Math for ML

Week 6.1: Central Limit Theorem, Distributions, and the MLE

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Logistics & Announcements

Lesson Overview

Gaussian Distribution. We define perhaps the most important "named" probability distribution, the Gaussian/"Normal" distribution, and go over some key properties.

Central Limit Theorem. We state and prove the central limit theorem, the statement that the sample average of *many* independent random variables converges in distribution to the Gaussian. It doesn't matter what distribution those random variables take!

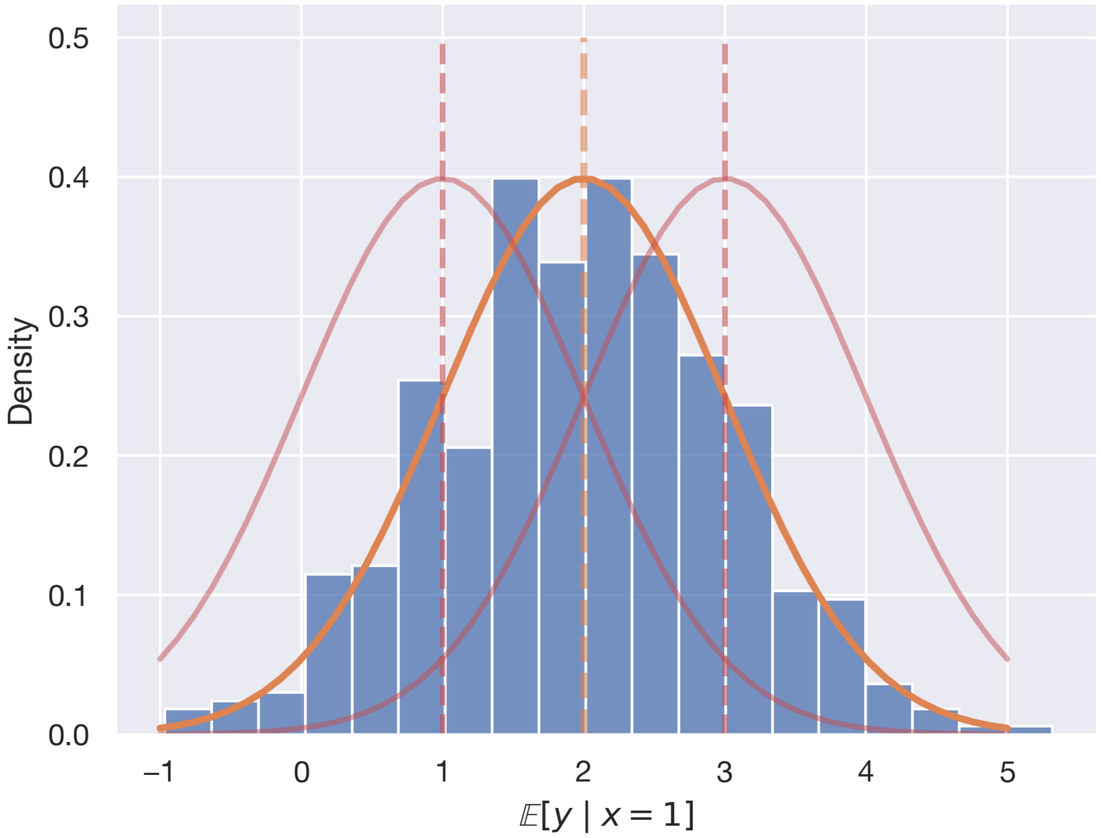
"Named" Distributions. We review other common "named" distributions for discrete and continuous random variables.

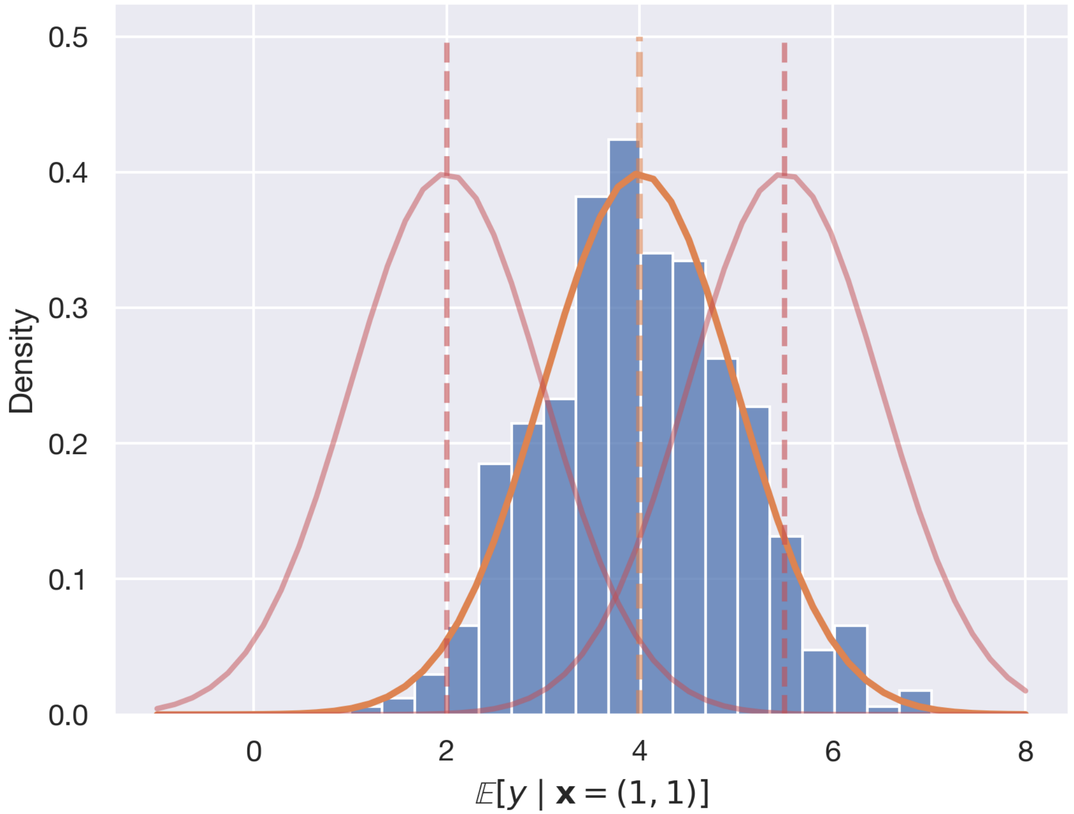
Maximum likelihood estimation. We define maximum likelihood estimation (MLE), a statistical/probabalistic perspective towards finding a well-generalizing model for data.

MLE and OLS. We explore the connection between MLE and OLS by defining the Gaussian error model. In this model, MLE and OLS correspond exactly, motivating our optimization problem another way.

Lesson Overview

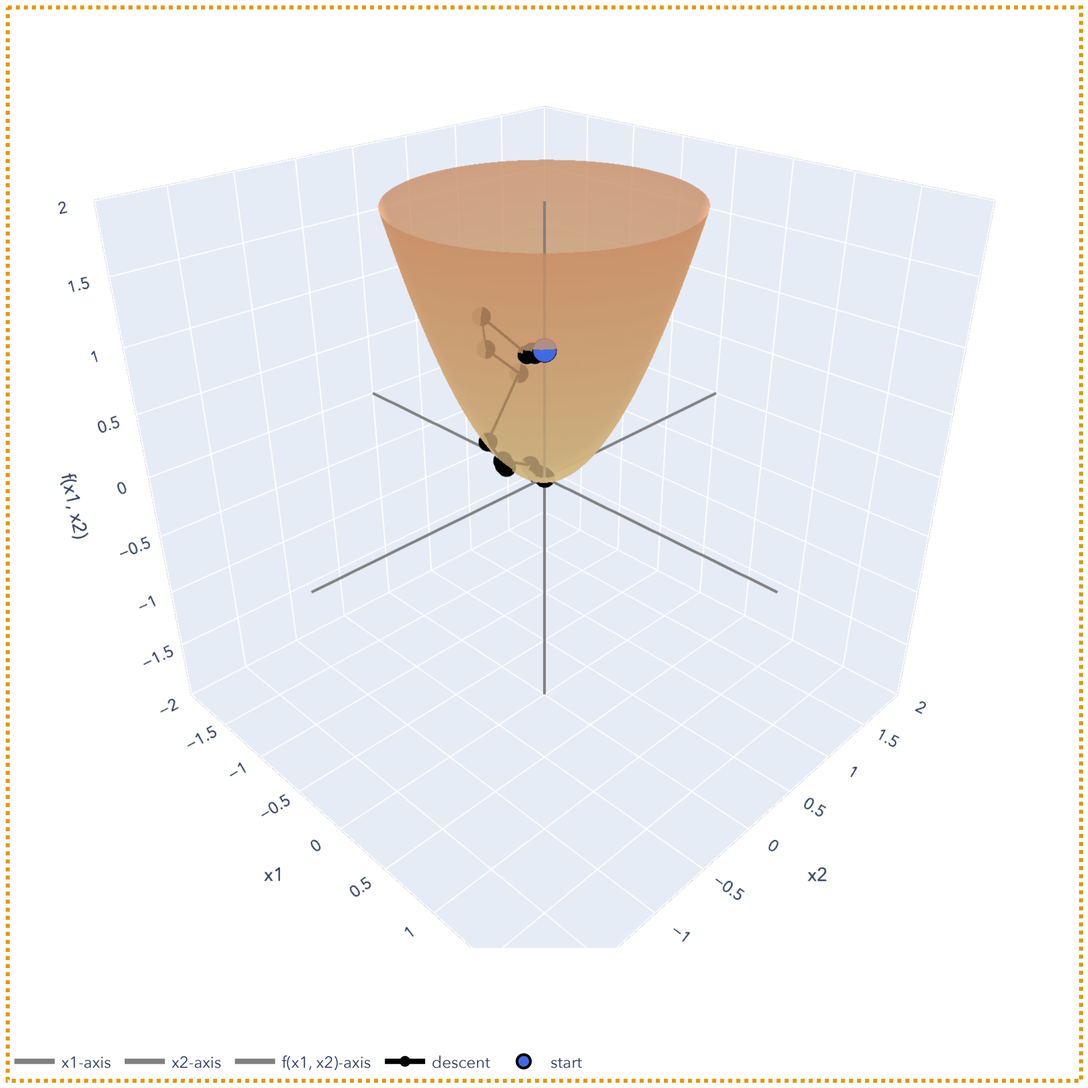
Big Picture: Least Squares

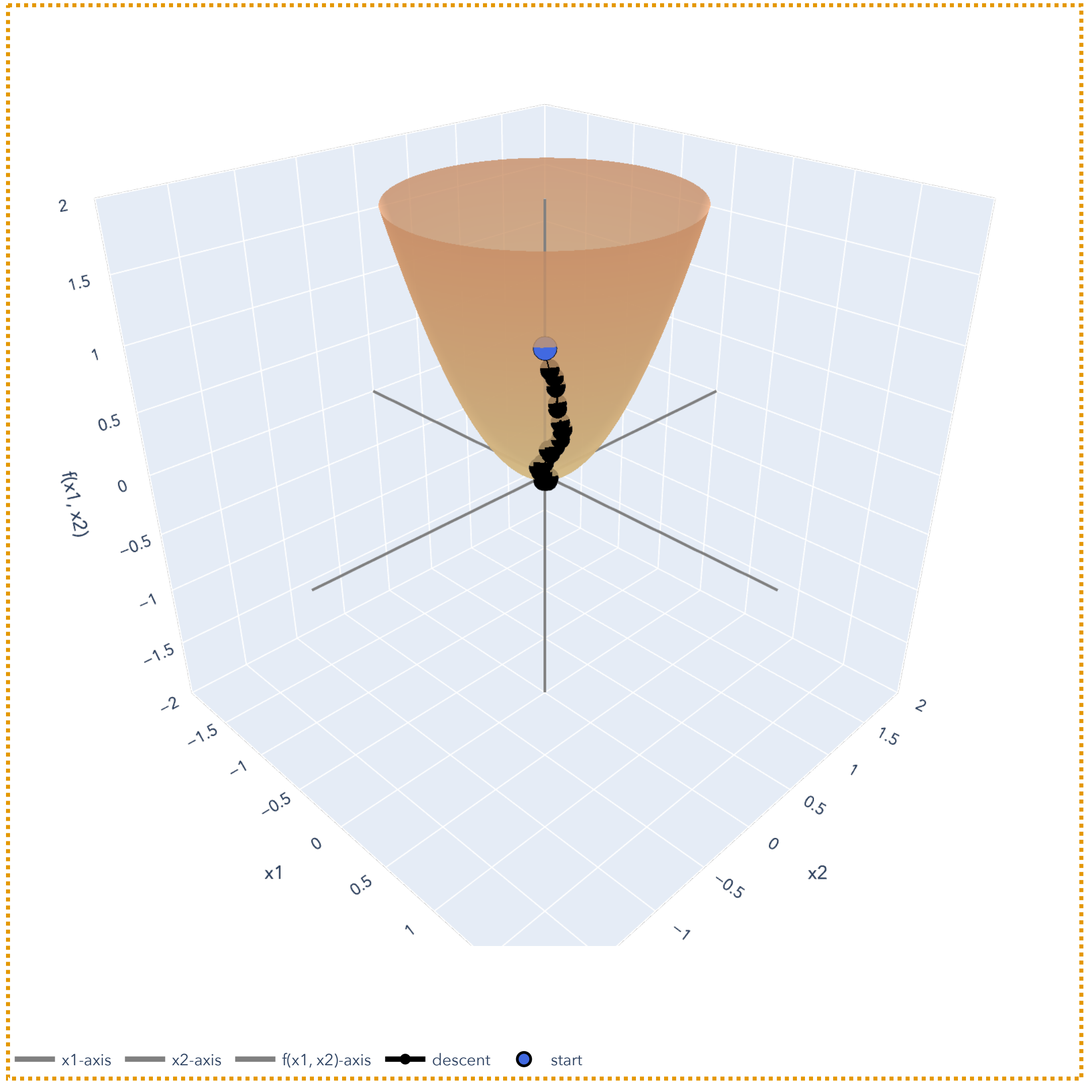




Lesson Overview

Big Picture: Gradient Descent





Probability Distributions

Review and Connection to Random Variables

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:

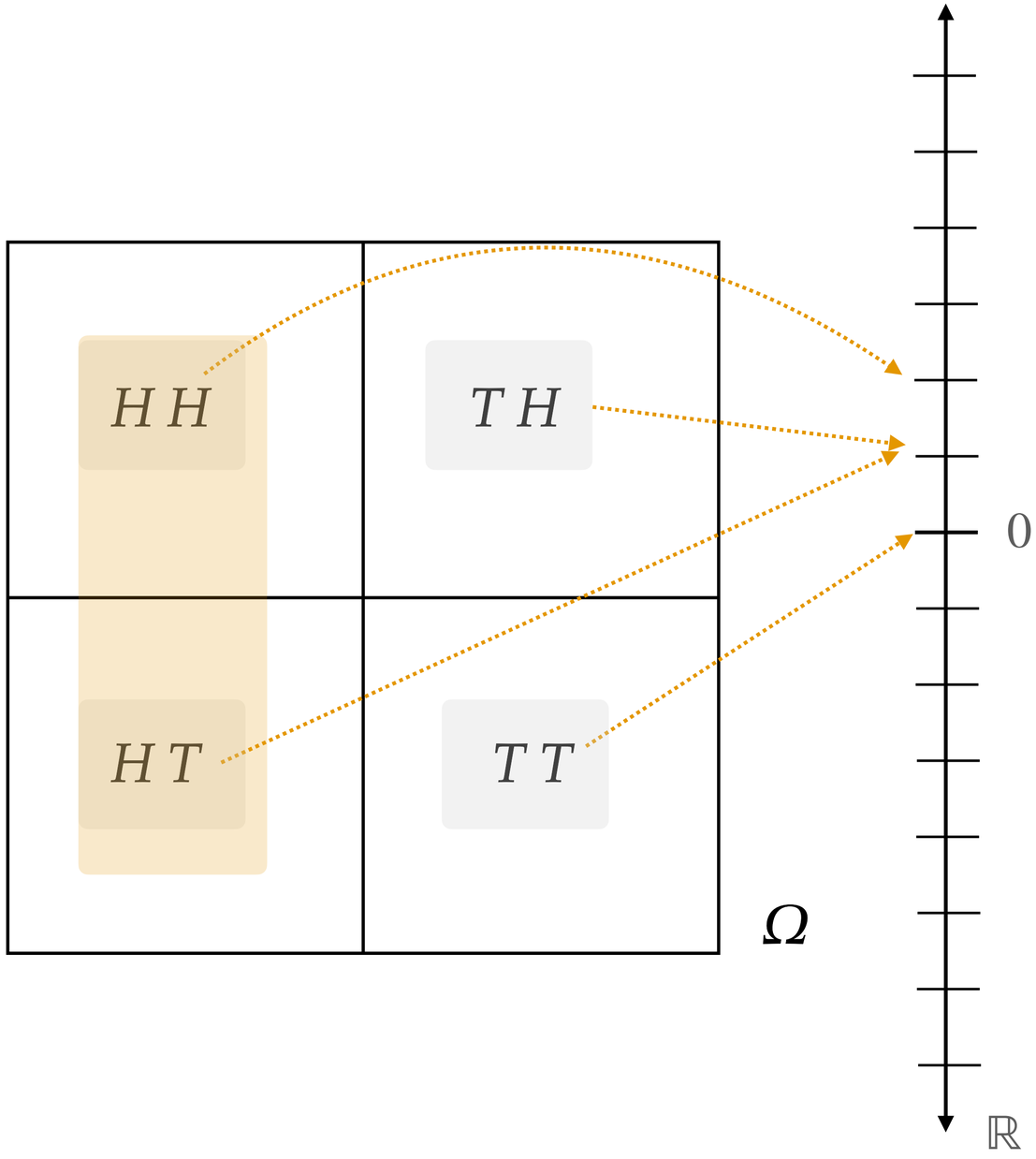
$$\mathscr{A} = \{\varnothing, \{HH\}, \{TT\}, \ldots, \{HH, HT, TH, TT\}\}$$

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 $(\Omega, \mathscr{A}, \mathbb{P})$ is a function $X : \Omega \to \mathbb{R}$ associating outcomes $\omega \in \Omega$ to numbers in $\mathbb{R}$:

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



Random Variables

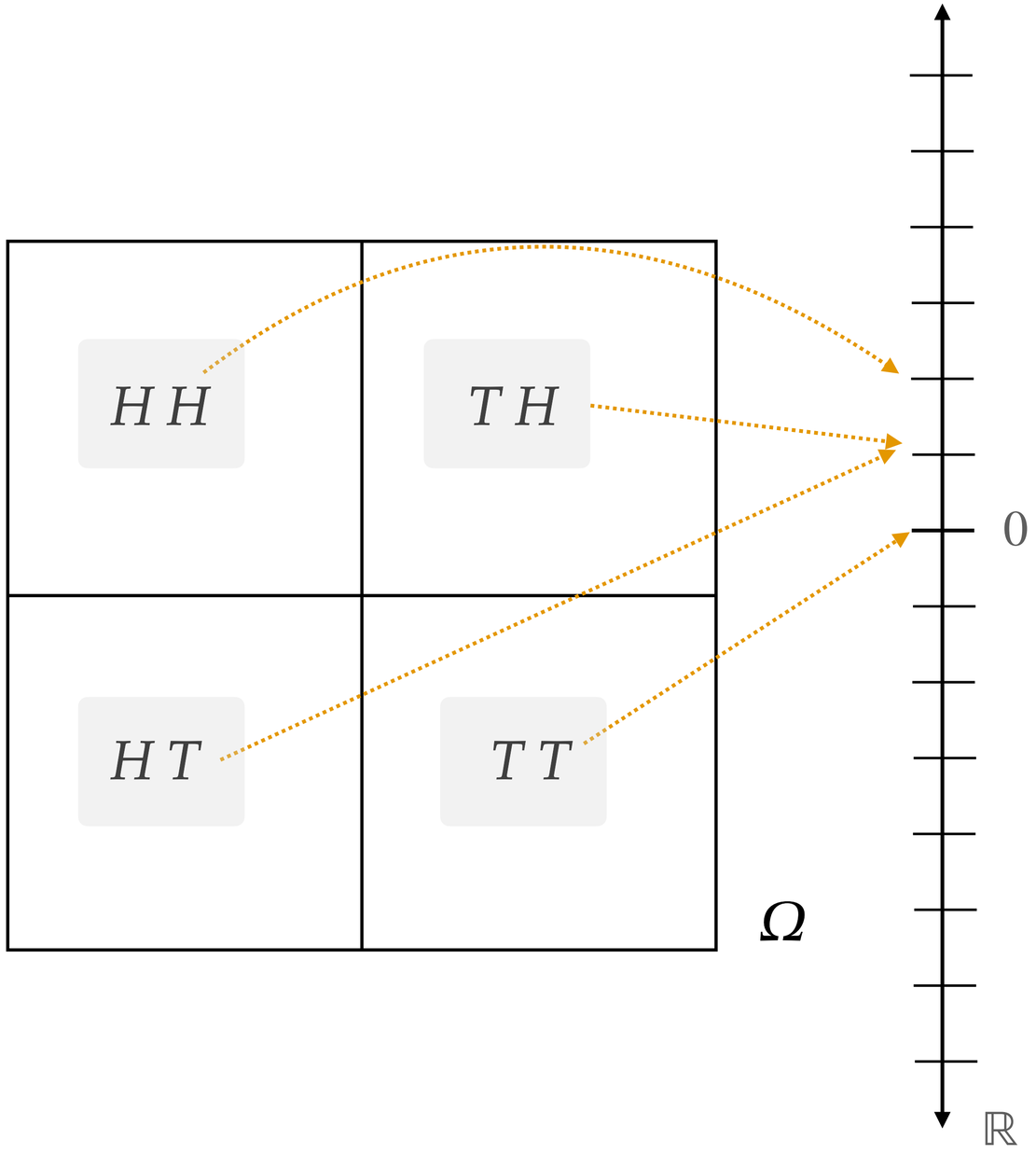
Discrete Base Measure

The probability measure is how we measure the "mass" of events (subsets).

The measure assigning outcomes as equally likely in a discrete space is:

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

Random variables "distribute" this mass over all of $\mathbb{R}$!



Random Variables

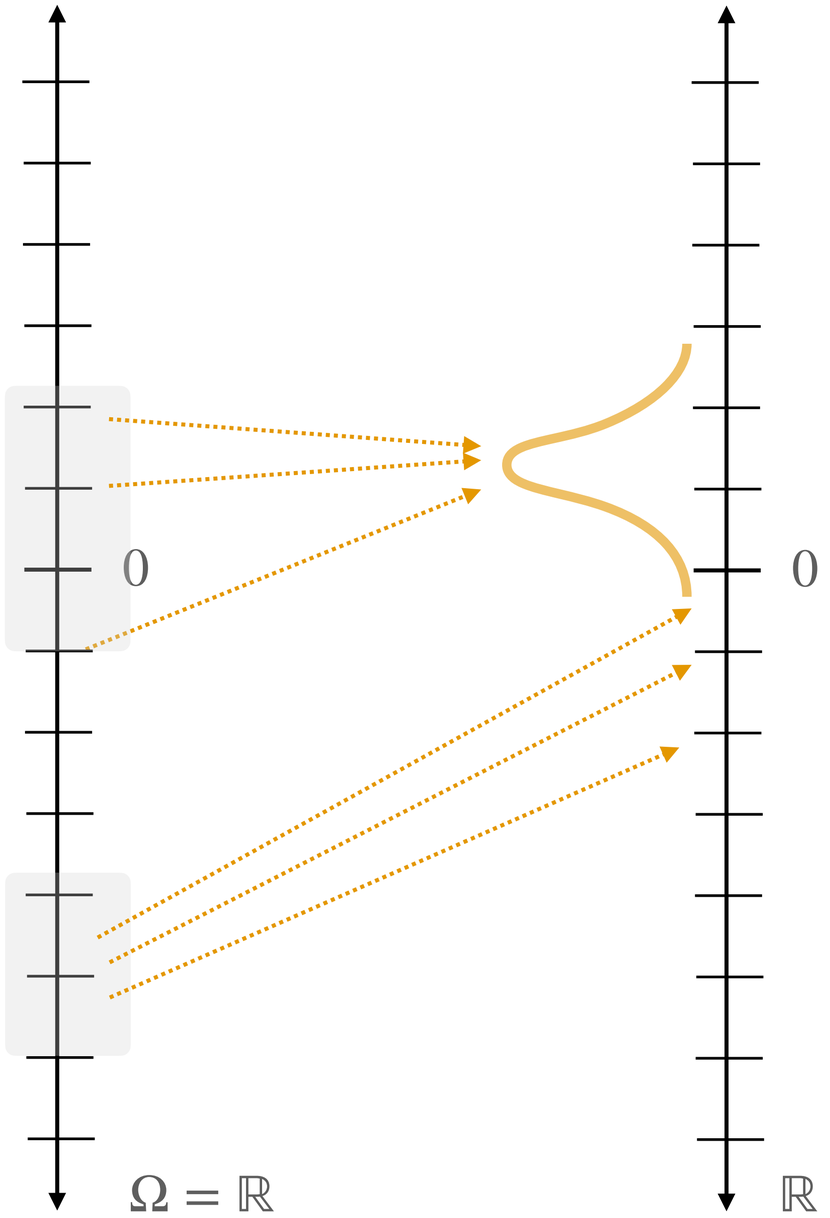
“Uncountable” Base Measure

The probability measure is how we measure the “mass” of events (subsets).

The measure assigning outcomes as equally likely in uncountable $\mathbb{R}$ is:

$$\mathbb{P}([a,b]) = \quad b - a \quad \text{for } [a,b] \subseteq \mathbb{R}.$$

Random variables “distribute” this mass over all of $\mathbb{R}$!



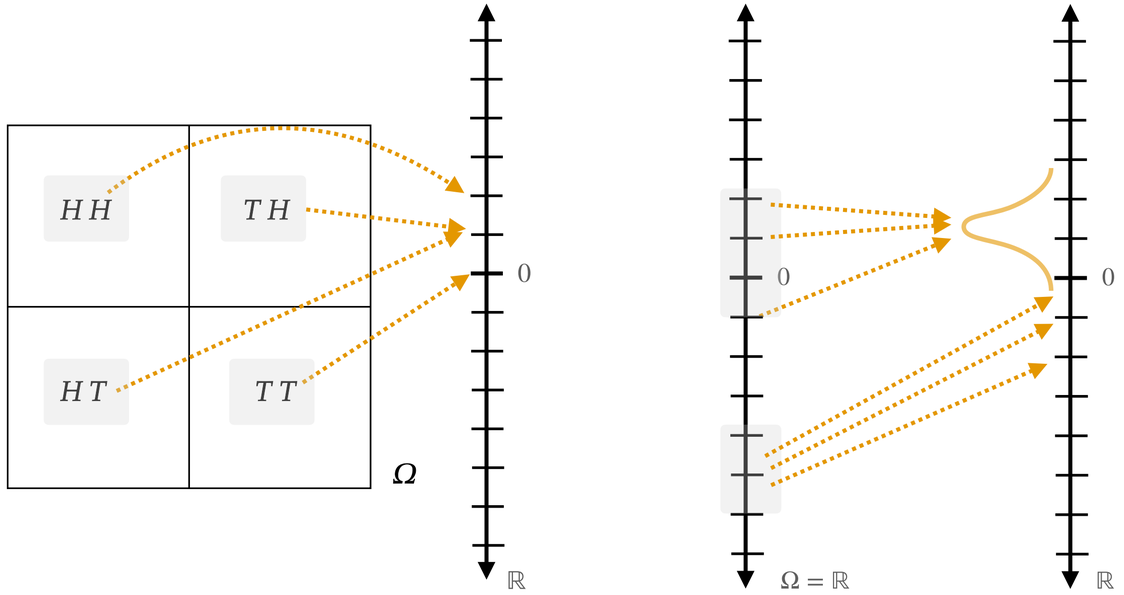
Random Variables

Connection to distributions

So a random variable $X : \Omega \to \mathbb{R}$ describes a way of "distributing" mass from Ω to $\mathbb{R}$.

If Ω is finite, this distribution is described by a probability mass function.

If Ω is uncountably infinite, this distribution is described by a probability density function.



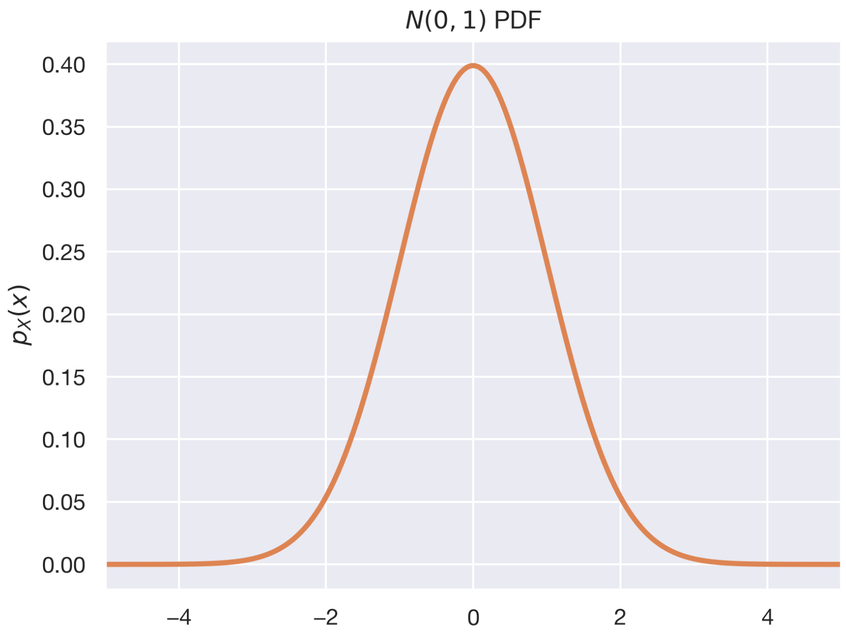
The Gaussian Distribution

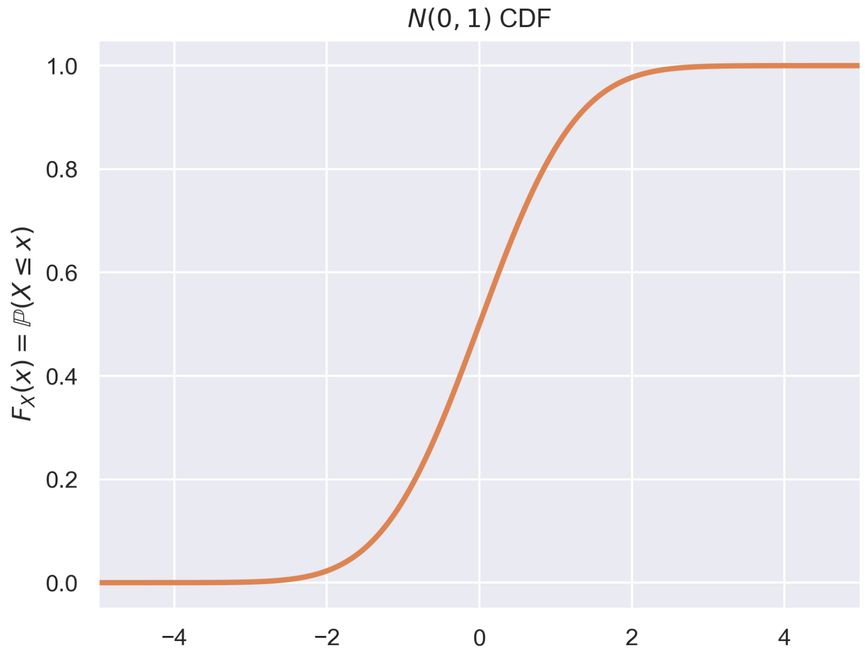
Definition and Properties

The Gaussian Distribution

Intuition and Shape

The Gaussian/Normal distribution with parameters μ and σ has a "bell-shaped" PDF centered at μ and "spread" depending on the parameter σ.





The Gaussian Distribution

Standard Gaussian Definition

A RV Z has a standard Gaussian/Normal distribution denoted $Z \sim N(0,1)$ if it has PDF:

$$p_Z(z) = \frac{1}{\sqrt{2\pi}} e^{-z^2/2}, \text{ for all } z \in \mathbb{R}.$$

This random variable has mean $\mathbb{E}[Z] = 0$ and variance $\mathrm{Var}(Z) = 1$.

Traditionally, standard Gaussians are denoted with Z, PDF $\phi(z)$, and CDF $\Phi(z)$.

The Gaussian Distribution

General Definition

A random variable X has a Gaussian/Normal distribution with parameters μ and σ, denoted $X \sim N(\mu, \sigma^2)$ if it has PDF:

$$p_X(x) = \frac{1}{\sigma\sqrt{2\pi}} \exp\left\{ -\frac{1}{2\sigma^2}(x-\mu)^2 \right\}, \text{ for all } x \in \mathbb{R}.$$

This random variable has mean $\mathbb{E}[X] = \mu$ and variance $\mathrm{Var}(X) = \sigma^2$.

The Gaussian Distribution

Properties of Gaussians

Standardization. If $X \sim N(\mu, \sigma^2)$, then $Z = (X - \mu)/\sigma \sim N(0,1)$. As a result:

$$\begin{aligned}\mathbb{P}(a < X < b) &= \mathbb{P}\left(\frac{a-\mu}{\sigma} < Z < \frac{b-\mu}{\sigma}\right) \\ &= \Phi\left(\frac{b-\mu}{\sigma}\right) - \Phi\left(\frac{a-\mu}{\sigma}\right)\end{aligned}$$

Standard to general. If $Z \sim N(0,1)$, then $X = \mu + \sigma Z \sim N(\mu, \sigma^2)$.

Sums of Gaussians. If $X_i \sim N(\mu_i, \sigma_i^2)$ for $i = 1, \ldots, n$ are independent, then

$$\sum_{i=1}^{n} X_i \sim N\left(\sum_{i=1}^{n} \mu_i, \sum_{i=1}^{n} \sigma_i^2\right).$$

Central Limit Theorem

Intuition and Simulations

Statistical Estimation

Intuition

In **probability theory**, we assumed we knew some data generating process (as a *distribution*) $\mathbb{P}_{\mathbf{x}}$, and we analyzed observed data under that process.

$$\mathbb{P}_{\mathbf{x}} \implies \mathbf{x}_1, \ldots, \mathbf{x}_n.$$

Statistics can be thought of as the "reverse process." We see some data and we try to make inferences about the process that generated the data.

$$\mathbf{x}_1, \ldots, \mathbf{x}_n \implies \mathbb{P}_{\mathbf{x}}$$

In order to do so, we need to formalize the notion that "collecting a lot of data" gives us a peek at the underlying process!

Law of Large Numbers

Theorem Statement

Theorem (Weak Law of Large Numbers). Let $X_1, \ldots, X_n$ be independent and identically distributed (i.i.d.) random variables with finite mean $\mu := \mathbb{E}[X_i]$. Let their *sample average* be denoted as

$$\overline{X}_n := \frac{1}{n} \sum_{i=1}^{n} X_i.$$

Then, for any $\epsilon > 0$,

$$\lim_{n \to \infty} \mathbb{P}\left(\left| \overline{X}_n - \mu \right| < \epsilon \right) = 1.$$

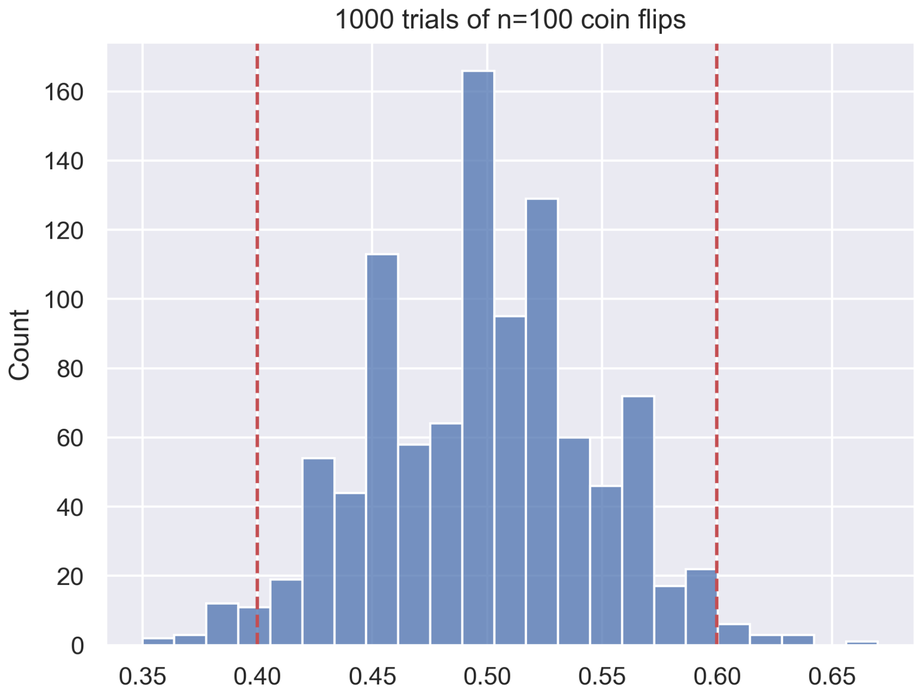
Law of Large Numbers

Example: Mean Estimator for Coins

Example. Let X_i be a random variable denoting the outcome of a single fair coin toss, with $X_i = 0$ for tails and $X_i = 1$ for heads. Clearly, $\mu := \mathbb{E}[X_i] = 1/2$.

Law of large numbers states that for *any* $\epsilon > 0$, *no matter how small*:

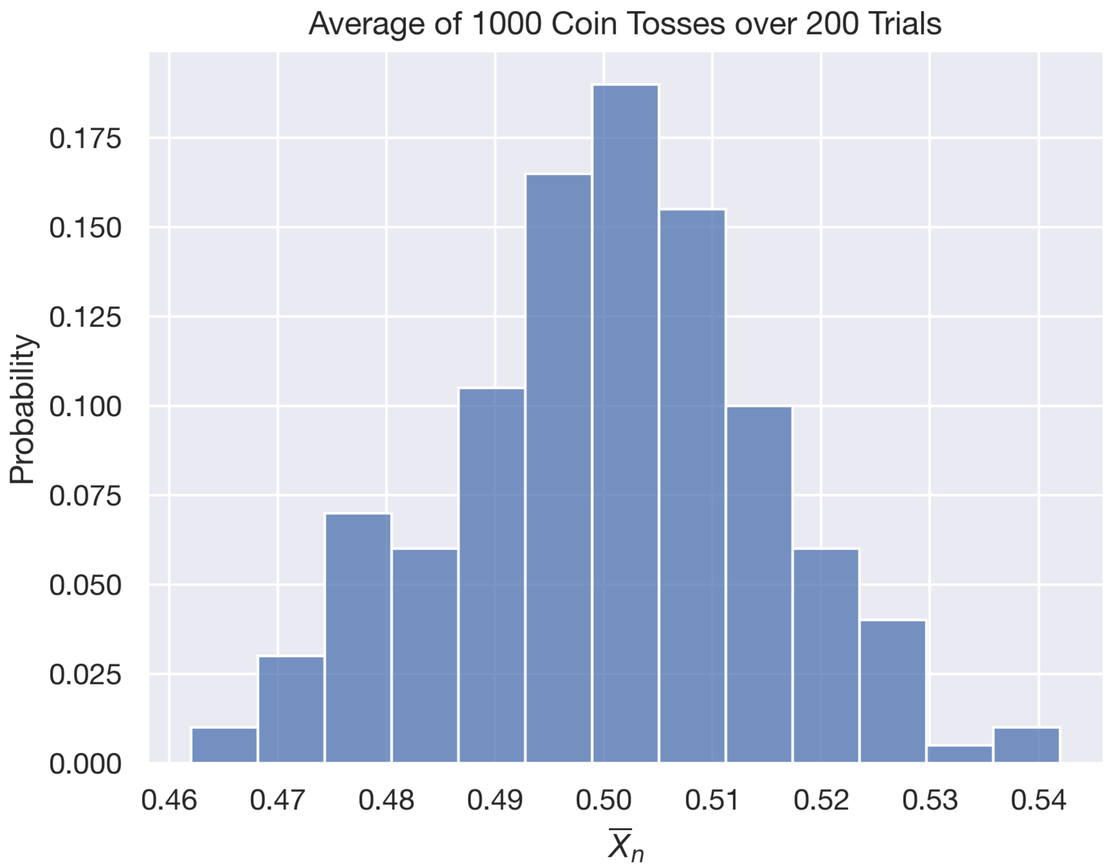
$$\lim_{n \to \infty} \mathbb{P}(\ \overline{X}_n - 1/2\ \ < \epsilon) = 1$$

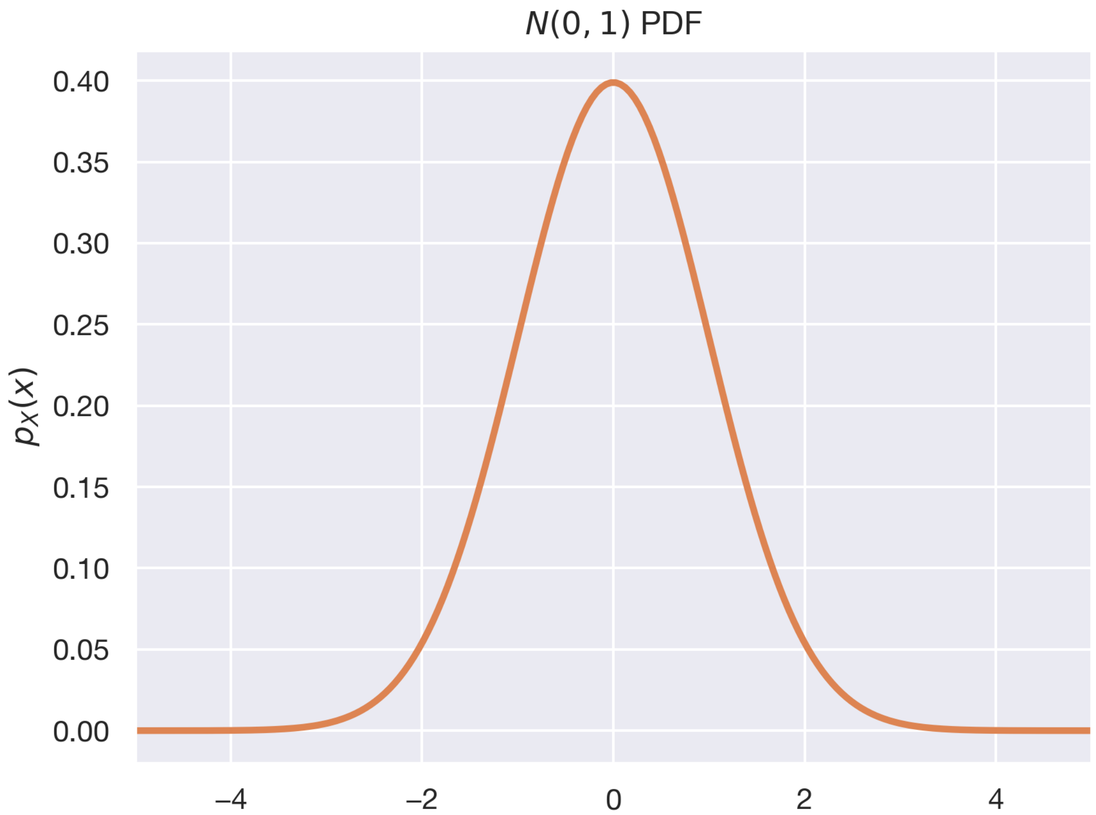


But can we say something more about the distribution *of the random variable* $\overline{X}_n$*?*

Central Limit Theorem

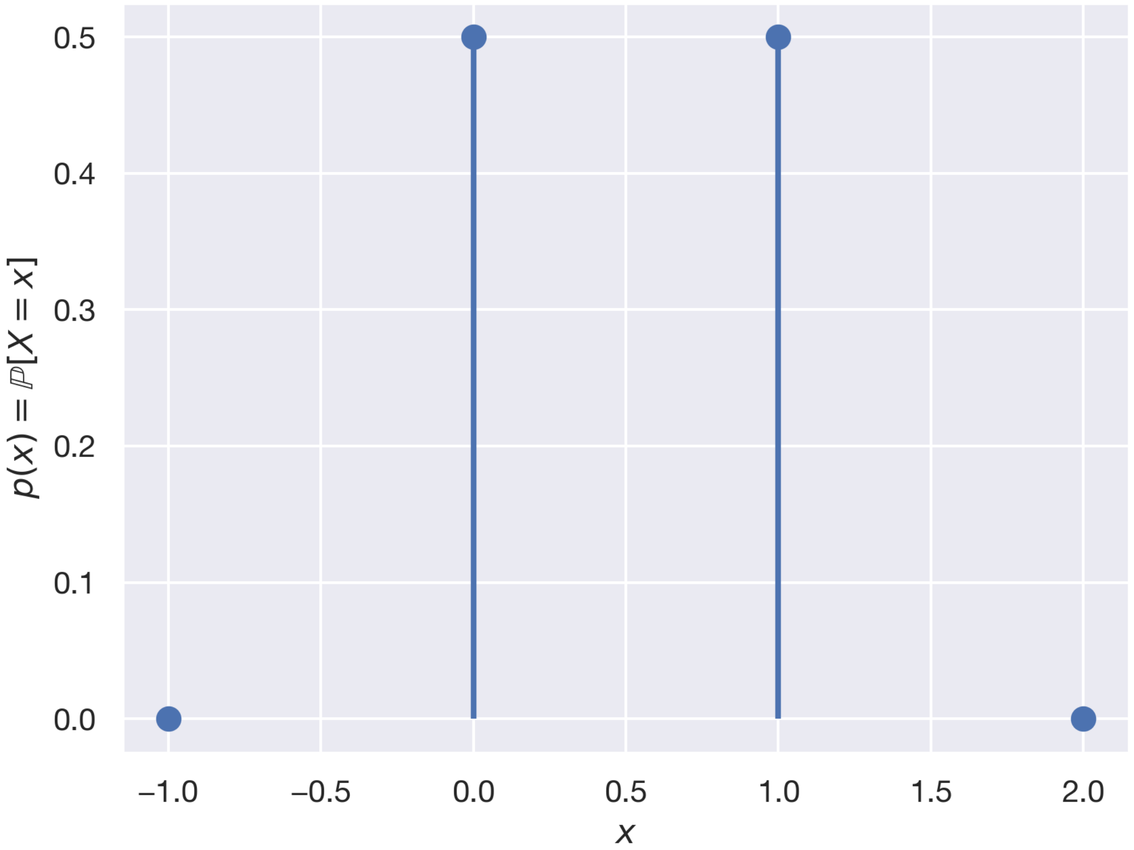
Intuition

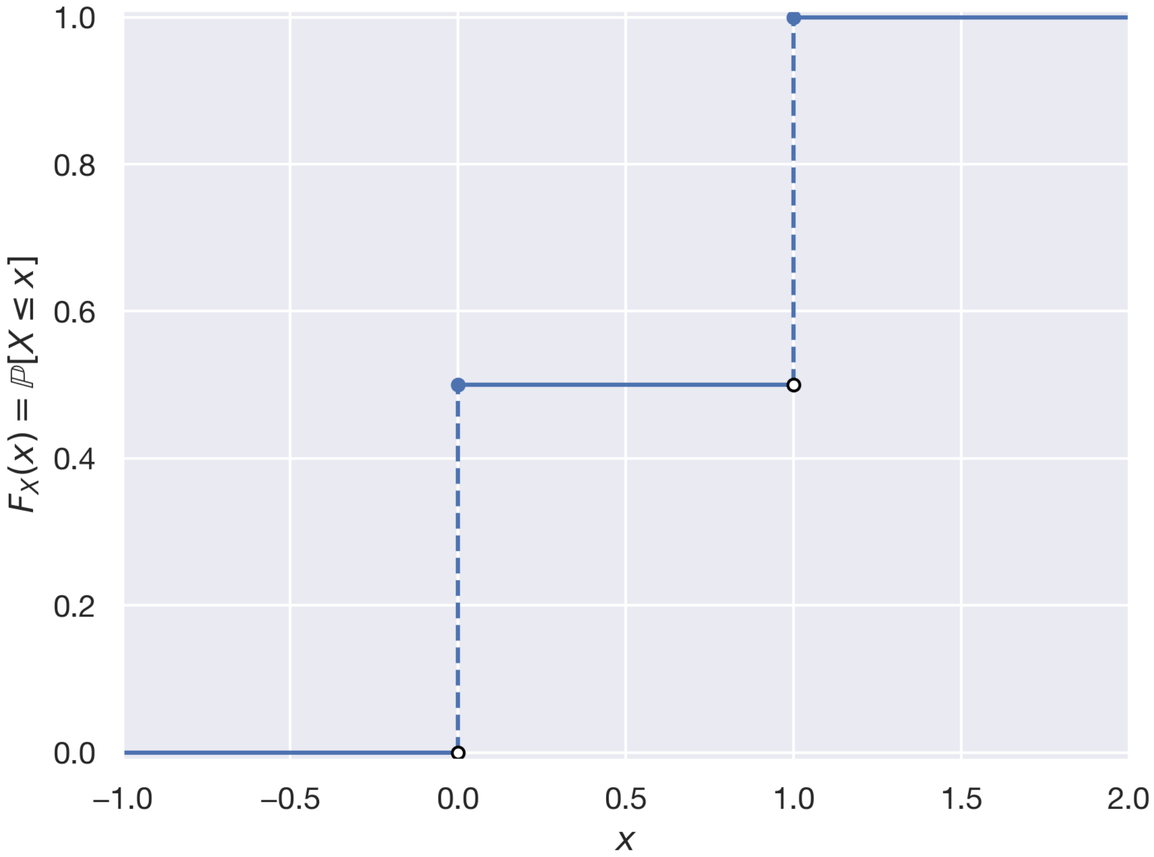




Central Limit Theorem

Experiment: Coin Tosses





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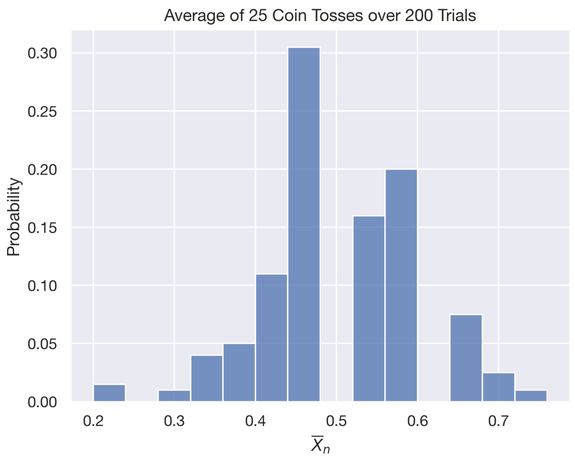

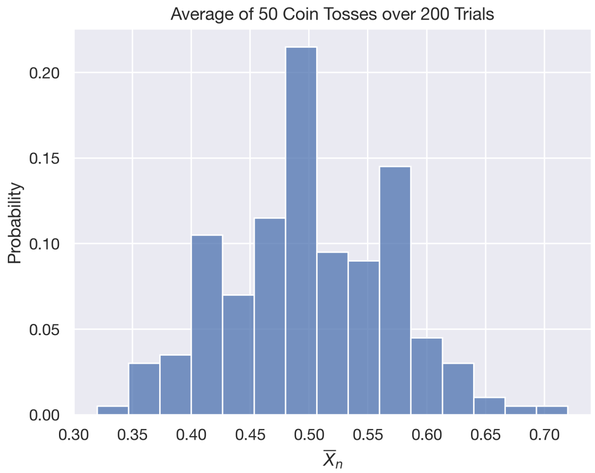

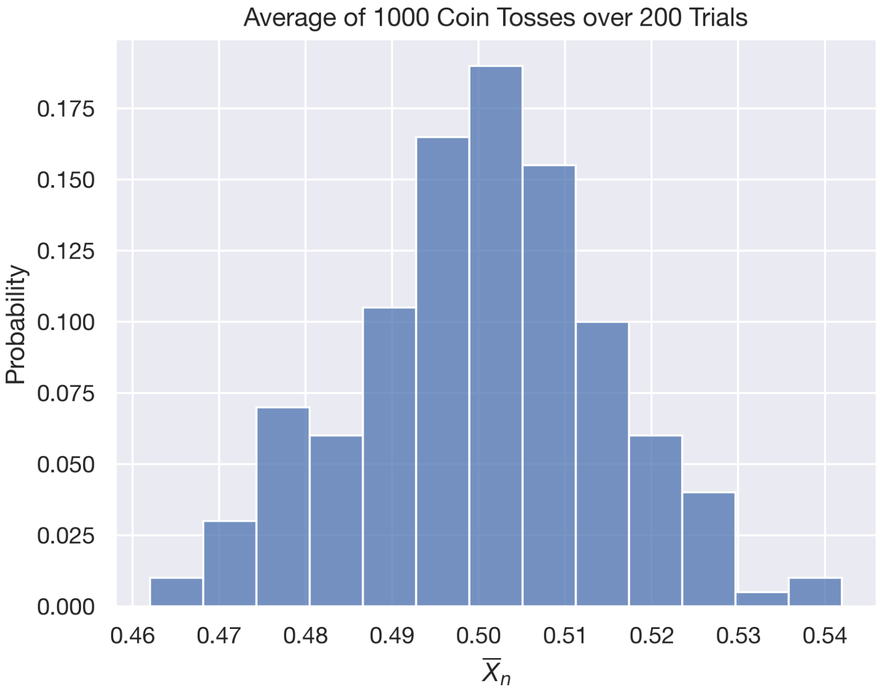

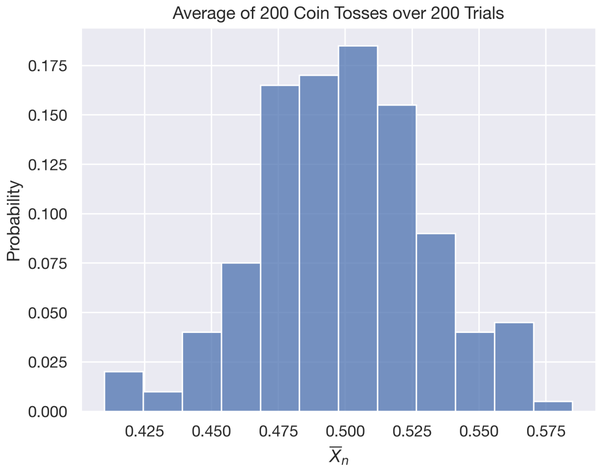

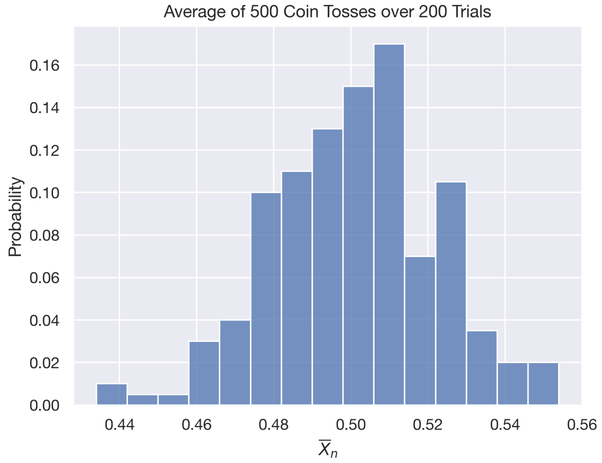

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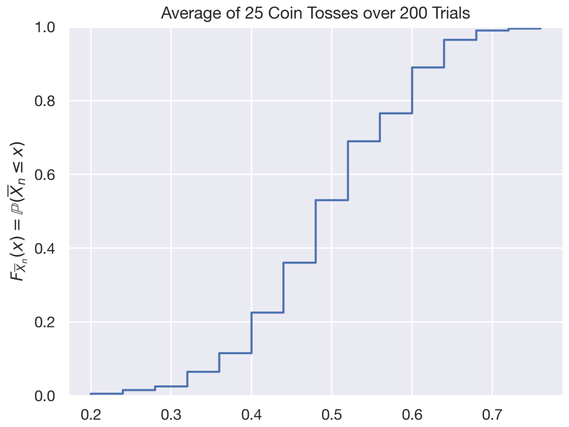
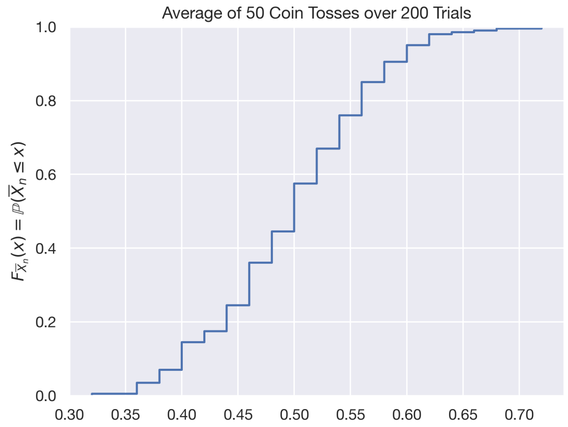
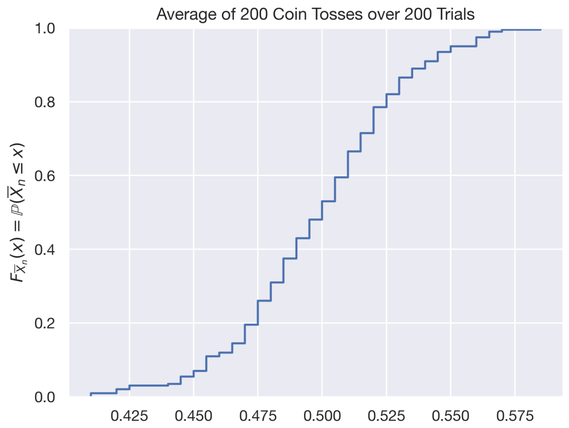
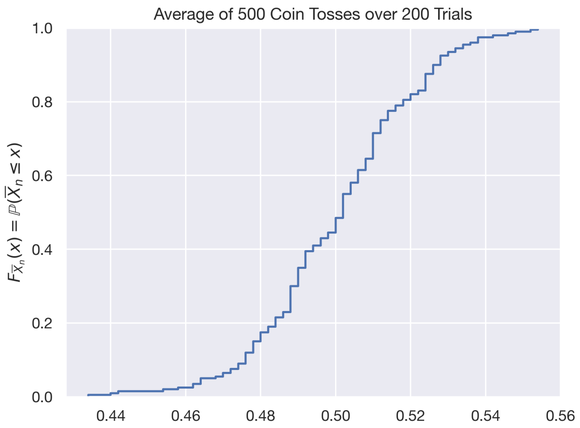
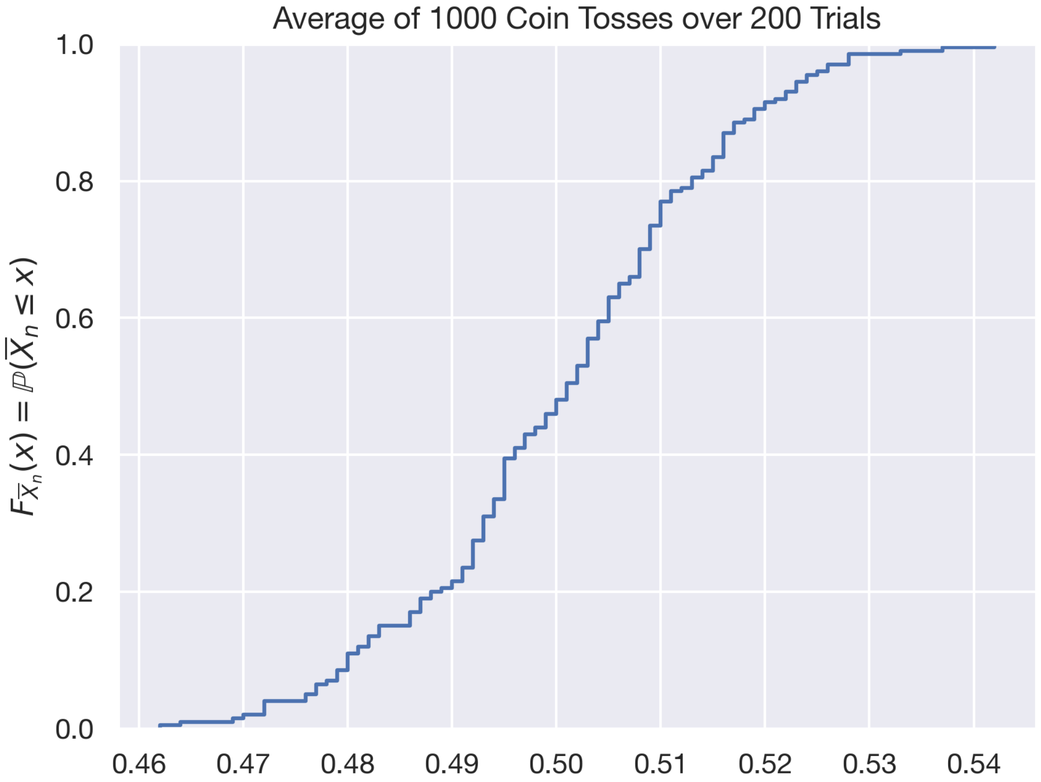




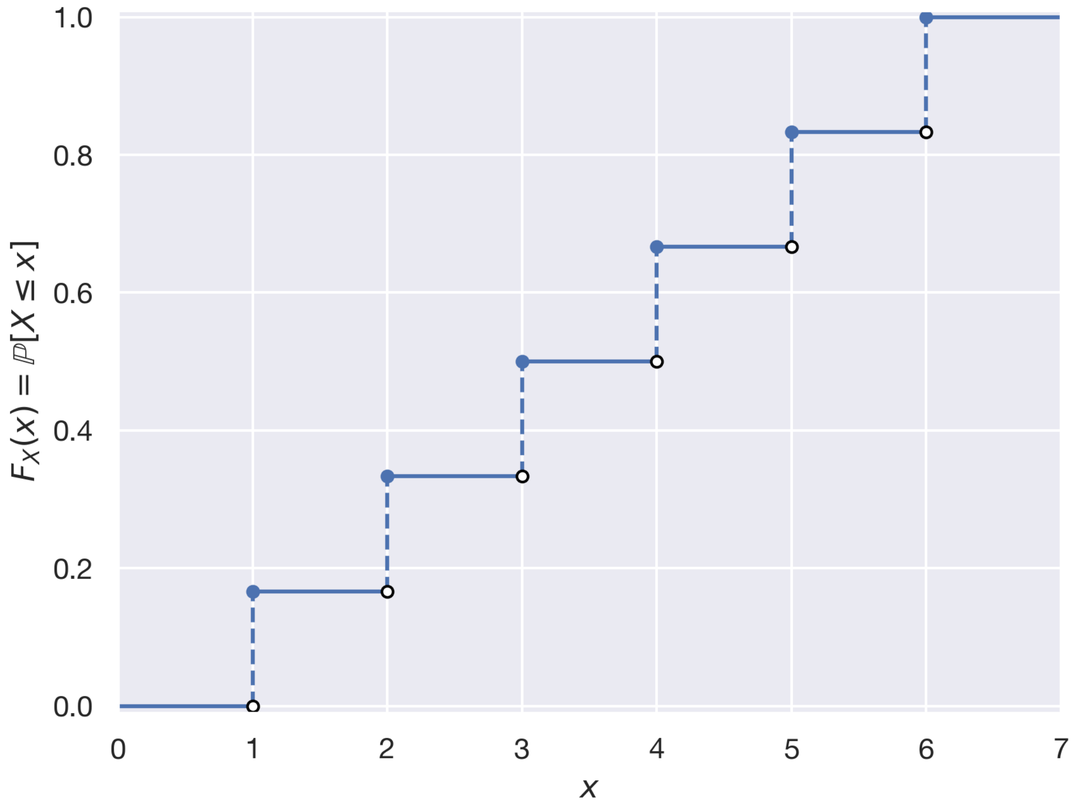


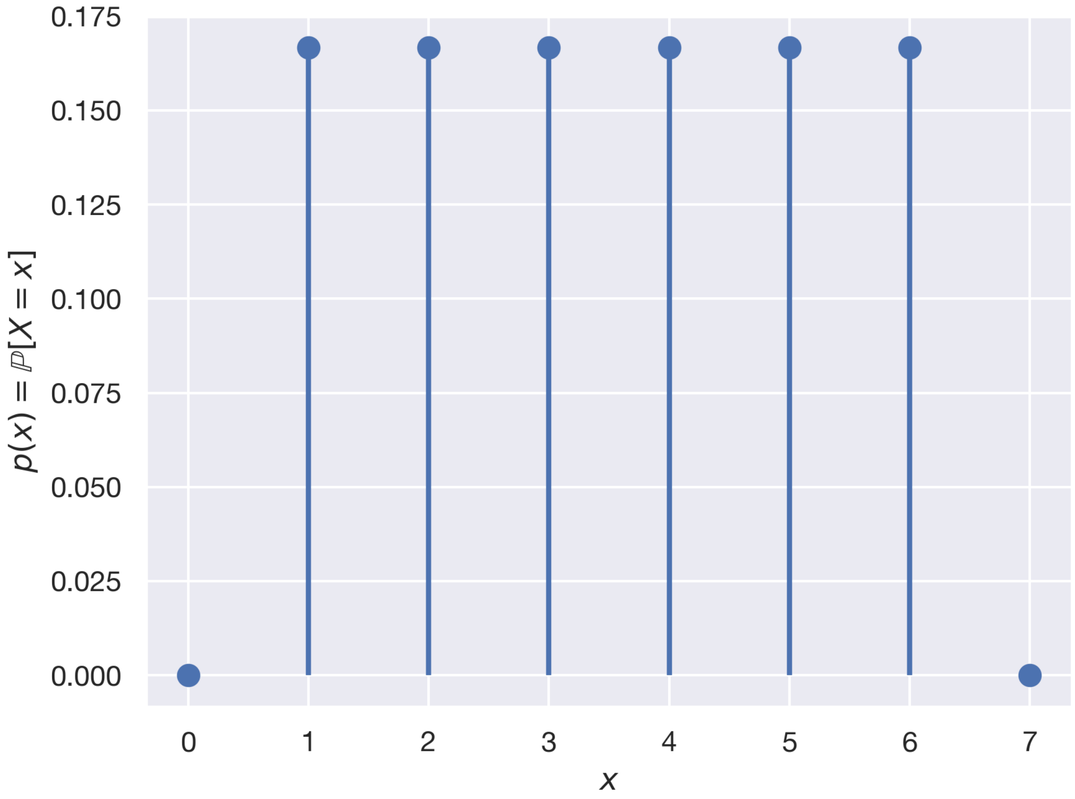




Central Limit Theorem

Experiment: Die Rolls





Central Limit Theorem

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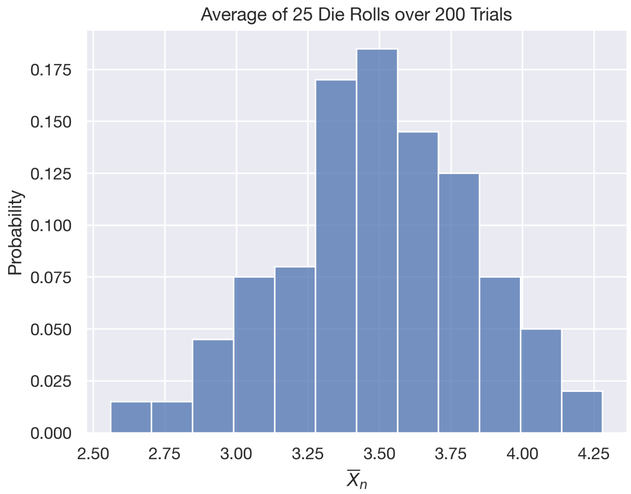
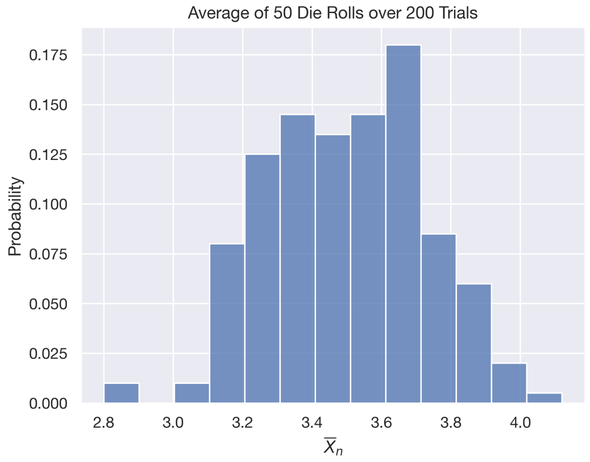
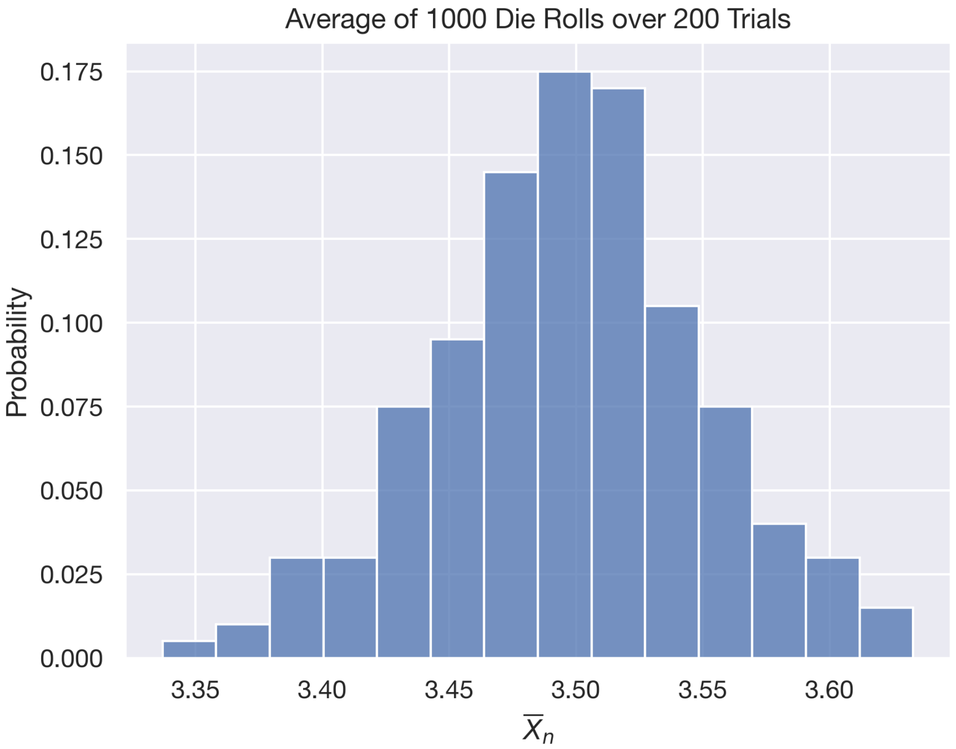
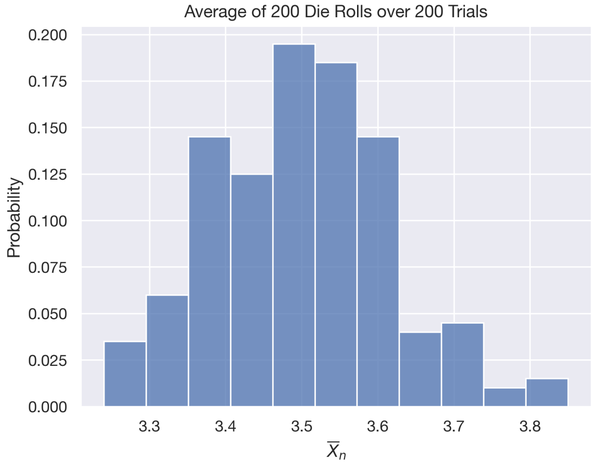
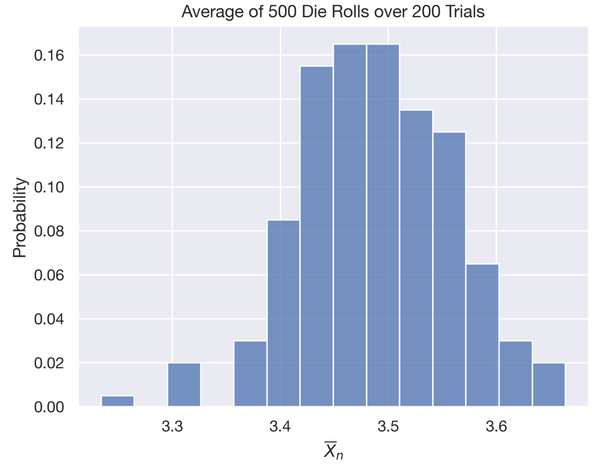




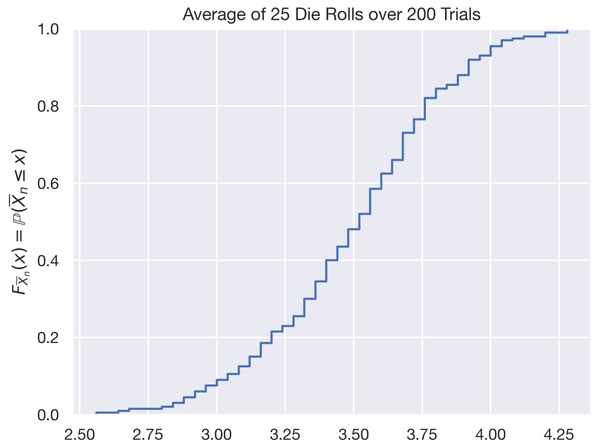


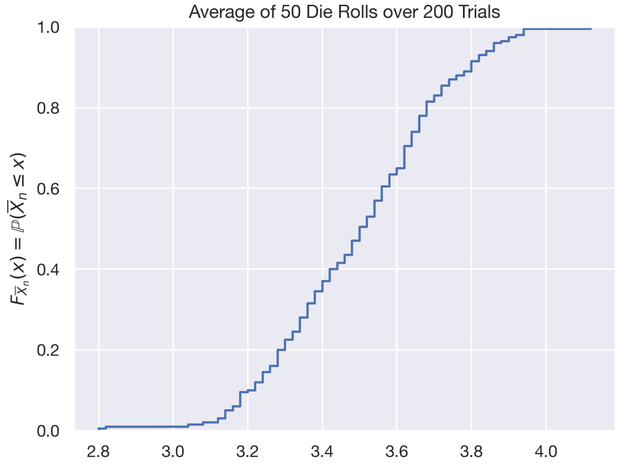


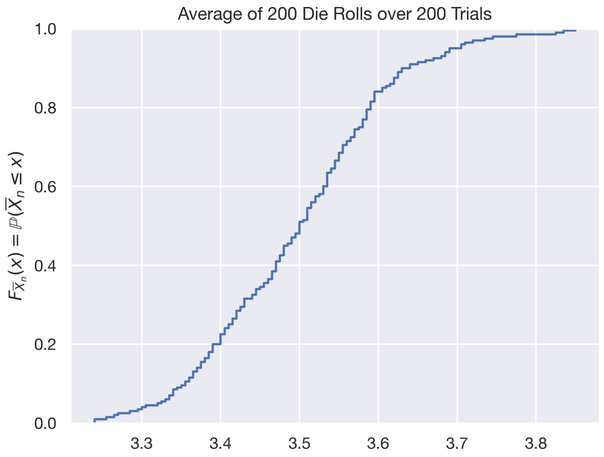


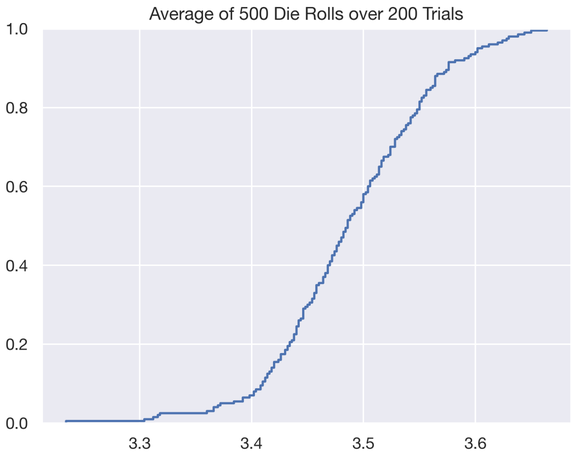
Central Limit Theorem

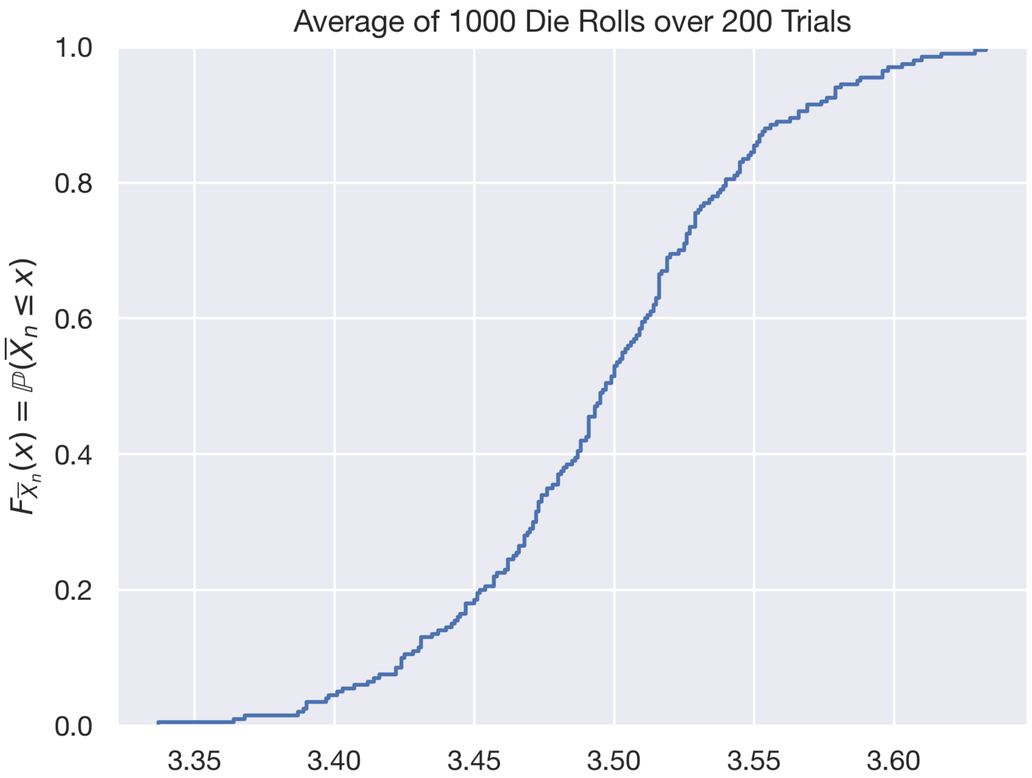
Experiment: Die Rolls





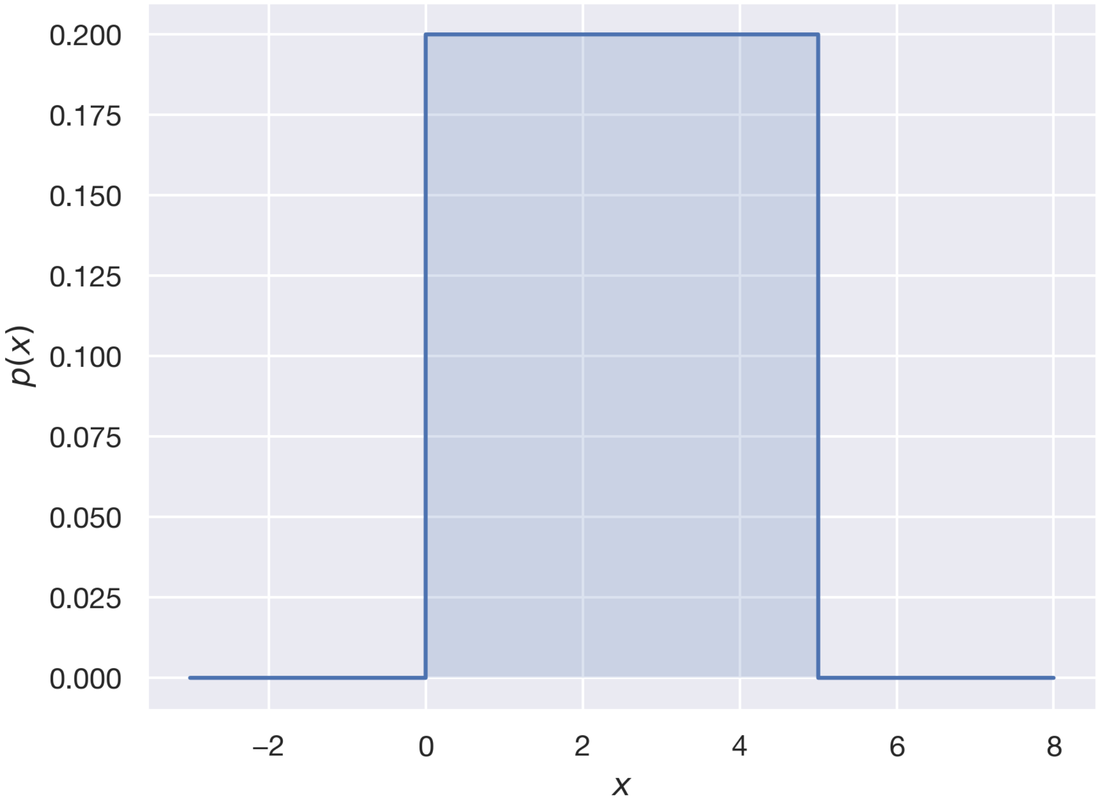


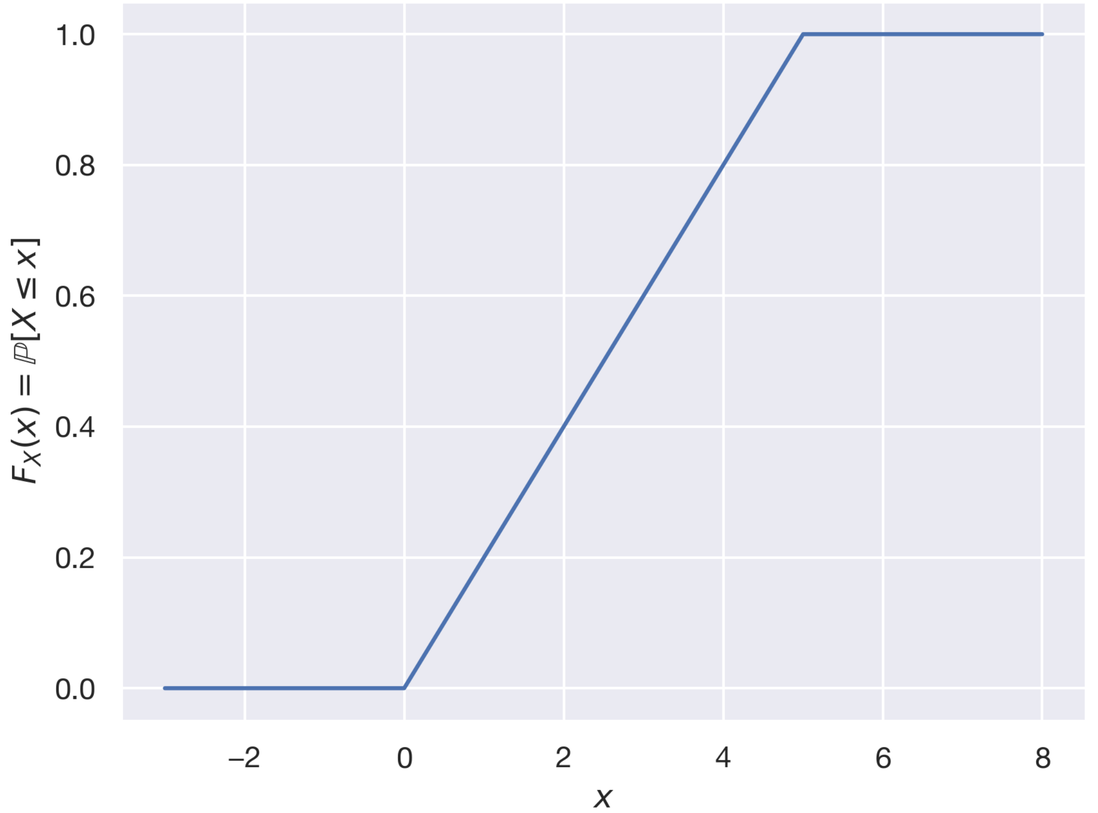




Central Limit Theorem

Experiment: Drawing uniform real value





Central Limit Theorem

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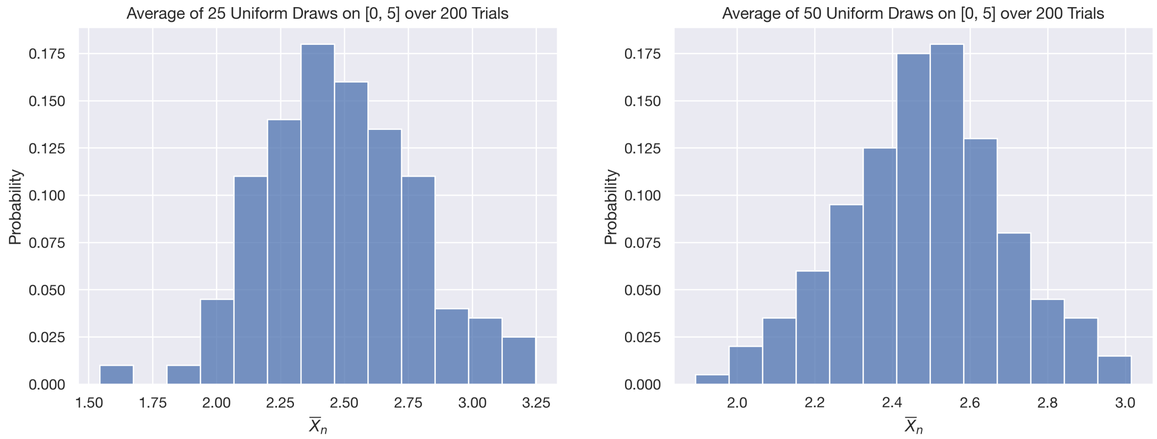

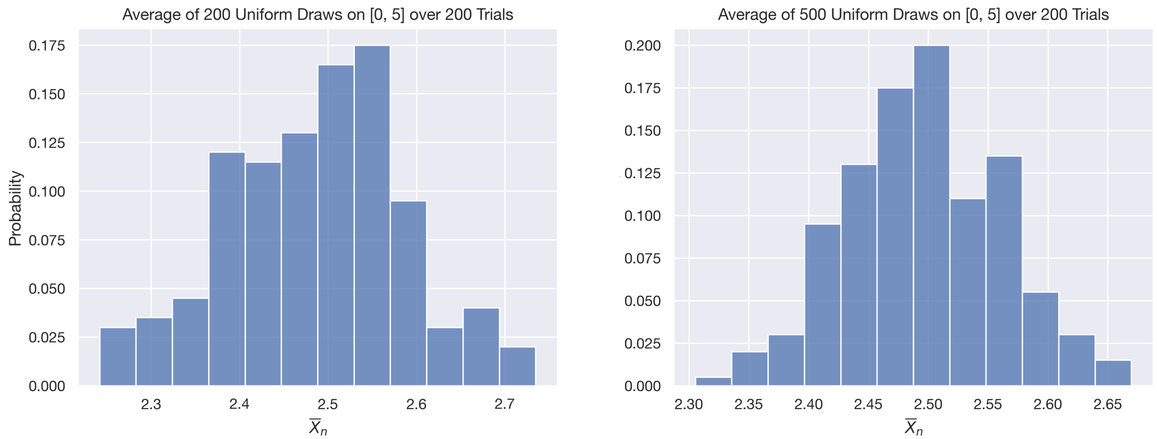

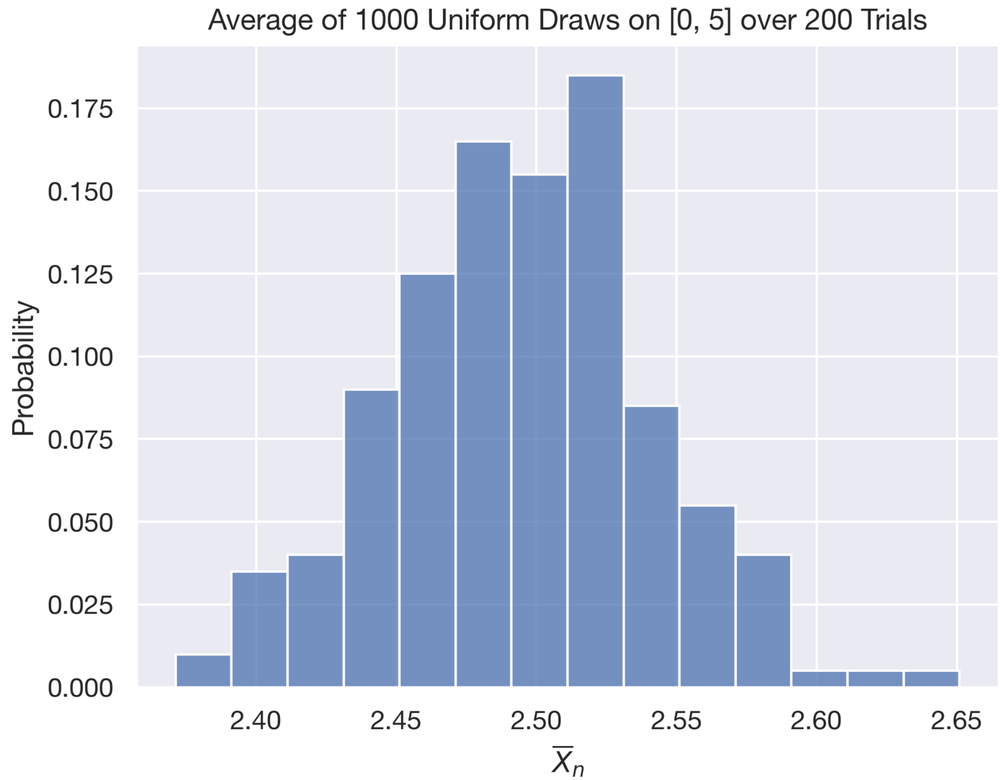

Central Limit Theorem

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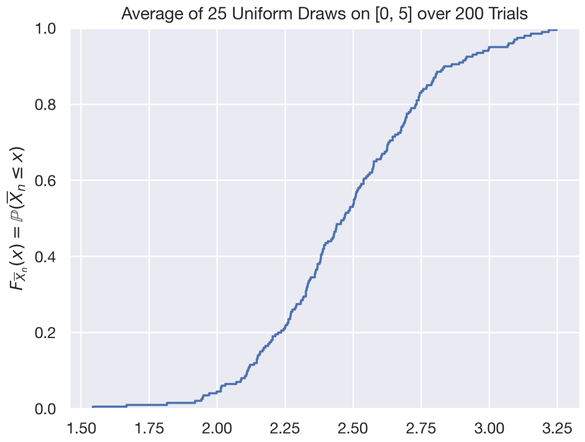

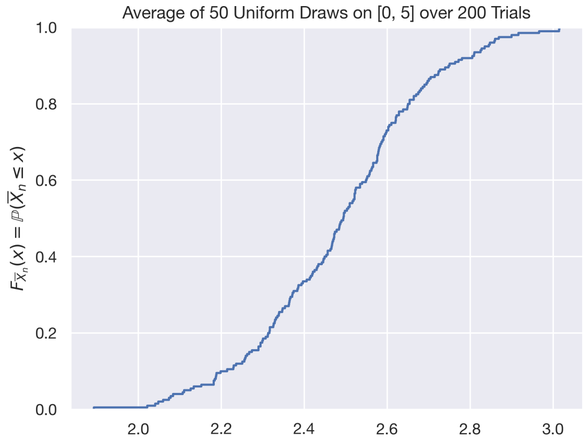

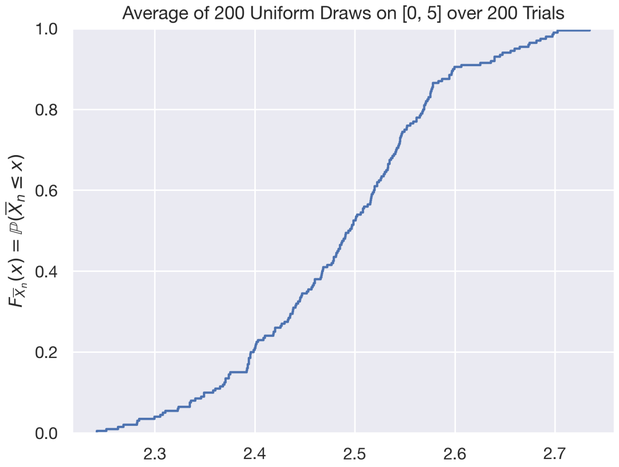

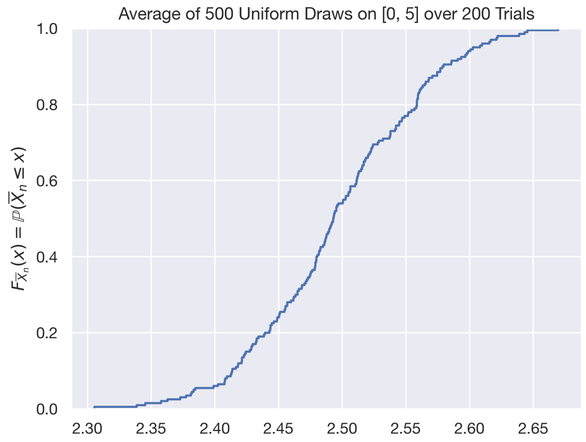

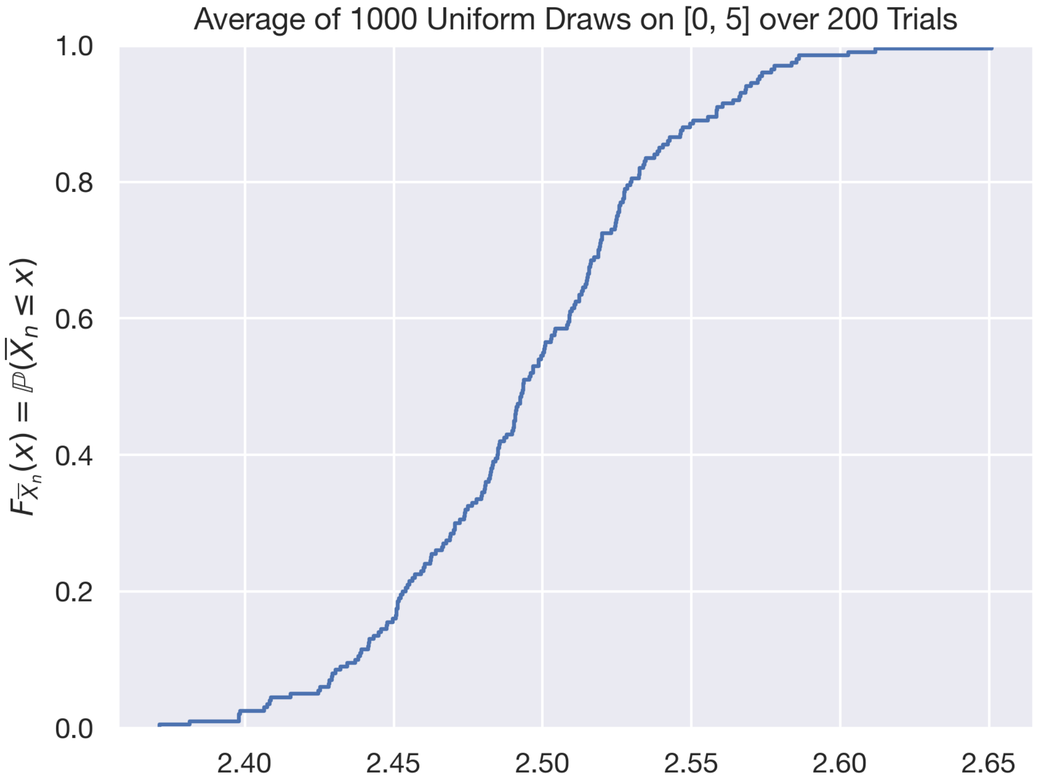

Convergence and MGFs

Tools for CLT Proof

Moment Generating Function

Intuition

The moment generating function (MGF) packs all the "moment" information of a random variable X into the Taylor-expandable function e^{tX}.

$$e^X = 1 + X + \frac{X^2}{2} + \frac{X^3}{3!} + \dots$$

$$e^{tX} = 1 + tX + \frac{t^2X^2}{2} + \frac{t^3X^3}{3!} + \dots$$

$$\mathbb{E}[e^{tX}] = 1 + t\mathbb{E}[X] + t^2\frac{\mathbb{E}[X^2]}{2} + t^3\frac{\mathbb{E}[X^3]}{3!} + \dots$$

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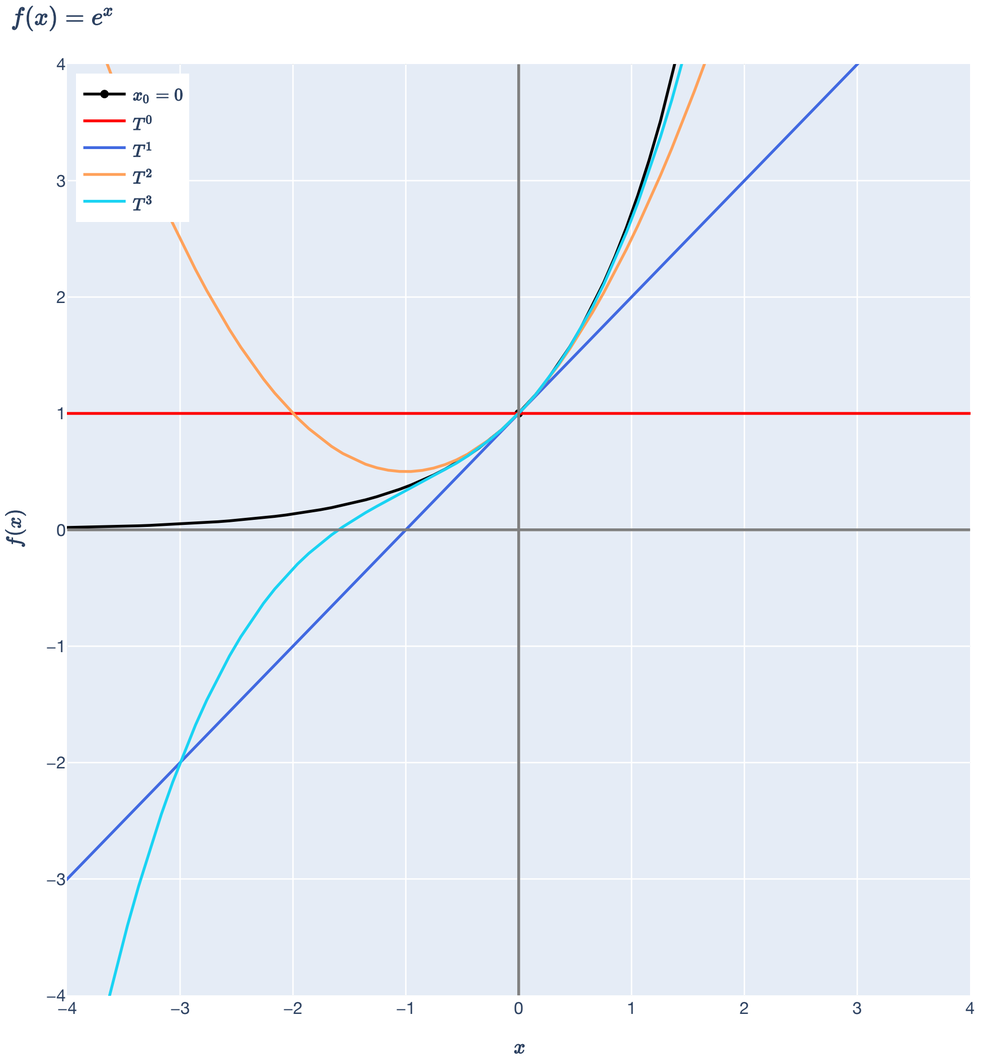

Moment Generating Function

Definition

The moment generating function (MGF) of a random variable X is the function $M_X : \mathbb{R} \to \mathbb{R}$ defined:

$$M_X(t) := \mathbb{E}[e^{tX}] = \int e^{tx} dF_X(x).$$

If M_X is well-defined in an interval around $t = 0$,

$$M_X'(0) = \left[\frac{d}{dt}\mathbb{E}[e^{tX}]\right]_{t=0} = \mathbb{E}\left[\frac{d}{dt}e^{tX}\right]_{t=0} = \mathbb{E}[Xe^{tX}]_{t=0} = \mathbb{E}[X].$$

Generally, the kth derivative at $t = 0$ gives the kth moment of X:

$$M^{(k)}(0) = \mathbb{E}[X^k].$$

Moment Generating Function

Properties

Theorem (MGF characterizes distributions). Let X and Y be random variables. If there exists some $\delta \in \mathbb{R}$ where $M_X(t) = M_Y(t)$ for all t in a neighborhood $B_\delta(0)$ around 0, then X and Y have the same distribution:

$$\mathbb{P}_X = \mathbb{P}_Y \text{ and } F_X(t) = F_Y(t) \text{ for their CDFs } F_X \text{ and } F_Y.$$

Theorem (MGF of Standard Normal). Let $Z \sim N(0,1)$. The MGF of Z exists and is given by:

$$M_Z(t) = e^{t^2/2}.$$

Theorem (Sums of independent RVs). If $X_1, \ldots, X_n$ are independent random variables and $S = \sum_{i=1}^{n} X_i$, then $M_S(t) = \prod_{i=1}^{n} M_{X_i}(t)$ where $M_{X_i}(t)$ is the MGF of X_i.

Central Limit Theorem

Proof and Implications

Central Limit Theorem

Theorem Statement

Theorem (Central Limit Theorem). Let $X_1, \ldots, X_n$ be independent and identically distributed (i.i.d.) random variables with finite mean $\mu := \mathbb{E}[X_i]$ and finite variance $\sigma^2 := \mathrm{Var}(X_i)$.

Let their *sample average* be denoted as $\overline{X}_n := \frac{1}{n}\sum_{i=1}^{n} X_i$ and let their "standardized" average be:

$$Z_n := \frac{\overline{X}_n - \mu}{\sqrt{\mathrm{Var}(\overline{X}_n)}} = \frac{\sqrt{n}(\overline{X}_n - \mu)}{\sigma}$$

Then, Z_n converge to $Z \sim N(0,1)$ in distribution. That is,

$$\lim_{n\to\infty} \mathbb{P}(Z_n \leq z) = \Phi(z) := \int_{-\infty}^{z} \frac{1}{\sqrt{2\pi}} e^{-x^2/2} dx = \mathbb{P}(Z \leq z).$$

Probability statements about $\overline{X}_n$ can be approximated using a Gaussian distribution!

Central Limit Theorem

Proof Sketch of CLT

Goal: Show the MGF of $Z_n := \sqrt{n}\overline{X}_n/\sigma$ approaches $M_Z(t) = e^{t^2/2}$.

Step 1: MGF property on sum of iid random variables to get an MGF for sample mean.

Step 2: Second-order approximation of MGF using Taylor's Theorem.

Step 3: We have first and second order information (mean $\mu = \mathbb{E}[X]$ and variance σ^2), so plug into Taylor expansion.

Step 4: Send $n \to \infty$ to show that Taylor's Theorem remainder is small.

The Gaussian Distribution

Properties of Gaussians

Standardization. If $X \sim N(\mu, \sigma^2)$, then $Z = (X - \mu)/\sigma \sim N(0,1)$. As a result:

$$\begin{aligned}\mathbb{P}(a < X < b) &= \mathbb{P}\left(\frac{a-\mu}{\sigma} < Z < \frac{b-\mu}{\sigma}\right) \\ &= \Phi\left(\frac{b-\mu}{\sigma}\right) - \Phi\left(\frac{a-\mu}{\sigma}\right)\end{aligned}$$

Standard to general. If $Z \sim N(0,1)$, then $X = \mu + \sigma Z \sim N(\mu, \sigma^2)$.

Sums of Gaussians. If $X_i \sim N(\mu_i, \sigma_i^2)$ for $i = 1, \ldots, n$ are independent, then

$$\sum_{i=1}^{n} X_i \sim N\left(\sum_{i=1}^{n} \mu_i, \sum_{i=1}^{n} \sigma_i^2\right).$$

Central Limit Theorem

Equivalent Approximations

For i.i.d. random variables $X_1, \ldots, X_n$, let:

$$\overline{X}_n := \frac{1}{n}\sum_{i=1}^{n} X_i$$

$$Z_n := \frac{\overline{X}_n - \mu}{\sqrt{\mathrm{Var}(\overline{X}_n)}} = \frac{\sqrt{n}(\overline{X}_n - \mu)}{\sigma}$$

$\Longrightarrow$

For large enough n, the CLT statement allows the equivalent approximations…

$$\overline{X}_n \approx N\left(\mu, \frac{\sigma^2}{n}\right)$$

$$\overline{X}_n - \mu \approx N\left(0, \frac{\sigma^2}{n}\right)$$

$$\sqrt{n}(\overline{X}_n - \mu) \approx N(0, \sigma^2)$$

$$\frac{\sqrt{n}(\overline{X}_n - \mu)}{\sigma} \approx N(0,1)$$

Central Limit Theorem

Two Implications

$$\overline{X}_n \approx N\left(\mu, \frac{\sigma^2}{n}\right) \text{ for large enough } n.$$

This says three things:

1. The mass of $\overline{X}_n$ centers to μ, the true mean of the i.i.d. random variables.

2. The spread of draws from $\overline{X}_n$ gets smaller and smaller as n grows.

3. The “shape” of this distribution is a bell-curve.

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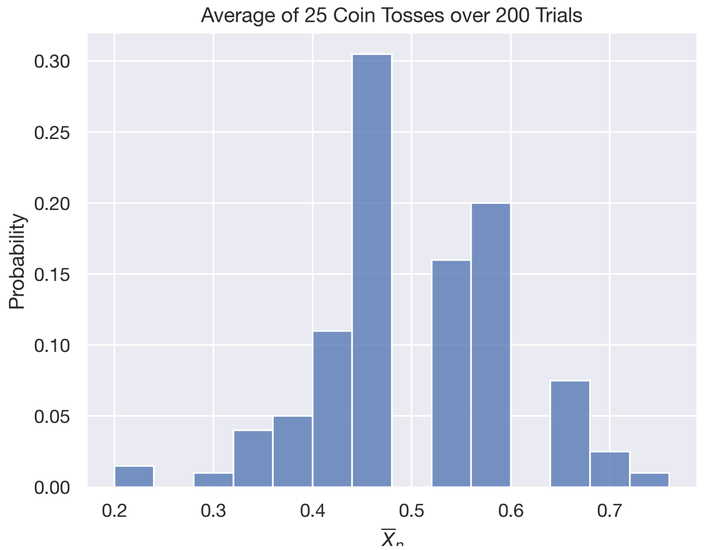

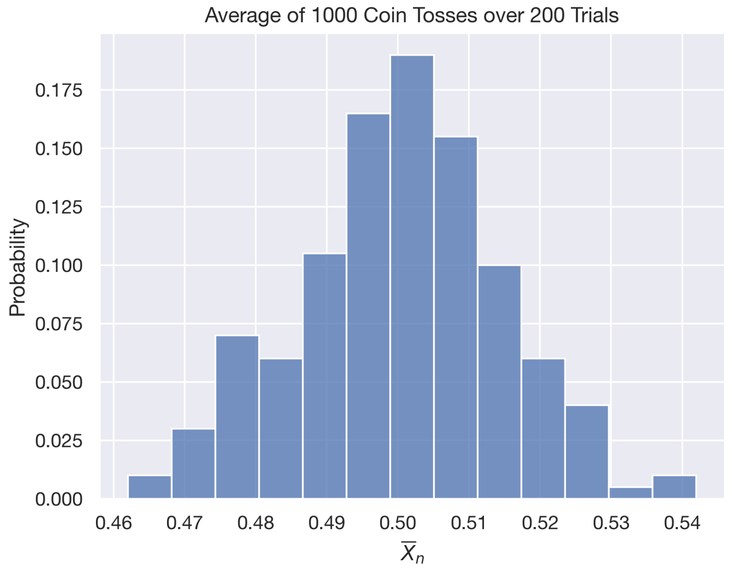

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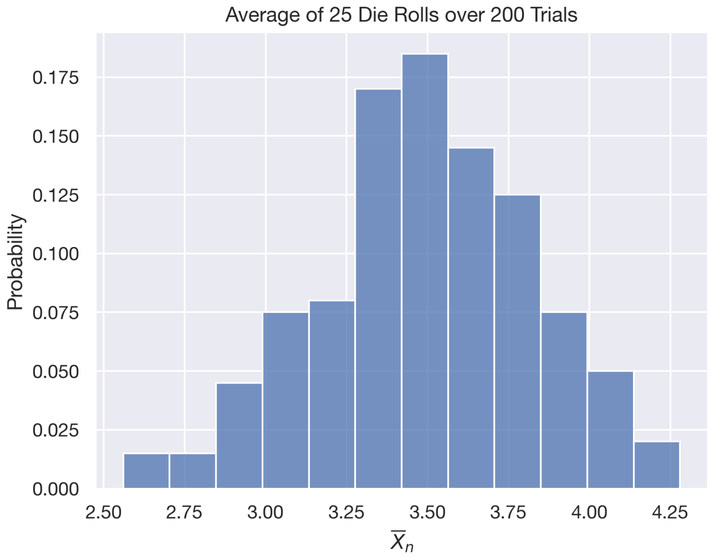

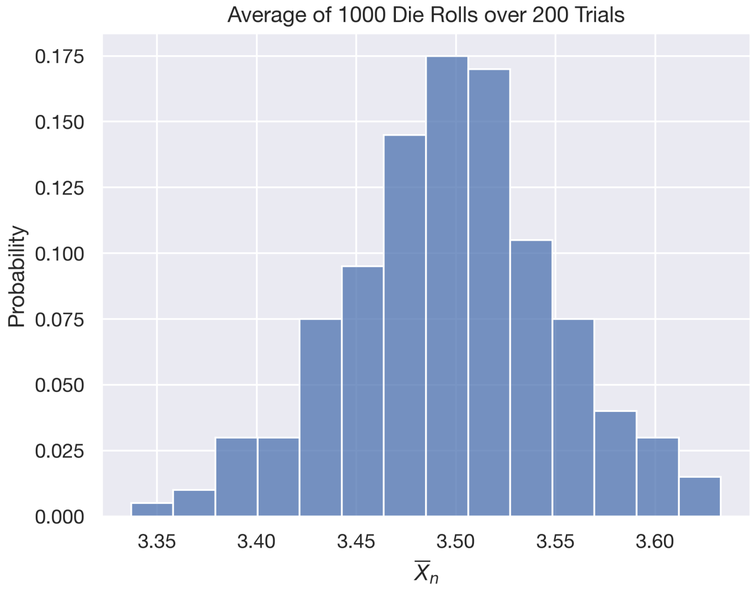

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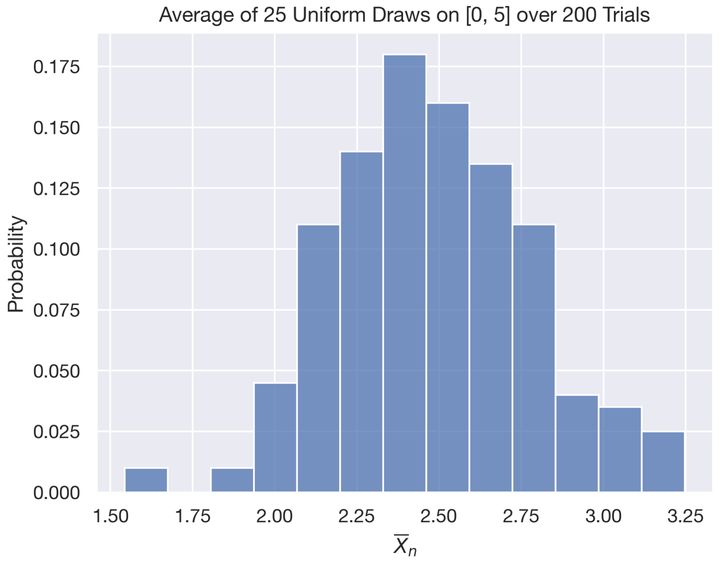
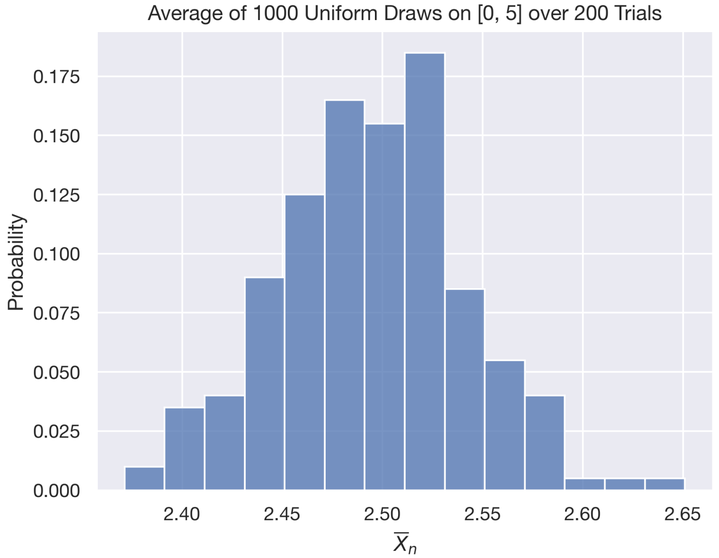




“Named” Distributions

Discrete Examples

Discrete Distributions

Discrete Random Variables

A discrete random variable X takes on a finite or countably infinite number of values.

CDF. $F_X(x) := \mathbb{P}(X \leq x)$**.**

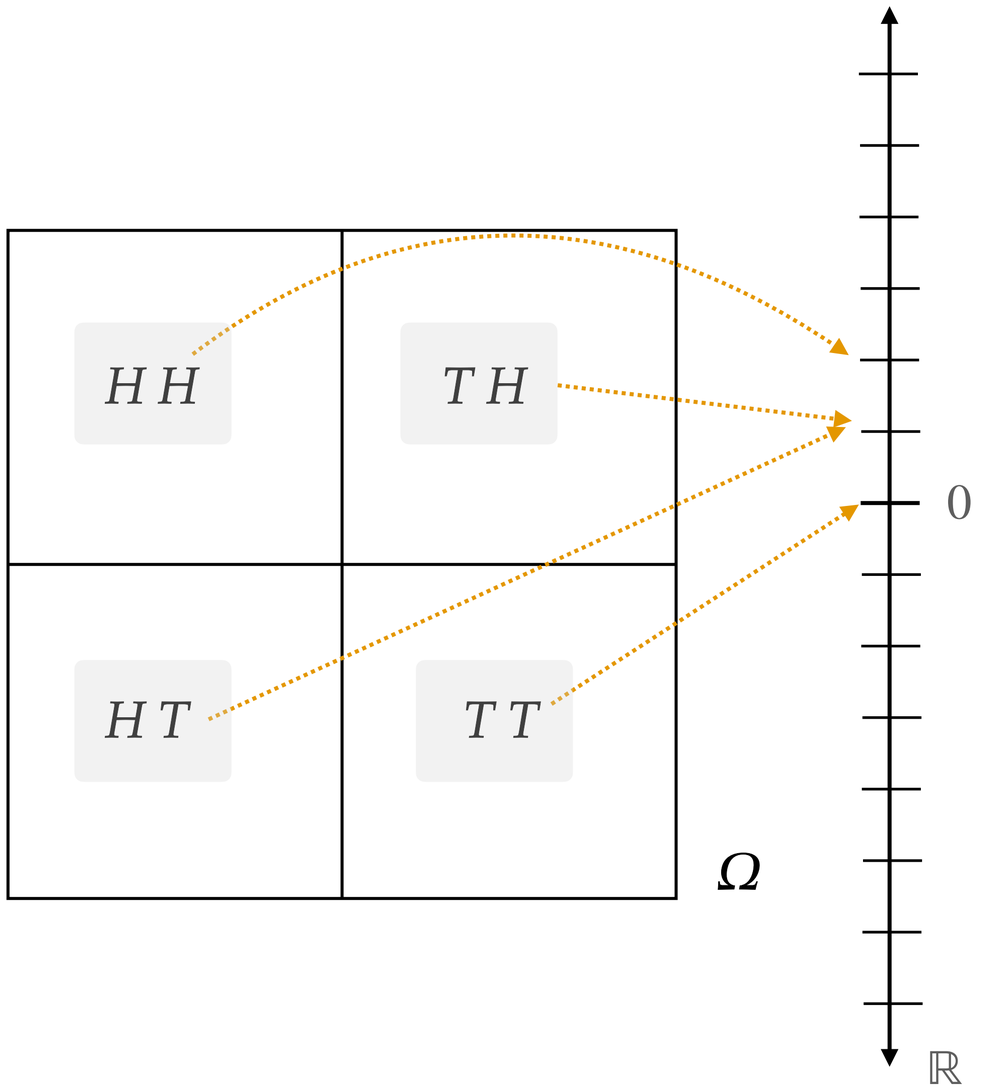
PMF. $p_X(x) = \mathbb{P}(X = x)$ and $\mathbb{P}(X \in A) = \sum_{x \in A} \mathbb{P}(X = x)$.

PMF is the height of the "jump" of F_X at x.

PMF is nonnegative.

PMF sums to 1.

Expectation. $\mathbb{E}(X) = \sum_x x p_X(x) = \sum_x x \mathbb{P}(X = x)$.



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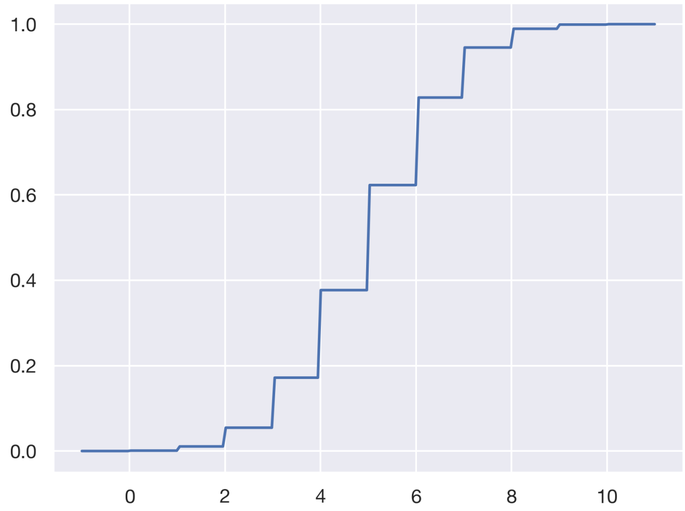
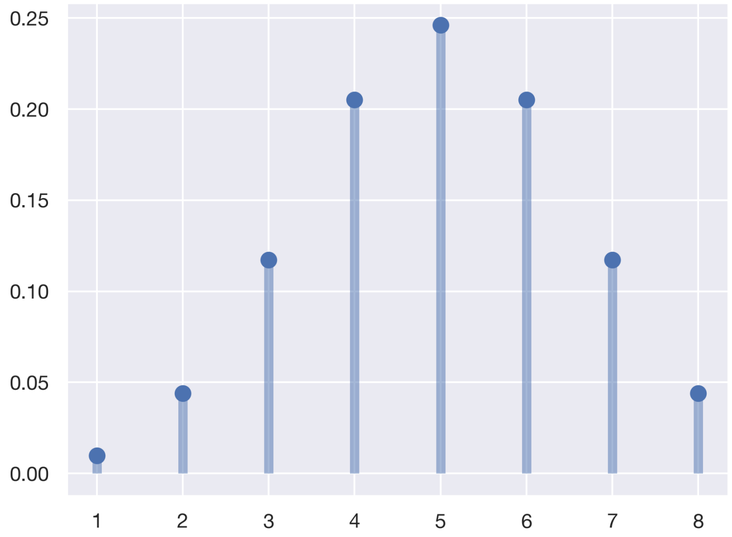




The Point Mass Distribution

"Story" of the Distribution

A single point $a \in \mathbb{R}$ has all the probability mass, every other point has zero mass.

Example. Let X be a random variable putting all its mass on $a = 1$.

The Point Mass Distribution

Properties

$$X \sim \delta_a$$

Parameters: $a \in \mathbb{R}$, the point mass.

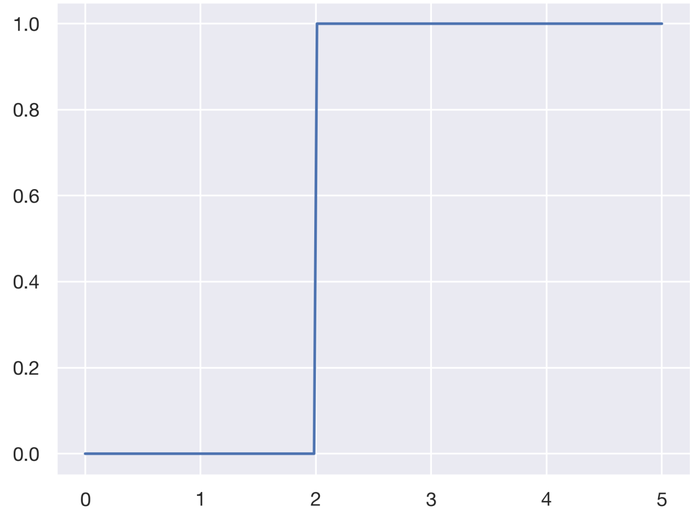
CDF: $F_X(x) = \begin{cases} 0 & x < a \\ 1 & x \geq a \end{cases}$

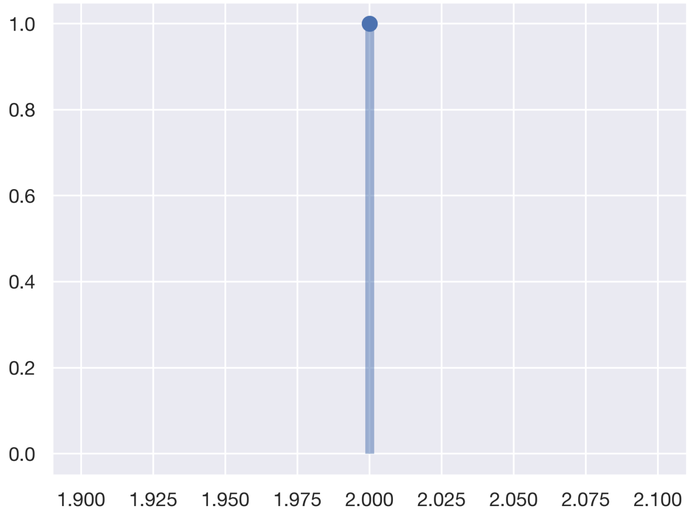
PMF: $p_X(x) = \begin{cases} 1 & x = a \\ 0 & x \neq a \end{cases}$

Mean: $\mathbb{E}[X] = a$.

Variance: $\mathrm{Var}(X) = 0$.

MGF: $M_X(t) = e^{ta}$.





The Discrete Uniform Distribution

"Story" of the Distribution

Randomly choose an element in a finite set S, with equal probability for each element.

Example. Let X be the number on the roll of a fair, six-sided die.

The Discrete Uniform Distribution

Properties

$$X \sim \text{Unif}(k)$$

Parameters: $k \in \mathbb{N}$, the number of possible states, denoted $\{1,2,\ldots,k\}$.

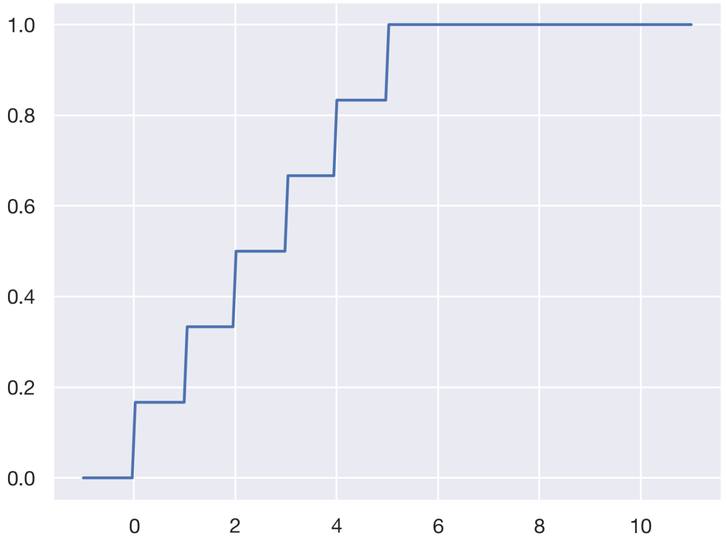
CDF: $F_X(x) = \dfrac{\lfloor k \rfloor}{n}$

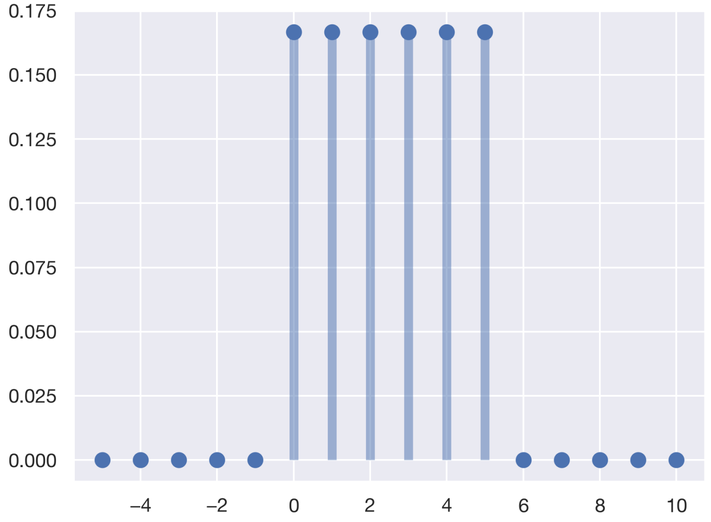
PMF: $p_X(x) = \begin{cases} 1/k & x = 1,\ldots,k \\ 0 & \text{otherwise} \end{cases}$

Mean: $\mathbb{E}[X] = \dfrac{k+1}{2}.$

Variance: $\text{Var}(X) = \dfrac{k^2-1}{12}.$

MGF: $M_X(t) = \dfrac{e^t(1-e^{kt})}{k(1-e^t)}.$





The Bernoulli Distribution

"Story" of the Distribution

Flip a coin that lands heads with probability p and tails with probability $1 - p$.

Example. Let X denote the outcome of a presidential election with two candidates and a tie-breaking mechanism, with 1 indicating Candidate A and 0 indicating Candidate B.

The Bernoulli Distribution

Properties

$$X \sim \text{Ber}(p)$$

Parameters: $p \in [0,1]$, the success probability.

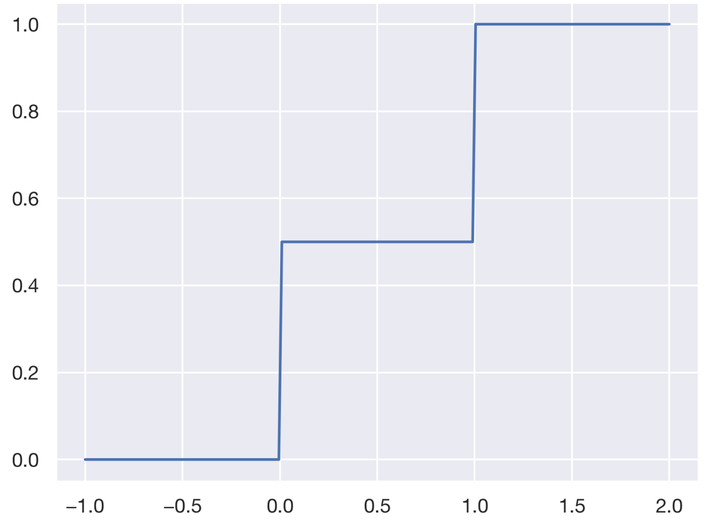
CDF: $F_X(x) = \begin{cases} 0 & x < 0 \\ 1-p & 0 \le x < 1 \\ 1 & x \ge 1 \end{cases}$

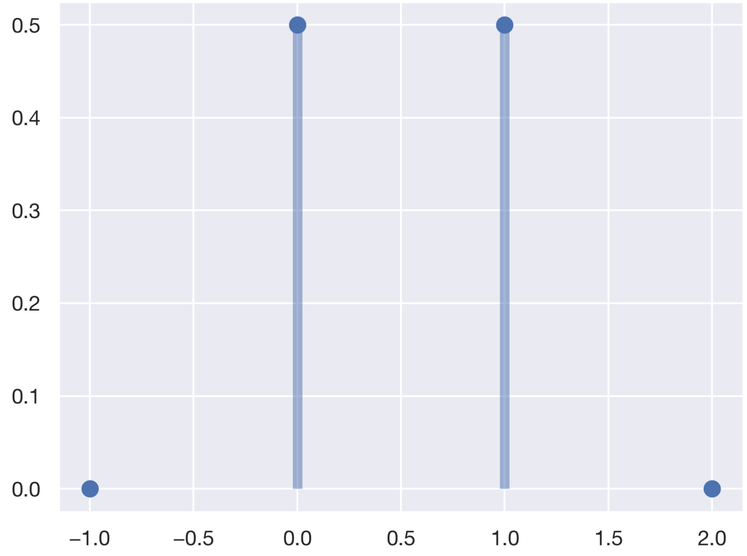
PMF: $p_X(x) = \begin{cases} 1-p & x = 0 \\ p & x = 1 \\ 0 & \text{otherwise} \end{cases}$

Mean: $\mathbb{E}[X] = p$.

Variance: $\text{Var}(X) = p(1-p)$.

MGF: $M_X(t) = 1 - p + pe^t$.





The Binomial Distribution

"Story" of the Distribution

Flip n independent coins, each landing heads with probability p and tails with probability $1-p$, and count the number of heads.

Example. Consider an urn with 7 orange balls and 3 green balls. Let X count the total number of orange balls drawn after drawing $n = 10$ balls *with replacement* from the urn.

The Binomial Distribution

Properties

$X \sim \text{Bin}(n, p)$

Parameters: $n \in \{0,1,2,\ldots\}$, the number of trials. $p \in [0,1]$, the success probability.

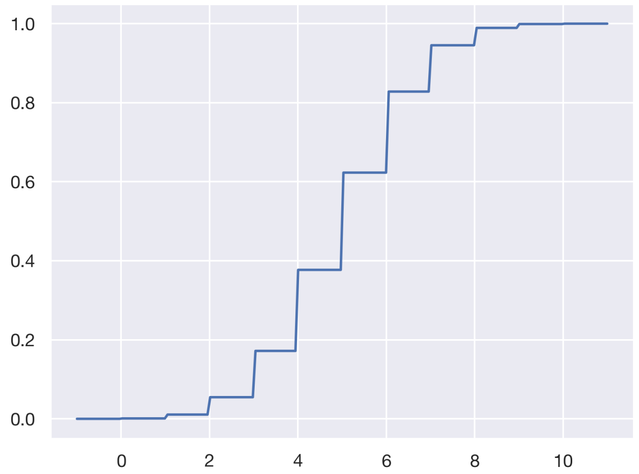
CDF: $F_X(x) = \sum_{i=0}^{\lfloor x \rfloor} \binom{n}{i} p^i (1-p)^{n-i}$

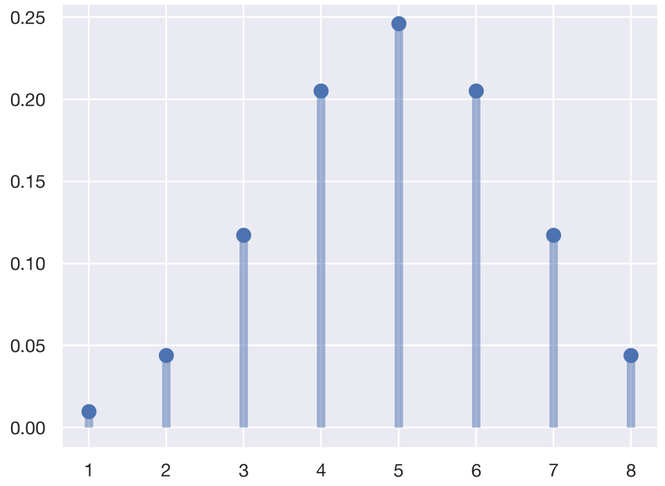
PMF: $p_X(x) = \binom{n}{x} p^k (1-p)^{n-x}$

Mean: $\mathbb{E}[X] = np.$

Variance: $\text{Var}(X) = np(1-p).$

MGF: $M_X(t) = (1 - p + pe^t)^n.$





The Geometric Distribution

"Story" of the Distribution

Flip coins, each landing heads with probability p and tails with probability $1-p$, until you see your first head. How many trials occurred?

Example. Let X be the number of rolls needed from repeatedly rolling a fair, six-sided die until 3 shows up.

The Geometric Distribution

Properties

$X \sim \text{Geom}(p)$

Parameters: $p \in [0,1]$, the success probability.

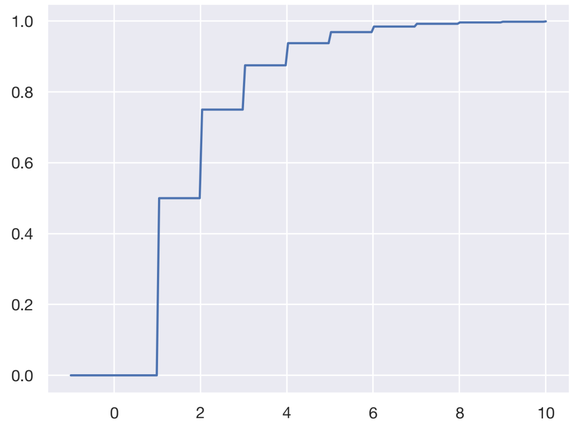
CDF: $F_X(x) = 1 - (1-p)^{\lfloor x \rfloor}$ if $x \geq 1$, 0 otherwise

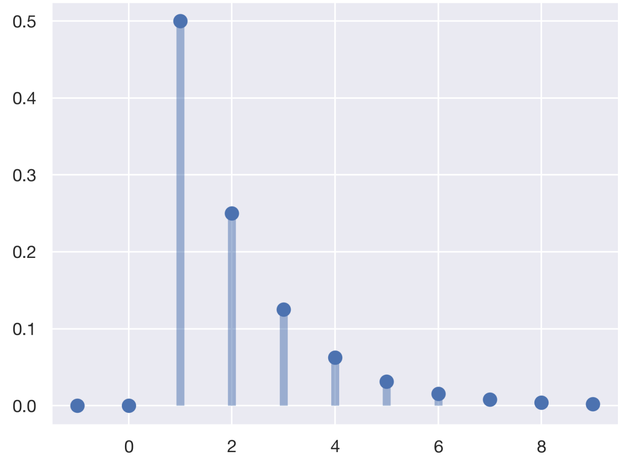
PMF: $p_X(x) = \begin{cases} (1-p)^{x-1}p & x \in \{1,2,3,\ldots,\} \\ 0 & \text{otherwise} \end{cases}$

Mean: $\mathbb{E}[X] = 1/p.$

Variance: $\text{Var}(X) = \dfrac{1-p}{p^2}.$

MGF: $M_X(t) = \dfrac{pe^t}{1-(1-p)e^2}$ for $t < -\ln(1-p).$





The Poisson Distribution

"Story" of the Distribution

Count the number of rare, "memoryless" events in a fixed time interval, if the average number of events in that interval is λ.

Example. Let X be the number of text messages you receive in a given hour if you receive an average of $\lambda = 3$ messages per hour.

Example. Let X count the number of times a raindrop hits a specific square inch in a minute, if that square inch receives an average of $\lambda = 10$ drops per minute.

Example. Let X count the number of V-2 missile impacts in *Gravity's Rainbow* per kilometer squared per fortnight, where each km^2 receives $\lambda = 0.3$ hits per fortnight.

The Poisson Distribution

Properties

$$X \sim \text{Pois}(\lambda)$$

Parameters: $\lambda \in (0,\infty)$, the success rate.

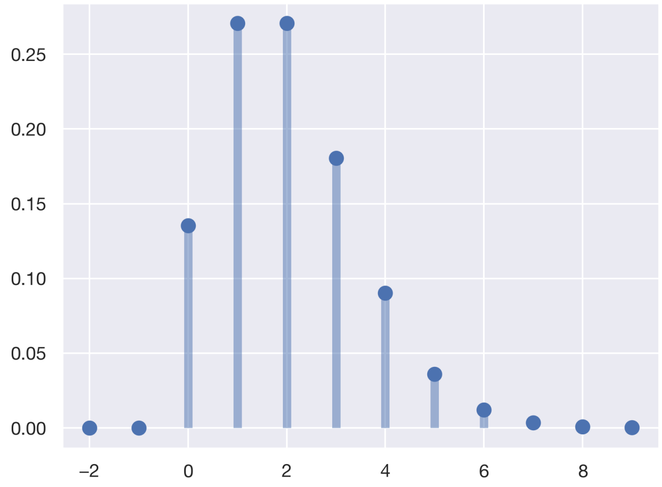
CDF: $F_X(x) = e^{-\lambda} \sum_{j=0}^{\lfloor x \rfloor} \frac{\lambda^j}{j!}$

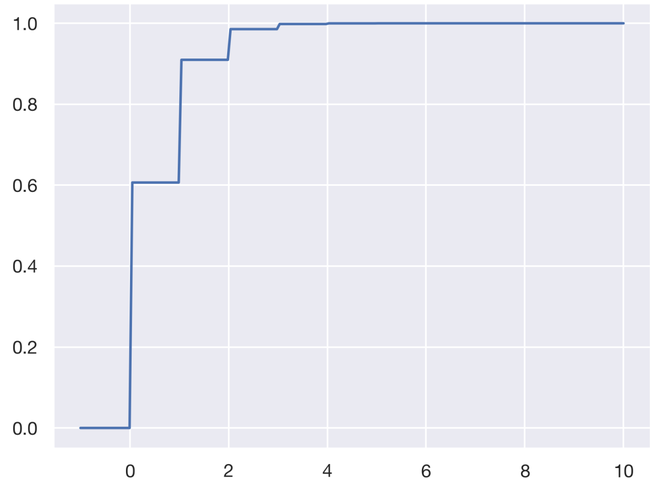
PMF: $p_X(x) = \frac{\lambda^k e^{-\lambda}}{k!}$

Mean: $\mathbb{E}[X] = \lambda$.

Variance: $\text{Var}(X) = \lambda$.

MGF: $M_X(t) = \exp(\lambda(e^t - 1))$.





“Named” Distributions

Continuous Examples

Continuous Distributions

Continuous Random Variables

A continuous random variable X takes on an uncountably infinite number of values. The probability at any point x is 0.

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

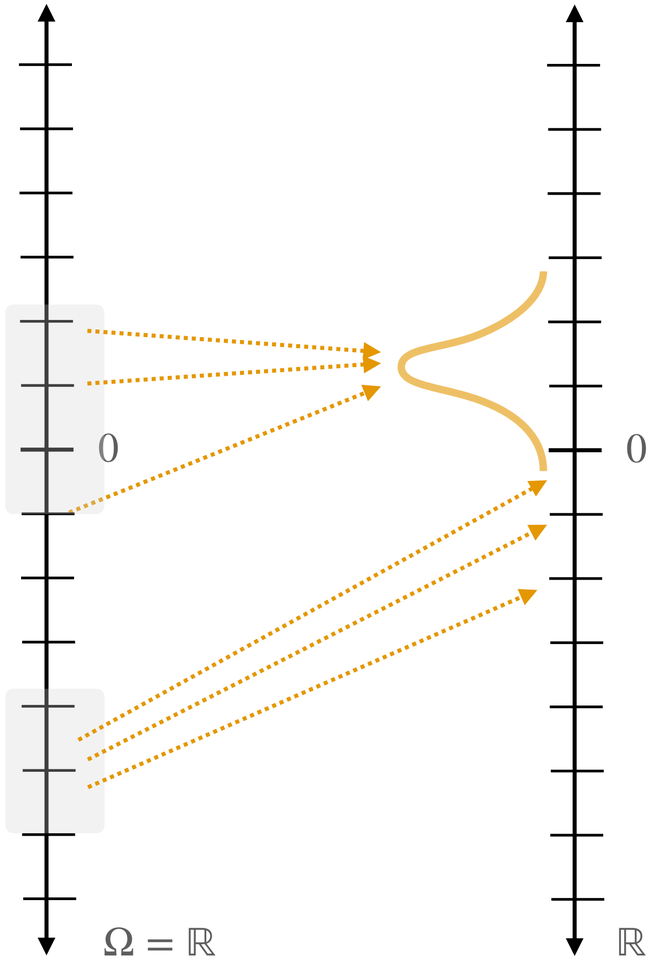
PDF. $p_X(x) = F'(x)$ and $\mathbb{P}(X \in A) = \int_A p_X(x)dx$.

PDF is the derivative of F.

PDF is nonnegative and integrates to 1.

PDF *does not* give probabilities at points.

Expectation. $\mathbb{E}(X) = \int_{-\infty}^{\infty} xp_X(x)dx$.



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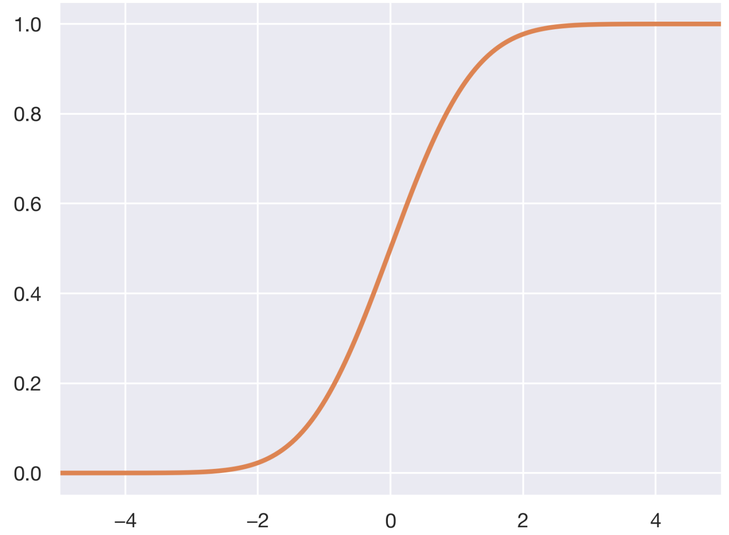
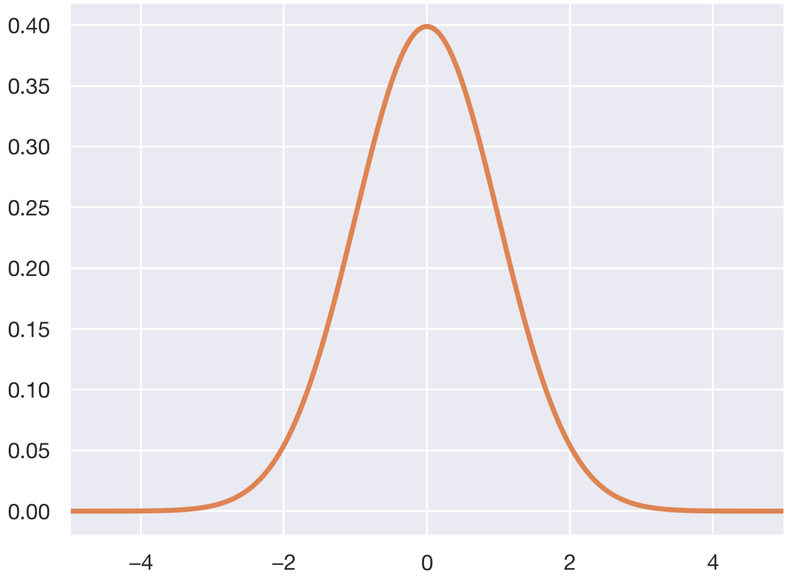
PDF *does not* give probabilities at points.

Expectation. $\mathbb{E}(X) = \int_{-\infty}^{\infty} xp_X(x)dx$.





The Uniform Distribution

"Story" of the Distribution

Draw a completely random number in the continuous interval from a to b.

Example. Let X be where you randomly break a stick of length $b = 20$ inches.

The Uniform Distribution

Properties

$$X \sim \text{Unif}(a, b)$$

Parameters: $-\infty < a < b < \infty$, the interval boundaries.

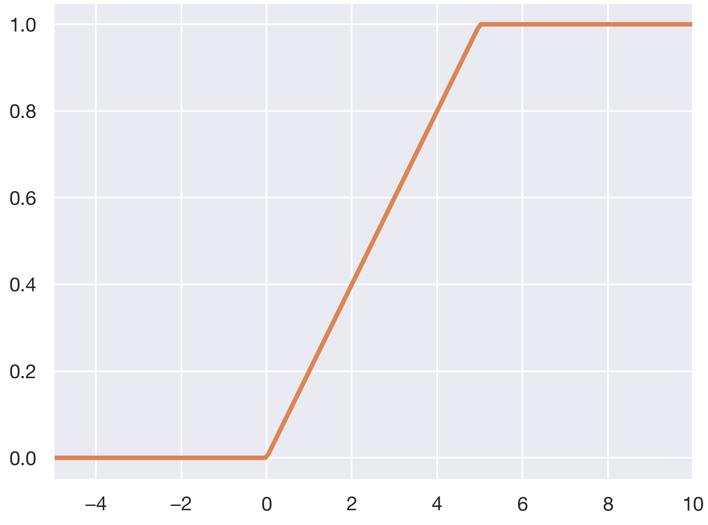
CDF: $F_X(x) = \begin{cases} 0 & x < a \\ \frac{x-a}{b-a} & x \in [a, b] \\ 1 & x > b \end{cases}$

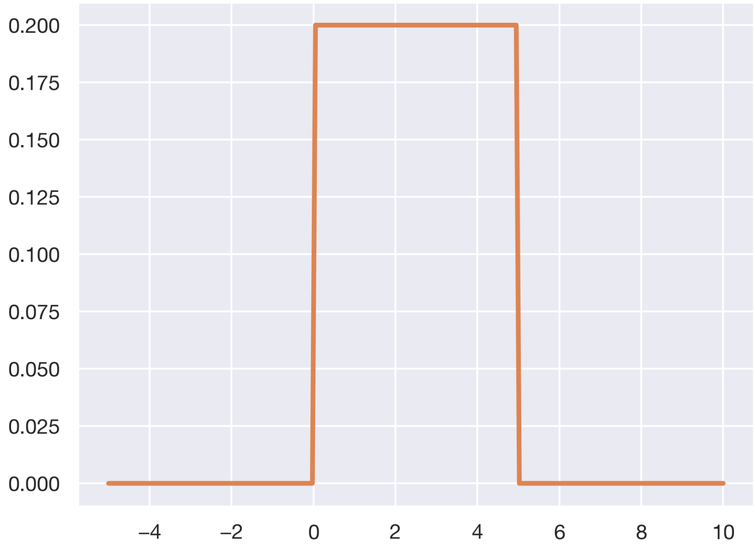
PDF: $p_X(x) = \begin{cases} \frac{1}{b-a} & x \in [a, b] \\ 0 & \text{otherwise} \end{cases}$

Mean: $\mathbb{E}[X] = \frac{1}{2}(a + b)$.

Variance: $\text{Var}(X) = \frac{1}{12}(b - a)^2$.

MGF: $M_X(t) = \frac{e^{tb} - e^{ta}}{t(b-a)}$ for $t \neq 0$ and $M_X(0) = 1$.





The Gaussian Distribution

"Story" of the Distribution

Draw a random number with probability distributed according to a "bell-shaped" curve.

Example. Let X be the height of a human male.

The Gaussian Distribution

Properties

$$X \sim N(\mu, \sigma^2)$$

Parameters: $\mu \in \mathbb{R}$ and $\sigma^2 \in \mathbb{R}_{>0}$.

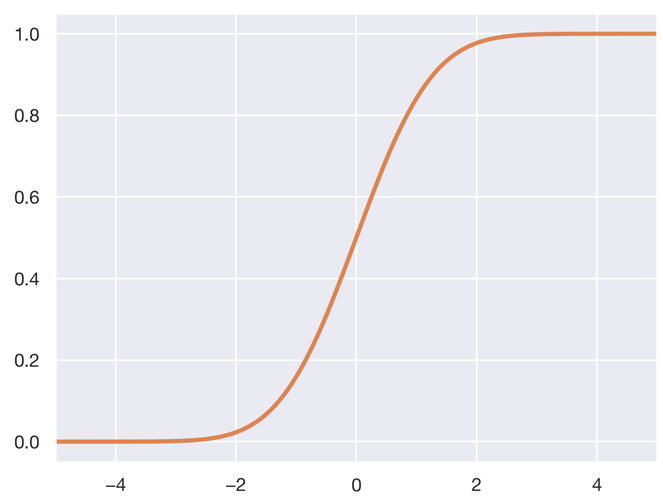
CDF: $F_X(x) = \int_{-\infty}^{x} p_X(x)dx = \Phi\left(\frac{x-\mu}{\sigma}\right)$ (no closed form)

PDF: $p_X(x) = \frac{1}{\sqrt{2\pi\sigma^2}} e^{-\frac{(x-\mu)^2}{2\sigma^2}}$

Mean: $\mathbb{E}[X] = \mu$.

Variance: $\mathrm{Var}(X) = \sigma^2$.

MGF: $M_X(t) = \exp(\mu t + \sigma^2 t^2/2)$.



The Chi-squared Distribution

"Story" of the Distribution

Add up k independent, squared standard Gaussian random variables.

Example. Let $\mathbf{z} = (z_1, z_2)$ be a random vector with independent entries $z_1 \sim N(0,1)$ and $z_2 \sim N(0,1)$. Then, $X = \|\mathbf{z}\|^2$ is a Chi-squared random variable with $k = 2$.

The Chi-squared Distribution

Properties

$$X \sim \chi^2(k)$$

Parameters: k, the "degrees of freedom."

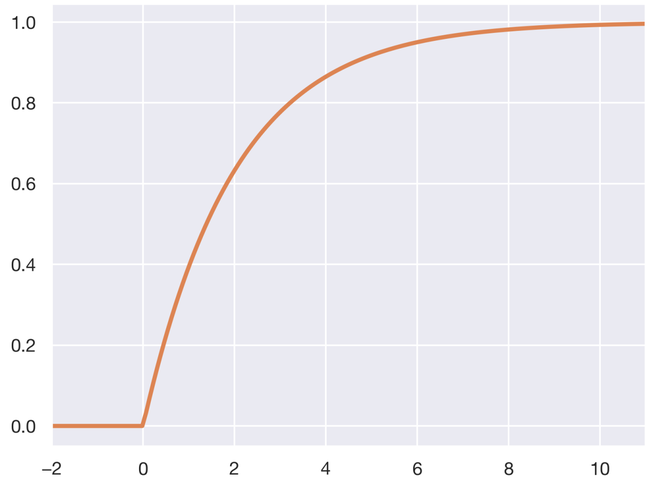
CDF: $F_X(x; 2) = 1 - e^{-x/2}$ (more complicated for $k \neq 2$)

PDF: $p_X(x) = \begin{cases} \frac{x^{k/2-1}e^{-x/2}}{2^{k/2}\int_0^\infty t^{k-1}e^{-t}dt} & x > 0 \\ 0 & \text{otherwise} \end{cases}$

Mean: $\mathbb{E}[X] = k$.

Variance: $\mathrm{Var}(X) = 2k$.

MGF: $M_X(t) = (1 - 2t)^{-k/2}$ for $t < 1/2$.



The Exponential Distribution

"Story" of the Distribution

The waiting time for a success in continuous time, where λ is the rate at which successes arrive.

Example. Let X be the time between receiving one text message and the next, where λ is the rate of text messages per unit time.

The Exponential Distribution

PDF, CDF, and MGF

$$X \sim \text{Expo}(\lambda)$$

Parameters: $\lambda > 0$, the success rate.

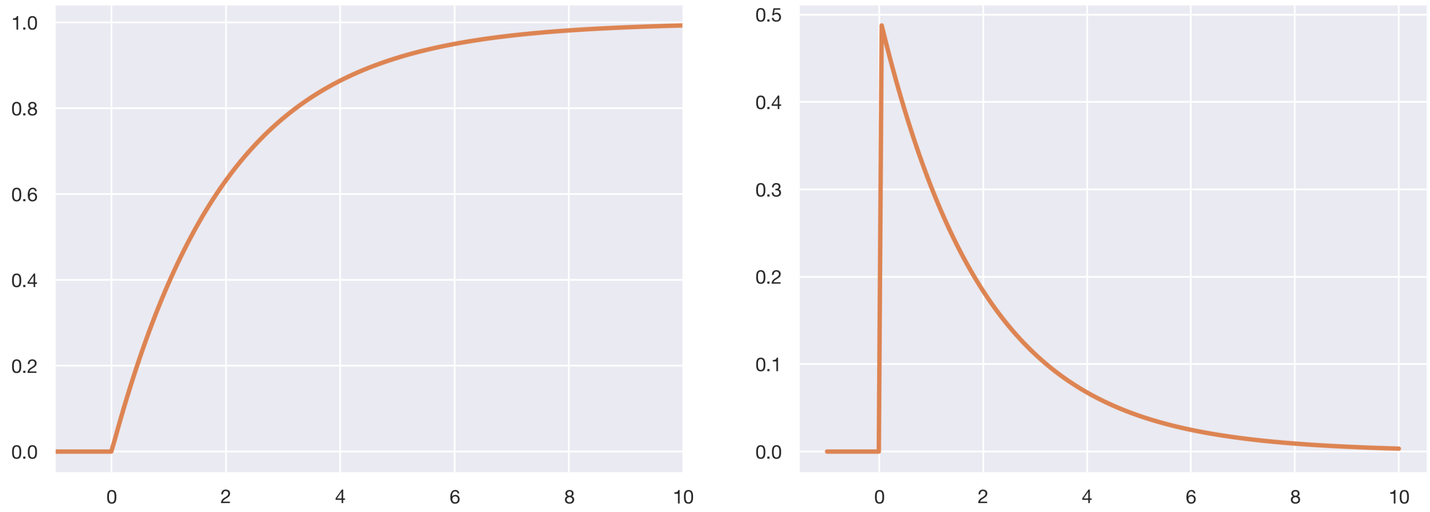
CDF: $F_X(x) = 1 - e^{-\lambda x}$

PDF: $p_X(x) = \lambda e^{-\lambda x}$

Mean: $\mathbb{E}[X] = 1/\lambda$.

Variance: $\text{Var}(X) = 1/\lambda^2$.

MGF: $M_X(t) = \dfrac{\lambda}{\lambda - t}$ for $t < \lambda$.



With certain parameters, equivalent to Chi-squared with 2 degrees of freedom.

Maximum Likelihood Estimation

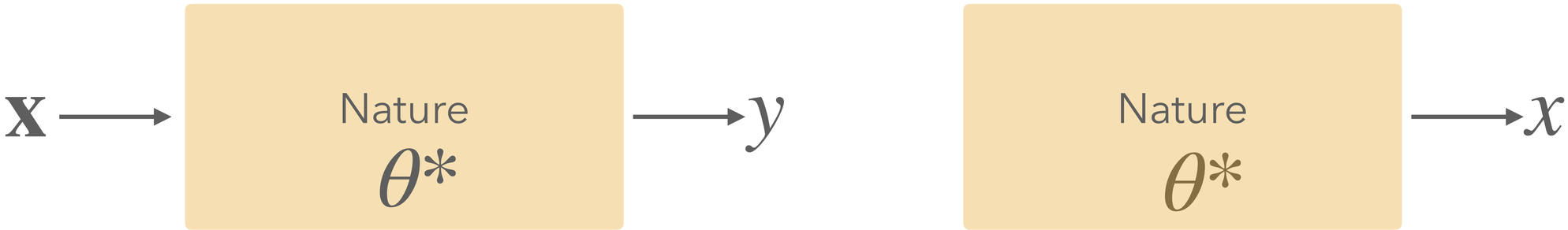
Intuition and Definition

Statistical Estimator

Intuition

A (statistical) estimator is a “best guess” at some (unknown) quantity of interest (the estimand) using observed data.

The quantity doesn’t have to be a single number; it could be, for example, a fixed vector, matrix, or function.



Statistical Estimator

Definition

Let $X_1, \ldots, X_n$ be n i.i.d. random variables drawn from some distribution $\mathbb{P}_X$ with parameter θ.

An estimator $\hat{\theta}_n$ of some fixed, unknown parameter θ is some function of $X_1, \ldots, X_n$:

$$\hat{\theta}_n = g(X_1, \ldots, X_n).$$

Defined similarly for random vectors.

Importantly: statistical estimators are functions of RVs, so they are *themselves* RVs!

Parametric Estimation vs. ERM

A different approach

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. There exists an **unknown** joint distribution $\mathbb{P}_{\mathbf{x},y}$ over $\mathbb{R}^d \times \mathbb{R}$, where we draw:

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

We then went on to minimize the empirical risk to get our model $f : \mathbb{R}^d \to \mathbb{R}$.

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

This uses no information about the distribution of the data (except iid)!

Parametric Estimation

Intuition

Suppose we have a good guess at the distribution generating some i.i.d. data $X_1, \ldots, X_n$.

"My data is probably generated from a Poisson distribution."

Then, we can restrict our attention to estimating a parametric model, a function $p(x; \theta)$ that depends on parameters $\theta = (\theta_1, \ldots, \theta_k)$ belonging to some parameter space $\Theta \subseteq \mathbb{R}^k$.

"Let's estimate $\lambda \in \mathbb{R}$ in the PMF $p(x; \lambda) = \dfrac{\lambda^k e^{-\lambda}}{k!}$."

If our assumption is good, then a good estimate $\hat{\theta}_n$ of θ might tell us everything we need to know about our data!

Parametric Estimation

Definition

A parametric model is a class of functions of the form:

$$\mathscr{F} := \{f(x;\theta) : \theta \in \Theta\},$$

where $\Theta \subseteq \mathbb{R}^k$ is the parameter space and $\theta = (\theta_1, \ldots, \theta_k)$ are the model parameters.

Example. The parameter space for the Gaussian distribution $N(\mu, \sigma^2)$ is

$$\Theta = \{(\mu, \sigma) : \mu \in \mathbb{R}, \sigma > 0\}.$$

Example. The parameter space for the Bernoulli distribution $\mathrm{Ber}(p)$ is

$$\Theta = \{p : 0 \leq p \leq 1\}.$$

Maximum Likelihood Estimation

Intuition

One way to do *parametric estimation* given i.i.d. data $X_1, \ldots, X_n$ is maximum likelihood estimation.

We assume that $X_1, \ldots, X_n$ are from a distribution with PDF $p(x; \theta)$ and parameter space $\Theta \subseteq \mathbb{R}^k$.

"Assume that the data come from a Gaussian with $p(x; \mu, \sigma) = \frac{1}{\sigma\sqrt{2\pi}} \exp\left\{ -\frac{1}{2\sigma^2}(x - \mu)^2 \right\}$*"*

We consider the likelihood function which maps from parameters Θ to some positive number: the "likelihood" of those parameters explaining the data.

Maximum Likelihood Estimation

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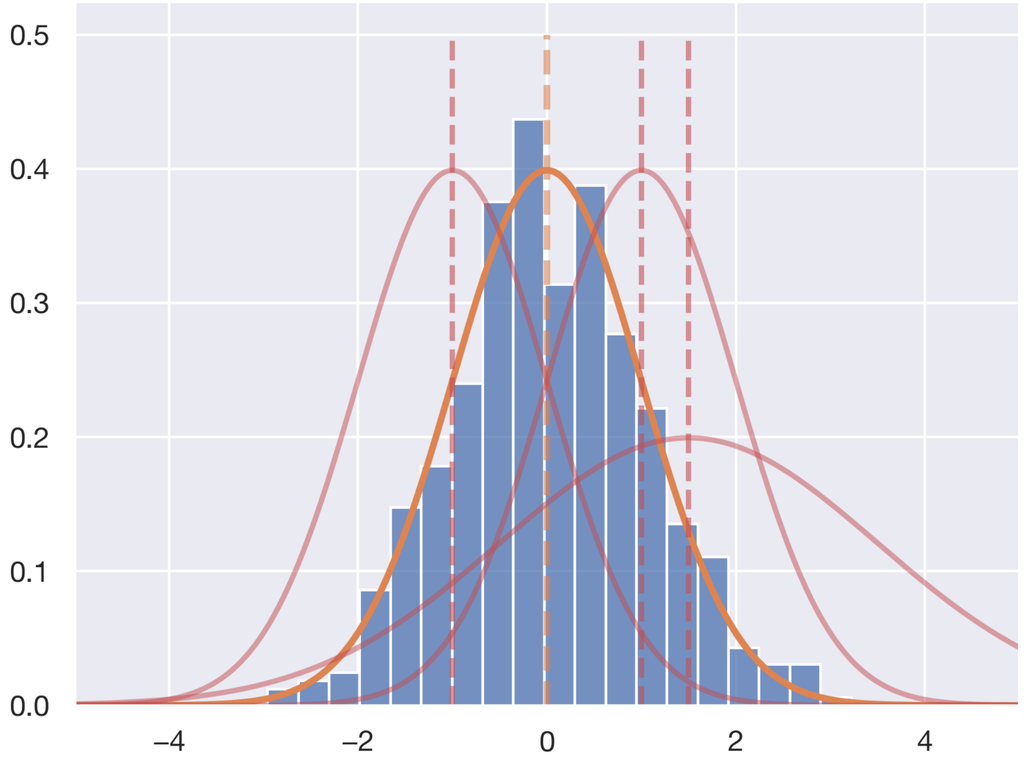

Maximum Likelihood Estimation

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One way to do *parametric estimation* given i.i.d. data $X_1, \ldots, X_n$ is maximum likelihood estimation.

We assume that $X_1, \ldots, X_n$ are from a distribution with PDF $p(x; \theta)$ and parameter space $\Theta \subseteq \mathbb{R}^k$.

"Assume that the data come from a Poisson distribution with $p_X(x) = \frac{\lambda^k e^{-\lambda}}{k!}$*"*

We consider the likelihood function which maps from parameters Θ to some positive number: the "likelihood" of those parameters explaining the data.

Maximum Likelihood Estimation

Definition

Consider the parametric model

$$\mathcal{F} := \{f(x;\theta) : \theta \in \Theta\}.$$

Let $X_1, \ldots, X_n$ be i.i.d. random variables (or random vectors $\mathbf{x}_1, \ldots, \mathbf{x}_n$). The likelihood function is the function $L_n : \Theta \to [0,\infty)$ defined by:

$$L_n(\theta) := \prod_{i=1}^{n} f(X_i;\theta).$$

Note that $X_1, \ldots, X_n$ are fixed here, so this is *just* a function of θ.

"How well does θ describe my data $X_1, \ldots, X_n$?"

Maximum Likelihood Estimation

Why log-likelihood?

The log-likelihood function is the function defined by:

$$\mathscr{L}_n(\theta) := \log L_n(\theta) = \sum_{i=1}^{n} \log f(X_i; \theta).$$

The maximum likelihood estimator $\hat{\theta}_{MLE}$ is the value of θ that maximizes $L_n(\theta)$.

$$\hat{\theta}_{MLE} = \arg\max_{\theta} L_n(\theta) = \arg\max_{\theta} \mathscr{L}_n(\theta).$$

$$\hat{\theta}_{MLE} = \arg\min_{\theta} -L_n(\theta) = \arg\min_{\theta} -\mathscr{L}_n(\theta)$$

$\log(\cdot)$ is a *monotonic* function, so the maximizer of $\log f$ corresponds to the maximizer of f.

MLE for Bernoulli

Step 1: Write down likelihood function

Example. Suppose $X_1, \ldots, X_n \sim \text{Ber}(p)$, so our parametric model is:

$$\mathcal{F} = \left\{ f(x; p) = p^x (1-p)^{1-x} : p \in [0,1] \right\}$$

$\Theta = \{p : 0 \leq p \leq 1\}$. The unknown parameter θ is p.

Likelihood function. The likelihood function is

$$L_n(\theta) = L_n(p) = \prod_{i=1}^{n} f(X_i; p) = \prod_{i=1}^{n} p^{X_i}(1-p)^{1-X_i} = p^{\sum_{i=1}^{n} X_i}(1-p)^{n-\sum_{i=1}^{n} X_i}.$$

Denote $S := \sum_{i=1}^{n} X_i$, and the likelihood function is:

$$L_n(p) = p^S (1-p)^{n-S}$$

MLE for Bernoulli

Step 2: Simplify using log-likelihood

Example. Suppose $X_1, \ldots, X_n \sim \mathrm{Ber}(p)$, so our parametric model is:

$$\mathcal{F} = \left\{ f(x;p) = p^x (1-p)^{1-x} : p \in [0,1] \right\}$$

$\Theta = \{p : 0 \leq p \leq 1\}$. The unknown parameter θ is p.

Likelihood function. Denote $S := \sum_{i=1}^{n} X_i$, and the likelihood function is:

$$L_n(p) = p^S (1-p)^{n-S}$$

Log-likelihood function. The log-likelihood is

$\mathscr{L}_n(p) = S \log p + (n-S)\log(1-p)$. Now optimize this with respect to p!

MLE for Bernoulli

Step 3: Optimize log-likelihood using calculus

Example. Suppose $X_1, \ldots, X_n \sim \mathrm{Ber}(p)$, so our parametric model is:

$$\mathscr{F} = \left\{ f(x; p) = p^x (1-p)^{1-x} : p \in [0,1] \right\}$$

$\Theta = \{p : 0 \leq p \leq 1\}$. The unknown parameter θ is p.

Optimizing the negative log-likelihood. We need to solve the optimization problem:

$$\underset{p \in [0,1]}{\text{minimize}} \quad -\mathscr{L}_n(p) = -S \log p + (S-n) \log(1-p).$$

First order condition: $\nabla_p \mathscr{L}_n(p) = -\frac{S}{p} - \frac{S-n}{1-p} = 0.$

Solving for p, we get: $\hat{p}_{MLE} = \frac{S}{n} = \frac{1}{n} \sum_{i=1}^{n} X_i.$

Maximum Likelihood Estimation

Example: Bernoulli

Example. Suppose $X_1, \ldots, X_n \sim \text{Ber}(p)$, so our parametric model is:

$$\mathscr{F} = \left\{ f(x;p) = p^x (1-p)^{1-x} : p \in [0,1] \right\}$$

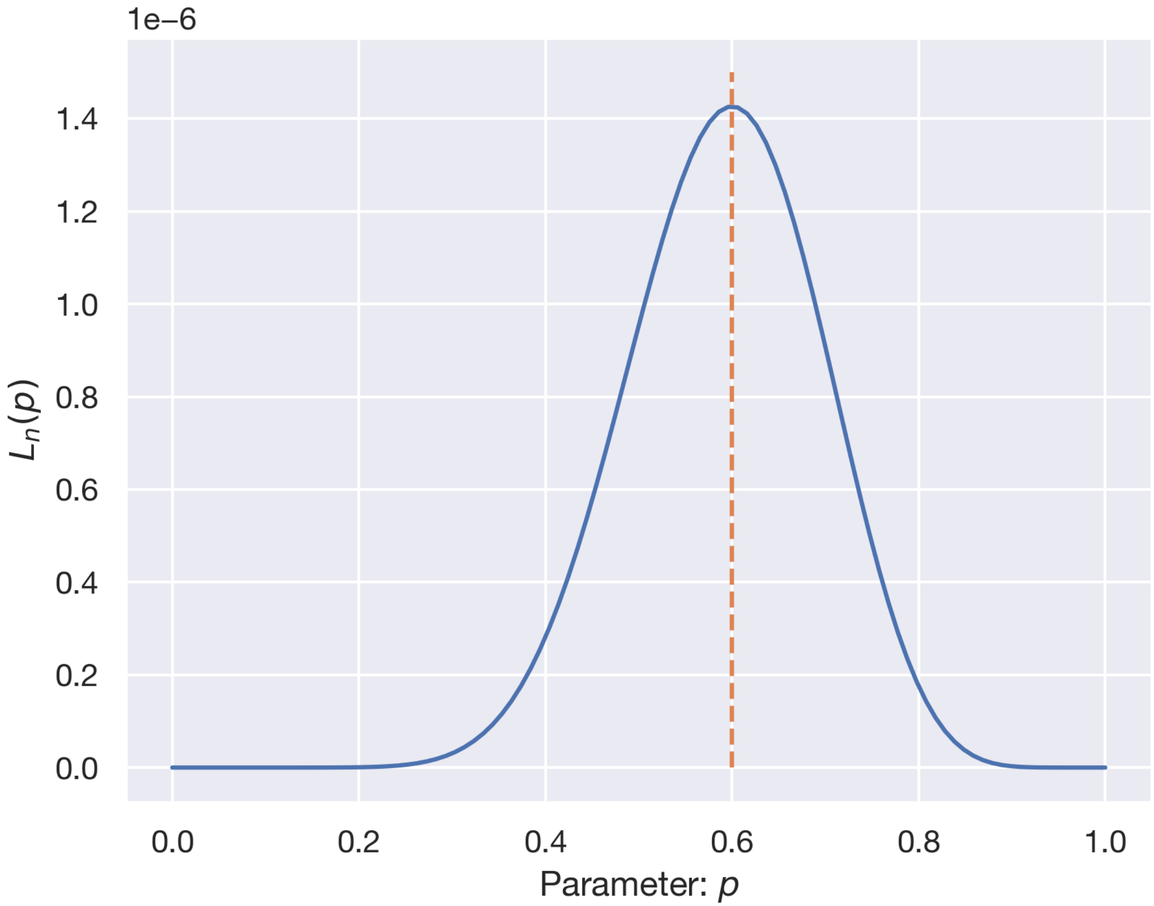
$\Theta = \{p : 0 \leq p \leq 1\}$. The unknown parameter θ is p.

The likelihood function is:

$$L_n(p) = p^{\sum_{i=1}^n X_i} (1-p)^{n - \sum_{i=1}^n X_i}$$

The maximum likelihood estimator of the estimand p is:

$$\hat{p}_{MLE} = \frac{S}{n} = \frac{1}{n} \sum_{i=1}^{n} X_i.$$



Maximum Likelihood Estimation

Properties of the MLE

Under certain conditions on the *statistical model* with true parameter θ, the MLE is…

Consistent. As $n \to \infty$, the MLE $\hat{\theta}_{MLE}$ satisfies $\mathbb{P}[\ \ \hat{\theta}_{MLE} - \theta\ \ > \epsilon] \to 0$.

Equivariant. If $\hat{\theta}_{MLE}$ is the MLE of θ, then $g(\hat{\theta}_{MLE})$ is the MLE of $g(\theta)$.

Asymptotically Normal. The random variable $(\hat{\theta} - \theta)/\sqrt{\hat{SE}} \to_D N(0,1)$, where $\hat{SE}$ is an estimate of the standard error.

Asymptotically optimal. Among all "well-behaved" estimators, the MLE has the smallest variance when $n \to \infty$.

Gaussian Error Model

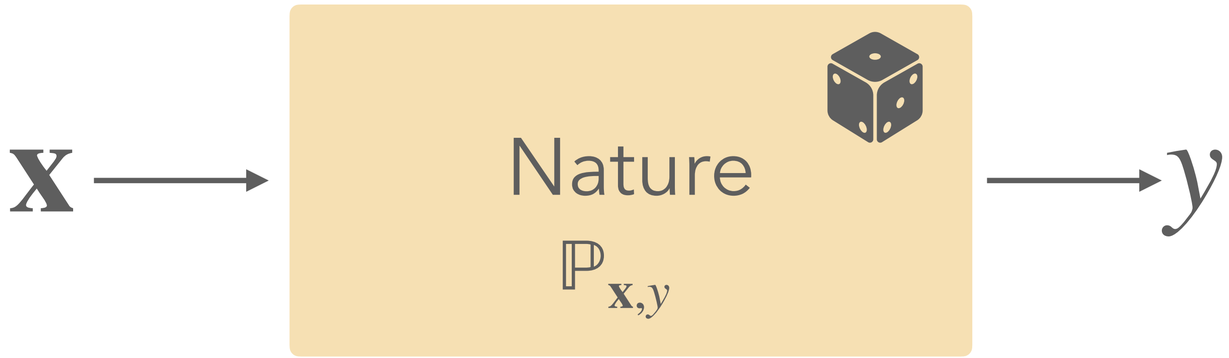
Further assumption on regression model

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 $\mathbf{x}_i$ with variance $\mathrm{Var}(\epsilon_i) = \sigma^2$.

$\mathbf{y} = \mathbf{X}\mathbf{w}^* + \epsilon$, where $\epsilon \in \mathbb{R}^n$ is a random vector with covariance matrix $\mathrm{Var}(\epsilon) = \sigma^2 \mathbf{I}$.



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 $y = \mathbf{x}^\top \mathbf{w}^* + \epsilon$, in the usual random error model.

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

Expectation: $\mathbb{E}[\hat{\mathbf{w}} \mid \mathbf{X}] = \mathbf{w}^*$ and $\mathbb{E}[\hat{\mathbf{w}}] = \mathbf{w}^*$, so $\mathbf{Bias}(\hat{\mathbf{w}}) = \mathbf{0}$.

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

Parameter MSE: $\mathrm{MSE}(\hat{\mathbf{w}}) = \mathbb{E}[\|\hat{\mathbf{w}} - \mathbf{w}^*\|^2] = \sigma^2 \mathbb{E}[\mathrm{tr}((\mathbf{X}^\top \mathbf{X})^{-1})]$

Risk (w.r.t. squared error): $R(\hat{\mathbf{w}}) = \mathbb{E}[(\hat{\mathbf{w}}^\top \mathbf{x} - y)^2] = \sigma^2 + \sigma^2 \mathbb{E}[\mathrm{tr}(\mathbf{\Sigma}(\mathbf{X}^\top \mathbf{X})^{-1})] \approx \sigma^2 + \dfrac{\sigma^2 d}{n}$.

Random error model

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

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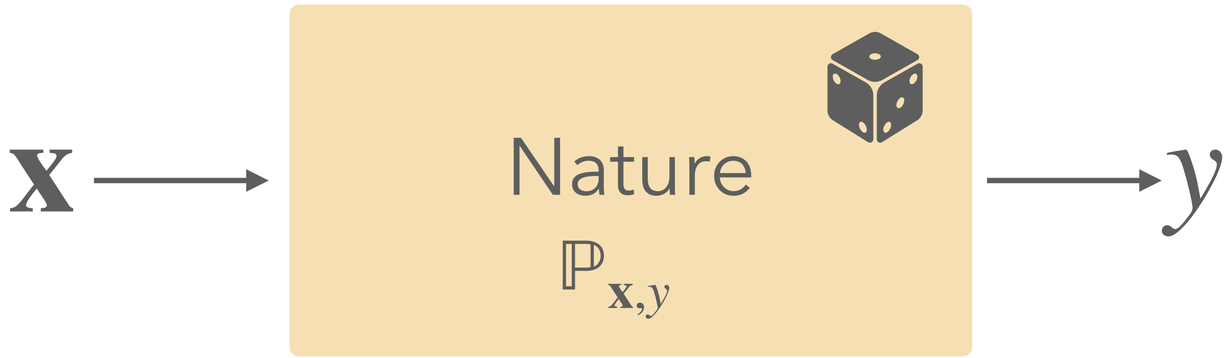


We can think of ϵ as the randomness from the "unexplained" errors in modeling the relationship of y to $\mathbf{x}$ with a linear model $\mathbf{w}^* \in \mathbb{R}^d$. Possibly very complex!

Gaussian Error Model

Motivation

We can think of ϵ as the randomness from the "unexplained" errors in modeling the relationship of y to $\mathbf{x}$ with a linear model $\mathbf{w}^* \in \mathbb{R}^d$. Possibly very complex!

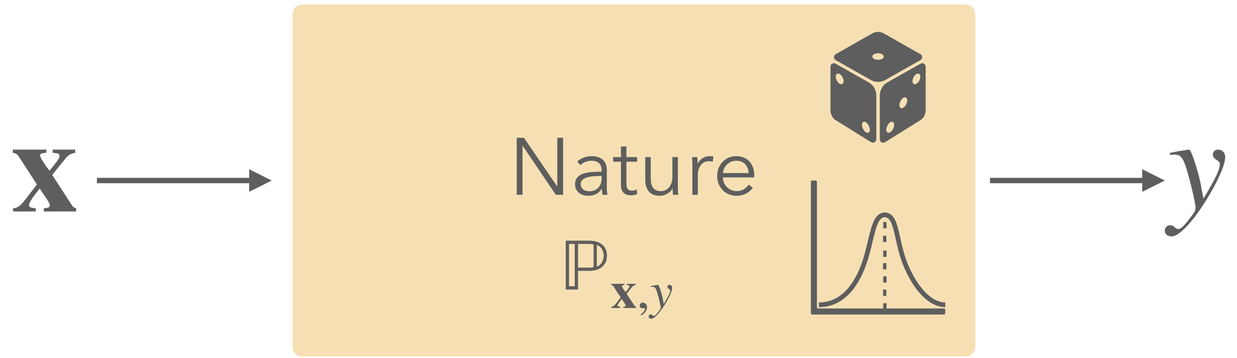
CLT: The distribution of the average of many random variables eventually looks Gaussian. Observable processes in Nature often arise from the sum of many "small contributions."

Random error model

Adding Gaussian assumption on ϵ

$$y_i = \mathbf{x}_i^\top \mathbf{w}^* + \epsilon_i, \text{ where } \epsilon_i \sim N(0,\sigma^2) \text{ and } \epsilon_i \text{ is independent of } \mathbf{x}_i.$$

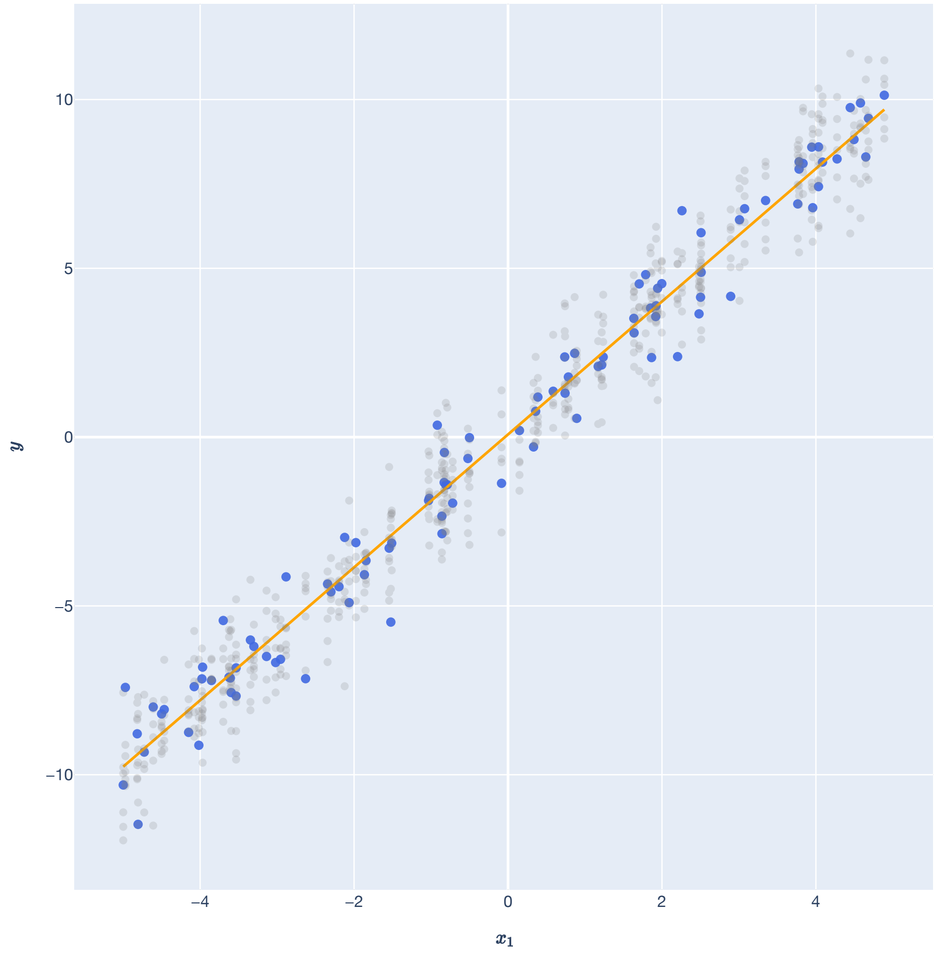
$$\mathbf{y} = \mathbf{X}\mathbf{w}^* + \epsilon, \text{ where } \epsilon \in \mathbb{R}^n \text{ is a Gaussian random vector with covariance matrix } \mathrm{Var}(\epsilon) = \sigma^2\mathbf{I}.$$

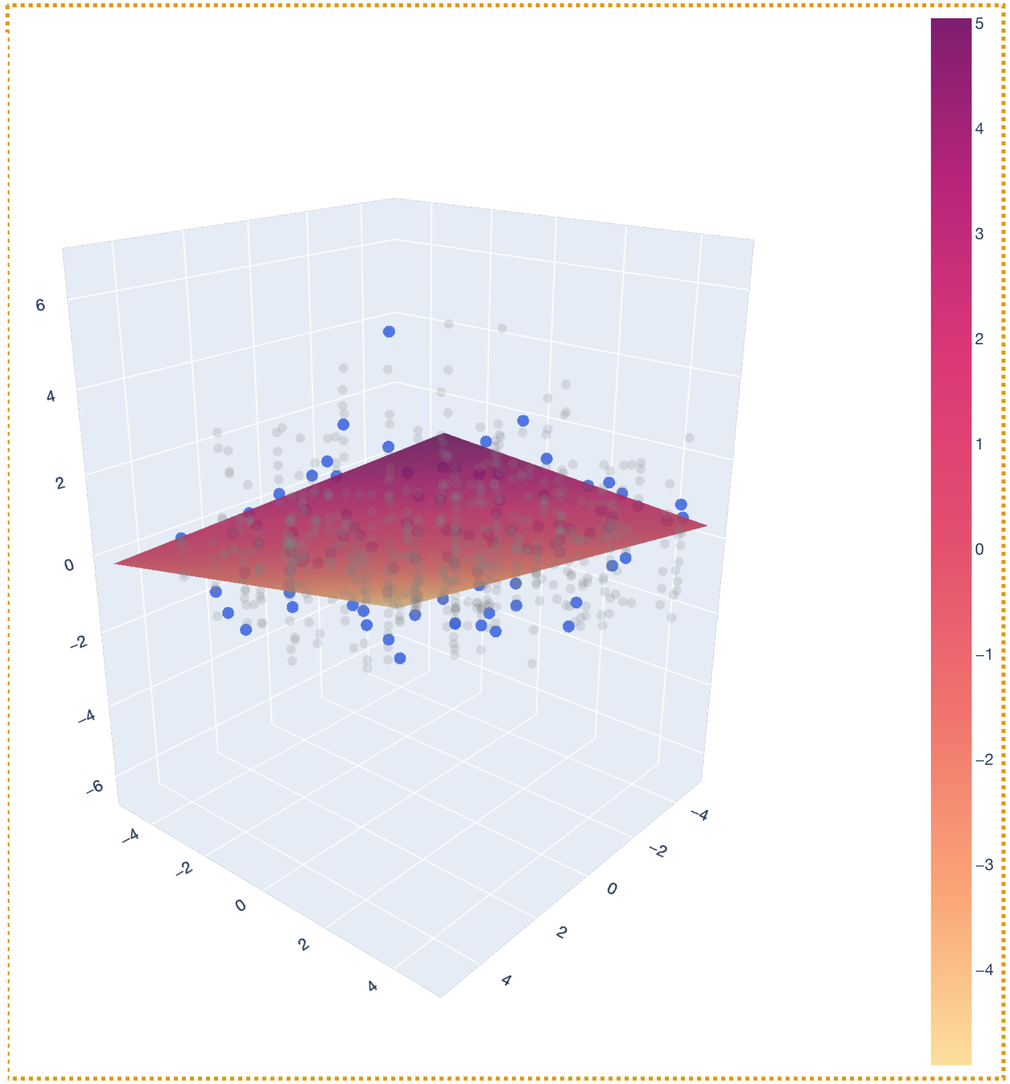


We can think of ϵ as the randomness from the "unexplained" errors in modeling the relationship of y to $\mathbf{x}$ with a linear model $\mathbf{w}^* \in \mathbb{R}^d$. Possibly very complex!

Gaussian Error Model

$d = 1$ and $d = 2$ case





OLS and MLE

Equivalence under Gaussian errors

Random error model

Adding Gaussian assumption on ϵ

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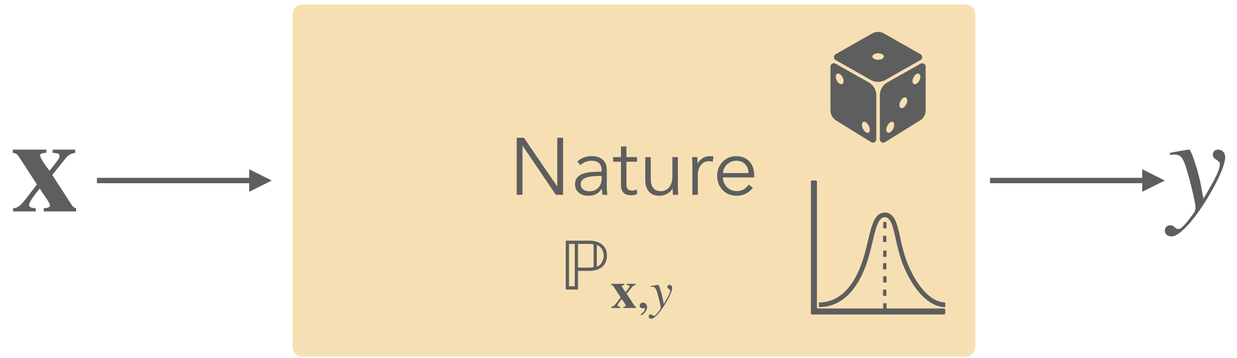
$$\mathbf{y} = \mathbf{X}\mathbf{w}^* + \epsilon, \text{ where } \epsilon \in \mathbb{R}^n \text{ is a Gaussian random vector with covariance matrix } \mathrm{Var}(\epsilon) = \sigma^2\mathbf{I}.$$



We can think of ϵ as the randomness from the "unexplained" errors in modeling the relationship of y to $\mathbf{x}$ with a linear model $\mathbf{w}^* \in \mathbb{R}^d$. Possibly very complex!

Problem Setup

Parametric Model

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

$\epsilon_i \sim N(0,\sigma^2)$ with $\mathbb{E}[\epsilon_i] = 0$ and $\mathrm{Var}(\epsilon_i) = \sigma^2$ all independent of $\mathbf{x}$ and each other.

This defines a *parametric model* on the *conditional* distribution $\mathbb{P}_{y|\mathbf{x}}$, with parameters $\theta = (\mathbf{w}^*, \sigma)$, with PDF:

$$p(y \mid \mathbf{x}; \mathbf{w}^*, \sigma) = \frac{1}{\sigma\sqrt{2\pi}} \exp\left\{-(y - \mathbf{x}^\top \mathbf{w}^*)^2/2\sigma^2\right\}.$$

Problem Setup

Log-Likelihood Function

Parametric model with parameters $\mathbf{w}^*$ and σ:

$$p(y \mid \mathbf{x}; \mathbf{w}^*, \sigma) = \frac{1}{\sigma\sqrt{2\pi}} \exp\left\{-(y - \mathbf{x}^\top \mathbf{w}^*)^2 / 2\sigma^2\right\}.$$

Given i.i.d. data $(\mathbf{x}_1, y_1), \ldots, (\mathbf{x}_n, y_n)$, the likelihood function is given by:

$$L_n(\mathbf{w}^*, \sigma) = \prod_{i=1}^{n} p(y_i \mid \mathbf{x}_i; \mathbf{w}^*, \sigma) = \left(\frac{1}{\sigma\sqrt{2\pi}}\right)^n \prod_{i=1}^{n} \exp\left\{-(y_i - \mathbf{x}_i^\top \mathbf{w}^*)^2 / 2\sigma^2\right\}$$

$$\mathscr{L}_n(\mathbf{w}^*, \sigma) = \log L_n(\mathbf{w}^*, \sigma) = n \log\left(\frac{1}{\sigma\sqrt{2\pi}}\right) - \sum_{i=1}^{n} \frac{(y_i - \mathbf{x}_i^\top \mathbf{w}^*)^2}{2\sigma^2}$$

Finding the MLE

Solving the MLE Optimization Problem

The log-likelihood function is given by:

$$\mathscr{L}_n(\mathbf{w}, \sigma) = \log L_n(\mathbf{w}, \sigma) = n \log \left(\frac{1}{\sigma\sqrt{2\pi}} \right) - \sum_{i=1}^{n} \frac{(y_i - \mathbf{x}_i^\top \mathbf{w})^2}{2\sigma^2}$$

We want to optimize and solve this for the estimand $\mathbf{w}$ (we don't care about estimating σ). To get $\hat{\mathbf{w}}_{MLE}$, we solve the optimization problem:

$$\underset{\mathbf{w} \in \mathbb{R}^d}{\text{maximize}} \ \mathscr{L}_n(\mathbf{w}) = n \log \left(\frac{1}{\sigma\sqrt{2\pi}} \right) - \sum_{i=1}^{n} \frac{(y_i - \mathbf{x}_i^\top \mathbf{w})^2}{2\sigma^2}$$

Finding the MLE

Solving the MLE Optimization Problem

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We want to optimize and solve this for the estimand $\mathbf{w}$ (we don't care about estimating σ). To get $\hat{\mathbf{w}}_{MLE}$, we solve the optimization problem:

$$\underset{\mathbf{w} \in \mathbb{R}^d}{\text{minimize}} \; -\mathscr{L}_n(\mathbf{w}) = -n \log \left(\frac{1}{\sigma\sqrt{2\pi}} \right) + \sum_{i=1}^{n} \frac{(y_i - \mathbf{x}_i^\top \mathbf{w})^2}{2\sigma^2}$$

Finding the MLE

Solving the MLE Optimization Problem

$$\underset{\mathbf{w}\in\mathbb{R}^d}{\text{minimize}} \sum_{i=1}^{n} \frac{(y_i - \mathbf{x}_i^\top \mathbf{w})^2}{2\sigma^2} = \frac{1}{2\sigma^2} \sum_{i=1}^{n} (y_i - \mathbf{x}_i^\top \mathbf{w})^2.$$

In matrix-vector form, this is the same as the optimization problem:

$$\underset{\mathbf{w}\in\mathbb{R}^d}{\text{minimize}} \ \frac{1}{2\sigma^2} \|\mathbf{X}\mathbf{w} - \mathbf{y}\|^2.$$

But $1/2\sigma^2$ is just a constant, so this is equivalent to OLS!

$$\underset{\mathbf{w}\in\mathbb{R}^d}{\text{minimize}} \ \|\mathbf{X}\mathbf{w} - \mathbf{y}\|^2$$

OLS and MLE

Theorem Statement

Theorem (OLS and MLE). Suppose that $(\mathbf{x}_1, y_1), \ldots, (\mathbf{x}_n, y_n)$ are i.i.d. samples in $\mathbb{R}^d \times \mathbb{R}$ with conditional distribution $\mathbb{P}_{y|\mathbf{x}}$ defined by:

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

where $\epsilon_i \sim N(0, \sigma^2)$ and each ϵ_i is independent. Let $\mathbf{X} \in \mathbb{R}^{n \times d}$ and $\mathbf{y} \in \mathbb{R}^n$ contain all the i.i.d. samples. Then, the maximum likelihood estimate (MLE) $\hat{\mathbf{w}}_{MLE}$ of the parameter $\mathbf{w}^*$ is given by the OLS estimator:

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

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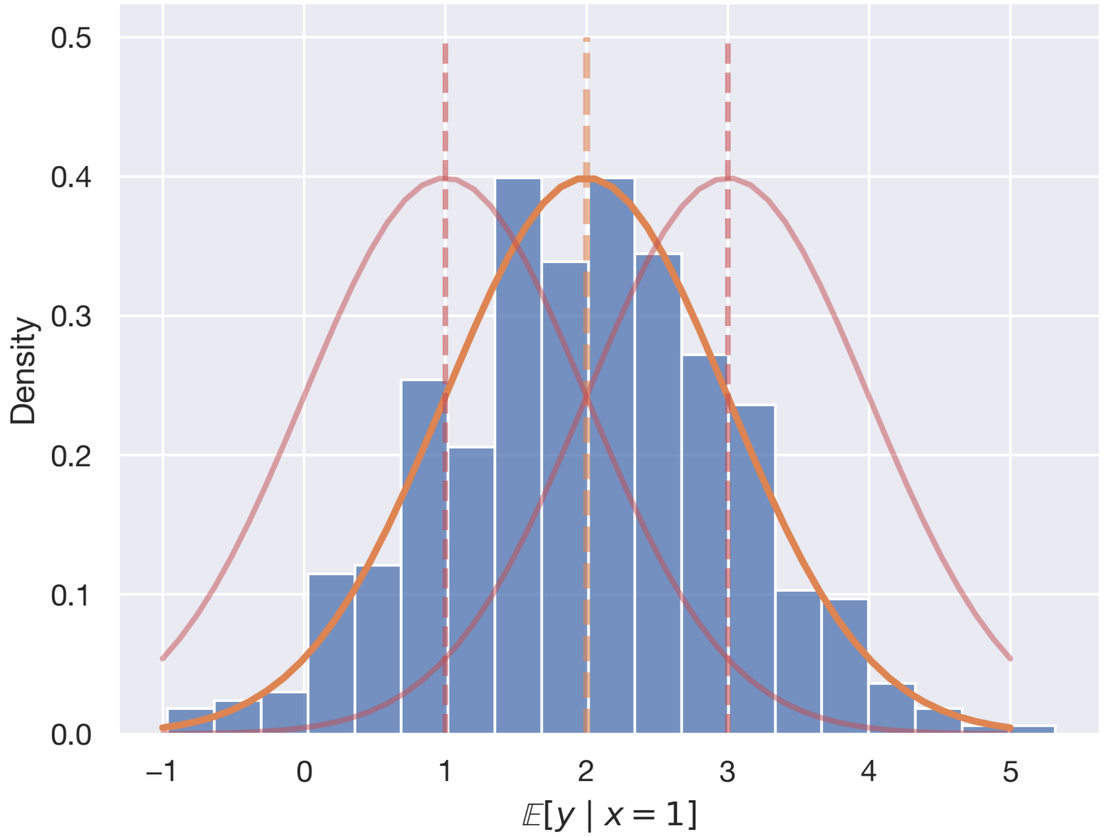

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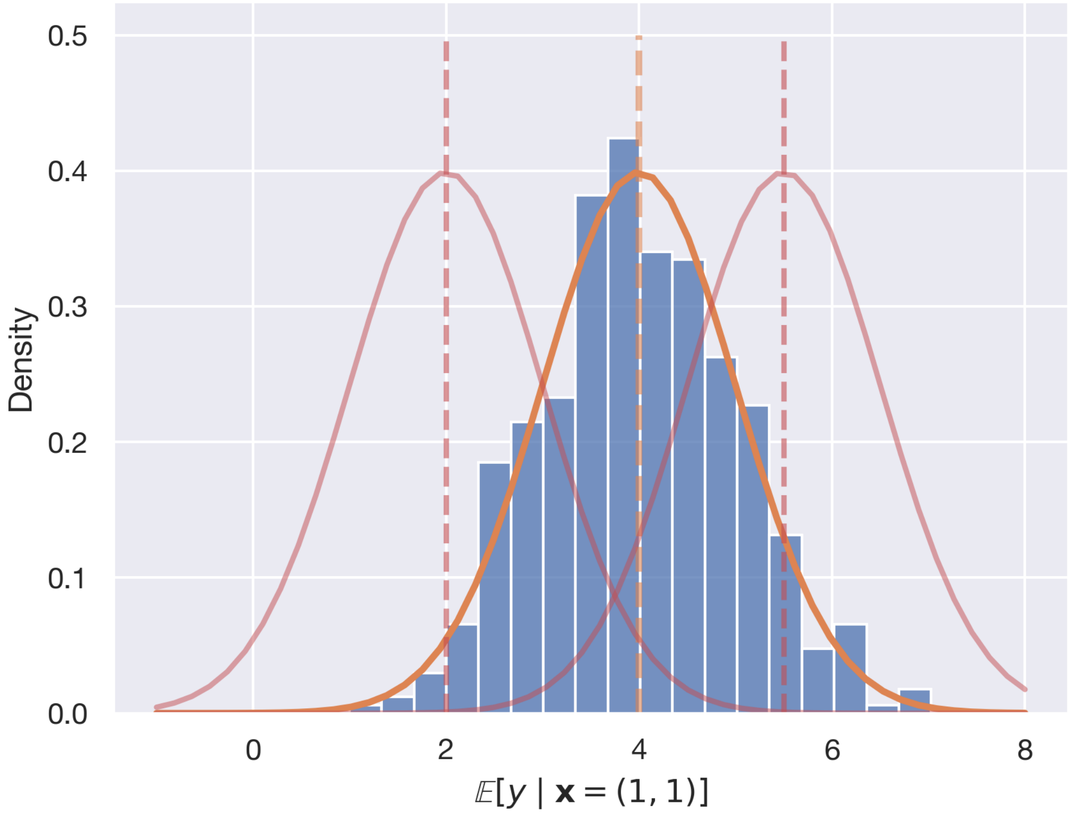


Recap

Lesson Overview

Gaussian Distribution. We define perhaps the most important "named" probability distribution, the Gaussian/"Normal" distribution, and go over some key properties.

Central Limit Theorem. We state and prove the central limit theorem, the statement that the sample average of *many* independent random variables converges in distribution to the Gaussian. It doesn't matter what distribution those random variables take!

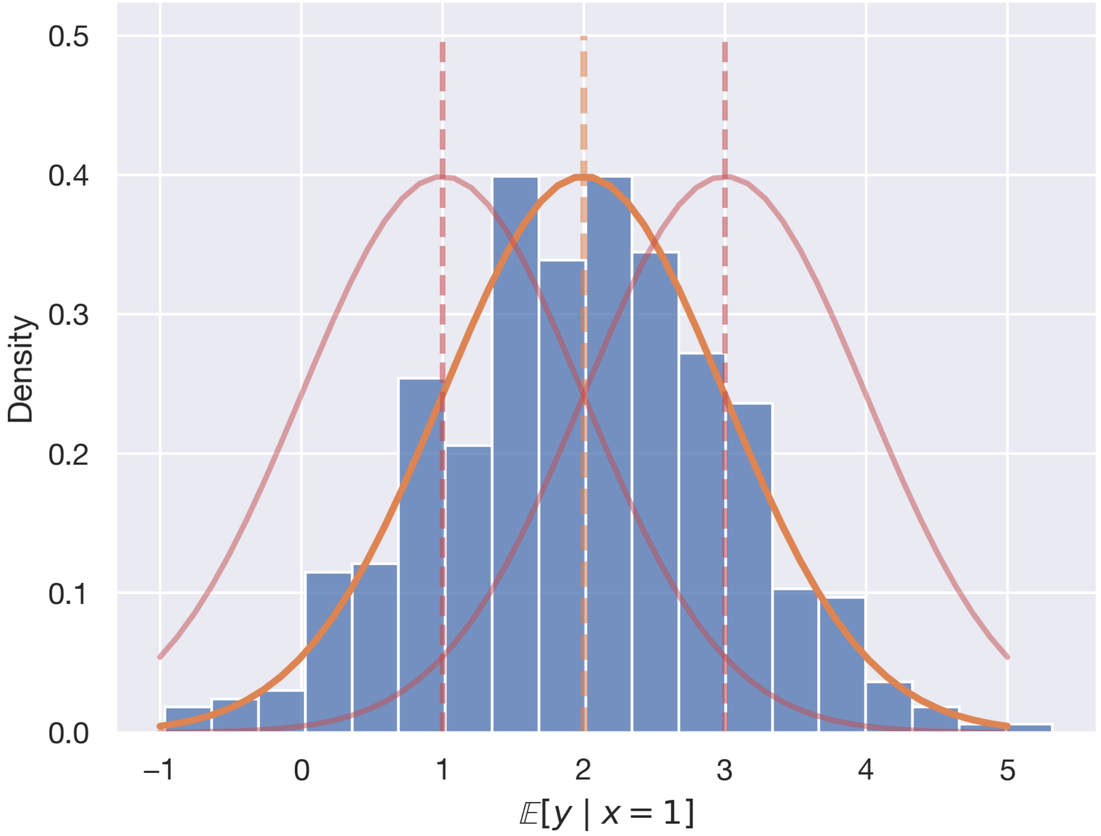
"Named" Distributions. We review other common "named" distributions for discrete and continuous random variables.

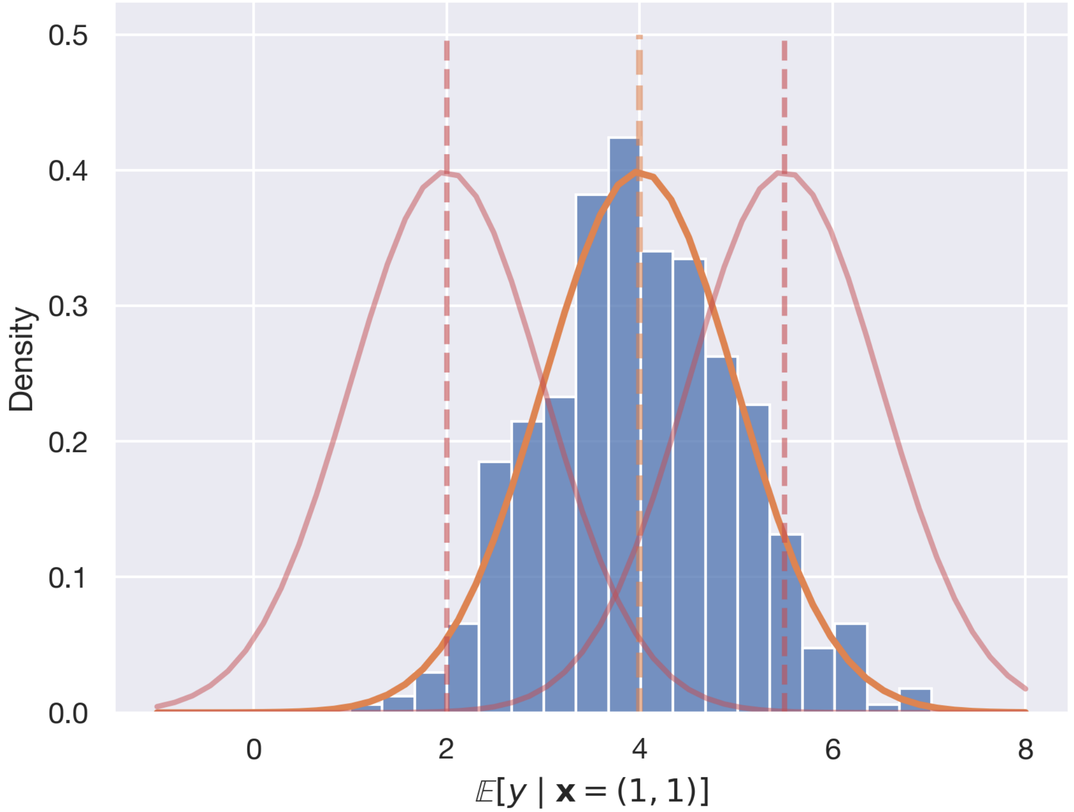
Maximum likelihood estimation. We define maximum likelihood estimation (MLE), a statistical/probabalistic perspective towards finding a well-generalizing model for data.

MLE and OLS. We explore the connection between MLE and OLS by defining the Gaussian error model. In this model, MLE and OLS correspond exactly, motivating our optimization problem another way.

Lesson Overview

Big Picture: Least Squares





Lesson Overview

Big Picture: Gradient Descent