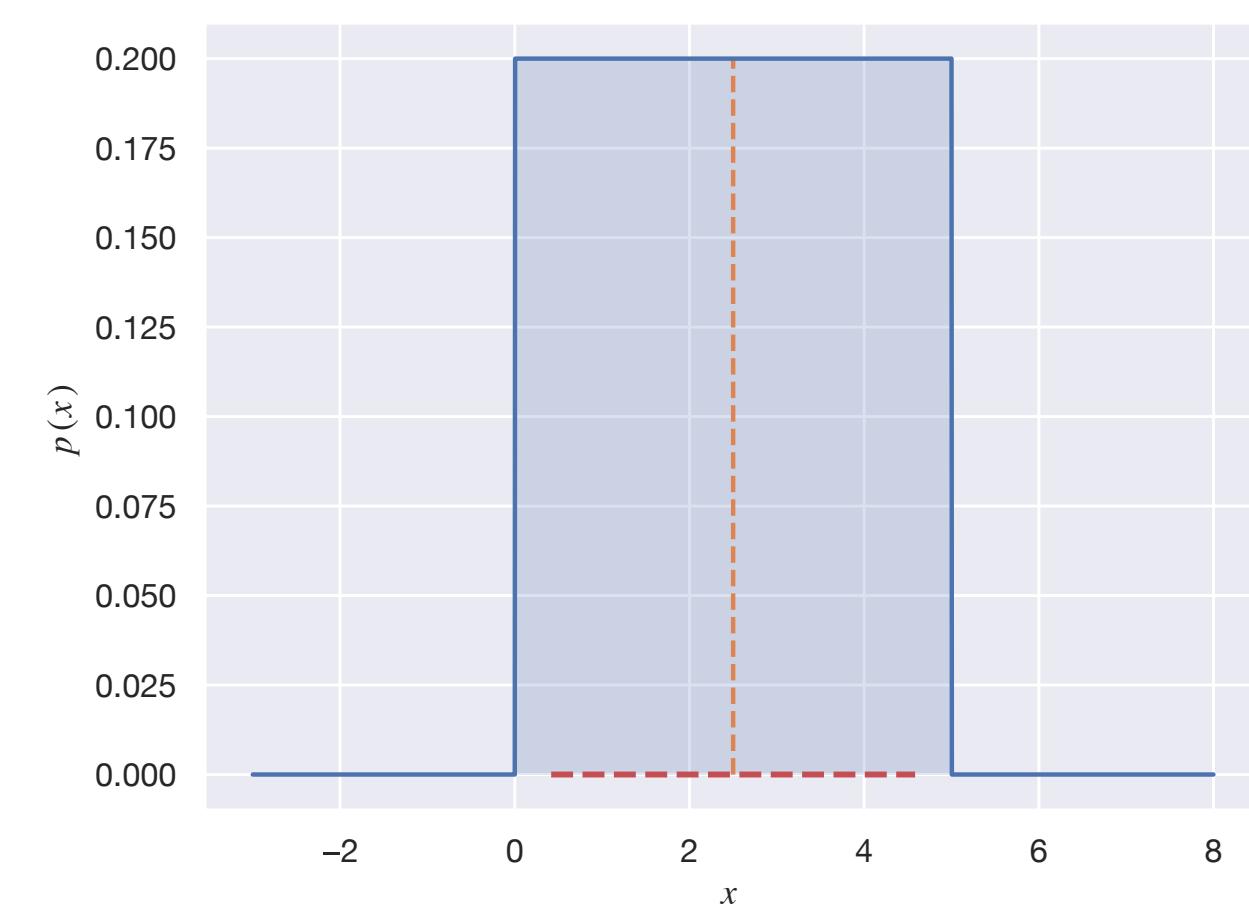
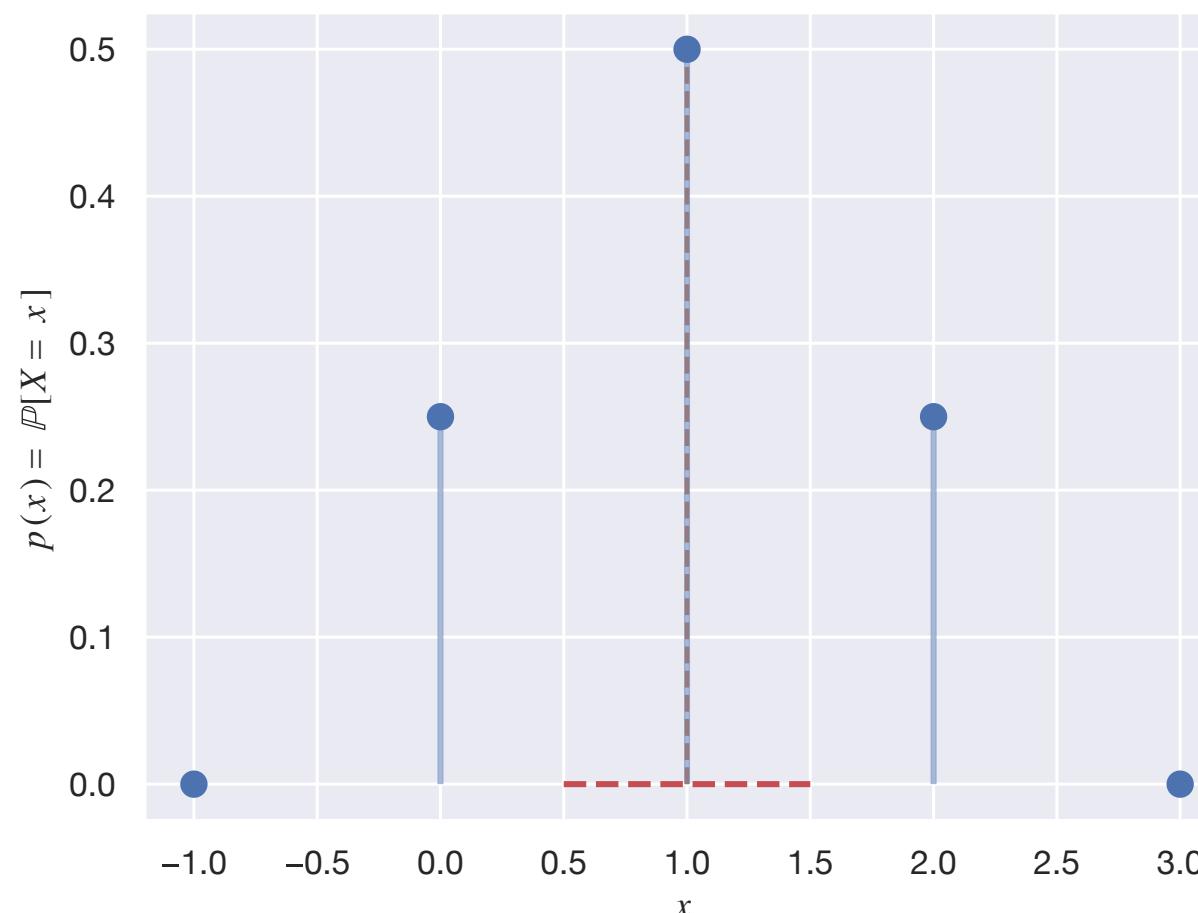
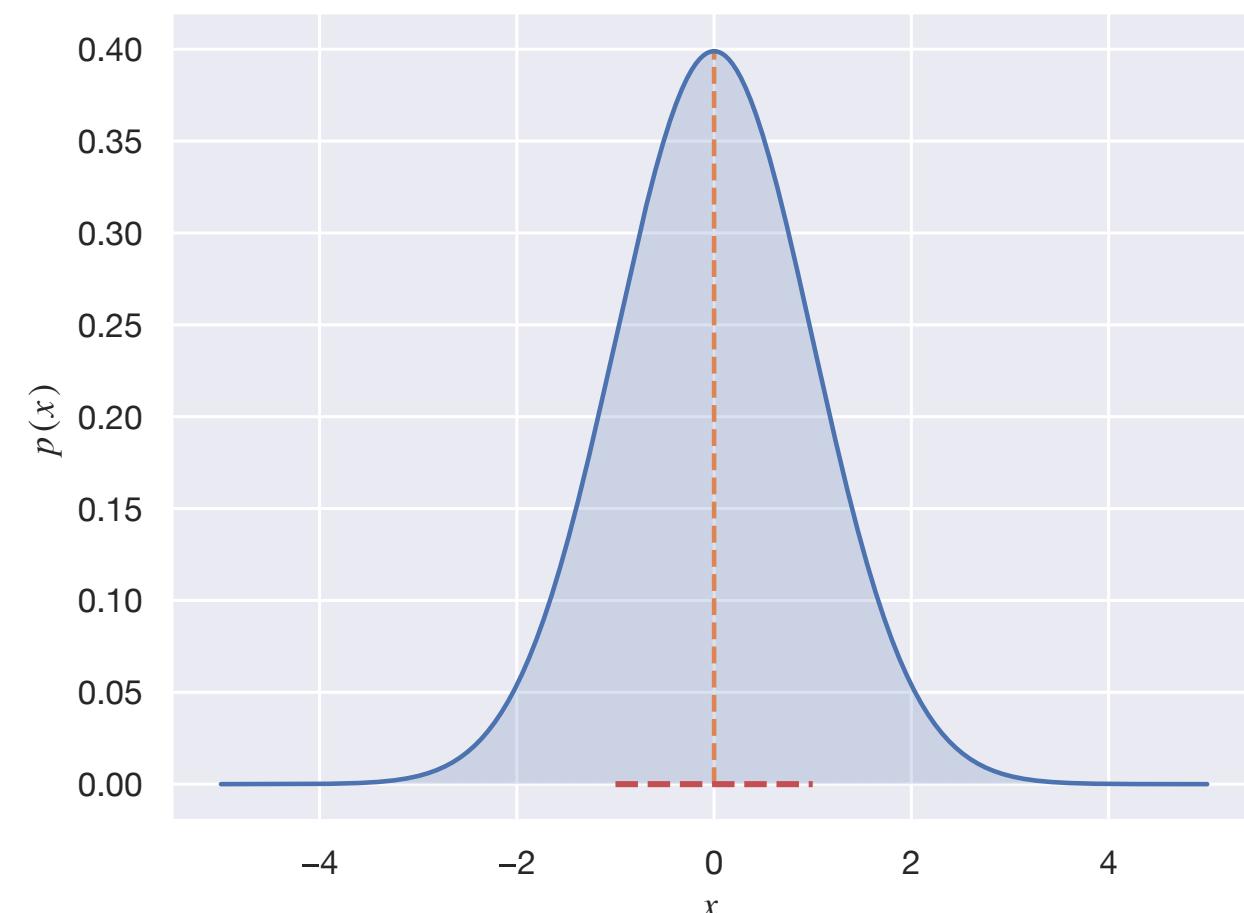
$$\text{Cov}(\alpha X + \beta Y, Z) = \alpha \text{Cov}(X, Z) + \beta \text{Cov}(Y, Z).$$

Covariance follows the “positive definiteness” property:

$$\text{Cov}(X, X) = \text{Var}(X) \geq 0.$$

Summary Statistics

Expectation, Variance, and Covariance



Random Vectors

Multivariate Random Variables

Random Vectors

Definition

So far, we have only been talking about single-variable distributions.

We can talk about multivariable distributions by considering random vectors:

$$\mathbf{X} = \begin{bmatrix} X_1 \\ X_2 \\ \vdots \\ X_n \end{bmatrix}$$

Random Vectors

Expectation

The expectation of a random vector just comes from taking the entry-wise expectation:

$$\mathbb{E}[\mathbf{X}] = \begin{bmatrix} \mathbb{E}[X_1] \\ \mathbb{E}[X_2] \\ \vdots \\ \mathbb{E}[X_n] \end{bmatrix}$$

Random Vectors

Variance and Covariance Matrix

The variance of a random vector generalizes to the [covariance matrix](#)

In the $d = 2$ case, where $\mathbf{X} = (X_1, X_2)$:

$$\Sigma = \begin{bmatrix} \text{Var}(X_1) & \text{Cov}(X_1, X_2) \\ \text{Cov}(X_2, X_1) & \text{Var}(X_2) \end{bmatrix}.$$

What do you notice about this matrix?

Random Vectors

Variance and Covariance Matrix

The variance of a random vector generalizes to the covariance matrix

$$\Sigma = \mathbb{E}[(\mathbf{X} - \mathbb{E}[\mathbf{X}])(\mathbf{X} - \mathbb{E}[\mathbf{X}])^\top] = \begin{bmatrix} \text{Var}(X_1) & \text{Cov}(X_1, X_2) & \dots & \text{Cov}(X_1, X_n) \\ \text{Cov}(X_2, X_1) & \text{Var}(X_2) & \dots & \text{Cov}(X_2, X_n) \\ \vdots & \vdots & \ddots & \vdots \\ \text{Cov}(X_n, X_1) & \text{Cov}(X_n, X_2) & \dots & \text{Var}(X_n) \end{bmatrix}$$

In general, $\Sigma_{i,j} = \text{Cov}(X_i, X_j)$.

In this class, a random vector's variance *is* its covariance:

$$\text{Var}(\mathbf{x}) := \Sigma = \mathbb{E}[(\mathbf{X} - \mathbb{E}[\mathbf{X}])(\mathbf{X} - \mathbb{E}[\mathbf{X}])^\top]$$

Random Vectors

Properties of the variance

The covariance matrix is **symmetric**.

$$\Sigma = \Sigma^T.$$

The covariance matrix is also **positive semidefinite**.

$$\mathbf{x}^T \Sigma \mathbf{x} \geq 0 \text{ for all } \mathbf{x} \in \mathbb{R}^d.$$

Covariance Matrix

In machine learning

Suppose $\mathbf{x} \sim \mathbb{P}_{\mathbf{x}}$ (i.e. \mathbf{x} is drawn from a distribution \mathbb{P} over \mathbb{R}^d)...

$\mathbf{x} = (x_1, x_2, \dots, x_d)$ a random vector of d random variables.

Then, if \mathbf{x} is centered (i.e. $\mathbb{E}[\mathbf{x}] = \mathbf{0}$), the covariance matrix (variance of \mathbf{x}) of $\mathbb{P}_{\mathbf{x}}$ is given by:

$$\Sigma = \mathbb{E}[\mathbf{x}\mathbf{x}^T] = \begin{bmatrix} x_1^2 & x_1x_2 & \dots & x_1x_d \\ x_2x_1 & x_2^2 & \dots & x_2x_d \\ \vdots & \dots & \ddots & \vdots \\ x_dx_1 & x_dx_2 & \dots & x_d^2 \end{bmatrix} \in \mathbb{R}^{d \times d}$$

A property of the true distribution, $\mathbb{P}_{\mathbf{x}}$.

Empirical Covariance Matrix

In machine learning

Suppose we draw n examples $\mathbf{x}_1, \dots, \mathbf{x}_n \sim \mathbb{P}_{\mathbf{x}}$ a distribution over \mathbb{R}^d ...

$\mathbf{x}_i = (x_1, x_2, \dots, x_d)$ a random vector of d random variables.

Arrange them into a matrix $\mathbf{X} \in \mathbb{R}^{n \times d}$, where \mathbf{x}_i^\top are the rows.

Then, if each \mathbf{x}_i is centered (i.e. $\mathbb{E}[\mathbf{x}_i] = \mathbf{0}$), the empirical covariance matrix is:

$$\hat{\Sigma}_n := \frac{1}{n} \mathbf{X}^\top \mathbf{X} \in \mathbb{R}^{d \times d}.$$

A property of the a specific observed dataset, $\mathbf{x}_1, \dots, \mathbf{x}_n$.

Empirical Covariance Matrix

In machine learning

If each \mathbf{x}_i is centered (i.e. $\mathbb{E}[\mathbf{x}_i] = \mathbf{0}$), the empirical covariance matrix is:

$$\hat{\Sigma}_n := \frac{1}{n} \mathbf{X}^\top \mathbf{X} \in \mathbb{R}^{d \times d}.$$

If not, we can center the columns by subtracting off their empirical mean:

$$\bar{\mathbf{x}}_j = \mathbf{x}_j - \frac{1}{n} \sum_{i=1}^n \mathbf{x}_j \text{ for all } j \in [d].$$

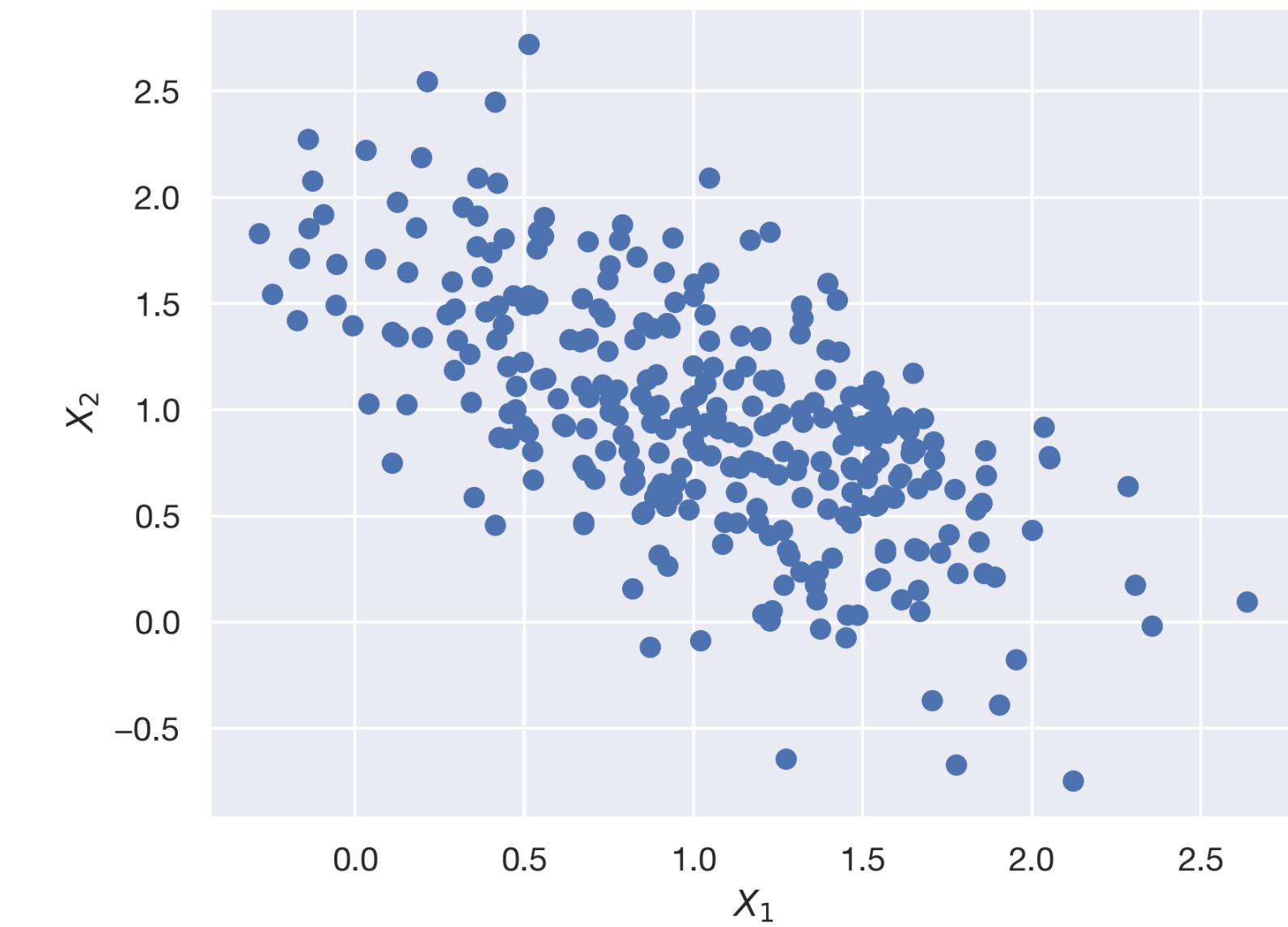
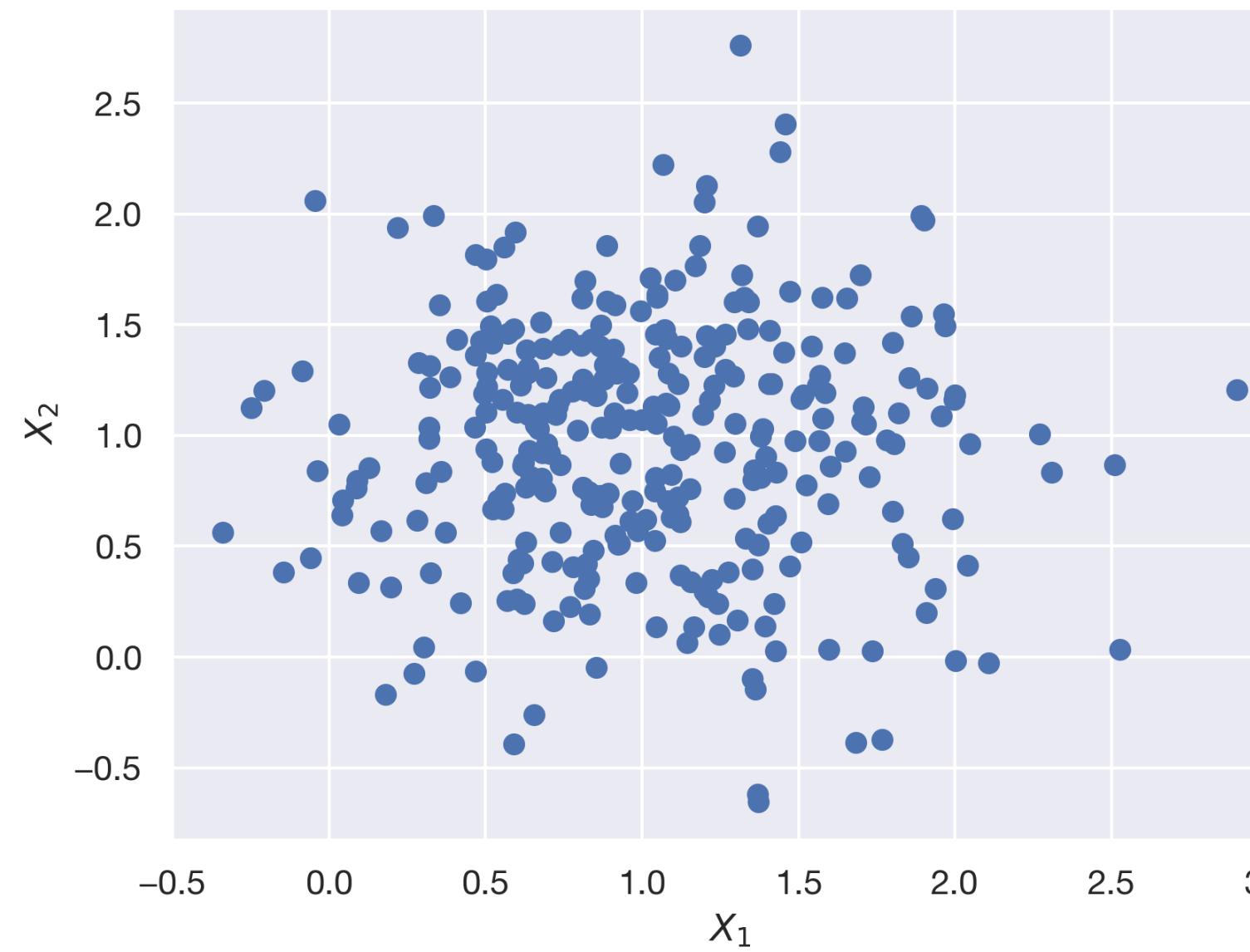
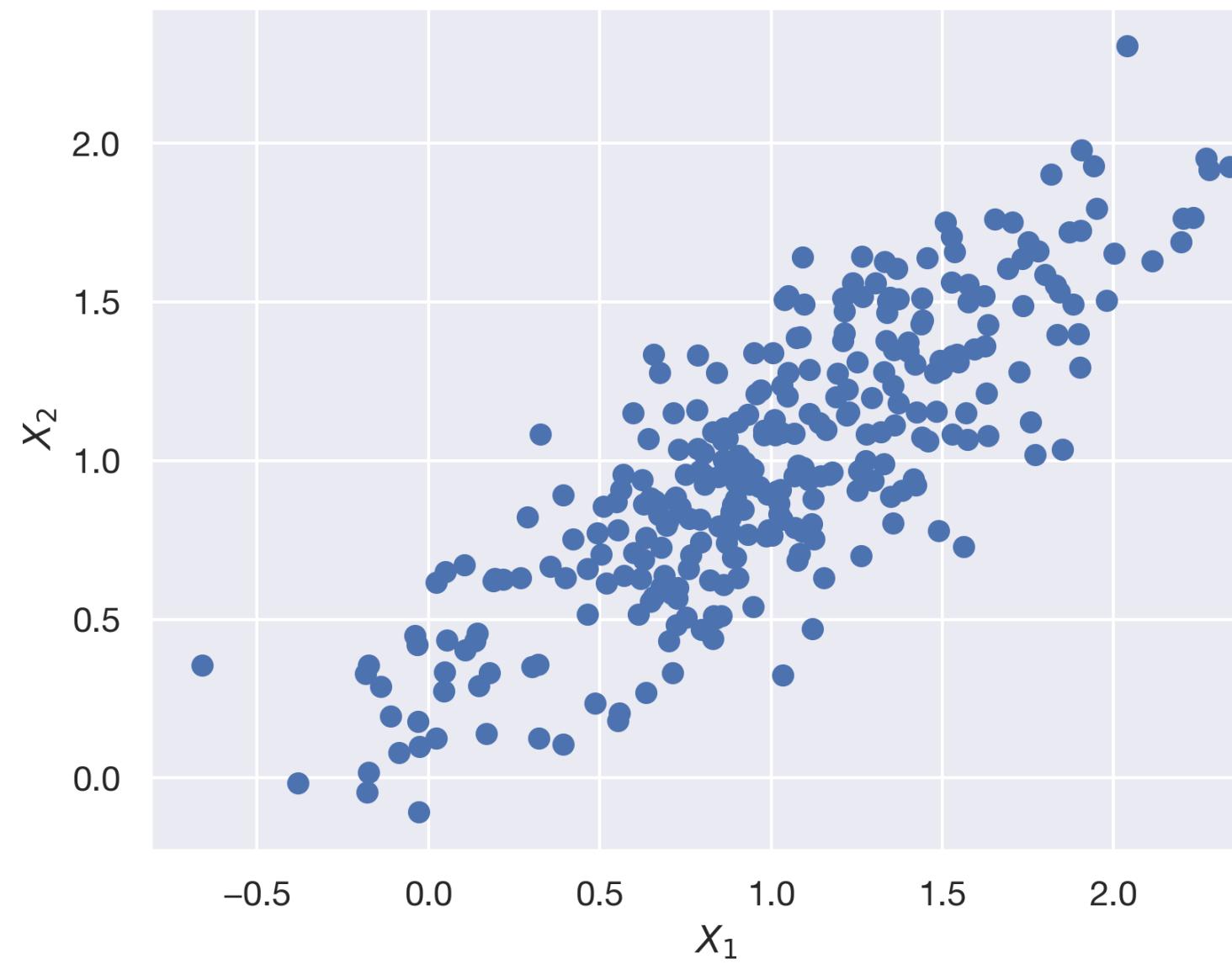
Construct $\bar{\mathbf{X}} \in \mathbb{R}^{n \times d}$ using the $\bar{\mathbf{x}}_j$ as columns.

Empirical Covariance Matrix

Relationship to eigendecomposition

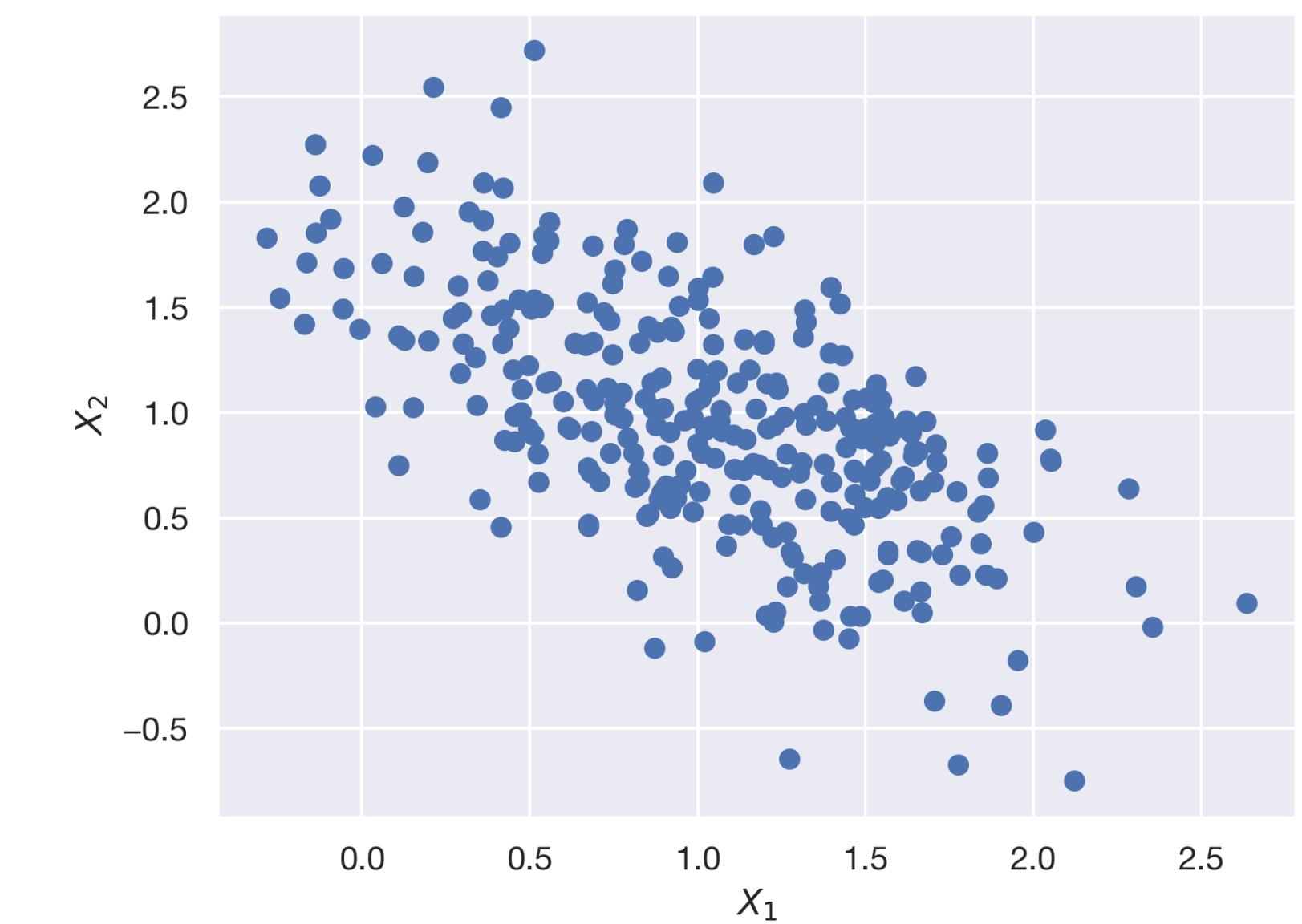
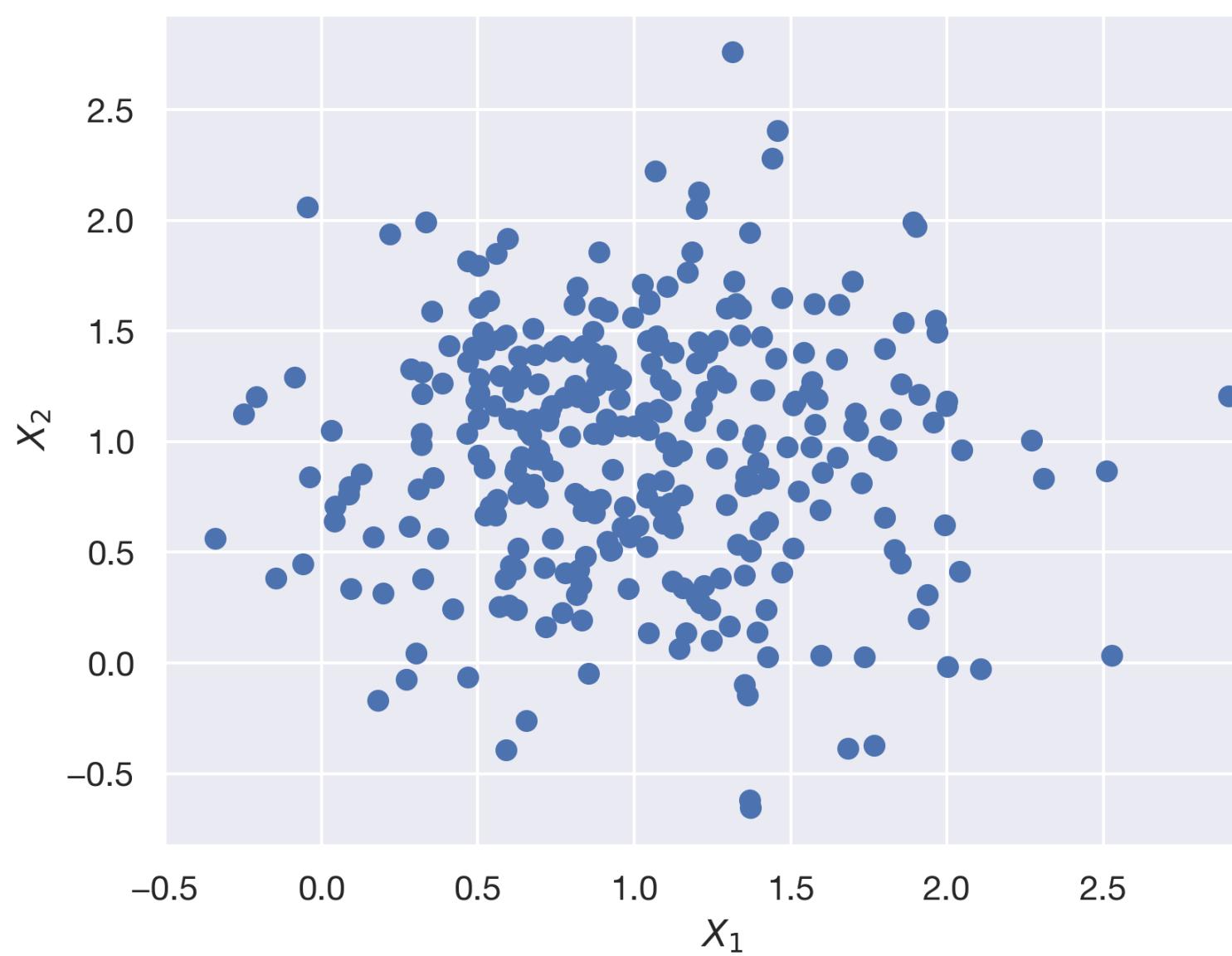
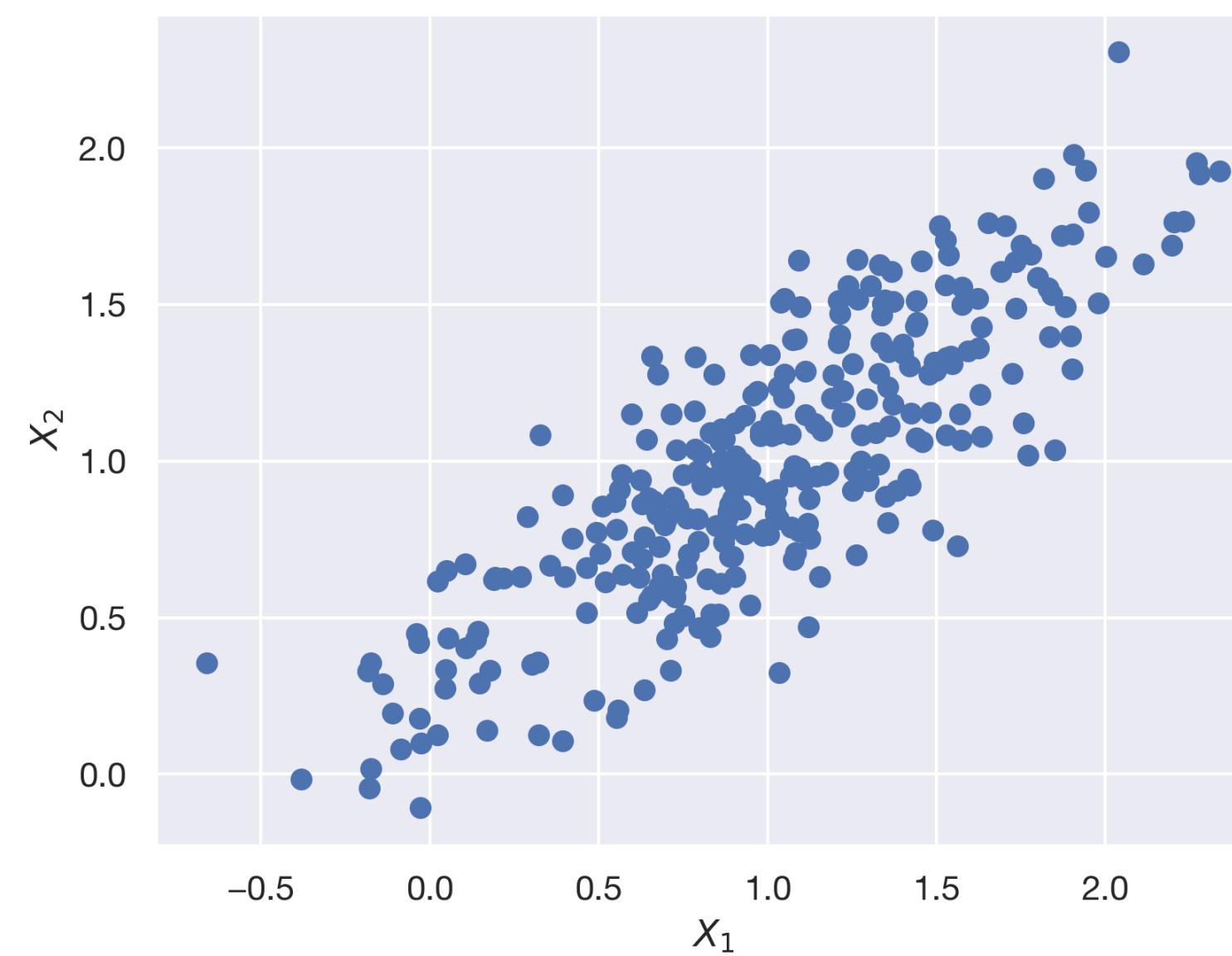
$$\hat{\Sigma}_n := \frac{1}{n} \mathbf{X}^\top \mathbf{X} = \frac{1}{n} \mathbf{V} \Lambda \mathbf{V}^\top$$

Eigendecomposition tells us geometry of the “shape” of the data cloud.



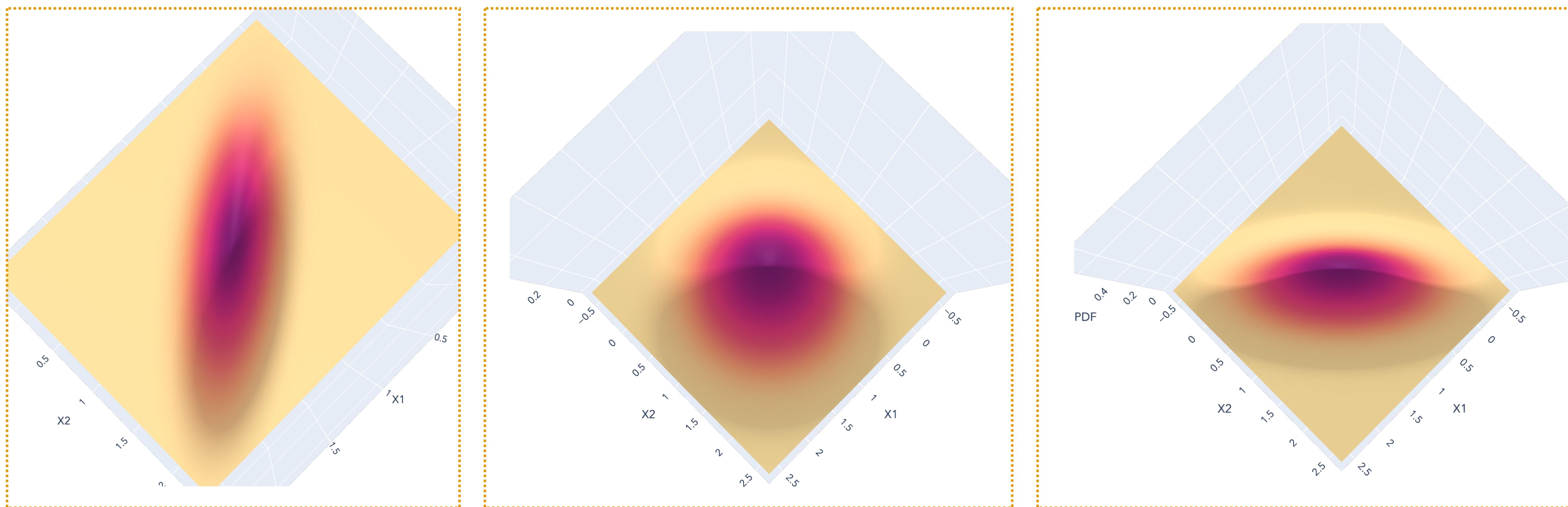
Empirical Covariance Matrix

Relationship to true covariance



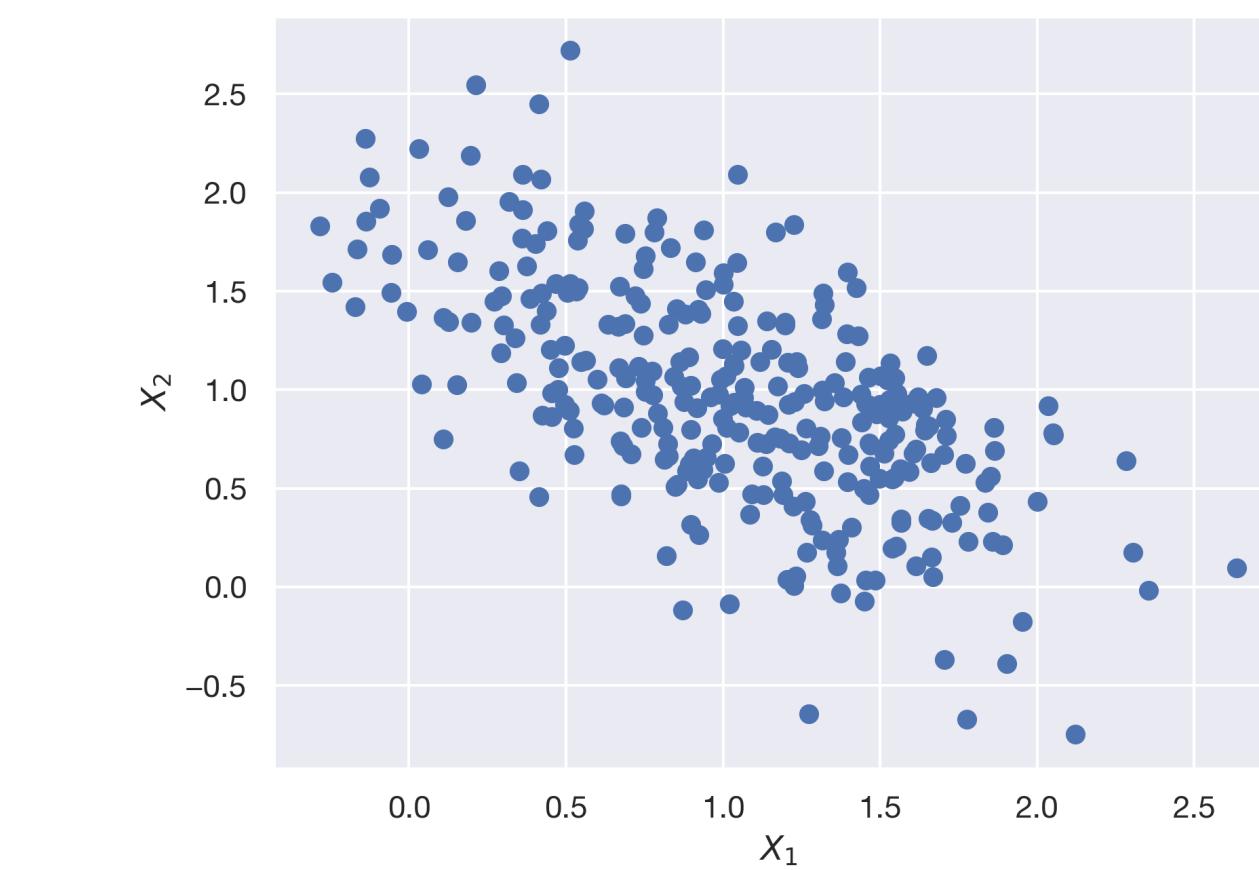
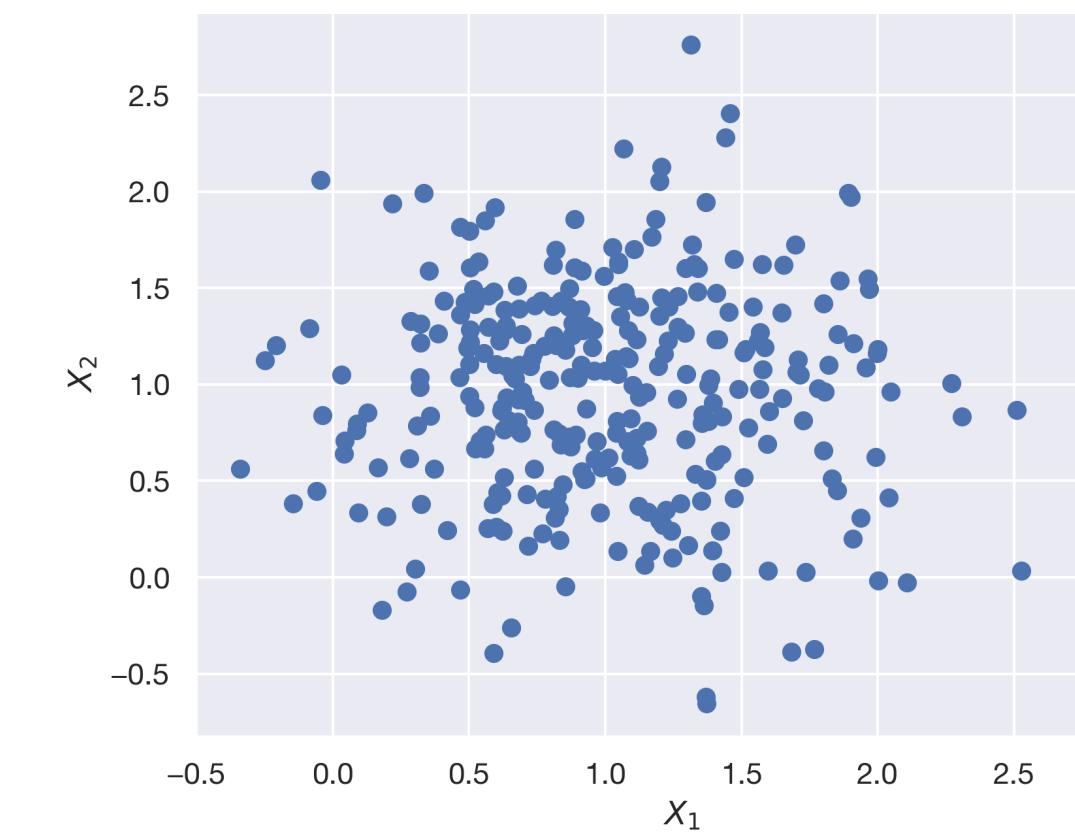
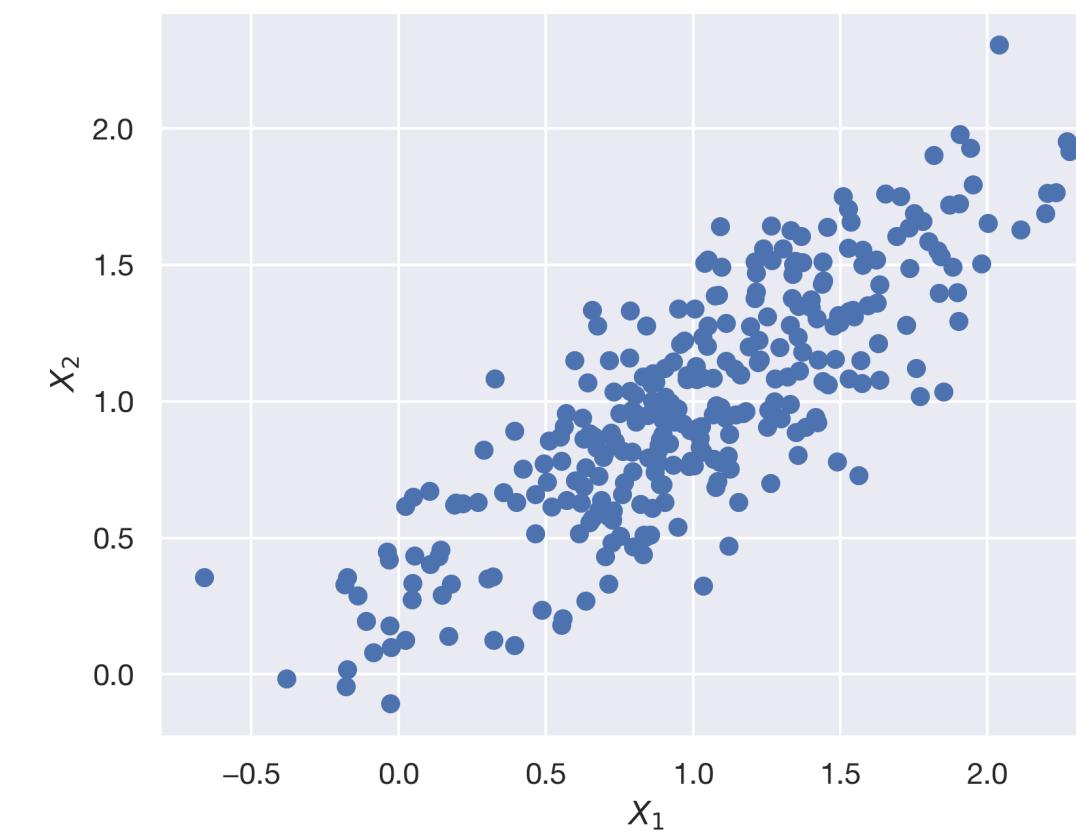
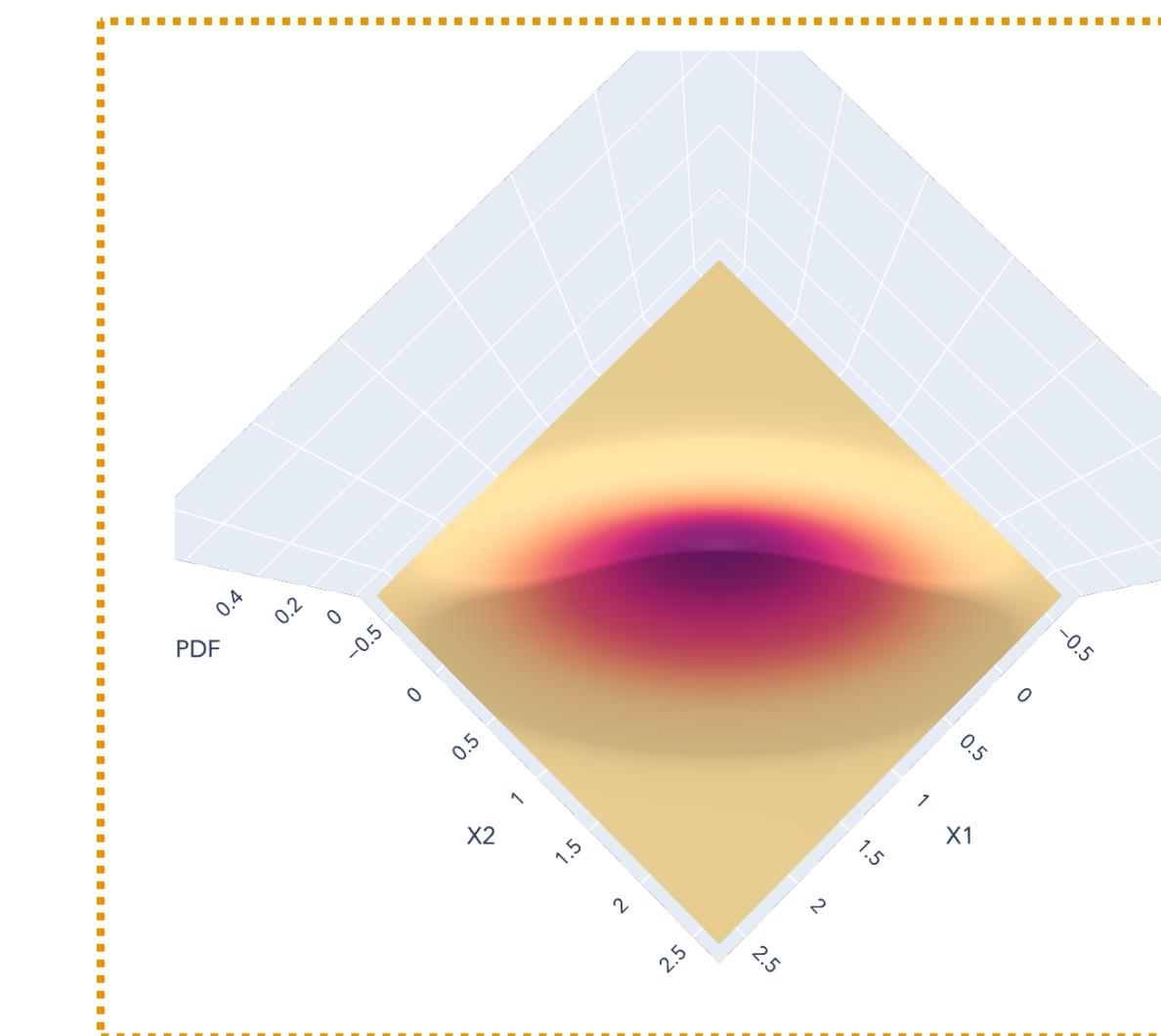
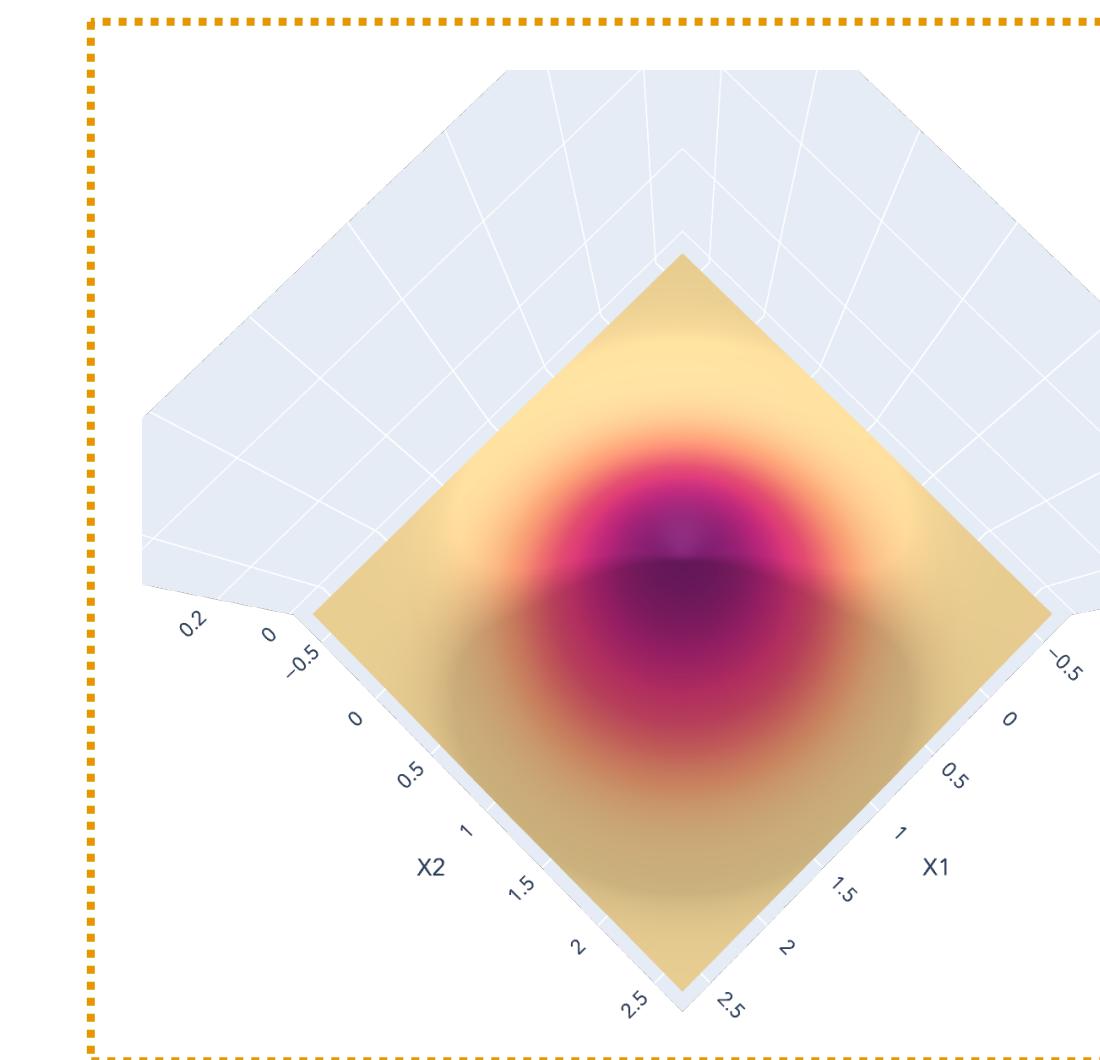
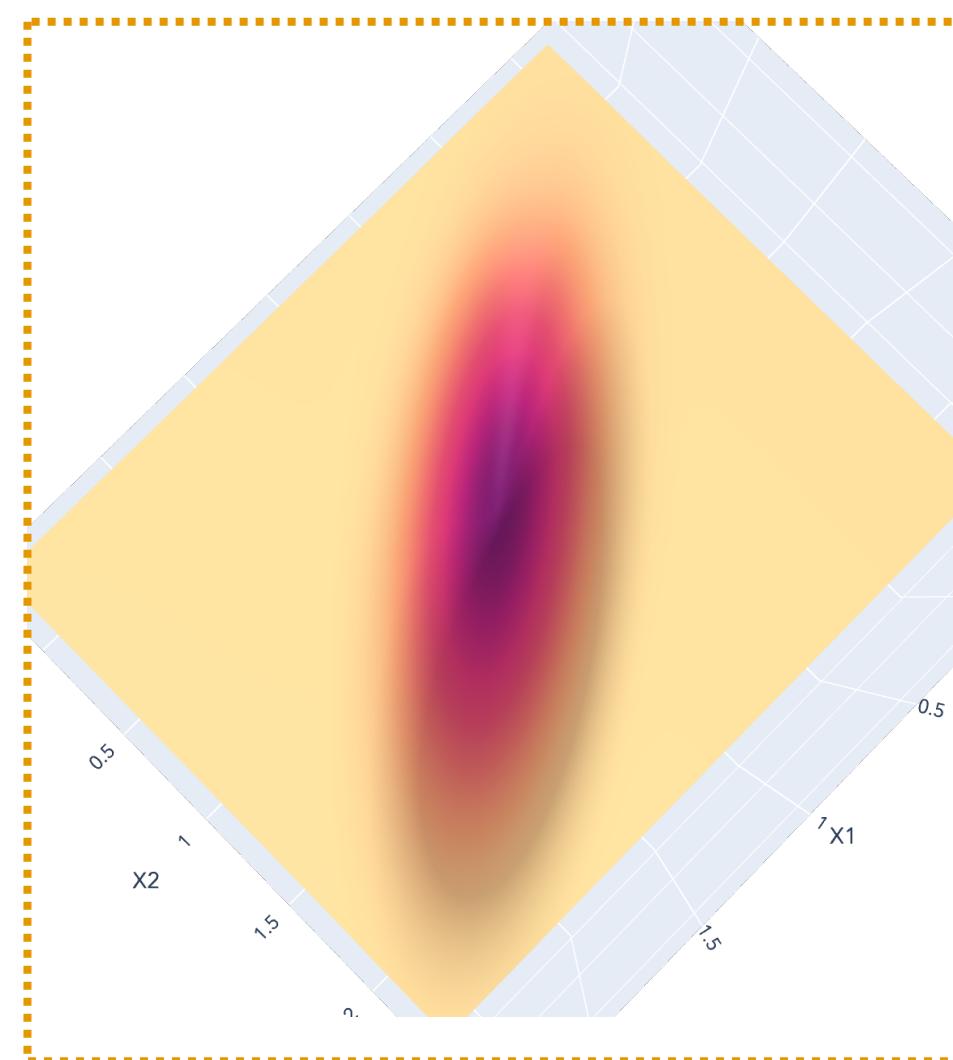
Empirical Covariance Matrix

Relationship to true covariance



Empirical Covariance Matrix

Relationship to true covariance

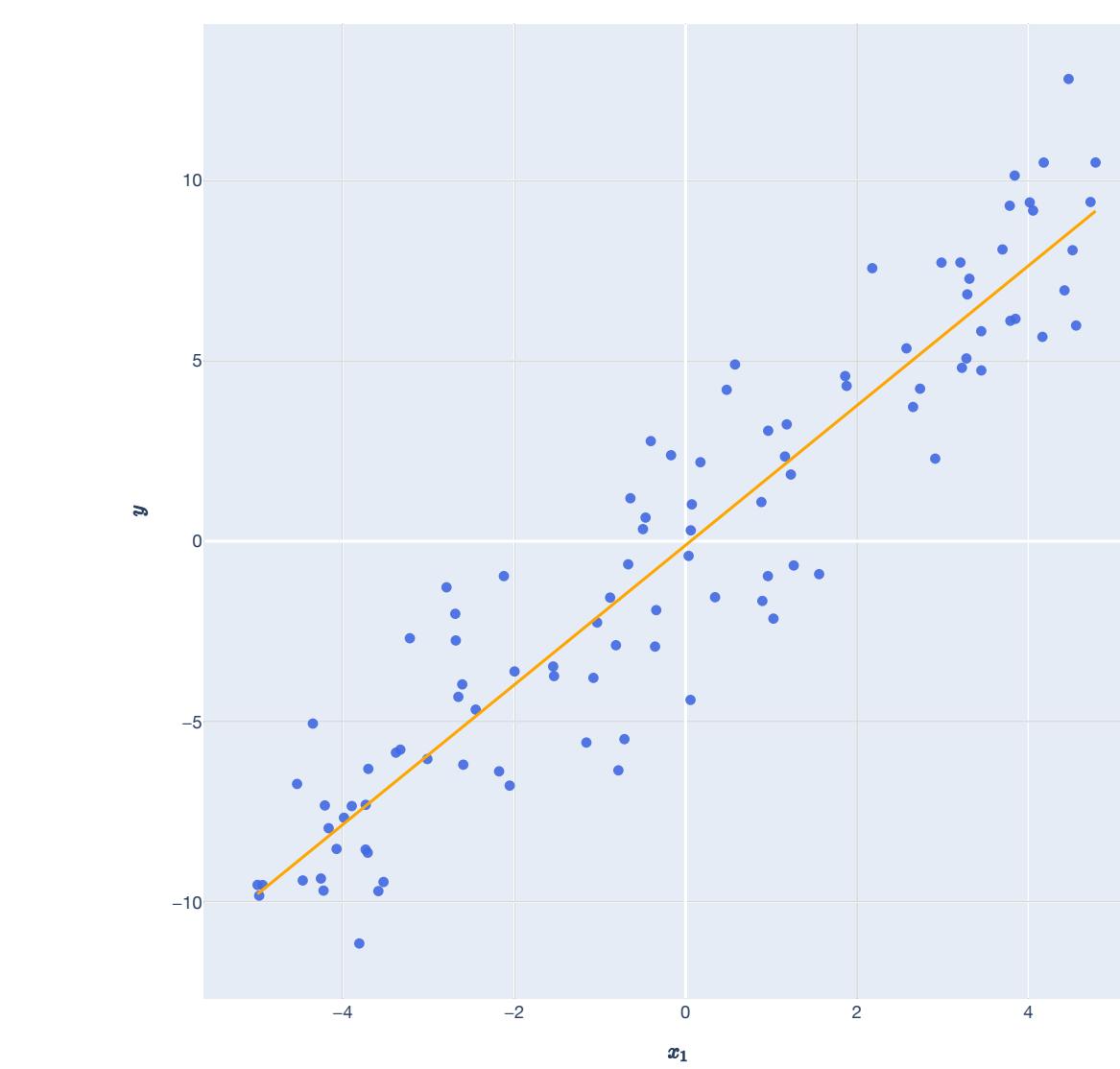
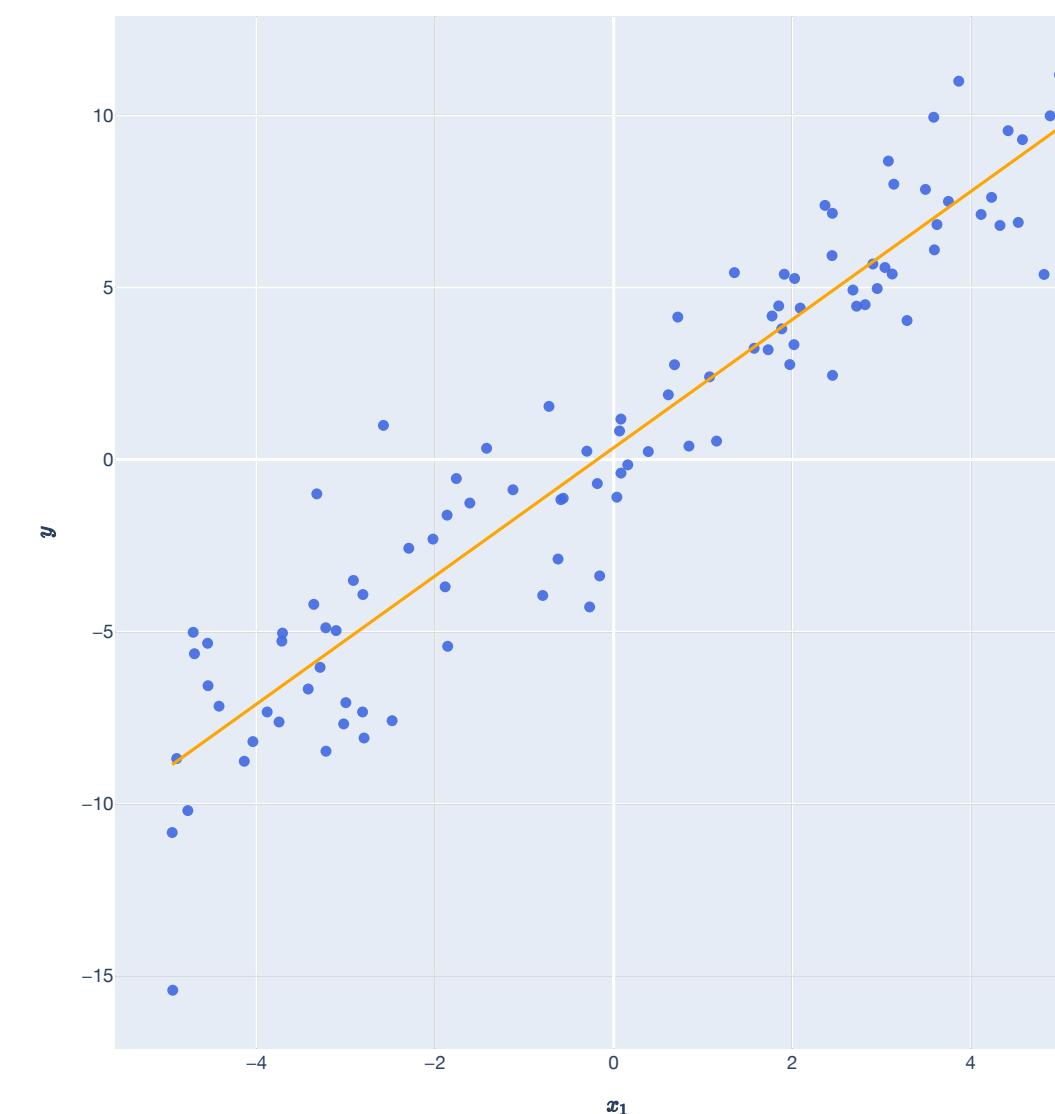
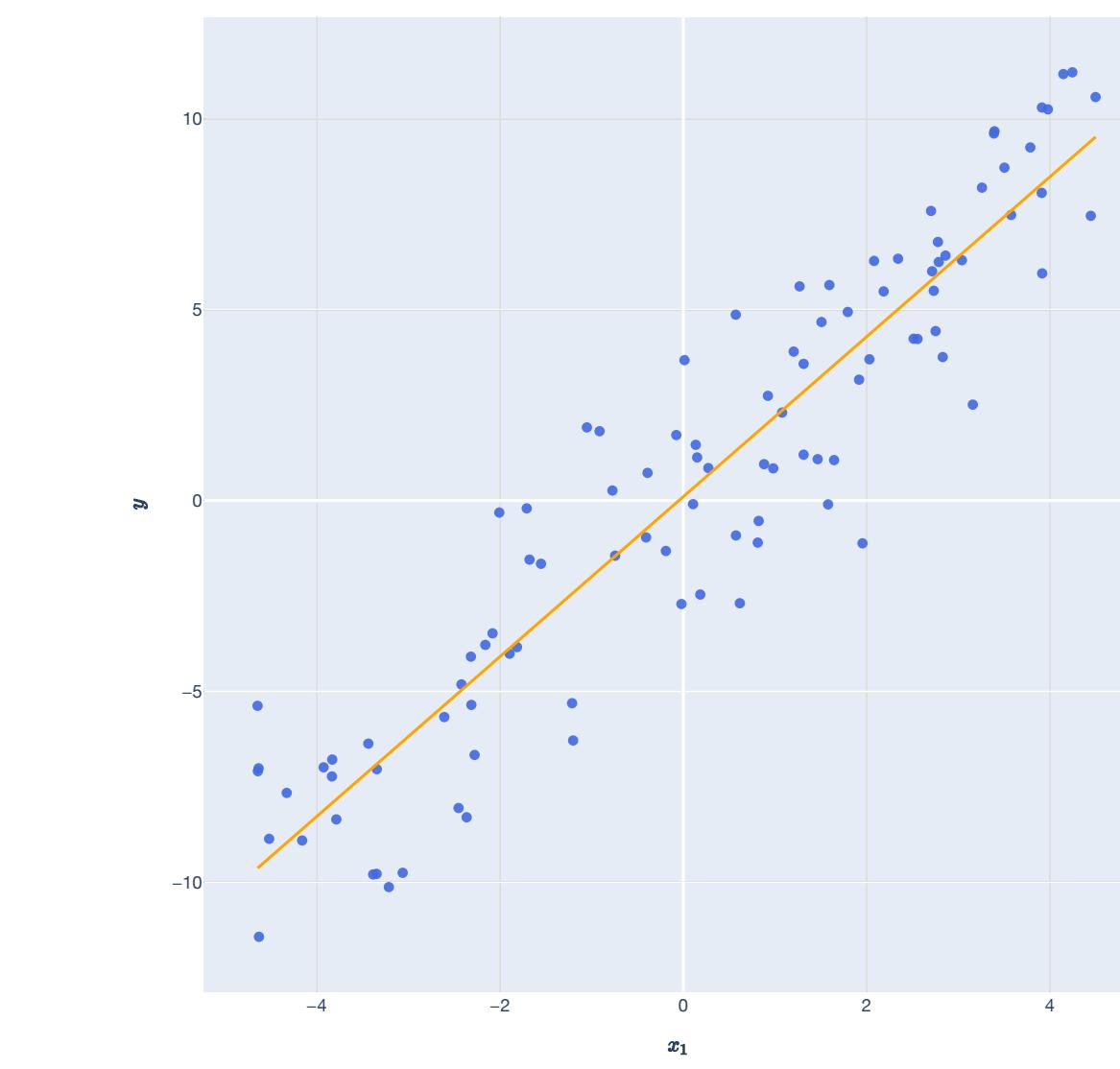
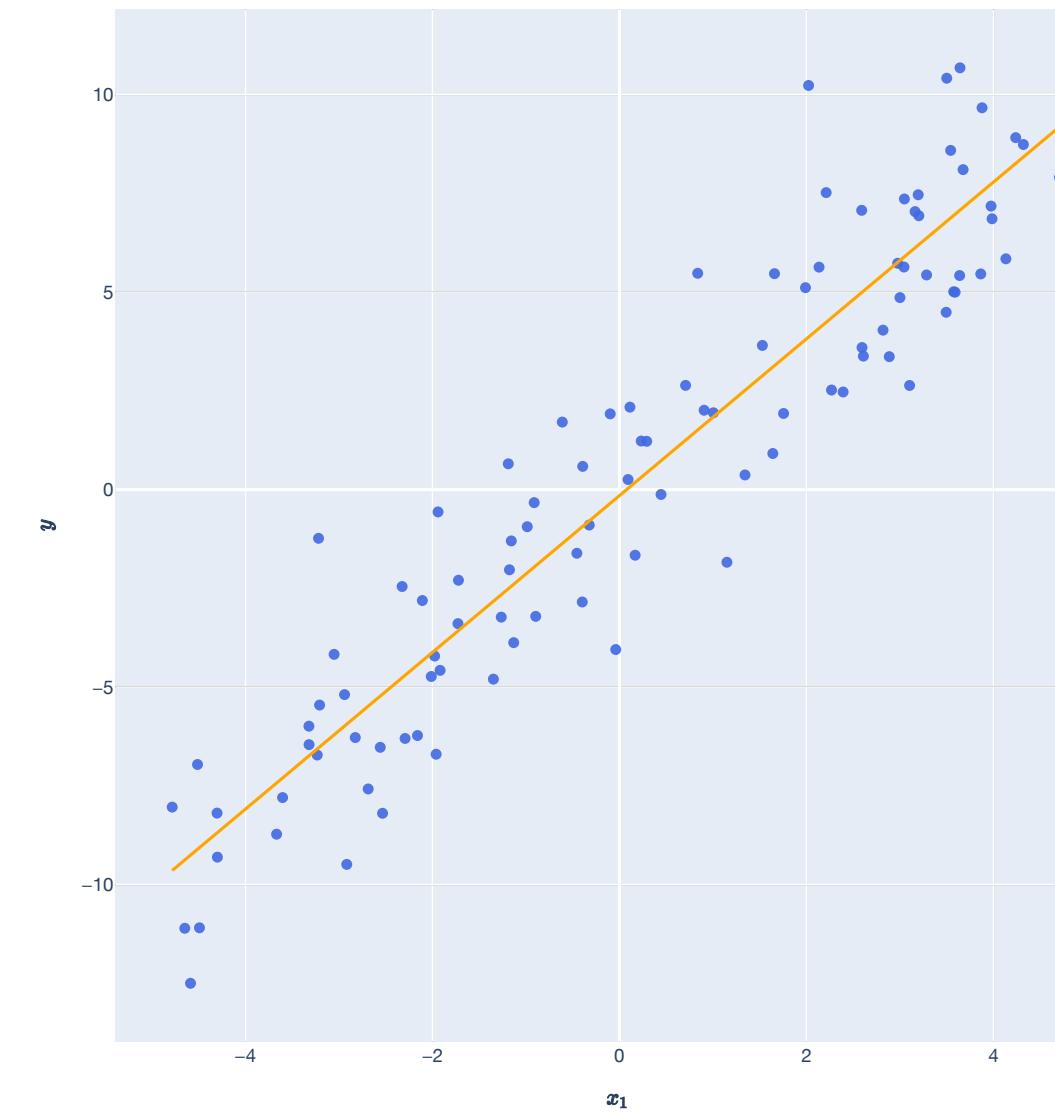
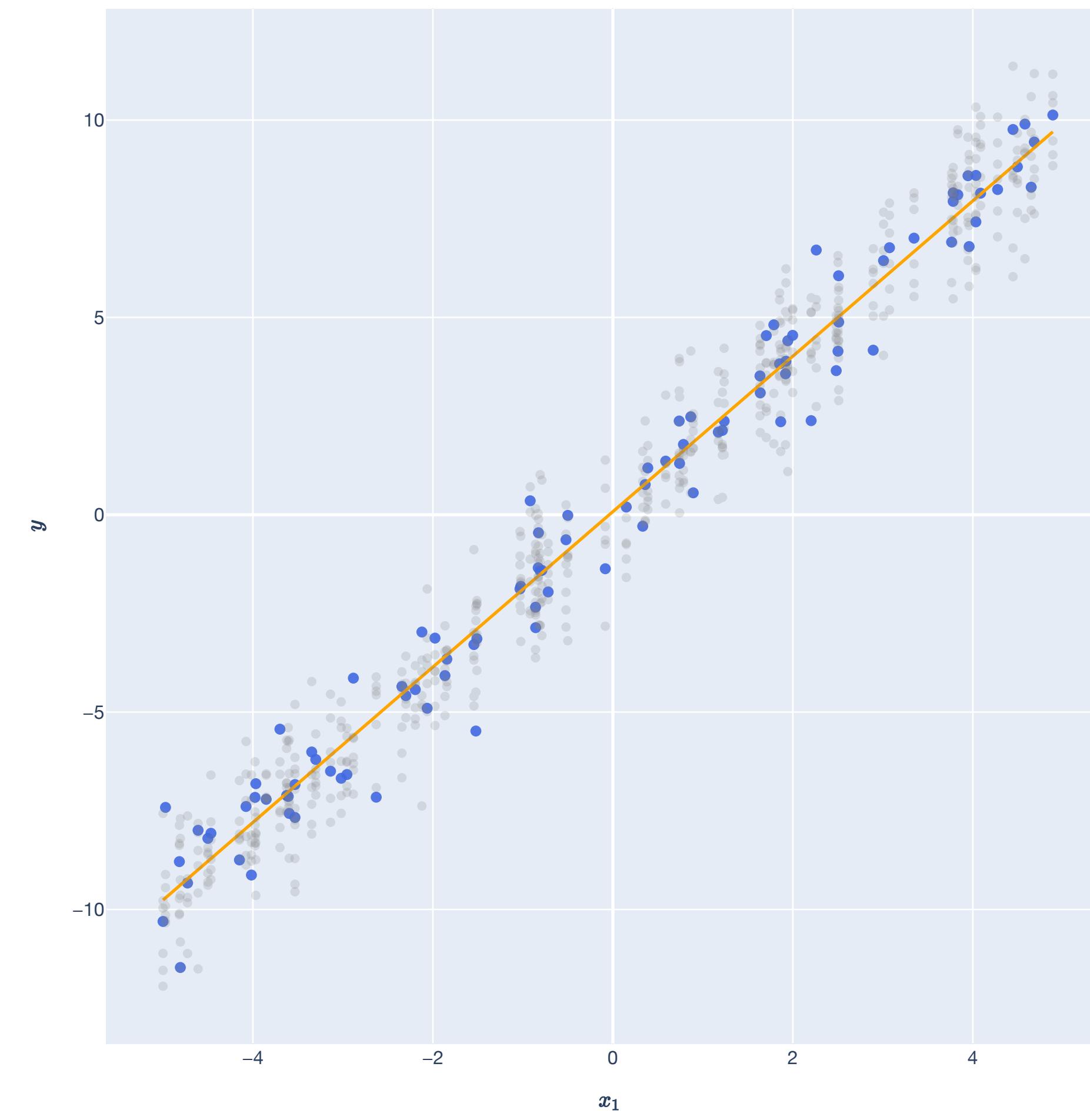


Data as random

Modeling regression with probability

Regression

Modeling randomness



Regression

Setup (Example View)

Observed: Matrix of *training samples* $\mathbf{X} \in \mathbb{R}^{n \times d}$ and vector of *training labels* $\mathbf{y} \in \mathbb{R}^n$.

$$\mathbf{X} = \begin{bmatrix} \leftarrow & \mathbf{x}_1^\top & \rightarrow \\ & \vdots & \\ \leftarrow & \mathbf{x}_n^\top & \rightarrow \end{bmatrix} \quad \mathbf{y} = \begin{bmatrix} y_1 \\ \vdots \\ y_n \end{bmatrix}, \text{ where } \mathbf{x}_1, \dots, \mathbf{x}_n \in \mathbb{R}^d.$$

Unknown: *Weight vector* $\mathbf{w} \in \mathbb{R}^d$ with weights w_1, \dots, w_d .

Goal: For each $i \in [n]$, we predict: $\hat{y}_i = \mathbf{w}^\top \mathbf{x}_i = w_1 x_{i1} + \dots + w_d x_{id} \in \mathbb{R}$.

Choose a weight vector that “fits the training data”: $\mathbf{w} \in \mathbb{R}^d$ such that $y_i \approx \hat{y}_i$ for $i \in [n]$, or:

$$\mathbf{X}\mathbf{w} = \hat{\mathbf{y}} \approx \mathbf{y}.$$

Regression

Setup (Feature View)

Observed: Matrix of *training samples* $\mathbf{X} \in \mathbb{R}^{n \times d}$ and vector of *training labels* $\mathbf{y} \in \mathbb{R}^n$.

$$\mathbf{X} = \begin{bmatrix} \uparrow & & \uparrow \\ \mathbf{x}_1 & \dots & \mathbf{x}_d \\ \downarrow & & \downarrow \end{bmatrix} \quad \mathbf{y} = \begin{bmatrix} y_1 \\ \vdots \\ y_n \end{bmatrix}, \text{ where } \mathbf{x}_1, \dots, \mathbf{x}_d \in \mathbb{R}^n.$$

Unknown: *Weight vector* $\mathbf{w} \in \mathbb{R}^d$ with weights w_1, \dots, w_d .

Choose a weight vector that "fits the training data": $\mathbf{w} \in \mathbb{R}^d$ such that $y_i \approx \hat{y}_i$ for $i \in [n]$, or:

$$\mathbf{X}\mathbf{w} = \hat{\mathbf{y}} \approx \mathbf{y}.$$

Regression

Setup

Ultimate Goal: Given a new, unseen $(\mathbf{x}_0, y_0) \in \mathbb{R}^d \times \mathbb{R}$, we wanted to generalize:

$$\hat{\mathbf{w}}^\top \mathbf{x}_0 \approx y_0.$$

To do this, we fit the “training data”: $\hat{\mathbf{w}} \in \mathbb{R}^d$ such that $y_i \approx \hat{y}_i$ for $i \in [n]$, or:

$$\mathbf{X}\hat{\mathbf{w}} = \hat{\mathbf{y}} \approx \mathbf{y}.$$

To find $\hat{\mathbf{w}}$, we follow the *principle of least squares*.

$$\hat{\mathbf{w}} = \arg \min_{\mathbf{w} \in \mathbb{R}^d} \|\mathbf{X}\mathbf{w} - \mathbf{y}\|^2$$

Regression

Setup

Least squares expanded is just:

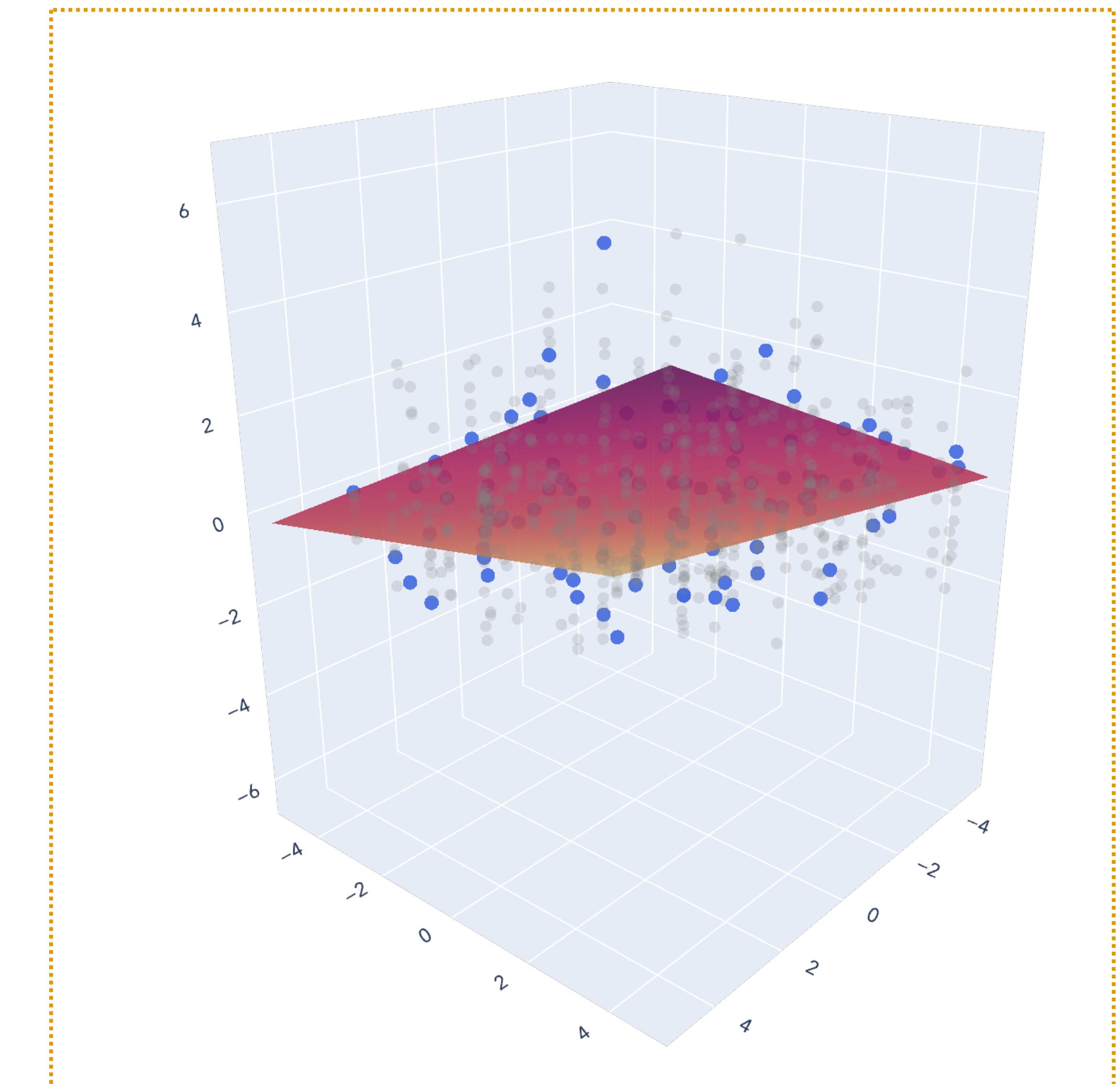
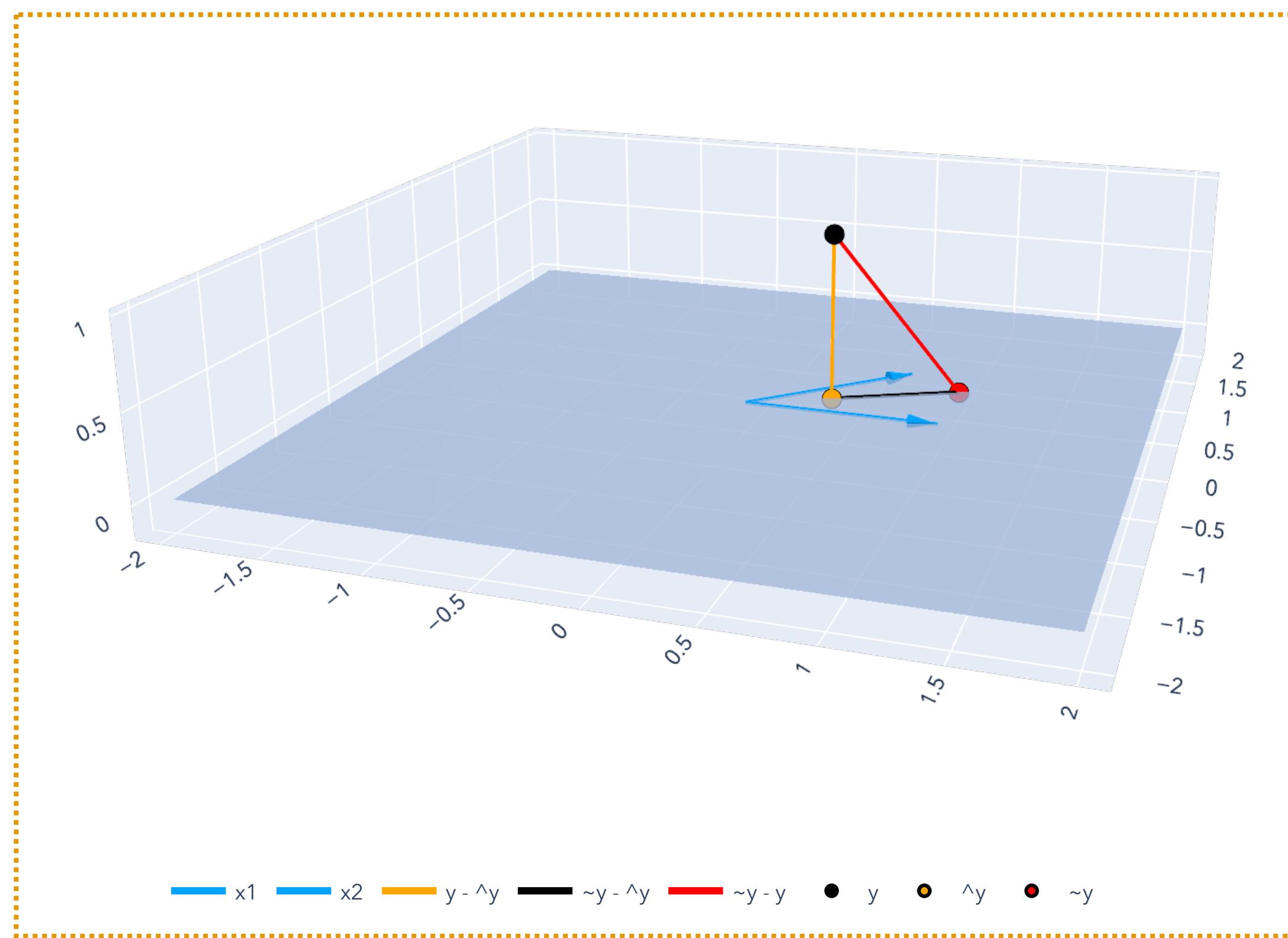
$$\|\mathbf{X}\mathbf{w} - \mathbf{y}\|^2 = \sum_{i=1}^n (\mathbf{w}^\top \mathbf{x}_i - y_i)^2$$

Put a $1/n$ in front, and it looks like we're minimizing an average:

$$\frac{1}{n} \|\mathbf{X}\mathbf{w} - \mathbf{y}\|^2 = \frac{1}{n} \sum_{i=1}^n (\mathbf{w}^\top \mathbf{x}_i - y_i)^2$$

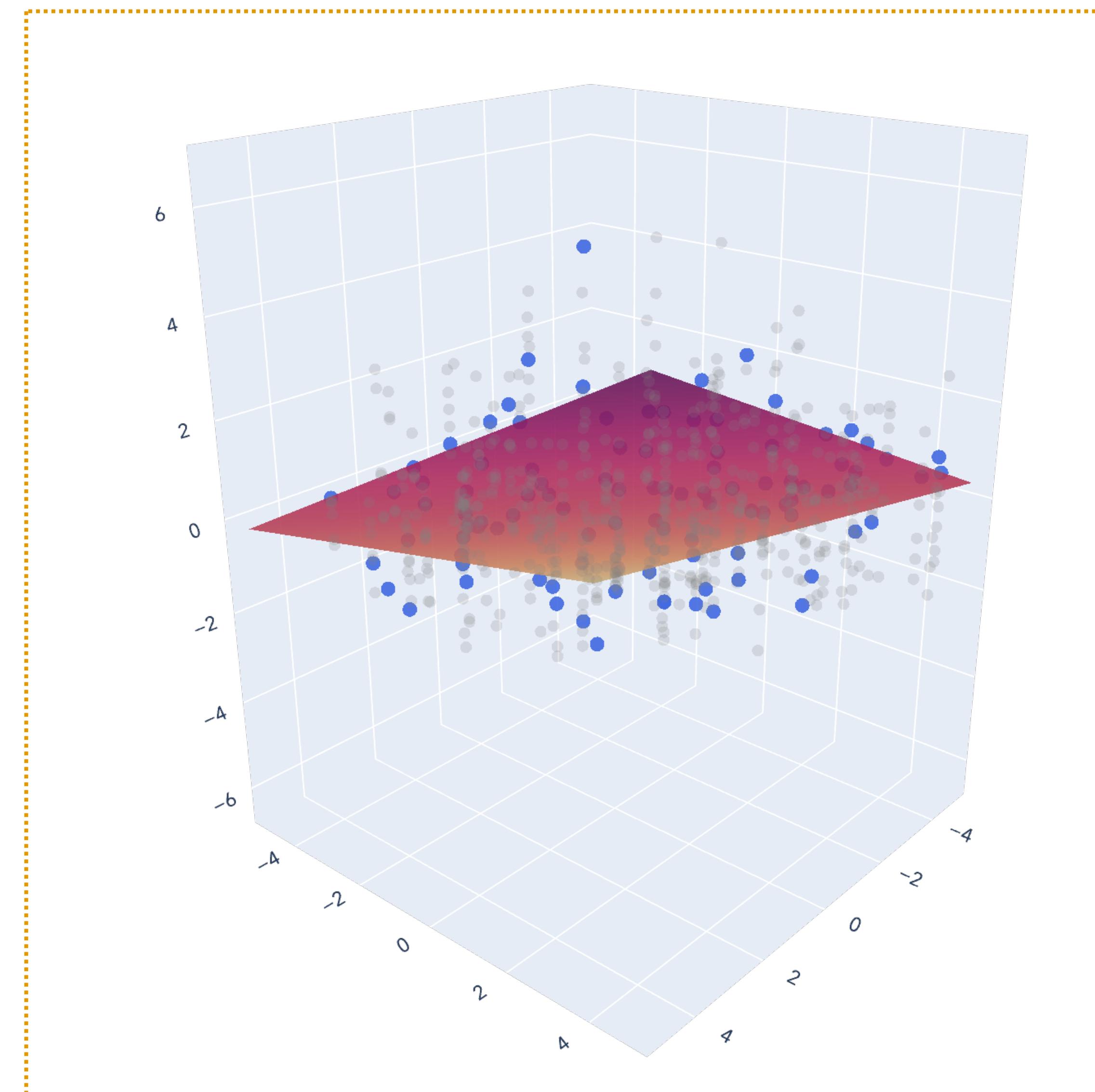
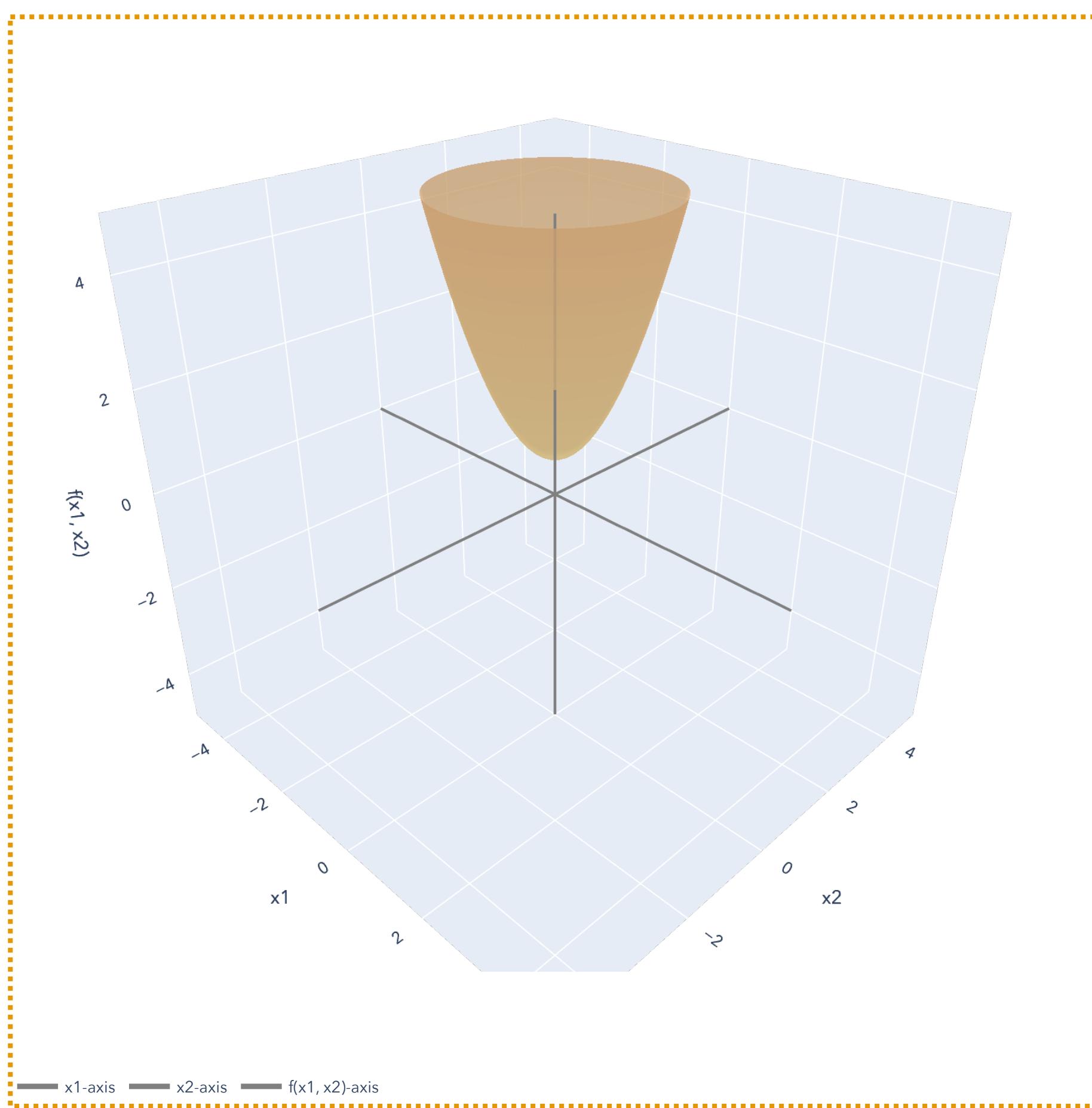
Regression

A note on \hat{w}



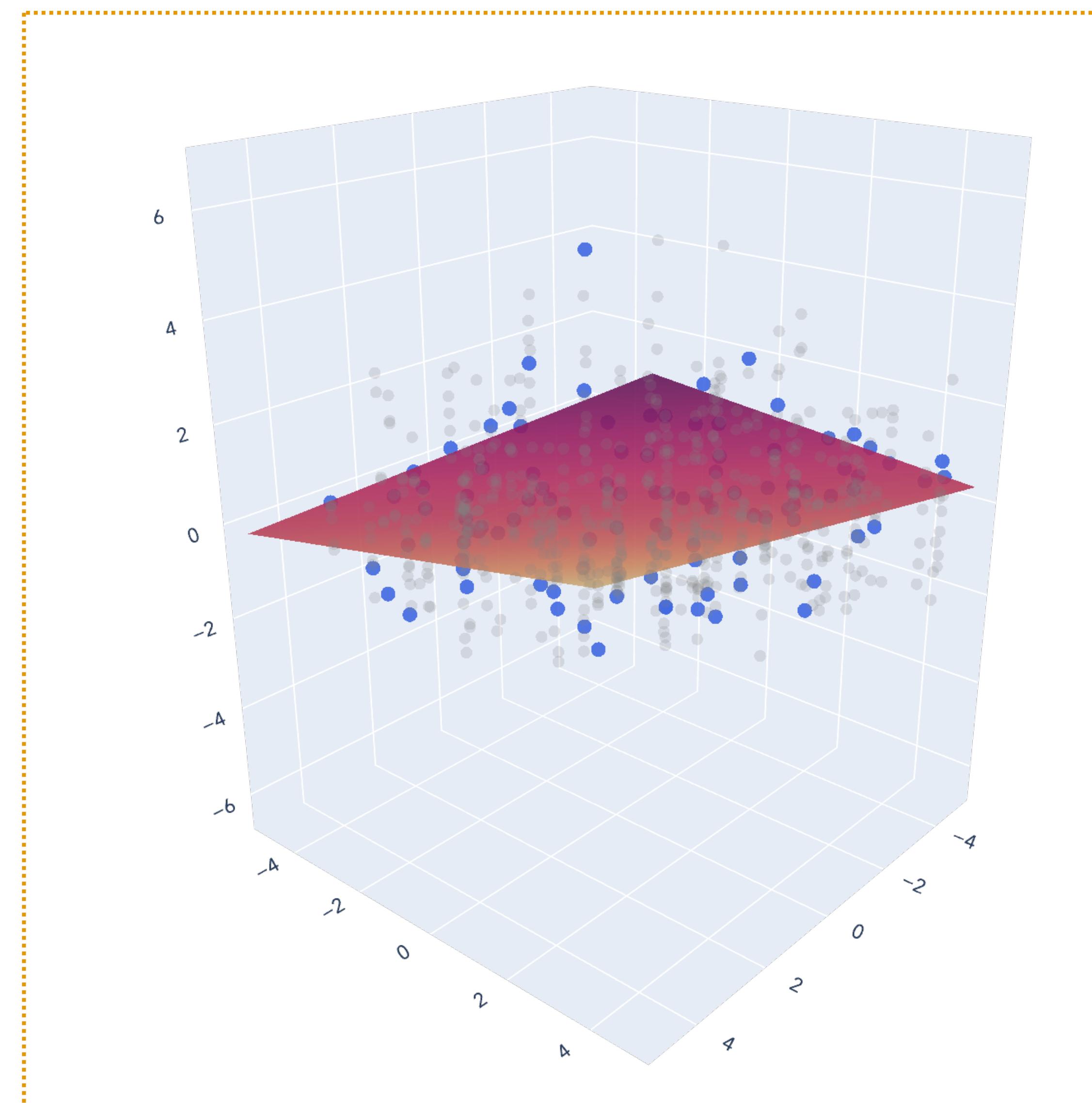
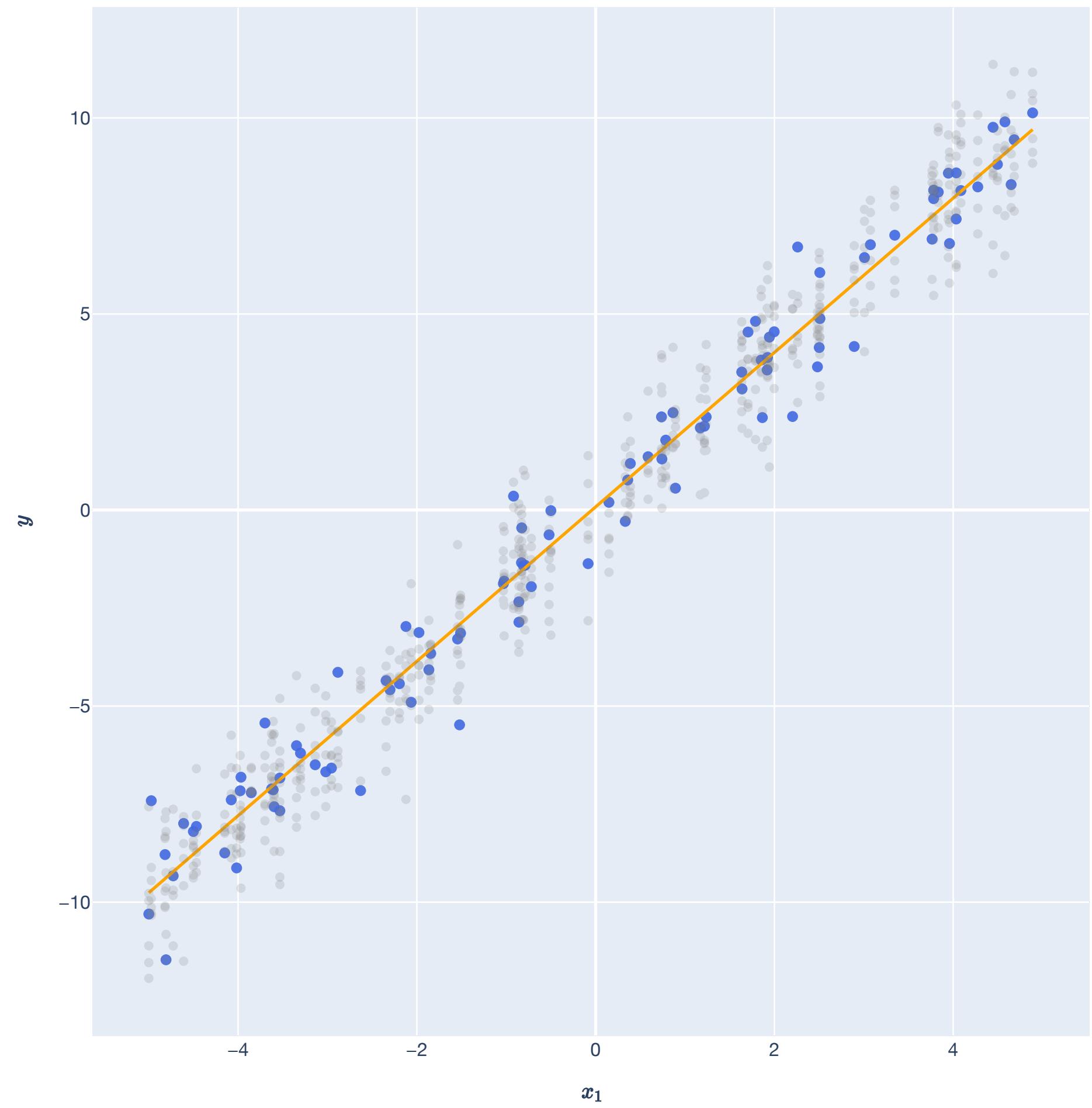
Regression

A note on \hat{w}



Regression

A note on \hat{w}



Regression

Setup, with randomness

Observed: Matrix of *training samples* $\mathbf{X} \in \mathbb{R}^{n \times d}$ and vector of *training labels* $\mathbf{y} \in \mathbb{R}^n$.

Random vector $\mathbf{x}_i \in \mathbb{R}^d$

$$\mathbf{X} = \begin{bmatrix} \mathbf{x}_1^\top & \\ \vdots & \\ \mathbf{x}_n^\top & \end{bmatrix}$$

Random variable y_i

$$\mathbf{y} = \begin{bmatrix} y_1 \\ \vdots \\ y_n \end{bmatrix}, \text{ where } \mathbf{x}_1, \dots, \mathbf{x}_n \in \mathbb{R}^d.$$

... from the joint distribution $\mathbb{P}_{\mathbf{x}, y}$ over $\mathbb{R}^d \times \mathbb{R}$!

Unknown: Weight vector $\mathbf{w} \in \mathbb{R}^d$ with weights w_1, \dots, w_d .

Goal: For each $i \in [n]$, we predict: $\hat{y}_i = \mathbf{w}^\top \mathbf{x}_i = w_1 x_{i1} + \dots + w_d x_{id} \in \mathbb{R}$.

Our "model", a function that we hope "generalizes" well to new datapoint (\mathbf{x}_0, y_0) .

Choose a weight vector that "fits the training data": $\mathbf{w} \in \mathbb{R}^d$ such that $y_i \approx \hat{y}_i$ for $i \in [n]$, or:

$$\mathbf{X}\mathbf{w} = \hat{\mathbf{y}} \approx \mathbf{y}.$$

Because we assume that $(\mathbf{x}_0, y_0) \sim \mathbb{P}_{\mathbf{x}, y}$ as well!

Regression with randomness

Part 1: Random data from probability distribution

Each row $\mathbf{x}_i^\top \in \mathbb{R}^d$ for $i \in [n]$ is a random vector.

Each $y_i \in \mathbb{R}$ is a random variable.

We will now assume there exists a joint distribution $\mathbb{P}_{\mathbf{x},y}$ over $\mathbb{R}^d \times \mathbb{R}$, where we draw:

$$(\mathbf{x}_i, y_i) \sim \mathbb{P}_{\mathbf{x},y}.$$

Regression with randomness

Part 1: Random data from probability distribution

Random vector Random variable

$$\mathbf{X} = \begin{bmatrix} & \leftarrow \mathbf{x}_1^\top \rightarrow \\ & \vdots \\ & \leftarrow \mathbf{x}_n^\top \rightarrow \end{bmatrix} \quad \mathbf{y} = \begin{bmatrix} y_1 \\ \vdots \\ y_n \end{bmatrix}, \text{ where } \mathbf{x}_1, \dots, \mathbf{x}_n \in \mathbb{R}^d.$$

... from the joint distribution $\mathbb{P}_{\mathbf{x},y}$ over $\mathbb{R}^d \times \mathbb{R}$!

Regression with randomness

Part 2: Notion of error and linear model

We want to find a model of the data, a function $f: \mathbb{R}^d \rightarrow \mathbb{R}$ that generalizes well to a newly drawn, unseen $(\mathbf{x}_0, y_0) \sim \mathbb{P}_{\mathbf{x}, y}$.

Our notion of error is the squared loss:

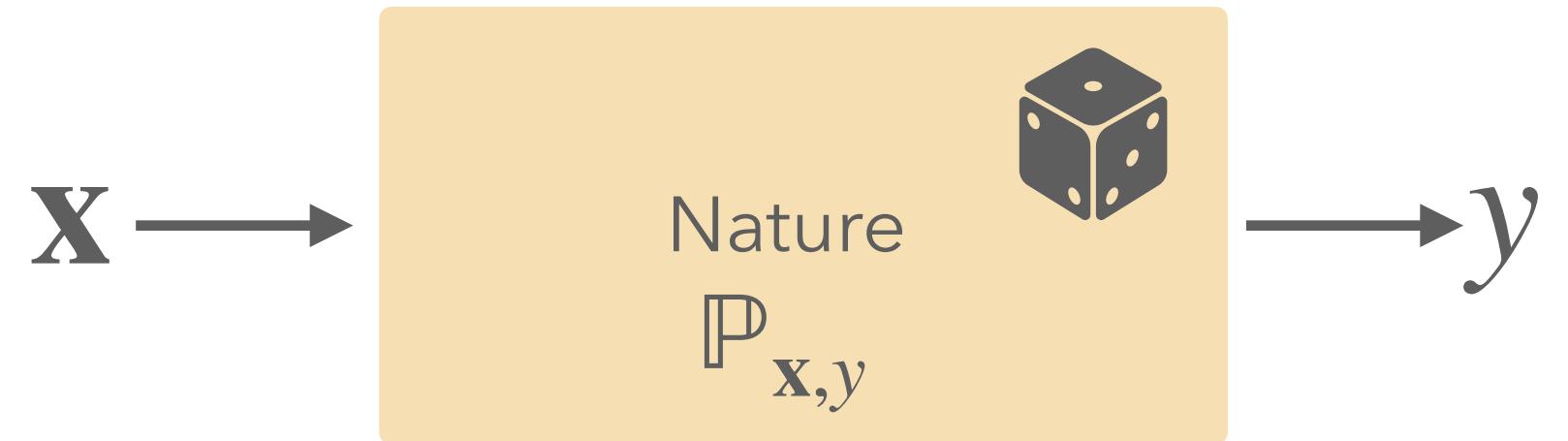
$$\ell(f(\mathbf{x}), y) := (y - f(\mathbf{x}))^2.$$

In our case, $f: \mathbb{R}^d \rightarrow \mathbb{R}$ is a *linear functional* of the features.

$$f_{\mathbf{w}}(\mathbf{x}) = \mathbf{w}^\top \mathbf{x}$$

Regression with randomness

Part 2: Notion of error and linear model



Assume further: $(\mathbf{x}_i, y_i) \in \mathbb{R}^d \times \mathbb{R}$ pair is drawn from a *joint distribution*, $\mathbb{P}_{\mathbf{x},y}$

$$y_i = f^*(\mathbf{x}_i) + \epsilon_i$$

Some *deterministic* function $f^* : \mathbb{R}^d \rightarrow \mathbb{R}$ explains as much as it can.

Some *randomness* ϵ_i models the unexplained relationship, where we assume

$$\mathbb{E}[\epsilon_i] = 0 \text{ and } \epsilon_i \text{ is independent of } \mathbf{x}_i.$$

Regression with randomness

Part 2: Notion of error and linear model

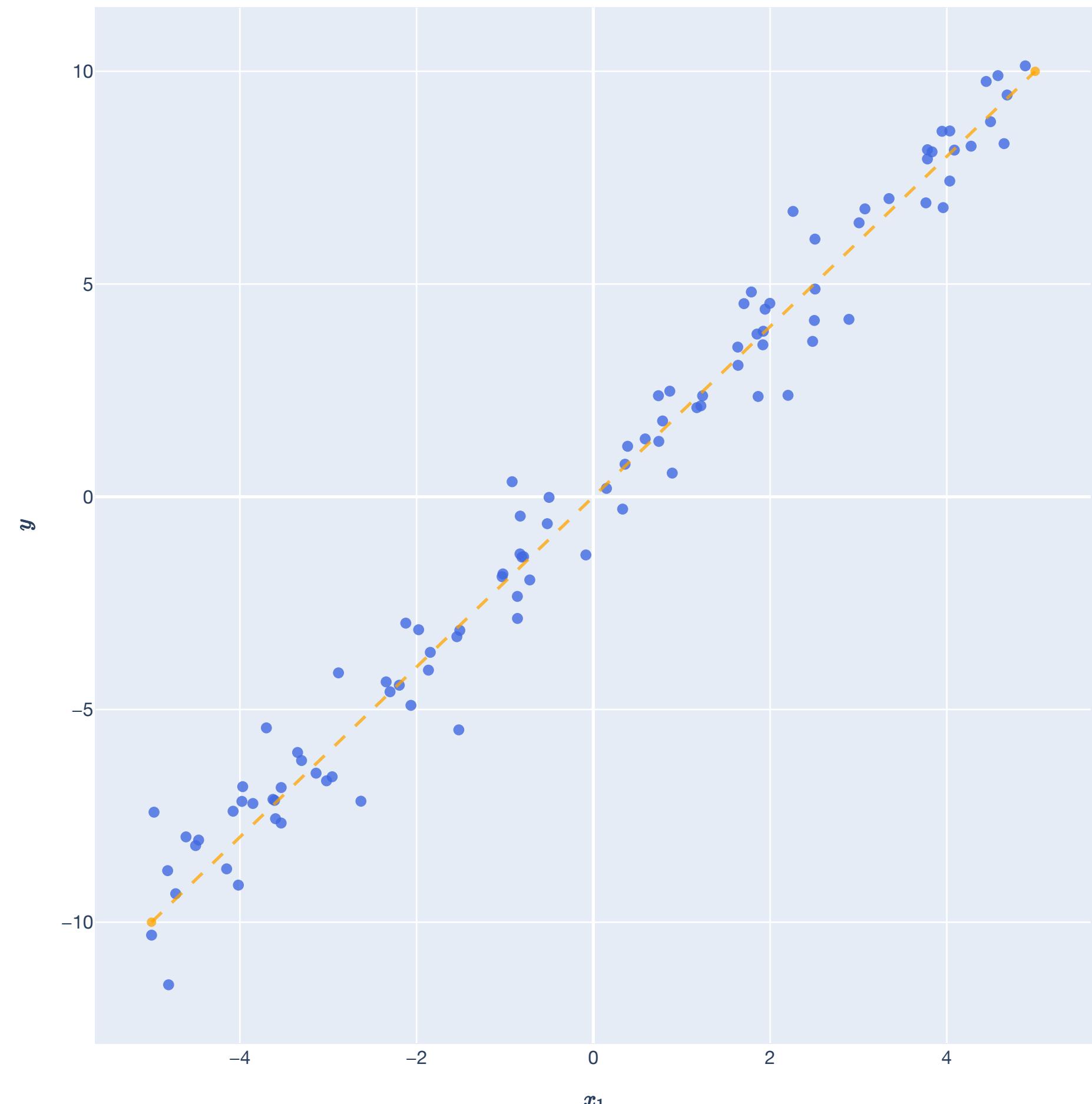
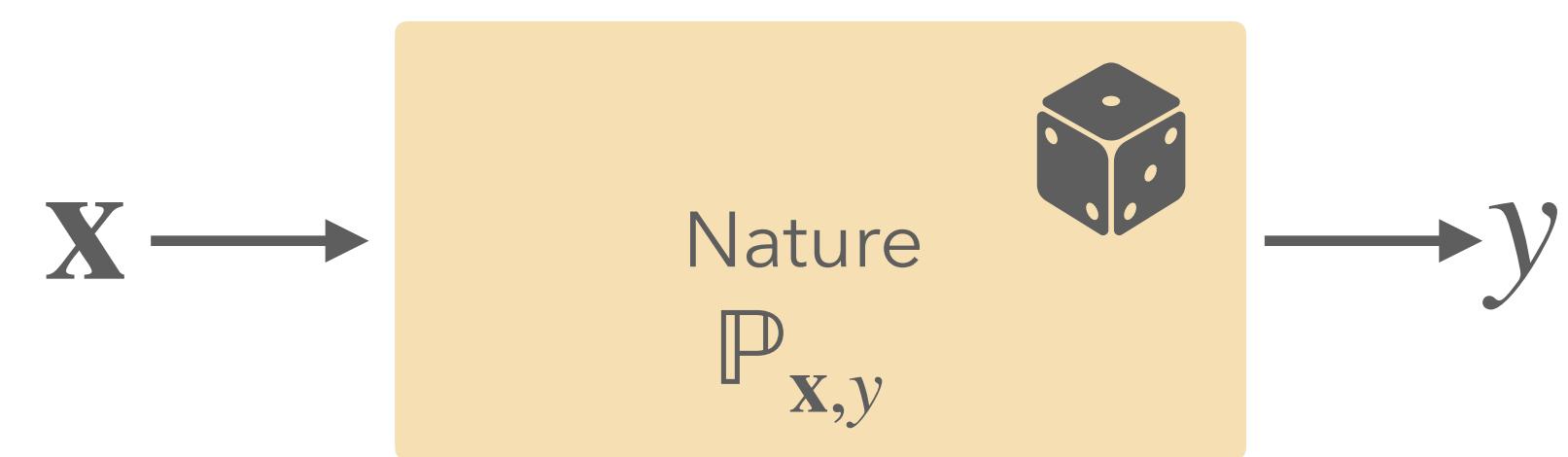
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Regression with randomness

Part 2: Notion of error and linear model

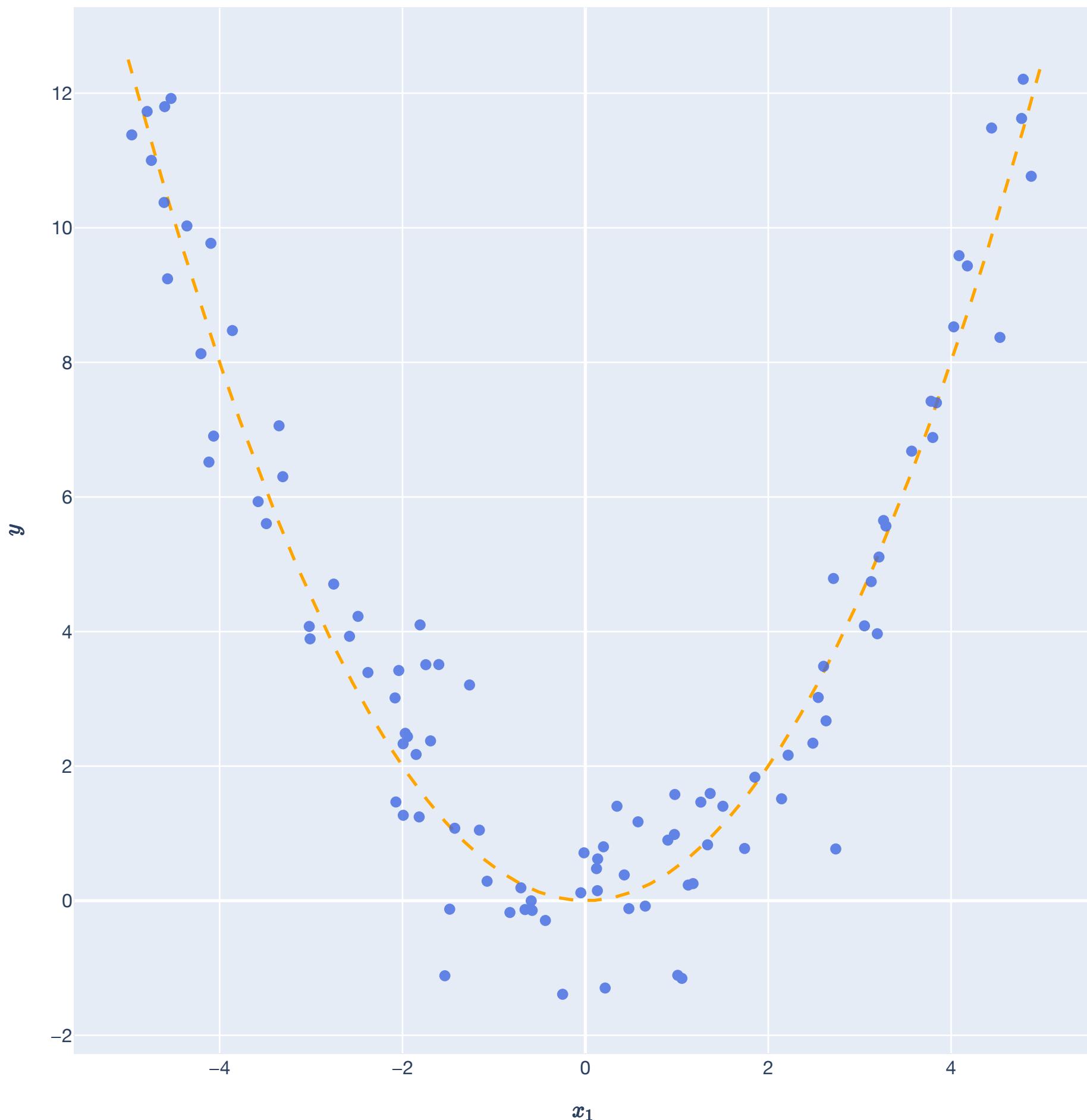
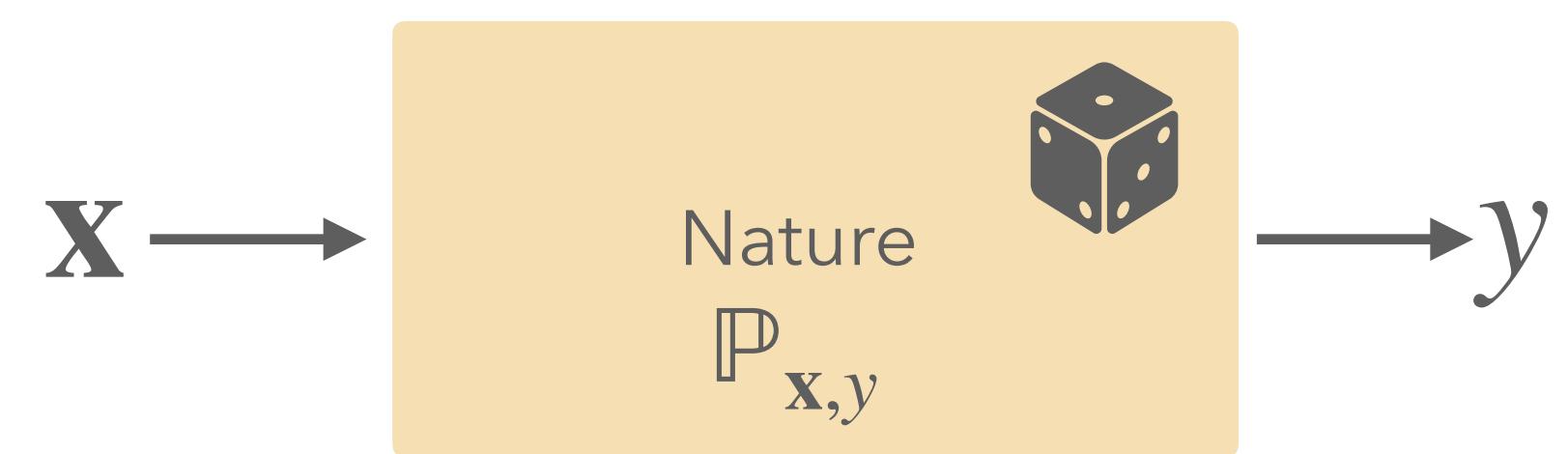
Assume further: $(\mathbf{x}_i, y_i) \in \mathbb{R}^d \times \mathbb{R}$ pair is drawn from a joint distribution, $\mathbb{P}_{\mathbf{x},y}$

$$y_i = f^*(\mathbf{x}_i) + \epsilon_i$$

Some deterministic function $f^* : \mathbb{R}^d \rightarrow \mathbb{R}$ explains as much as it can.

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Regression with randomness

Part 2: Notion of error and linear model

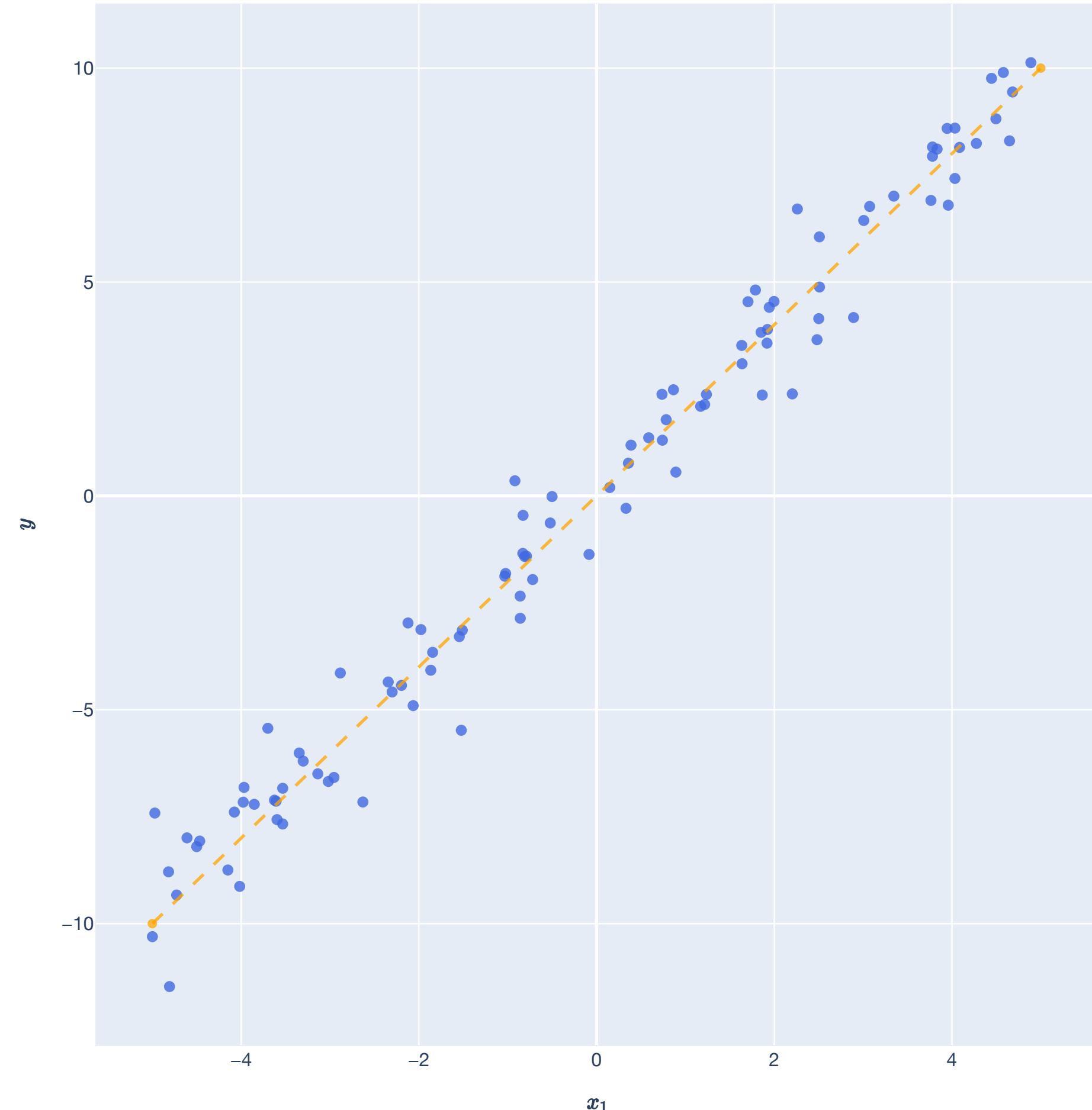
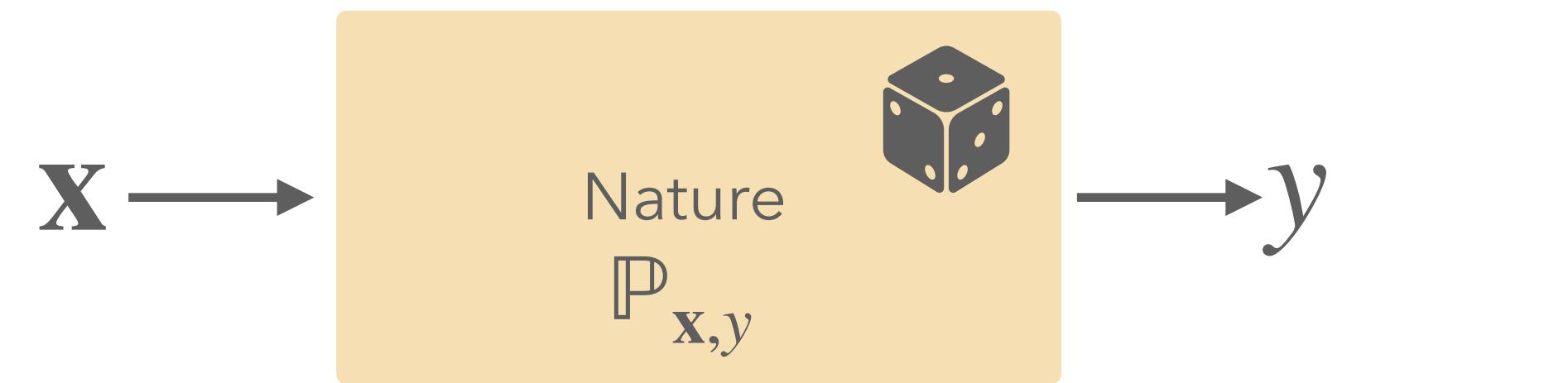
Assume further: $(\mathbf{x}_i, y_i) \in \mathbb{R}^d \times \mathbb{R}$ pair is drawn from a joint distribution, $\mathbb{P}_{\mathbf{x},y}$

$$y_i = \mathbf{x}_i^\top \mathbf{w}^* + \epsilon_i$$

Some *linear* function $f_{\mathbf{w}^*}(\mathbf{x}) = \mathbf{x}^\top \mathbf{w}^*$ explains linear relationship between \mathbf{x} and y .

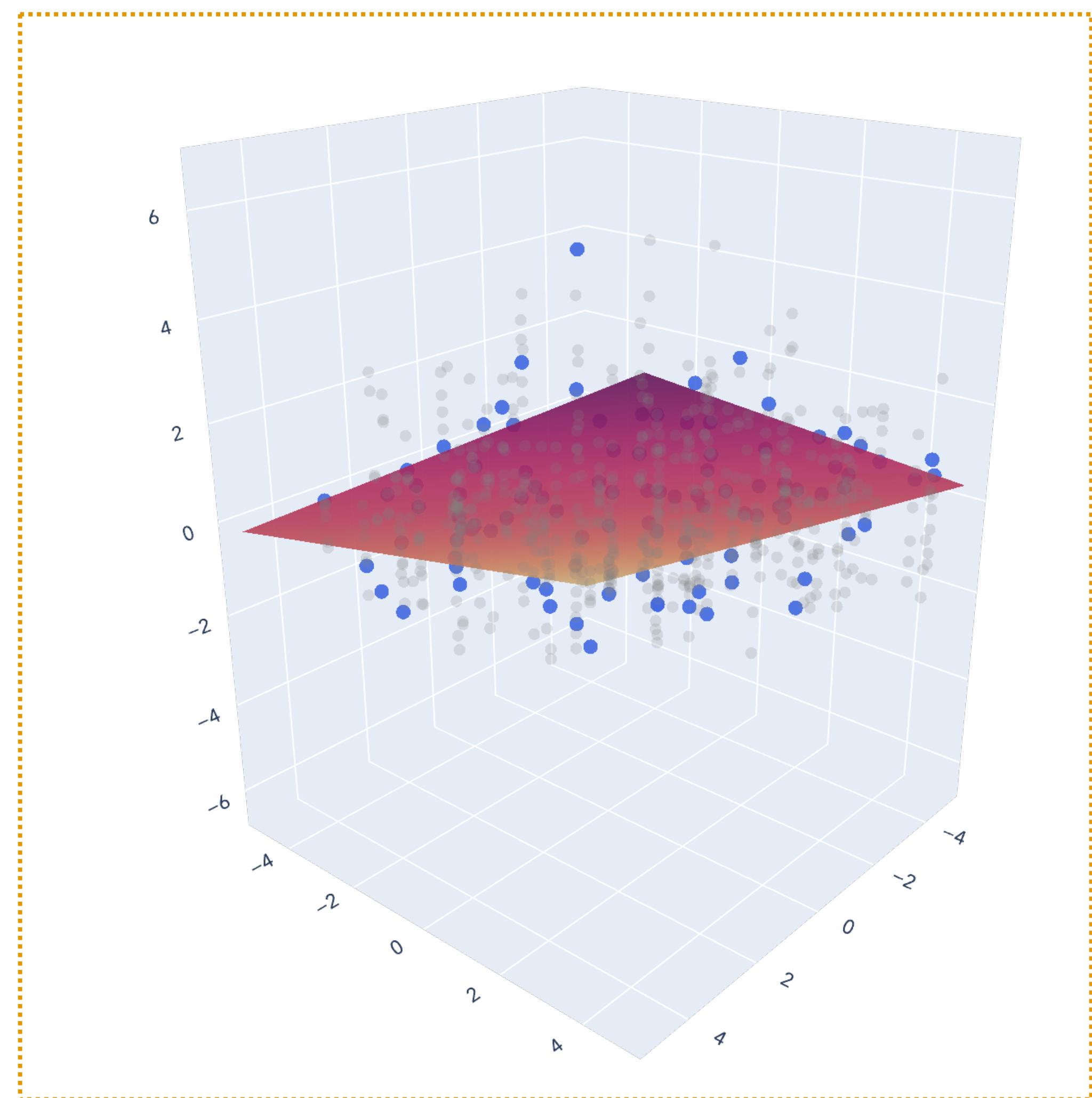
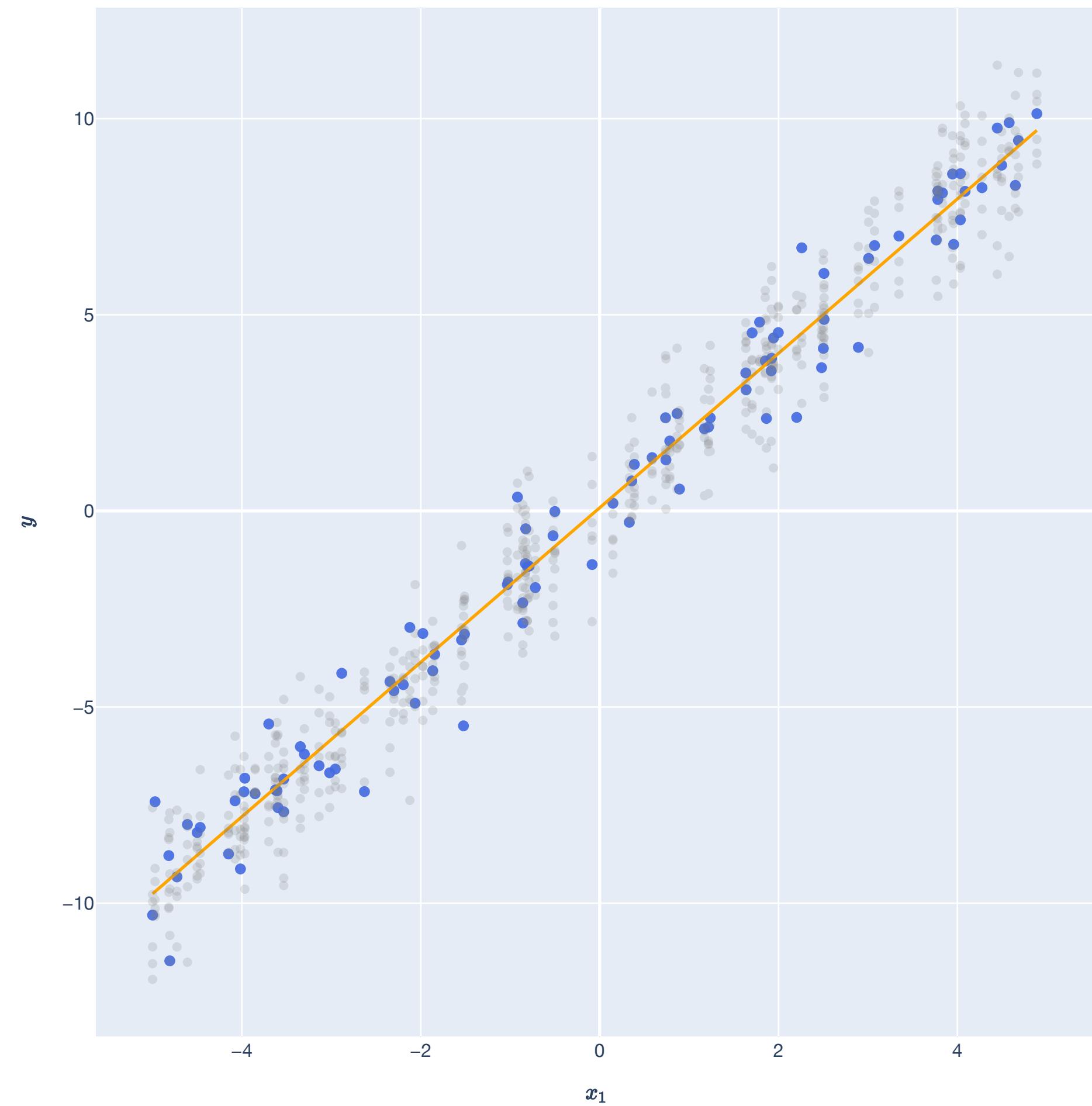
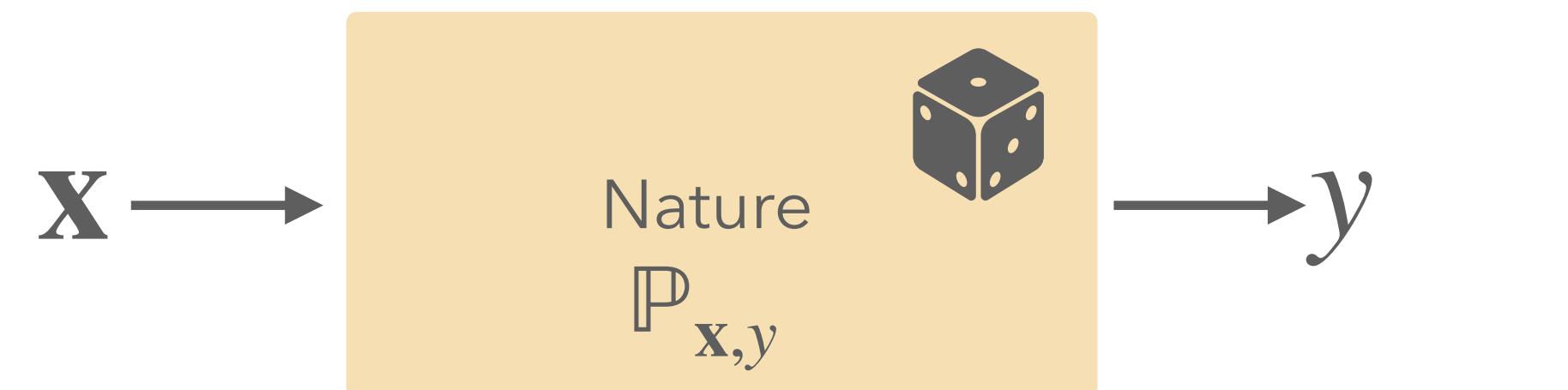
Some *randomness* ϵ_i models the unexplained relationship, where we assume

$$\mathbb{E}[\epsilon_i] = 0 \text{ and } \epsilon_i \text{ is independent of } \mathbf{x}_i.$$



Regression with randomness

Part 2: Notion of error and linear model



Regression with randomness

Part 2: Notion of error and linear model

Each $(\mathbf{x}_i, y_i) \in \mathbb{R}^d \times \mathbb{R}$ pair is drawn from a *joint distribution*, $\mathbb{P}_{\mathbf{x},y}$

$$y_i = \mathbf{x}_i^\top \mathbf{w}^* + \epsilon_i, \text{ where } \mathbb{E}[\epsilon_i] = 0 \text{ and } \epsilon_i \text{ is independent of } \mathbf{x}_i.$$

This gives us $\mathbf{X} \in \mathbb{R}^{n \times d}$ and $\mathbf{y} \in \mathbb{R}^n$, so we can also write:

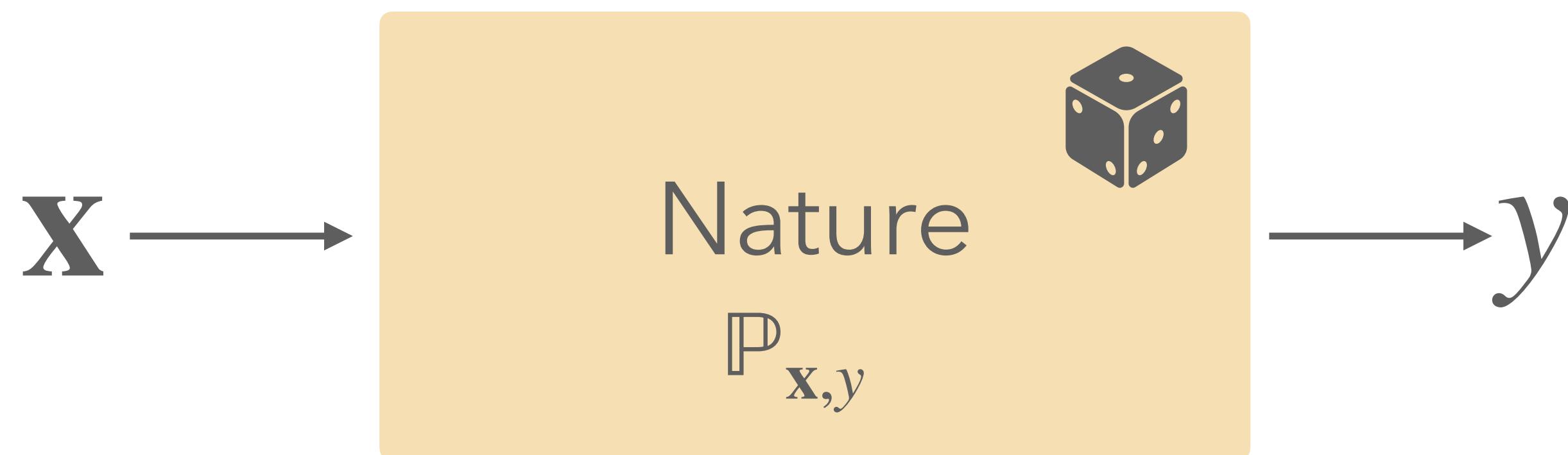
$$\mathbf{y} = \mathbf{X}\mathbf{w}^* + \boldsymbol{\epsilon}, \text{ where } \boldsymbol{\epsilon} \in \mathbb{R}^n \text{ is a random vector.}$$

Random error model

Our main assumption on $\mathbb{P}_{\mathbf{x},y}$

$y_i = \mathbf{x}_i^\top \mathbf{w}^* + \epsilon_i$ where $\mathbb{E}[\epsilon_i] = 0$ and ϵ_i is independent of \mathbf{x}_i .

$\mathbf{y} = \mathbf{X}\mathbf{w}^* + \boldsymbol{\epsilon}$, where $\boldsymbol{\epsilon} \in \mathbb{R}^n$ is a random vector.



Regression with randomness

Part 2: Notion of error and linear model

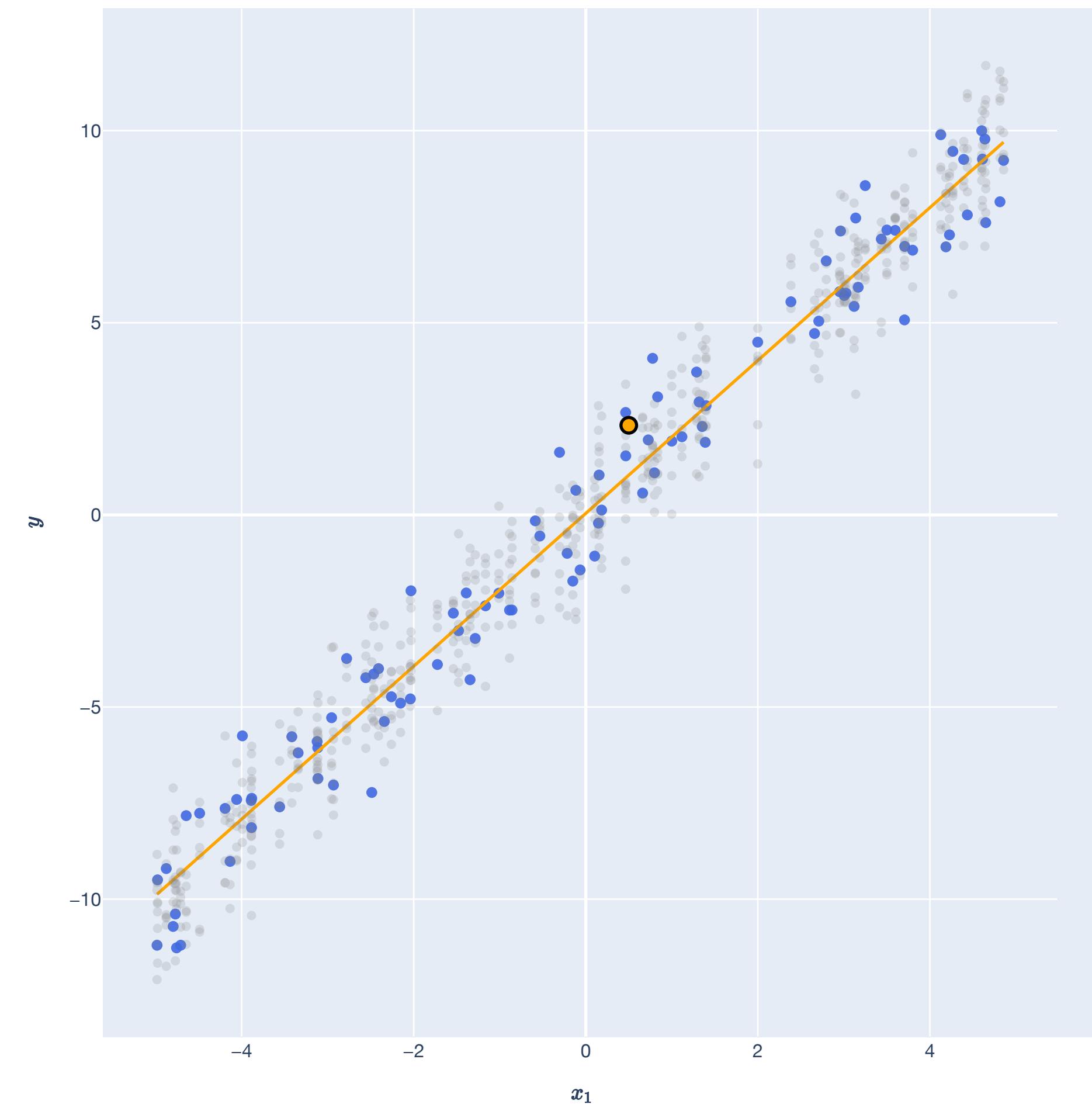
Each $(\mathbf{x}_i, y_i) \in \mathbb{R}^d \times \mathbb{R}$ pair is drawn from a *joint distribution*, $\mathbb{P}_{\mathbf{x},y}$

Draw a new (\mathbf{x}_0, y_0) from the distribution $\mathbb{P}_{\mathbf{x},y}$.

Our model $\hat{f}: \mathbb{R}^d \rightarrow \mathbb{R}$ should predict well on new examples.

Notion of error for new (\mathbf{x}_0, y_0) is still squared loss

$$\ell(\hat{f}(\mathbf{x}_0), y_0) := (y_0 - \hat{f}(\mathbf{x}_0))^2.$$



Regression with randomness

Part 2: Notion of error and linear model

Random vector $\mathbf{X} = \begin{bmatrix} \leftarrow \mathbf{x}_1^\top \rightarrow \\ \vdots \\ \leftarrow \mathbf{x}_n^\top \rightarrow \end{bmatrix}$ Random variable $\mathbf{y} = \begin{bmatrix} y_1 \\ \vdots \\ y_n \end{bmatrix}$, where $\mathbf{x}_1, \dots, \mathbf{x}_n \in \mathbb{R}^d$ from the joint distribution $\mathbb{P}_{\mathbf{x}, y}$ over $\mathbb{R}^d \times \mathbb{R}$!

Unknown: Weight vector $\mathbf{w} \in \mathbb{R}^d$ with weights w_1, \dots, w_d .

Our “model”, a function that we hope “generalizes” well to new datapoint (\mathbf{x}_0, y_0) .

Goal: For each $i \in [n]$, we predict: $\hat{y}_i = \mathbf{w}^\top \mathbf{x}_i = w_1 x_{i1} + \dots + w_d x_{id} \in \mathbb{R}$.

Regression with randomness

Part 3: Risk and empirical risk

Each $(\mathbf{x}_i, y_i) \in \mathbb{R}^d \times \mathbb{R}$ pair is drawn from a *joint distribution*, $\mathbb{P}_{\mathbf{x},y}$

We want to find a linear function $f: \mathbb{R}^d \rightarrow \mathbb{R}$ for predicting on this new example:

$$f(\mathbf{x}) = \mathbf{w}^\top \mathbf{x}$$

New (\mathbf{x}_0, y_0) is also from $\mathbb{P}_{\mathbf{x},y}$ and notion of error is **squared loss**:

$$\ell(f(\mathbf{x}_0), y_0) := (y_0 - f(\mathbf{x}_0))^2.$$

To make a decision, we care about the *expected loss* (**risk**):

$$R(f) := \mathbb{E}_{(\mathbf{x}_0, y_0)}[(y_0 - f(\mathbf{x}_0))^2] = \mathbb{E}_{(\mathbf{x}_0, y_0)}[(y_0 - \mathbf{w}^\top \mathbf{x}_0)^2] = R(\mathbf{w})$$

Regression with randomness

Part 3: Risk and empirical risk

Ultimate goal: Find $f(\mathbf{x}) = \mathbf{w}^\top \mathbf{x}$ that generalizes on a new $(\mathbf{x}_0, y_0) \sim \mathbb{P}_{\mathbf{x}, y}$:

$$R(f) := \mathbb{E}_{(\mathbf{x}_0, y_0)}[(y_0 - f(\mathbf{x}_0))^2] = \mathbb{E}_{(\mathbf{x}_0, y_0)}[(y_0 - \mathbf{w}^\top \mathbf{x}_0)^2] = R(\mathbf{w})$$

Intermediary goal: Find $f(\mathbf{x}) = \mathbf{w}^\top \mathbf{x}$ that does well on the training samples:

$$\hat{R}(\hat{f}) := \frac{1}{n} \sum_{i=1}^n (\hat{f}(\mathbf{x}_i) - y_i)^2 = \frac{1}{n} \sum_{i=1}^n (\mathbf{w}^\top \mathbf{x}_i - y_i)^2 = \hat{R}(\mathbf{w}).$$

As long as (\mathbf{x}_0, y_0) from same distribution, these are close as $n \rightarrow \infty$!

Regression with randomness

Part 3: Risk and empirical risk

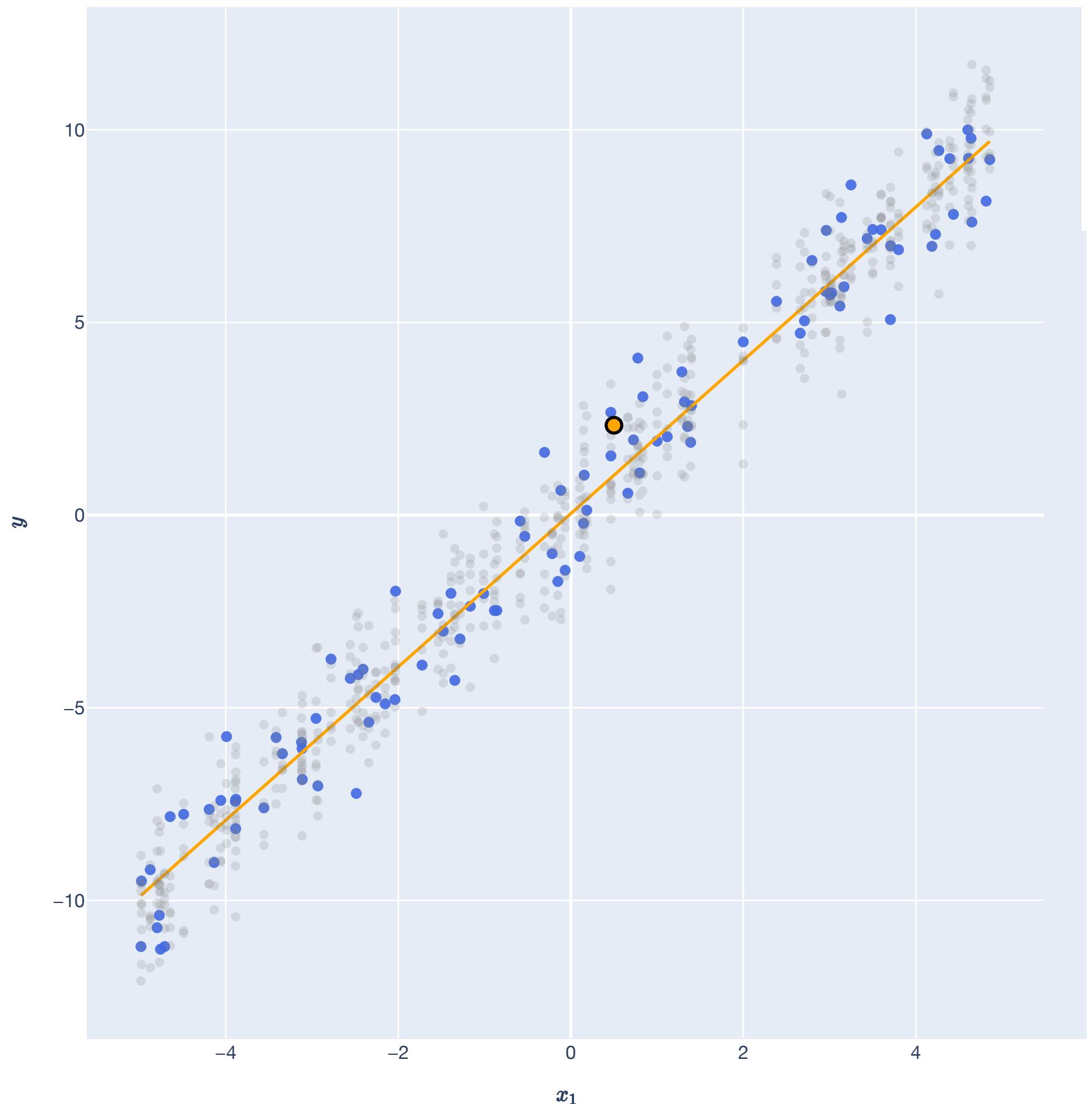
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Intermediary goal: Find $f(\mathbf{x}) = \mathbf{w}^\top \mathbf{x}$ that does well on the training samples:

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As long as (\mathbf{x}_0, y_0) from same distribution, these are close as $n \rightarrow \infty!$



Regression with randomness

Part 3: Risk and empirical risk

Observed: Matrix of *training samples* $\mathbf{X} \in \mathbb{R}^{n \times d}$ and vector of *training labels* $\mathbf{y} \in \mathbb{R}^n$.

Random vector \mathbf{x}_i

$$\mathbf{X} = \begin{bmatrix} \leftarrow & \mathbf{x}_1^\top & \rightarrow \\ & \vdots & \\ \leftarrow & \mathbf{x}_n^\top & \rightarrow \end{bmatrix}$$

Random variable y_i

$$\mathbf{y} = \begin{bmatrix} y_1 \\ \vdots \\ y_n \end{bmatrix}, \text{ where } \mathbf{x}_1, \dots, \mathbf{x}_n \in \mathbb{R}^d.$$

... from the joint distribution $\mathbb{P}_{\mathbf{x}, y}$ over $\mathbb{R}^d \times \mathbb{R}$!

Unknown: Weight vector $\mathbf{w} \in \mathbb{R}^d$ with weights w_1, \dots, w_d .

Goal: For each $i \in [n]$, we predict: $\hat{y}_i = \mathbf{w}^\top \mathbf{x}_i = w_1 x_{i1} + \dots + w_d x_{id} \in \mathbb{R}$.

Our "model", a function that we hope "generalizes" well to new datapoint (\mathbf{x}_0, y_0) .

Choose a weight vector that "fits the training data": $\mathbf{w} \in \mathbb{R}^d$ such that $y_i \approx \hat{y}_i$ for $i \in [n]$, or:

$$\mathbf{X}\mathbf{w} = \hat{\mathbf{y}} \approx \mathbf{y}. \quad \text{Because we assume that } (\mathbf{x}_0, y_0) \sim \mathbb{P}_{\mathbf{x}, y} \text{ as well!}$$

Statistics of the OLS Estimator

Bias and Variance

Statistics of the Error Model

Setup

Let $\mathbf{x} \in \mathbb{R}^d$ be a *random vector* and $y \in \mathbb{R}$ be *random variable* be drawn from the *joint distribution* $\mathbb{P}_{\mathbf{x},y}$, where

$$y = \mathbf{x}^\top \mathbf{w}^* + \epsilon,$$

where ϵ is a *random variable* with $\mathbb{E}[\epsilon] = 0$ and $\text{Var}(\epsilon) = \sigma^2$, with ϵ independent of \mathbf{x} .

Statistics of the Error Model

Conditional Expectation

$$y = \mathbf{x}^\top \mathbf{w}^* + \epsilon$$

$\mathbb{E}[\epsilon | \mathbf{x}] = 0$, because errors are independent of \mathbf{x} .

$\text{Var}(\epsilon | \mathbf{x}) = \sigma^2$, because errors are independent of \mathbf{x} .

$\mathbb{E}[y | \mathbf{x}] = \mathbf{x}^\top \mathbf{w}^*$, the regression function.

This is the target we're aiming for!

Statistics of OLS

Using OLS to minimize empirical risk

$$y = \mathbf{x}^\top \mathbf{w}^* + \epsilon$$

Find $f(\mathbf{x}) := \hat{\mathbf{w}}^\top \mathbf{x}$ that does well on training samples, minimizing empirical risk:

$$\hat{R}(\hat{f}) := \frac{1}{n} \sum_{i=1}^n (\hat{f}(\mathbf{x}_i) - y_i)^2 = \frac{1}{n} \|\mathbf{X}\hat{\mathbf{w}} - \mathbf{y}\|^2$$

Obtain the least squares estimator the same way:

$$\hat{\mathbf{w}} = (\mathbf{X}^\top \mathbf{X})^{-1} \mathbf{X}^\top \mathbf{y}.$$

Statistics of OLS

Conditional expectation and variance

$$y = \mathbf{x}^\top \mathbf{w}^* + \epsilon$$

Obtain the least squares estimator the same way:

$$\hat{\mathbf{w}} = (\mathbf{X}^\top \mathbf{X})^{-1} \mathbf{X}^\top \mathbf{y}.$$

This $\hat{\mathbf{w}} \in \mathbb{R}^d$ is a random vector now!

If we condition on $\mathbf{X} \in \mathbb{R}^{n \times d}$, we can get statistics on this random vector.

Expectation: $\mathbb{E}[\hat{\mathbf{w}} | \mathbf{X}] = \mathbf{w}^*$.

Variance: $\text{Var}[\hat{\mathbf{w}} | \mathbf{X}] = (\mathbf{X}^\top \mathbf{X})^{-1} \sigma^2$.

Statistics of OLS

Intuition

$$y = \mathbf{x}^\top \mathbf{w}^* + \epsilon$$

Obtain the least squares estimator the same way:

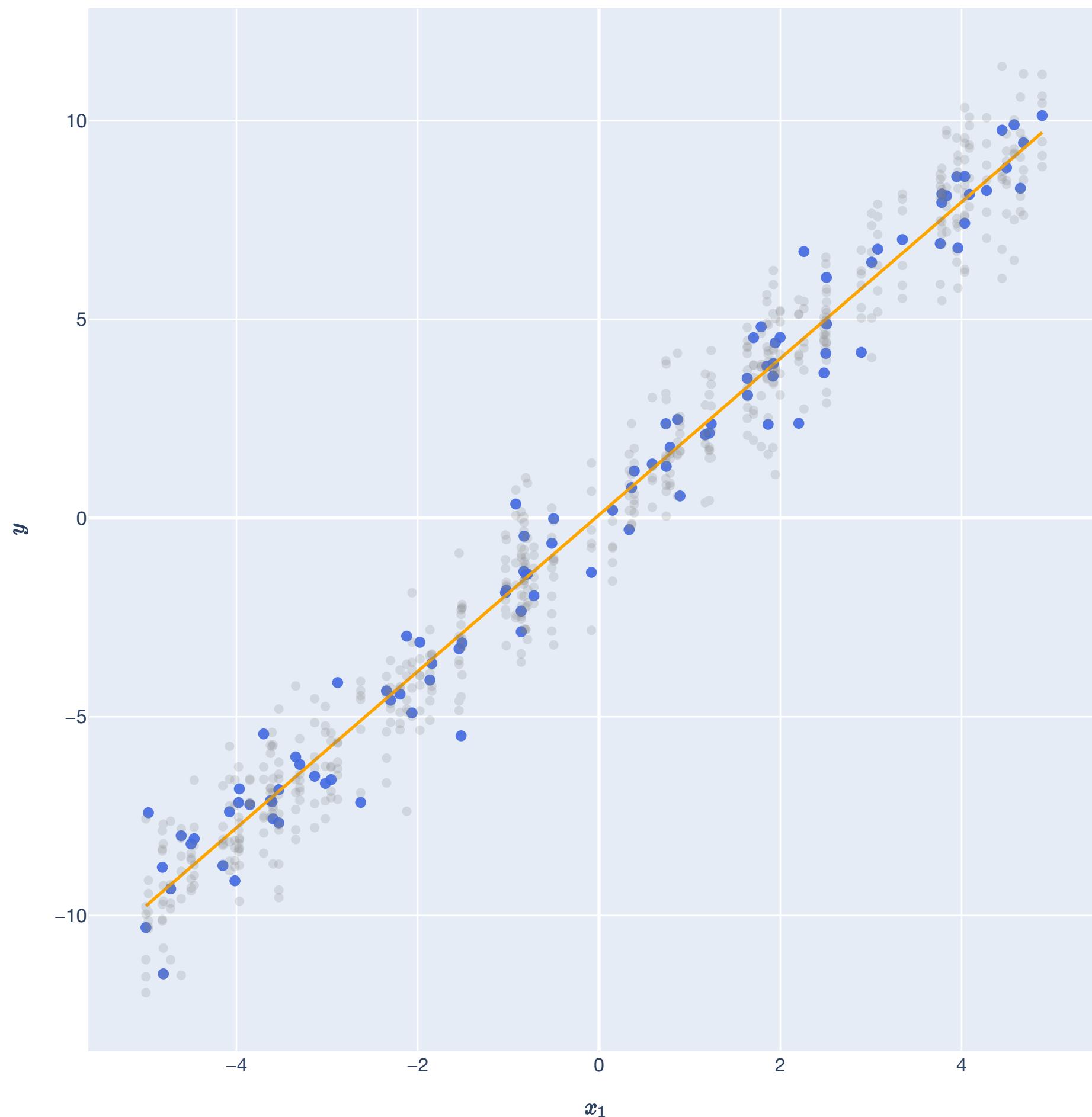
$$\hat{\mathbf{w}} = (\mathbf{X}^\top \mathbf{X})^{-1} \mathbf{X}^\top \mathbf{y}.$$

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Statistics of OLS

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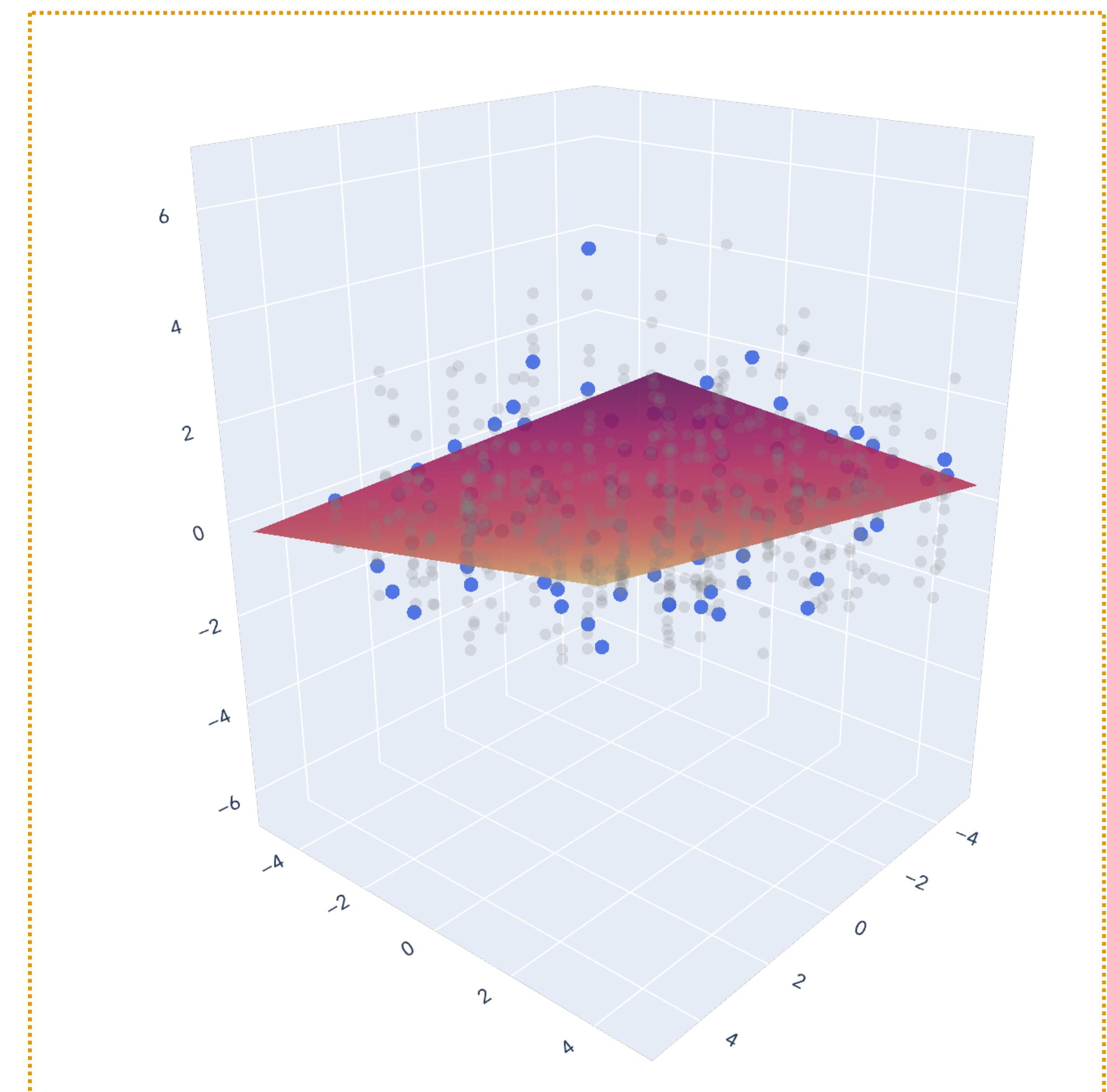
$$\hat{\mathbf{w}} = (\mathbf{X}^\top \mathbf{X})^{-1} \mathbf{X}^\top \mathbf{y}.$$

This $\hat{\mathbf{w}} \in \mathbb{R}^d$ is a random vector now!

If we condition on $\mathbf{X} \in \mathbb{R}^{n \times d}$, we can get statistics on this random vector.

Expectation: $\mathbb{E}[\hat{\mathbf{w}} | \mathbf{X}] = \mathbf{w}^*$.

Variance: $\text{Var}[\hat{\mathbf{w}} | \mathbf{X}] = (\mathbf{X}^\top \mathbf{X})^{-1} \sigma^2$.



Statistics of OLS

Theorem

Theorem (Statistical properties of OLS). Let $\mathbb{P}_{\mathbf{x},y}$ be a joint distribution $\mathbb{R}^d \times \mathbb{R}$ such that

$$y = \mathbf{x}^\top \mathbf{w}^* + \epsilon,$$

where $\mathbf{w}^* \in \mathbb{R}^d$ and ϵ is a random variable with $\mathbb{E}[\epsilon] = 0$ and $\text{Var}(\epsilon) = \sigma^2$, independent of \mathbf{x} . Let $\mathbf{X} \in \mathbb{R}^{n \times d}$ and $\mathbf{y} \in \mathbb{R}^n$ by drawing n random examples (\mathbf{x}_i, y_i) from $\mathbb{P}_{\mathbf{x},y}$.

Then, the OLS estimator $\hat{\mathbf{w}} = (\mathbf{X}^\top \mathbf{X})^{-1} \mathbf{X}^\top \mathbf{y}$ has the following statistical properties:

Expectation: $\mathbb{E}[\hat{\mathbf{w}} | \mathbf{X}] = \mathbf{w}^*$ and $\mathbb{E}[\hat{\mathbf{w}}] = \mathbf{w}^*$.

Variance: $\text{Var}[\hat{\mathbf{w}} | \mathbf{X}] = (\mathbf{X}^\top \mathbf{X})^{-1} \sigma^2$ and $\text{Var}[\hat{\mathbf{w}}] = \sigma^2 \mathbb{E}[(\mathbf{X}^\top \mathbf{X})^{-1}]$

Proof of OLS Expectation

Use conditional expectation and error model, then tower rule

$$y_i = \mathbf{x}_i^\top \mathbf{w}^* + \epsilon_i \text{ so } \mathbf{y} = \mathbf{X}\mathbf{w}^* + \boldsymbol{\epsilon}, \text{ where } \mathbf{X} \in \mathbb{R}^{n \times d}, \mathbf{y} \in \mathbb{R}^n \text{ and } \boldsymbol{\epsilon} \in \mathbb{R}^n$$

Goal: $\mathbb{E}[\hat{\mathbf{w}} | \mathbf{X}] = \mathbf{w}^*$ and $\mathbb{E}[\hat{\mathbf{w}}] = \mathbf{w}^*$.

Take *conditional* expectation of OLS estimator and use the error model assumption on \mathbf{y} :

$$\mathbb{E}[\hat{\mathbf{w}} | \mathbf{X}] = \mathbb{E}[(\mathbf{X}^\top \mathbf{X})^{-1} \mathbf{X}^\top \mathbf{y} | \mathbf{X}]$$

$$= \mathbb{E}[(\mathbf{X}^\top \mathbf{X})^{-1} \mathbf{X}^\top (\mathbf{X}\mathbf{w}^* + \boldsymbol{\epsilon}) | \mathbf{X}] \quad \text{Replace } \mathbf{y} \text{ with error model assumption.}$$

$$= \mathbb{E}[(\mathbf{X}^\top \mathbf{X})^{-1} \mathbf{X}^\top \mathbf{X}\mathbf{w}^* + (\mathbf{X}^\top \mathbf{X})^{-1} \boldsymbol{\epsilon} | \mathbf{X}]$$

$$= \mathbb{E}[\mathbf{w}^* + (\mathbf{X}^\top \mathbf{X})^{-1} \boldsymbol{\epsilon} | \mathbf{X}] = \mathbf{w}^* \implies \mathbb{E}[\hat{\mathbf{w}}] = \mathbb{E}[\mathbb{E}[\hat{\mathbf{w}} | \mathbf{X}]] = \mathbf{w}^*$$

“Pulling out what’s known” property of cond. expectation.

Tower rule/law of total expectation property.

Proof of OLS Variance

Part 1: Take conditional variance and use error model

$$y_i = \mathbf{x}_i^\top \mathbf{w}^* + \epsilon_i \text{ so } \mathbf{y} = \mathbf{X}\mathbf{w}^* + \boldsymbol{\epsilon}, \text{ where } \mathbf{X} \in \mathbb{R}^{n \times d}, \mathbf{y} \in \mathbb{R}^n \text{ and } \boldsymbol{\epsilon} \in \mathbb{R}^n$$

Variance: $\text{Var}[\hat{\mathbf{w}} | \mathbf{X}] = (\mathbf{X}^\top \mathbf{X})^{-1} \sigma^2$ and $\text{Var}[\hat{\mathbf{w}}] = \sigma^2 \mathbb{E}[(\mathbf{X}^\top \mathbf{X})^{-1}]$

Take *conditional* variance of OLS estimator and use the error model assumption on \mathbf{y} :

Definition of OLS $\hat{\mathbf{w}}$ and error model

From previous proof: expectation of $\hat{\mathbf{w}}$.

$$\begin{aligned} \text{Var}[\hat{\mathbf{w}} | \mathbf{X}] &= \mathbb{E}[(\hat{\mathbf{w}} - \mathbb{E}[\hat{\mathbf{w}} | \mathbf{X}]) (\hat{\mathbf{w}} - \mathbb{E}[\hat{\mathbf{w}} | \mathbf{X}])^\top | \mathbf{X}] \\ &= \mathbb{E}[((\mathbf{X}^\top \mathbf{X})^{-1} \mathbf{X}^\top (\mathbf{X}\mathbf{w}^* + \boldsymbol{\epsilon}) - \mathbf{w}^*) ((\mathbf{X}^\top \mathbf{X})^{-1} \mathbf{X}^\top (\mathbf{X}\mathbf{w}^* + \boldsymbol{\epsilon}) - \mathbf{w}^*)^\top | \mathbf{X}] \\ &= \mathbb{E}[(\mathbf{w}^* + (\mathbf{X}^\top \mathbf{X})^{-1} \mathbf{X}^\top \boldsymbol{\epsilon} - \mathbf{w}^*) (\mathbf{w}^* + (\mathbf{X}^\top \mathbf{X})^{-1} \mathbf{X}^\top \boldsymbol{\epsilon} - \mathbf{w}^*)^\top | \mathbf{X}] \\ &= \mathbb{E}[(\mathbf{X}^\top \mathbf{X})^{-1} \mathbf{X}^\top \boldsymbol{\epsilon} \boldsymbol{\epsilon}^\top \mathbf{X} (\mathbf{X}^\top \mathbf{X})^{-1} | \mathbf{X}] = (\mathbf{X}^\top \mathbf{X})^{-1} \mathbf{X}^\top \mathbb{E}[\boldsymbol{\epsilon} \boldsymbol{\epsilon}^\top | \mathbf{X}] \mathbf{X} (\mathbf{X}^\top \mathbf{X})^{-1} \end{aligned}$$

Cond. expectation property: taking out what's known.

Proof of OLS Variance

Part 2: Understand variance (covariances) of $\epsilon\epsilon^\top$

$y_i = \mathbf{x}_i^\top \mathbf{w}^* + \epsilon_i$ so $\mathbf{y} = \mathbf{X}\mathbf{w}^* + \boldsymbol{\epsilon}$, where $\mathbf{X} \in \mathbb{R}^{n \times d}$, $\mathbf{y} \in \mathbb{R}^n$ and $\boldsymbol{\epsilon} \in \mathbb{R}^n$

Variance: $\text{Var}[\hat{\mathbf{w}} | \mathbf{X}] = (\mathbf{X}^\top \mathbf{X})^{-1} \sigma^2$ and $\text{Var}[\hat{\mathbf{w}}] = \sigma^2 \mathbb{E}[(\mathbf{X}^\top \mathbf{X})^{-1}]$

Remains to understand the expectation of the matrix $\boldsymbol{\epsilon}\boldsymbol{\epsilon}^\top \in \mathbb{R}^{n \times n}$:

$$\text{Var}[\hat{\mathbf{w}} | \mathbf{X}] = (\mathbf{X}^\top \mathbf{X})^{-1} \mathbf{X}^\top \mathbb{E}[\boldsymbol{\epsilon}\boldsymbol{\epsilon}^\top | \mathbf{X}] \mathbf{X} (\mathbf{X}^\top \mathbf{X})^{-1}$$

For $n = 3$, this looks like:

$$\boldsymbol{\epsilon}\boldsymbol{\epsilon}^\top = \begin{bmatrix} \epsilon_1^2 & \epsilon_1\epsilon_2 & \epsilon_1\epsilon_3 \\ \epsilon_2\epsilon_1 & \epsilon_2^2 & \epsilon_2\epsilon_3 \\ \epsilon_3\epsilon_1 & \epsilon_3^2 & \epsilon_3\epsilon_3 \end{bmatrix}$$

ϵ are indep. of \mathbf{X} in error model.

$$\text{so } \mathbb{E}[\boldsymbol{\epsilon}\boldsymbol{\epsilon}^\top | \mathbf{X}] = \mathbb{E}[\boldsymbol{\epsilon}\boldsymbol{\epsilon}^\top]$$

$$\mathbb{E}[\epsilon_i^2] = \mathbb{E}[(\epsilon_i - 0)(\epsilon_i - 0)] = \text{Cov}(\epsilon_i, \epsilon_i) = \text{Var}(\epsilon_i) = \sigma^2$$

$$\begin{bmatrix} \mathbb{E}\epsilon_1^2 & \mathbb{E}\epsilon_1\epsilon_2 & \mathbb{E}\epsilon_1\epsilon_3 \\ \mathbb{E}\epsilon_2\epsilon_1 & \mathbb{E}\epsilon_2^2 & \mathbb{E}\epsilon_2\epsilon_3 \\ \mathbb{E}\epsilon_3\epsilon_1 & \mathbb{E}\epsilon_3\epsilon_2 & \mathbb{E}\epsilon_3^2 \end{bmatrix} = \begin{bmatrix} \sigma^2 & 0 & 0 \\ 0 & \sigma^2 & 0 \\ 0 & 0 & \sigma^2 \end{bmatrix} = \sigma^2 \mathbf{I}$$

For $i \neq j$, $\mathbb{E}[\epsilon_i\epsilon_j] = \mathbb{E}[(\epsilon_i - 0)(\epsilon_j - 0)] = \text{Cov}(\epsilon_i, \epsilon_j) = 0$ by independence

Random Vectors

Variance and Covariance Matrix

The variance of a random vector generalizes to the covariance matrix

$$\Sigma = \mathbb{E}[(\mathbf{X} - \mathbb{E}[\mathbf{X}])(\mathbf{X} - \mathbb{E}[\mathbf{X}])^\top] = \begin{bmatrix} \text{Var}(X_1) & \text{Cov}(X_1, X_2) & \dots & \text{Cov}(X_1, X_n) \\ \text{Cov}(X_2, X_1) & \text{Var}(X_2) & \dots & \text{Cov}(X_2, X_n) \\ \vdots & \vdots & \ddots & \vdots \\ \text{Cov}(X_n, X_1) & \text{Cov}(X_n, X_2) & \dots & \text{Var}(X_n) \end{bmatrix}$$

In general, $\Sigma_{i,j} = \text{Cov}(X_i, X_j)$.

In this class, a random vector's variance *is* its covariance:

$$\text{Var}(\mathbf{x}) := \Sigma = \mathbb{E}[(\mathbf{X} - \mathbb{E}[\mathbf{X}])(\mathbf{X} - \mathbb{E}[\mathbf{X}])^\top]$$

Proof of OLS Variance

Part 3: Cancel out inverse and use law of total variance

$y_i = \mathbf{x}_i^\top \mathbf{w}^* + \epsilon_i$ so $\mathbf{y} = \mathbf{X}\mathbf{w}^* + \boldsymbol{\epsilon}$, where $\mathbf{X} \in \mathbb{R}^{n \times d}$, $\mathbf{y} \in \mathbb{R}^n$ and $\boldsymbol{\epsilon} \in \mathbb{R}^n$

Variance: $\text{Var}[\hat{\mathbf{w}} | \mathbf{X}] = (\mathbf{X}^\top \mathbf{X})^{-1} \sigma^2$ and $\text{Var}[\hat{\mathbf{w}}] = \sigma^2 \mathbb{E}[(\mathbf{X}^\top \mathbf{X})^{-1}]$

Remains to understand the expectation of the matrix $\boldsymbol{\epsilon} \boldsymbol{\epsilon}^\top \in \mathbb{R}^{n \times n}$:

$$\text{Var}[\hat{\mathbf{w}} | \mathbf{X}] = (\mathbf{X}^\top \mathbf{X})^{-1} \mathbf{X}^\top \mathbb{E}[\boldsymbol{\epsilon} \boldsymbol{\epsilon}^\top | \mathbf{X}] \mathbf{X} (\mathbf{X}^\top \mathbf{X})^{-1}$$

Therefore, $\mathbb{E}[\boldsymbol{\epsilon} \boldsymbol{\epsilon}^\top | \mathbf{X}] = \sigma^2 \mathbf{I}$.

Uses inverse!

So conclude: $\text{Var}[\hat{\mathbf{w}} | \mathbf{X}] = (\mathbf{X}^\top \mathbf{X})^{-1} \mathbf{X}^\top \sigma^2 \mathbf{I} \mathbf{X} (\mathbf{X}^\top \mathbf{X})^{-1} = \sigma^2 (\mathbf{X}^\top \mathbf{X})^{-1}$

and $\text{Var}[\hat{\mathbf{w}}] = \mathbb{E}[\text{Var}[\hat{\mathbf{w}} | \mathbf{X}]] + \text{Var}[\mathbb{E}[\hat{\mathbf{w}} | \mathbf{X}]] = \mathbb{E}[\sigma^2 (\mathbf{X}^\top \mathbf{X})^{-1}] + \text{Var}[\mathbf{w}^*] = \sigma^2 \mathbb{E}[(\mathbf{X}^\top \mathbf{X})^{-1}]$

Law of total variance (PS5).

From first part (expectation of $\hat{\mathbf{w}}$)

Statistics of OLS

Theorem

Theorem (Statistical properties of OLS). Let $\mathbb{P}_{\mathbf{x},y}$ be a joint distribution $\mathbb{R}^d \times \mathbb{R}$ such that

$$y = \mathbf{x}^\top \mathbf{w}^* + \epsilon,$$

where $\mathbf{w}^* \in \mathbb{R}^d$ and ϵ is a random variable with $\mathbb{E}[\epsilon] = 0$ and $\text{Var}(\epsilon) = \sigma^2$, independent of \mathbf{x} . Let $\mathbf{X} \in \mathbb{R}^{n \times d}$ and $\mathbf{y} \in \mathbb{R}^n$ by drawing n random examples (\mathbf{x}_i, y_i) from $\mathbb{P}_{\mathbf{x},y}$.

Then, the OLS estimator $\hat{\mathbf{w}} = (\mathbf{X}^\top \mathbf{X})^{-1} \mathbf{X}^\top \mathbf{y}$ has the following statistical properties:

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Variance: $\text{Var}[\hat{\mathbf{w}} | \mathbf{X}] = (\mathbf{X}^\top \mathbf{X})^{-1} \sigma^2$ and $\text{Var}[\hat{\mathbf{w}}] = \sigma^2 \mathbb{E}[(\mathbf{X}^\top \mathbf{X})^{-1}]$

Recap

Lesson Overview

Probability Spaces. We'll review the basic axioms and components of probability: sample space, events, and probability measures. This allows us to ditch these notions and introduce *random variables*.

Random variables. Review of the definition of a random variable, its *distribution/law*, its PDF/PMF/CDF, and joint distributions of several RVs.

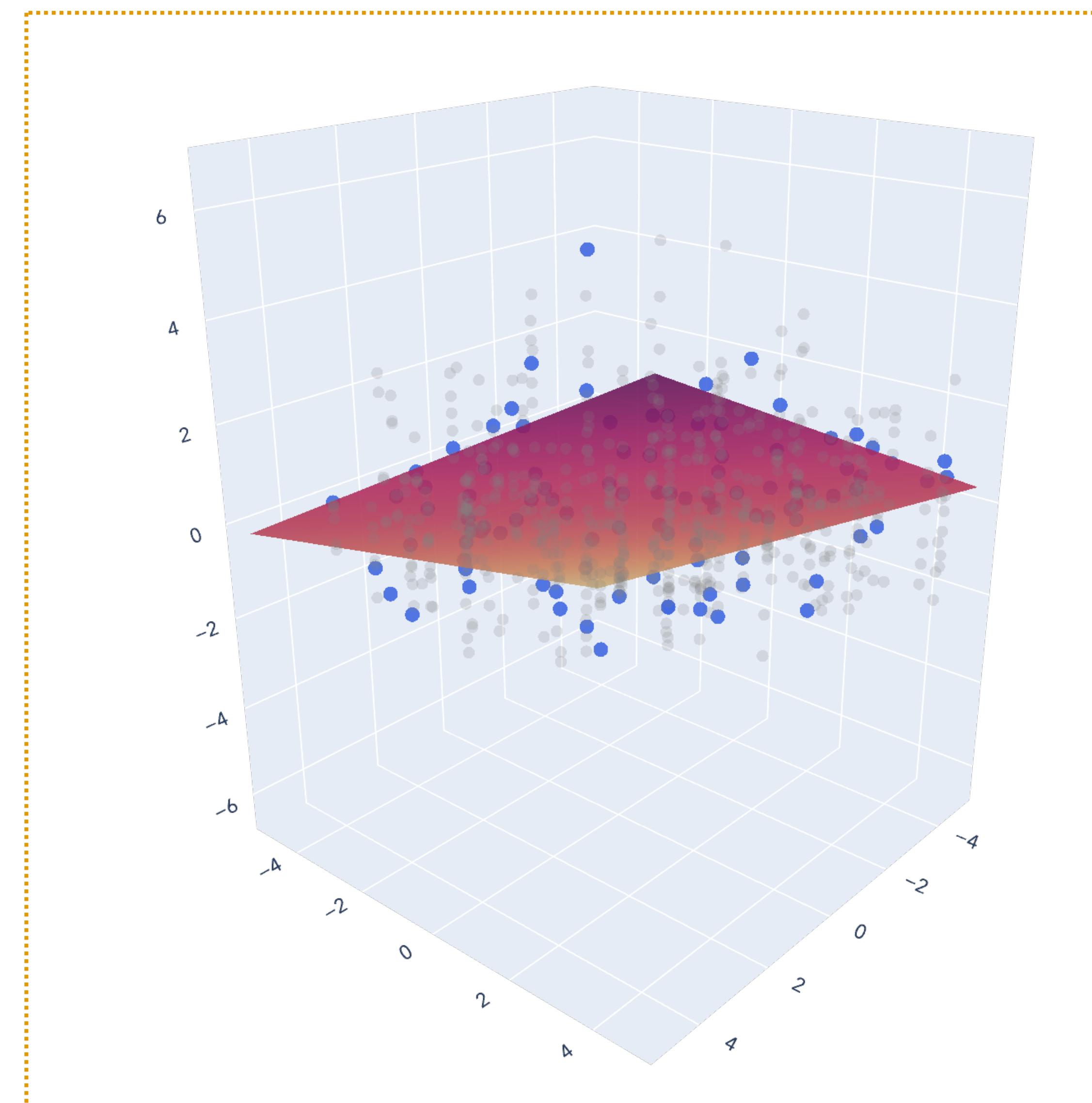
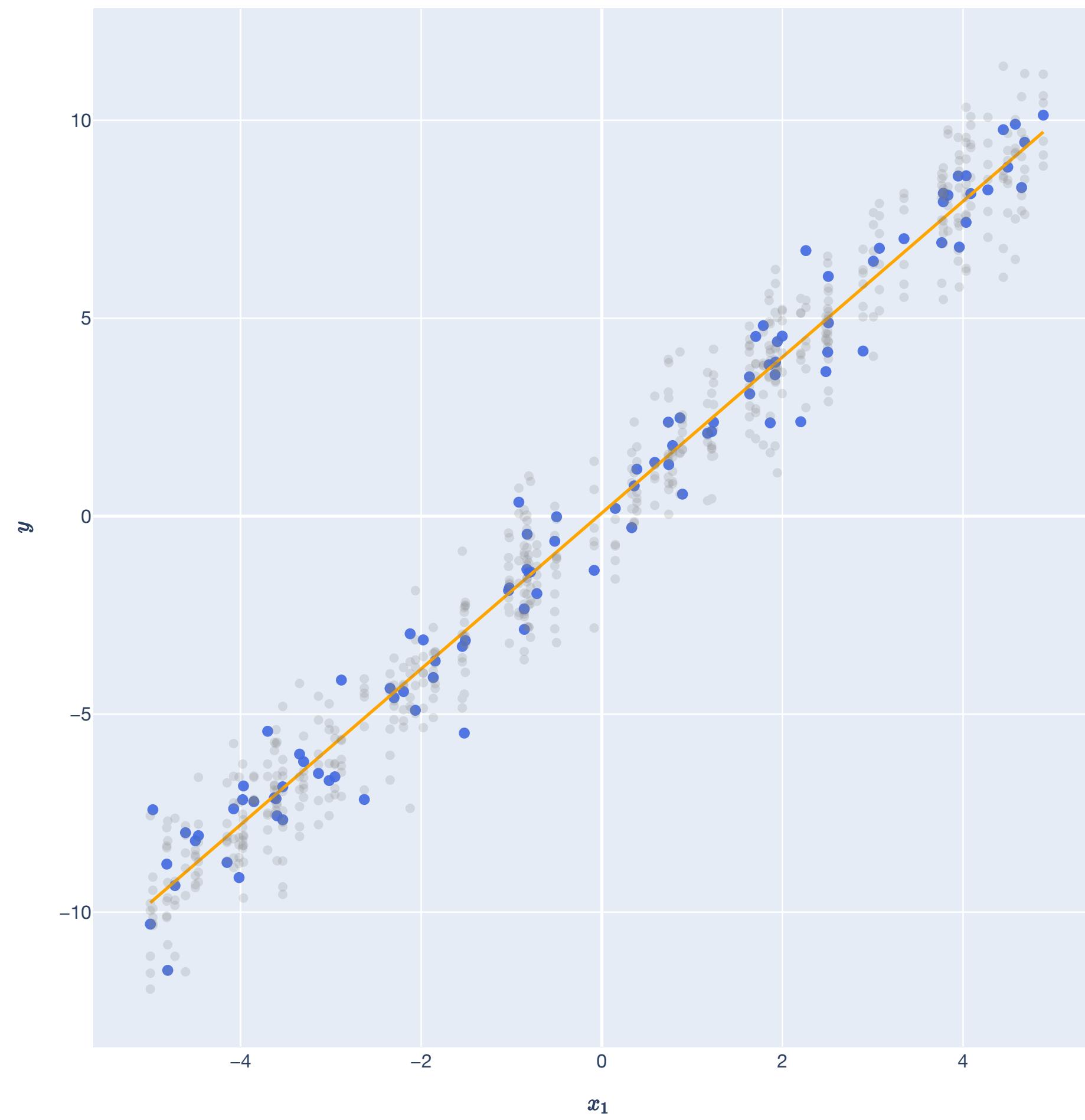
Expectation, variance, and covariance. Review of these basic summary statistics of random variables and common properties.

Random vectors. Introduce the idea of a *random vector*, which is just a list of multiple random variables. Discuss generalizations of expectation and variance to random vectors.

Data as random, statistical model of ML. Introduce a statistical model of ML and the random error model. Introduce *modeling assumptions*. State and prove basic statistical properties of the OLS estimator.

Lesson Overview

Big Picture: Least Squares



Lesson Overview

Big Picture: Gradient Descent

