



Computer  
Science

# **CSC696H: Probabilistic Methods in ML**

**Probability and Statistics : Review**

Prof. Jason Pacheco

# Outline

- Random Variables and Discrete Probability
- Fundamental Rules of Probability
- Expected Value and Moments
- Continuous Probability
- Bayesian Inference

# Outline

- **Random Variables and Discrete Probability**
- Fundamental Rules of Probability
- Expected Value and Moments
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# Random Variables

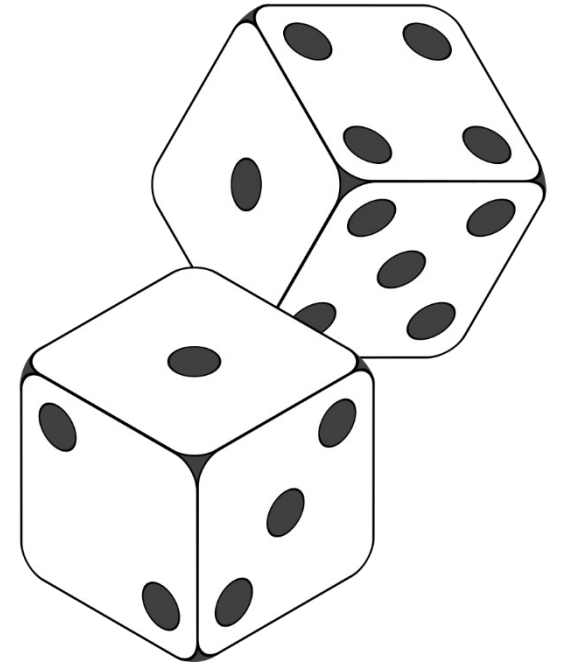
*(Informally) A random variable is an unknown quantity whose value depends on the outcome of a random process*

**Example** Roll 2 dice and let random variable  $X$  represent their sum. It takes values,

$$X \in \{2, 3, 4, \dots, 12\}$$

**Example** Flip a coin and let random variable  $Y$  represent the outcome,

$$Y \in \{\text{Heads}, \text{Tails}\}$$



# Discrete vs. Continuous Probability

**Discrete** RVs take on a finite or countably infinite set of values

**Continuous** RVs take an uncountably infinite set of values

- Representing / interpreting / computing probabilities becomes more complicated in the continuous setting
- We will focus on discrete RVs for now...

# Random Variables and Probability

Capitol letters represent  
random variables

Lowercase letters are  
realized *values*

$$X = x$$

$X = x$  is the **event** that  $X$  takes the value  $x$

**Example** Let  $X$  be the random variable (RV) representing the sum of two dice with values,

$$X \in \{2, 3, 4, \dots, 12\}$$

$X=5$  is the *event* that the dice sum to 5.

# Probability Mass Function

A function  $p(X)$  is a **probability mass function (PMF)** of a discrete random variable if the following conditions hold:

(a) It is nonnegative for all values in the support,

$$p(X = x) \geq 0$$

(b) The sum over all values in the support is 1,

$$\sum_x p(X = x) = 1$$

**Intuition** Probability mass is conserved, just as in physical mass. Reducing probability mass of one event must increase probability mass of other events so that the definition holds...

# Probability Mass Function

**Example** Let  $X$  be the outcome of a single fair die. It has the PMF,

$$p(X = x) = \frac{1}{6} \quad \text{for } x = 1, \dots, 6 \quad \text{Uniform Distribution}$$

**Example** We can often represent the PMF as a vector. Let  $S$  be an RV that is the *sum of two fair dice*. The PMF is then,

**Observe that  $S$  does not follow a uniform distribution**

$$p(S) = \begin{pmatrix} p(S = 2) \\ p(S = 3) \\ p(S = 4) \\ \vdots \\ p(S = 12) \end{pmatrix} = \begin{pmatrix} 1/36 \\ 1/18 \\ 1/6 \\ \vdots \\ 1/36 \end{pmatrix}$$



# Functions of Random Variables

Any function  $f(X)$  of a random variable  $X$  is also a random variable and it has a probability distribution

**Example** Let  $X_1$  be an RV that represents the result of a fair die, and let  $X_2$  be the result of another fair die. Then,

$$S = X_1 + X_2$$

Is an RV that is the *sum of two fair dice* with PMF  $p(S)$ .

**NOTE** Even if we know the PMF  $p(X)$  and we know that the PMF  $p(f(X))$  exists, it is not always easy to calculate!

# PMF Notation

- We use  $p(X)$  to refer to the probability mass *function* (i.e. a function of the RV  $X$ )
- We use  $p(X=x)$  to refer to the probability of the *outcome*  $X=x$  (also called an “event”)
- We will often use  $p(x)$  as shorthand for  $p(X=x)$

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- Expected Value and Moments
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- Bayesian Inference

# Joint Probability

**Definition** Two (discrete) RVs  $X$  and  $Y$  have a *joint PMF* denoted by  $p(X, Y)$  and the probability of the event  $X=x$  and  $Y=y$  denoted by  $p(X = x, Y = y)$  where,

(a) It is nonnegative for all values in the support,

$$p(X = x, Y = y) \geq 0$$

(b) The sum over all values in the support is 1,

$$\sum_x \sum_y p(X = x, Y = y) = 1$$

# Joint Probability

Let  $X$  and  $Y$  be *binary RVs*. We can represent the joint PMF  $p(X,Y)$  as a 2x2 array (table):

		Y	
		0	1
X	0	0.04	0.36
	1	0.30	0.30

**All values are nonnegative**

# Joint Probability

Let  $X$  and  $Y$  be *binary RVs*. We can represent the joint PMF  $p(X,Y)$  as a 2x2 array (table):

		Y	
		0	1
X	0	0.04	0.36
	1	0.30	0.30

**The sum over all values is 1:  
 $0.04 + 0.36 + 0.30 + 0.30 = 1$**

# Joint Probability

Let  $X$  and  $Y$  be *binary RVs*. We can represent the joint PMF  $p(X, Y)$  as a 2x2 array (table):

		Y	
		0	1
X	0	0.04	0.36
	1	0.30	0.30

$$P(X=1, Y=0) = 0.30$$

# Fundamental Rules of Probability

Given two RVs  $X$  and  $Y$  the **conditional distribution** is:

$$p(X | Y) = \frac{p(X, Y)}{p(Y)} = \frac{p(X, Y)}{\sum_x p(X=x, Y)}$$

Multiply both sides by  $p(Y)$  to obtain the **probability chain rule**:

$$p(X, Y) = p(Y)p(X | Y)$$

For  $N$  RVs  $X_1, X_2, \dots, X_N$ :

$$p(X_1, X_2, \dots, X_N) = p(X_1)p(X_2 | X_1) \dots p(X_N | X_{N-1}, \dots, X_1)$$

Chain rule valid  
for any ordering

$$= p(X_1) \prod_{i=2}^N p(X_i | X_{i-1}, \dots, X_1)$$



# Fundamental Rules of Probability

## Law of total probability

$$p(Y) = \sum_x p(Y, X = x)$$

- $P(y)$  is a **marginal** distribution
- This is called **marginalization**

**Proof**

$$\begin{aligned} \sum_x p(Y, X = x) &= \sum_x p(Y) p(X = x | Y) && \text{( chain rule )} \\ &= p(Y) \sum_x p(X = x | Y) && \text{( distributive property )} \\ &= p(Y) && \text{( PMF sums to 1 )} \end{aligned}$$

*Generalization for conditionals:*

$$p(Y | Z) = \sum_x p(Y, X = x | Z)$$

# Tabular Method

Let  $X, Y$  be binary RVs with the joint probability table

For Binomial use K-by-K probability table.

		Y	
		$y_1$	$y_2$
X	$x_1$	0.04	0.36
	$x_2$	0.30	0.30

0.4  $P(x_1)$

0.6  $P(x_2)$

$P(x)$

$P(y_1) = P(x_1, y_1) + P(x_2, y_1)$   
 $P(y_2) = P(x_1, y_2) + P(x_2, y_2)$   
[i.e., sum down columns]

0.34  $P(y_1)$

0.66  $P(y_2)$

$P(y)$

$P(x_1) = P(x_1, y_1) + P(x_1, y_2)$   
 $P(x_2) = P(x_2, y_1) + P(x_2, y_2)$   
[i.e., sum across rows]

# Tabular Method

We don't care about event  $Y=y_2$

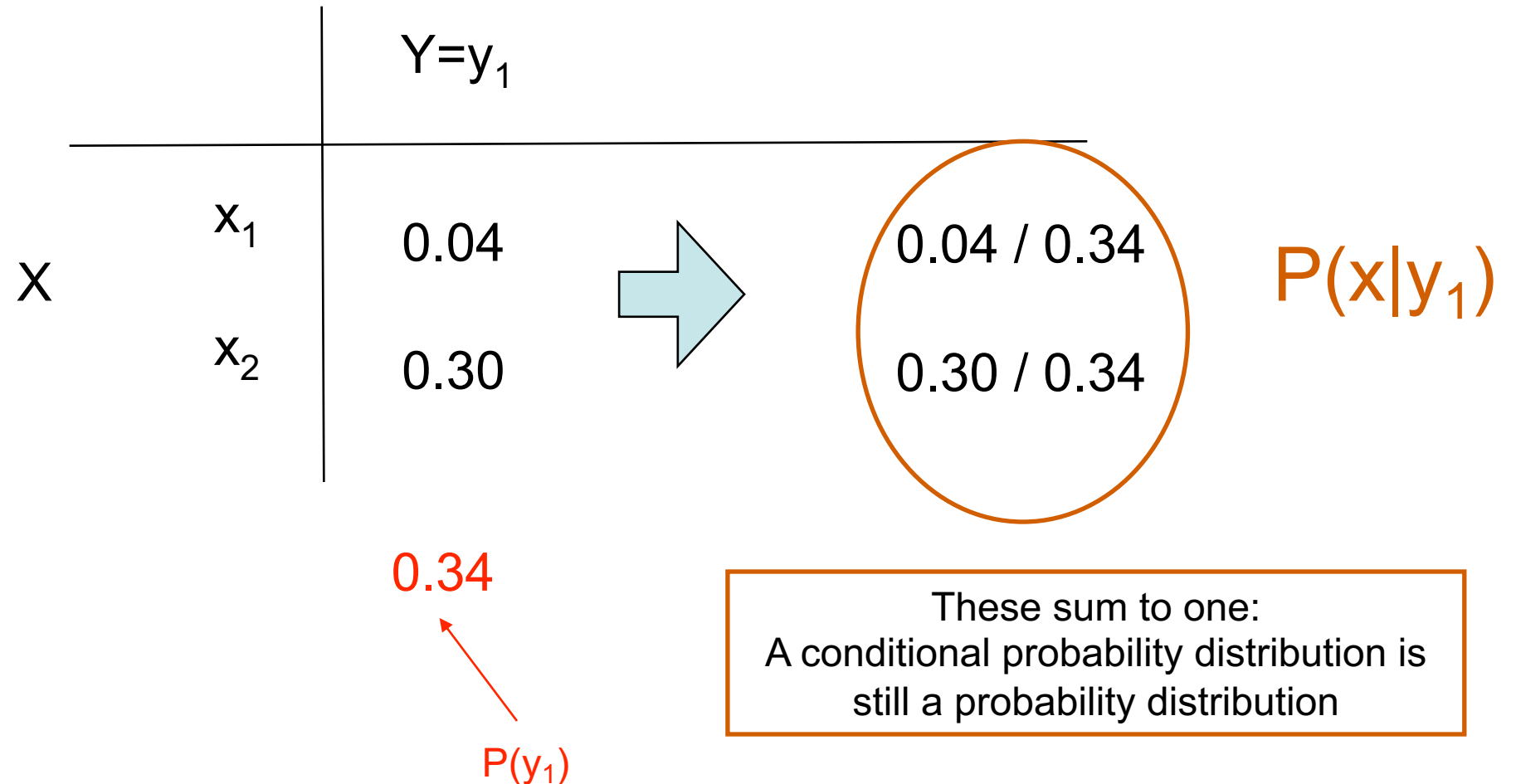
		Y	
		$y_1$	$y_2$
X	$x_1$	0.04	Censored!
	$x_2$	0.30	

$P(x|y_1)=?$

0.34

$P(y_1)$

# Tabular Method



# Summary

- A **random variable** is an unknown quantity whose value depends on the outcome a random process (informal definition)
- $X = x$  is an event with probability mass  $p(X = x)$

- $p(X)$  is a **probability mass function (PMF)** satisfying

$$p(X = x) \geq 0 \qquad \sum_x p(X = x) = 1$$

- Some fundamental rules of probability:

- Conditional:  $p(X | Y) = \frac{p(X, Y)}{p(Y)} = \frac{p(X, Y)}{\sum_x p(X=x, Y)}$
- Law of total probability:  $p(Y) = \sum_x p(Y, X = x)$
- Probability chain rule:  $p(X, Y) = p(Y)p(X | Y)$

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# Moments of RVs

**Definition** The expectation of a discrete RV  $X$ , denoted by  $\mathbf{E}[X]$ , is:

$$\mathbf{E}[X] = \sum_x x p(X = x)$$

Summation over all values in domain of  $X$

**Example** Let  $X$  be the sum of two fair dice, then:

$$\mathbf{E}[X] = \frac{1}{36} \cdot 2 + \frac{1}{18} \cdot 3 + \dots + \frac{1}{36} \cdot 12 = 7$$

**Theorem (Linearity of Expectations)** For any finite collection of discrete RVs  $X_1, X_2, \dots, X_N$  with finite expectations,

**Corollary** For any constant  $c$   
 $\mathbf{E}[cX] = c\mathbf{E}[X]$

$$\mathbf{E} \left[ \sum_{i=1}^N X_i \right] = \sum_{i=1}^N \mathbf{E}[X_i]$$

E.g. for two RVs  $X$  and  $Y$   
 $\mathbf{E}[X + Y] = \mathbf{E}[X] + \mathbf{E}[Y]$

# Moments of RVs

**Law of Total Expectation** *Let  $X$  and  $Y$  be discrete RVs with finite expectations, then:*

$$\mathbf{E}[X] = \mathbf{E}_Y[\mathbf{E}_X[X | Y]]$$

**Proof**

$$\begin{aligned}\mathbf{E}_Y[\mathbf{E}_X[X | Y]] &= \mathbf{E}_Y \left[ \sum_x x \cdot p(x | Y) \right] \\ &= \sum_y \left[ \sum_x x \cdot p(x | y) \right] \cdot p(y) && \text{( Definition of expectation )} \\ &= \sum_y \sum_x x \cdot p(x, y) && \text{( Probability chain rule )} \\ &= \sum_x x \sum_y p(x, y) && \text{( Linearity of expectations )} \\ &= \sum_x x \cdot p(x) = \mathbf{E}[X] && \text{( Law of total probability )}\end{aligned}$$



# Moments of RVs

**Definition** The conditional expectation of a discrete RV  $X$ , given  $Y$  is:

$$\mathbf{E}[X \mid Y = y] = \sum_x x p(X = x \mid Y = y)$$

**Example** Roll two standard six-sided dice and let  $X$  be the result of the first die and let  $Y$  be the sum of both dice, then:

$$\begin{aligned} \mathbf{E}[X_1 \mid Y = 5] &= \sum_{x=1}^4 x p(X_1 = x \mid Y = 5) \\ &= \sum_{x=1}^4 x \frac{p(X_1 = x, Y = 5)}{p(Y = 5)} = \sum_{x=1}^4 x \frac{1/36}{4/36} = \frac{5}{2} \end{aligned}$$

*Conditional expectation follows properties of expectation (linearity, etc.)*

# Moments of RVs

**Definition** The variance of a RV  $X$  is defined as,

$$\mathbf{Var}[X] = \mathbf{E}[(X - \mathbf{E}[X])^2] \quad \boxed{\text{(X-units)}^2}$$

The standard deviation is  $\sigma[X] = \sqrt{\mathbf{Var}[X]}$ . (X-units)

**Lemma** An equivalent form of variance is:

$$\mathbf{Var}[X] = \mathbf{E}[X^2] - (\mathbf{E}[X])^2$$

**Proof** Keep in mind that  $E[X]$  is a constant,

$$\begin{aligned} \mathbf{E}[(X - \mathbf{E}[X])^2] &= \mathbf{E}[X^2 - 2X\mathbf{E}[X] + \mathbf{E}[X]^2] && \text{(Distributive property)} \\ &= \mathbf{E}[X^2] - 2\mathbf{E}[X]\mathbf{E}[X] + \mathbf{E}[X]^2 && \text{(Linearity of expectations)} \\ &= \mathbf{E}[X^2] - \mathbf{E}[X]^2 && \text{(Algebra)} \end{aligned}$$

# Moments of RVs

**Definition** The covariance of two RVs  $X$  and  $Y$  is defined as,

$$\mathbf{Cov}(X, Y) = \mathbf{E}[(X - \mathbf{E}[X])(Y - \mathbf{E}[Y])]$$

**Lemma** For any two RVs  $X$  and  $Y$ ,

$$\mathbf{Var}[X + Y] = \mathbf{Var}[X] + \mathbf{Var}[Y] + 2\mathbf{Cov}(X, Y)$$

e.g. variance is not a linear operator.

**Proof**  $\mathbf{Var}[X + Y] = \mathbf{E}[(X + Y - \mathbf{E}[X + Y])^2]$

**(Linearity of expectation)**  $= \mathbf{E}[(X + Y - \mathbf{E}[X] - \mathbf{E}[Y])^2]$

**(Distributive property)**  $= \mathbf{E}[(X - \mathbf{E}[X])^2 + (Y - \mathbf{E}[Y])^2 + 2(X - \mathbf{E}[X])(Y - \mathbf{E}[Y])]$

**(Linearity of expectation)**  $= \mathbf{E}[(X - \mathbf{E}[X])^2] + \mathbf{E}[(Y - \mathbf{E}[Y])^2] + 2\mathbf{E}[(X - \mathbf{E}[X])(Y - \mathbf{E}[Y])]$

**(Definition of Var / Cov)**  $= \mathbf{Var}[X] + \mathbf{Var}[Y] + 2\mathbf{Cov}(X, Y)$

# Summary

## Moments and Expected Value

- Expected value of a discrete RV:

$$\mathbf{E}[X] = \sum_x x p(X = x)$$

- Expectation is a linear operator

$$\mathbf{E} \left[ \sum_{i=1}^N X_i \right] = \sum_{i=1}^N \mathbf{E}[X_i]$$

- Variance of a RV:

$$\mathbf{Var}[X] = \mathbf{E}[(X - \mathbf{E}[X])^2]$$

- Variance is **not** a linear operator

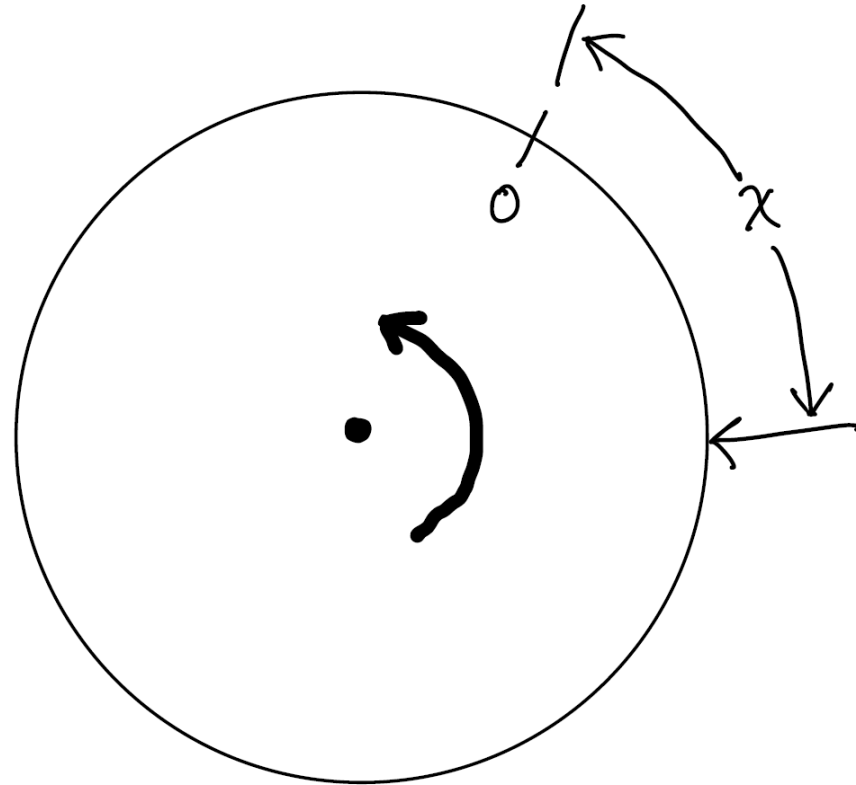
$$\mathbf{Var}[X + Y] = \mathbf{Var}[X] + \mathbf{Var}[Y] + 2\mathbf{Cov}(X, Y)$$

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# Continuous Probability

**Experiment** Spin continuous wheel and measure  $X$  displacement from 0



**Question** Assuming uniform probability, what is  $p(X = x)$ ?

# Continuous Probability

➤ Let  $p(X = x) = \pi$  be the probability of any single outcome

➤ Let  $S(k)$  be set of any  $k$  *distinct* points in  $[0, 1)$  then,

$$P(x \in S(k)) = k\pi$$

➤ Since  $0 < P(x \in S(k)) < 1$  by axioms of probability,  $k\pi < 1$  for any  $k$

➤ Therefore:  $\pi = 0$  and  $P(x \in S(k)) = p(X = x) = 0$

# Continuous Probability

- We have a well-defined event that  $x$  takes a value in set  $x \in S(k)$
- Clearly this event can happen... i.e. **it is possible**
- But we have shown it has zero probability of occurring,

$$P(x \in S(k)) = 0$$

- By the axioms of probability, the probability that it **doesn't happen** is,

$$P(x \notin S(k)) = 1 - P(x \in S(k)) = 1$$

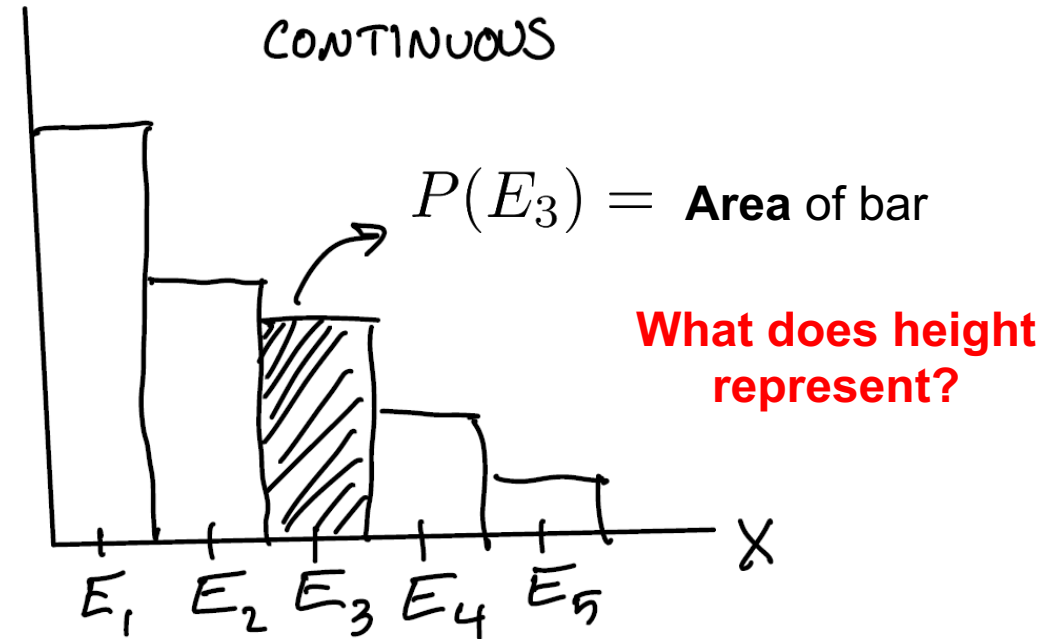
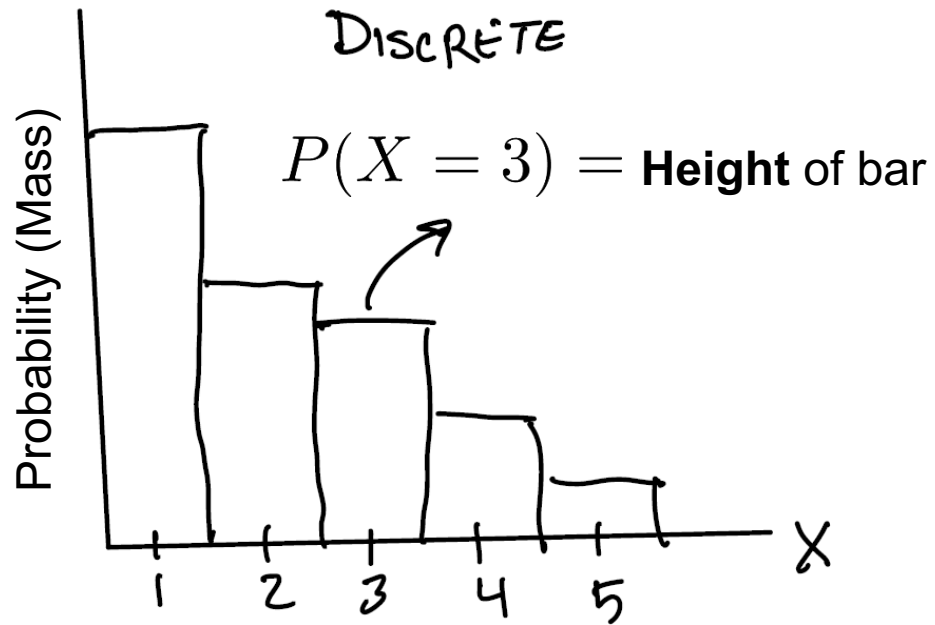
***We seem to have a paradox!***

**Solution** Rethink how we interpret probability in continuous setting

- Define events as *intervals* instead of discrete values
- Assign probability to those intervals



# Continuous Probability



Probability

$\Delta x$

Height =  $\frac{\text{Probability}}{\Delta x}$

Height represents *probability per unit* in the x-direction

We call this a **probability density** (as opposed to probability mass)

# Continuous Probability

➤ We denote the **probability density function** (PDF) as,  $p(X)$

➤ An event E corresponds to an *interval*  $a \leq X < b$

➤ The probability of an interval is given by the *area under the PDF*,

$$P(a \leq X < b) = \int_a^b p(X = x) dx$$

➤ Specific outcomes have zero probability  $P(X = 0) = P(x \leq X < x) = 0$

➤ But may have nonzero *probability density*  $p(X = x)$

# Continuous Probability Measures

**Definition** The cumulative distribution function (CDF) of a real-valued continuous RV  $X$  is the function given by,

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

Different ways to represent probability of interval, CDF is just a convention.

➤ Can easily measure probability of closed intervals,

$$P(a \leq X < b) = P(b) - P(a)$$

➤ If  $X$  is *absolutely continuous* (i.e. differentiable) then,

Fundamental Theorem of Calculus

$$p(x) = \frac{dP(x)}{dx} \quad \text{and} \quad P(t) = \int_{-\infty}^t p(x) dx$$

Where  $p(x)$  is the *probability density function (PDF)*

# Continuous Probability

*Most definitions for discrete RVs hold, replacing PMF with PDF/CDF...*

Two RVs  $X$  &  $Y$  are **independent** if and only if,

$$p(x, y) = p(x)p(y) \quad \text{or} \quad P(X \leq x, Y \leq y) = P(X \leq x)P(Y \leq y)$$

**Conditionally independent** given  $Z$  iff,

$$\text{Shorthand: } P(x) = P(X \leq x)$$

$$p(x, y | z) = p(x | z)p(y | z) \quad \text{or} \quad P(x, y | z) = P(x | z)P(y | z)$$

**Probability chain rule,**

$$p(x, y) = p(x)p(y | x) \quad \text{and} \quad P(x, y) = P(x)P(y | x)$$

# Continuous Probability

*...and by replacing summation with integration...*

**Law of Total Probability** for continuous distributions,

$$p(x) = \int_{\mathcal{Y}} p(x, y) dy$$

**Expectation** of a continuous random variable,

$$\mathbf{E}[X] = \int_{\mathcal{X}} x \cdot p(x) dx$$

**Covariance** of two continuous random variables X & Y,

$$\mathbf{Cov}(X, Y) = \mathbf{E}[(X - \mathbf{E}[X])(Y - \mathbf{E}[Y])] = \int_{\mathcal{X}} \int_{\mathcal{Y}} (x - \mathbf{E}[X])(y - \mathbf{E}[Y])p(x, y) dx dy$$

# Continuous Probability

**Caution** *Some technical subtleties arise in continuous spaces...*

For **discrete** RVs  $X$  &  $Y$ , the conditional

$P(Y=y)=0$  means impossible

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

is **undefined** when  $P(Y=y) = 0$  ... no problem.

For **continuous** RVs we have,

$$P(X \leq x | Y = y) = \frac{P(X \leq x, Y = y)}{P(Y = y)}$$

but numerator and denominator are 0/0.

$P(Y=y)=0$  means improbable,  
but not impossible

# Continuous Probability

Defining the conditional distribution as a limit fixes this...

$$P(X \leq x | Y = y) = \lim_{\delta \rightarrow 0} P(X \leq x | y \leq Y \leq y + \delta)$$

$$= \lim_{\delta \rightarrow 0} \frac{P(X \leq x, y \leq Y \leq y + \delta)}{P(y \leq Y \leq y + \delta)}$$

$$= \lim_{\delta \rightarrow 0} \frac{P(X \leq x, Y \leq y + \delta) - P(X \leq x, Y \leq y)}{P(Y \leq y + \delta) - P(Y \leq y)}$$

$$= \int_{-\infty}^x \lim_{\delta \rightarrow 0} \frac{\frac{\partial}{\partial x} P(u, y + \delta) - \frac{\partial}{\partial x} P(u, y)}{P(y + \delta) - P(y)} du$$

$$= \int_{-\infty}^x \lim_{\delta \rightarrow 0} \frac{(\frac{\partial}{\partial x} P(u, y + \delta) - \frac{\partial}{\partial x} P(u, y)) / \delta}{(P(y + \delta) - P(y)) / \delta} du$$

$$= \int_{-\infty}^x \frac{\frac{\partial^2}{\partial x \partial y} P(u, y)}{\frac{\partial}{\partial y} P(y)} du = \int_{-\infty}^x \frac{p(u, y)}{p(y)} du$$

**Definition** The conditional PDF is given by,

$$p(x | y) = \frac{p(x, y)}{p(y)}$$

( **Fundamental theorem of calculus** )

( **Assume interchange limit / integral** )

( **Multiply by  $\frac{\delta}{\delta} = 1$**  )

( **Definition of partial derivative** )

( **Definition PDF** )

# Useful Continuous Distributions

**Uniform** distribution on interval  $[a, b]$ ,

$$p(x) = \begin{cases} 0 & \text{if } x \leq a, \\ \frac{1}{b-a} & \text{if } a \leq x \leq b, \\ 0 & \text{if } b \leq x \end{cases} \quad P(X \leq x) = \begin{cases} 0 & \text{if } x \leq a, \\ \frac{x-a}{b-a} & \text{if } a \leq x \leq b, \\ 1 & \text{if } b \leq x \end{cases}$$

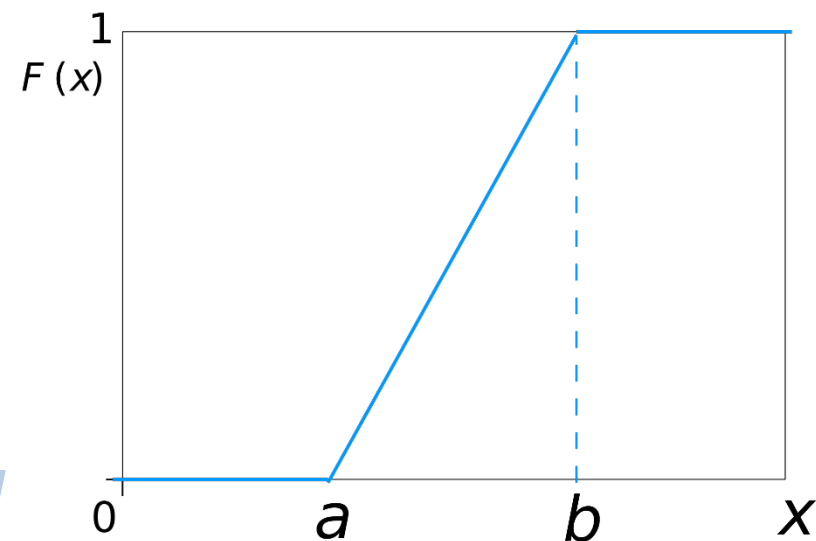
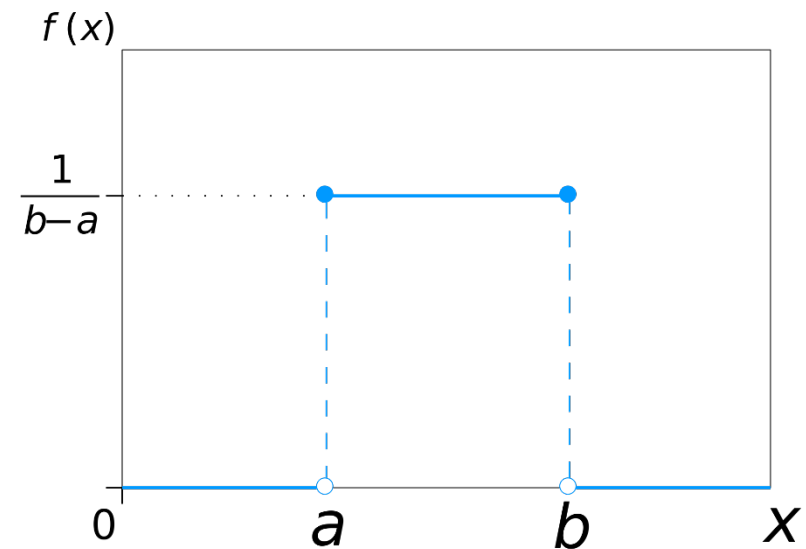
Say that  $X \sim U(a, b)$  whose moments are,

$$\mathbf{E}[X] = \frac{b+a}{2} \quad \mathbf{Var}[X] = \frac{(b-a)^2}{12}$$

Suppose  $X \sim U(0, 1)$  and we are told  $X \leq \frac{1}{2}$   
what is the conditional distribution?

$$P(X \leq x \mid X \leq \frac{1}{2}) = U(0, \frac{1}{2})$$

*Holds generally: Uniform closed under conditioning*





# Useful Continuous Distributions

**Exponential** distribution with scale  $\lambda$ ,

$$p(x) = \lambda e^{-\lambda x} \quad P(x) = 1 - e^{-\lambda x}$$

for  $X > 0$ . Moments given by,

$$\mathbf{E}[X] = \frac{1}{\lambda} \quad \mathbf{Var}[X] = \frac{2}{\lambda^2}$$

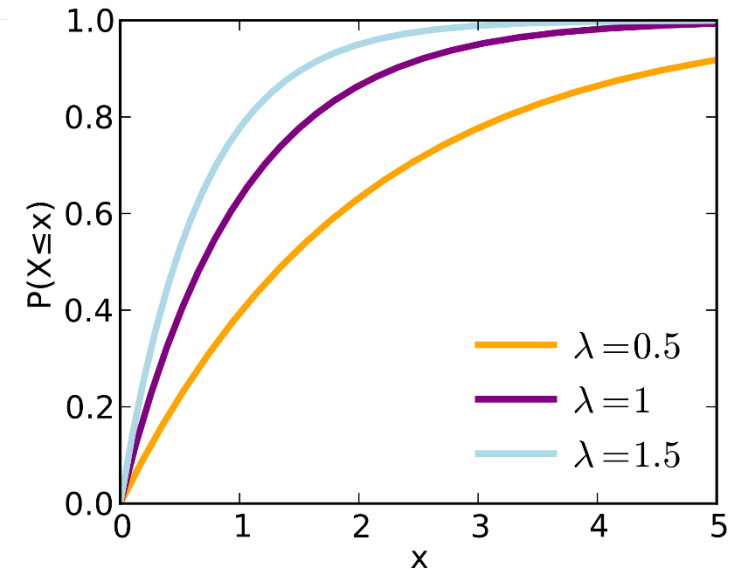
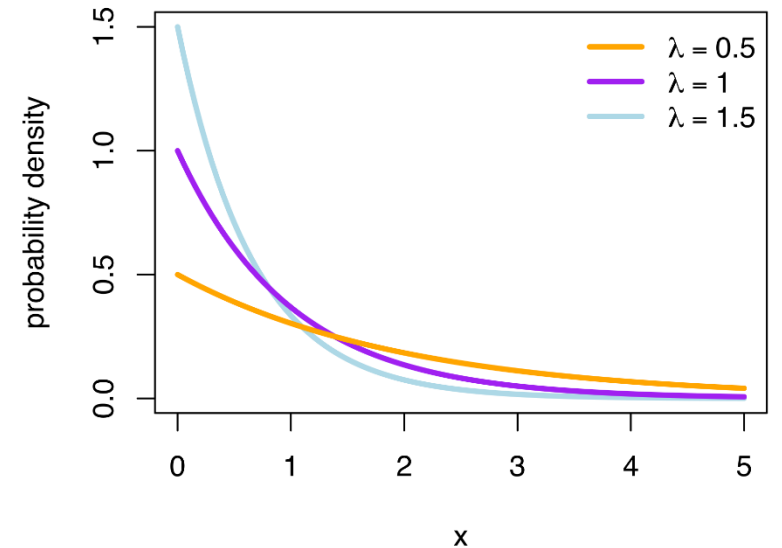
## Useful properties

- **Closed under conditioning** If  $X \sim \text{Exponential}(\lambda)$  then,

$$P(X \geq s + t \mid X \geq s) = P(X \geq s) = e^{-\lambda s}$$

- **Minimum** Let  $X_1, X_2, \dots, X_N$  be i.i.d. exponentially distributed with scale parameters  $\lambda_1, \lambda_2, \dots, \lambda_N$  then,

$$P(\min(X_1, X_2, \dots, X_N)) = \text{Exponential}(\sum_i \lambda_i)$$



# Useful Continuous Distributions

**Gaussian** (a.k.a. Normal) distribution with mean (location)  $\mu$  and variance (scale)  $\sigma^2$  parameters,

$$p(x) = \frac{1}{\sqrt{2\pi\sigma^2}} \exp -\frac{1}{2}(x - \mu)^2/\sigma^2$$

We say  $X \sim \mathcal{N}(\mu, \sigma^2)$ .

## Useful Properties

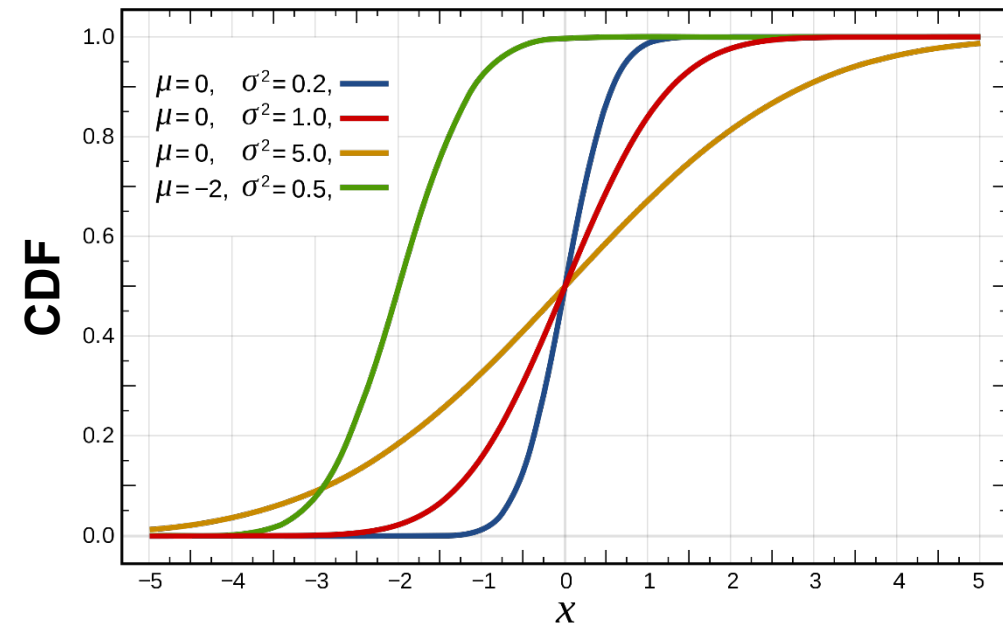
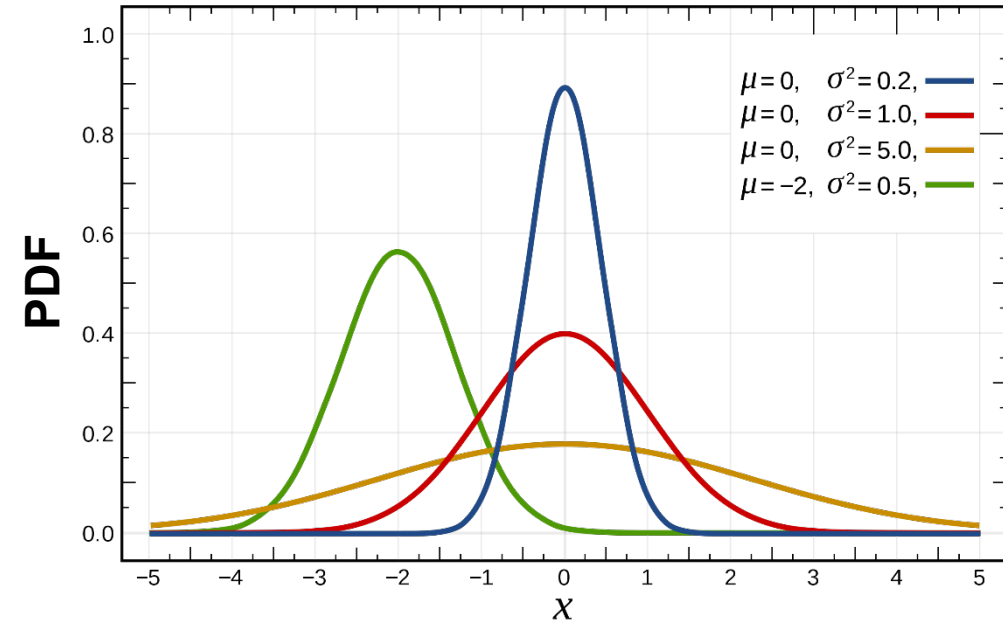
- Closed under additivity:

$$X \sim \mathcal{N}(\mu_x, \sigma_x^2) \quad Y \sim \mathcal{N}(\mu_y, \sigma_y^2)$$

$$X + Y \sim \mathcal{N}(\mu_x + \mu_y, \sigma_x^2 + \sigma_y^2)$$

- Closed under linear functions (a and b constant):

$$aX + b \sim \mathcal{N}(a\mu_x + b, a^2\sigma_x^2)$$



# Useful Continuous Distributions

**Multivariate Gaussian** On RV  $X \in \mathcal{R}^d$  with mean  $\mu \in \mathcal{R}^d$  and positive semidefinite covariance matrix  $\Sigma \in \mathcal{R}^{d \times d}$ ,

$$p(x) = |2\pi\Sigma|^{-1/2} \exp -\frac{1}{2}(x - \mu)^T \Sigma^{-1}(x - \mu)$$

Moments given by parameters directly.

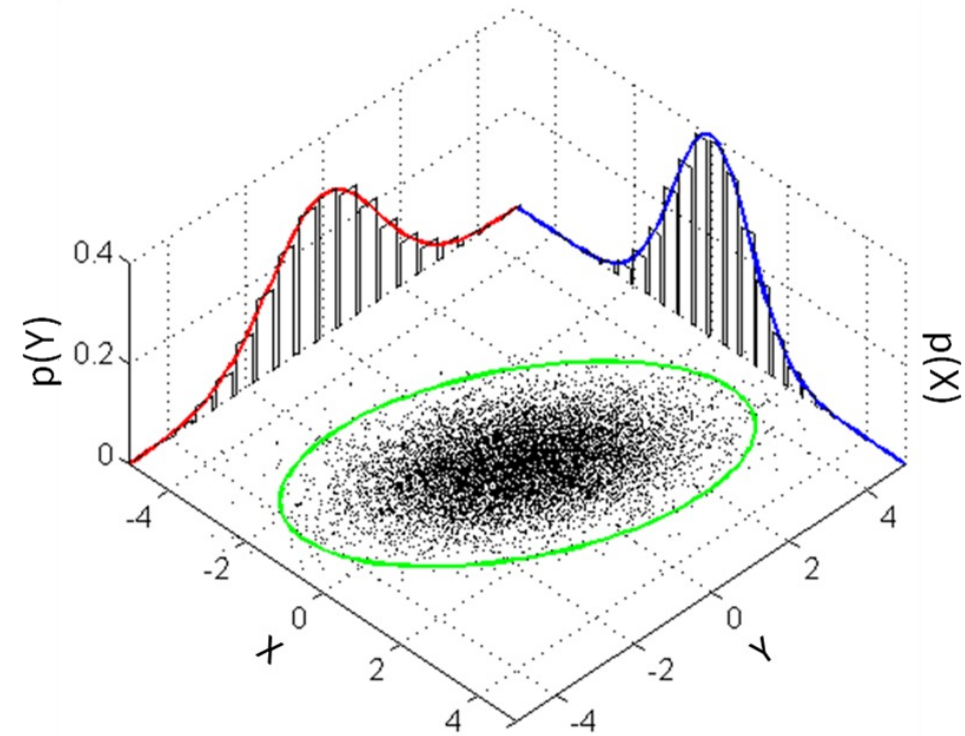
## Useful Properties

- Closed under additivity (same as univariate case)
- Closed under linear functions,

$$AX + b \sim \mathcal{N}(A\mu_x + b, A\Sigma A^T)$$

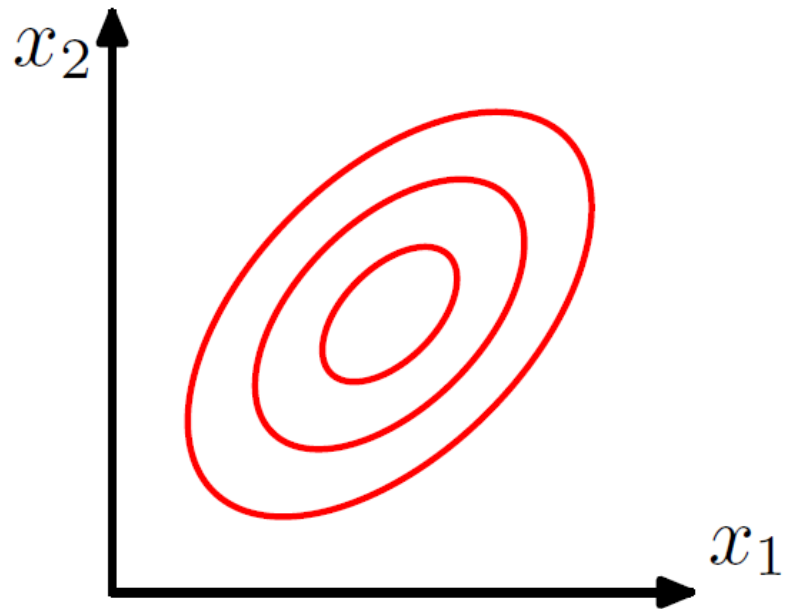
Where  $A \in \mathcal{R}^{m \times d}$  and  $b \in \mathcal{R}^m$  (output dimensions may change)

- Closed under conditioning and marginalization

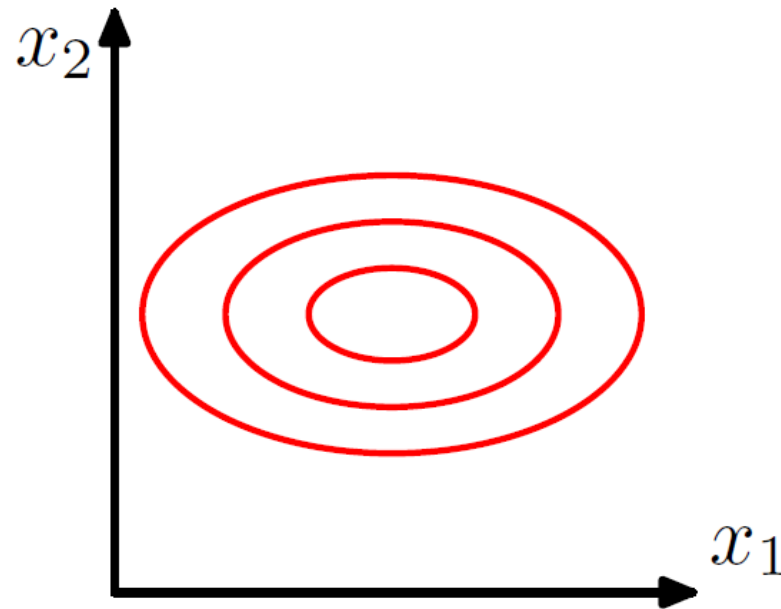


# Covariance

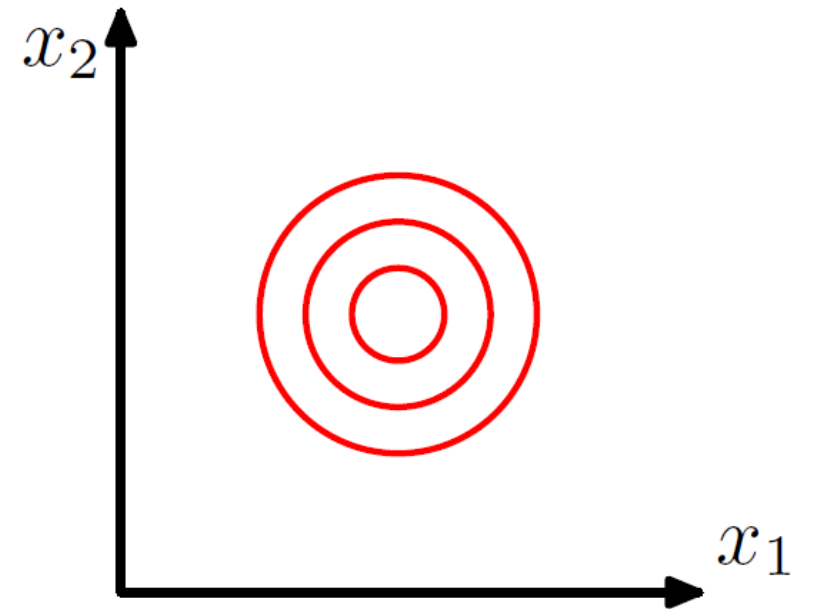
Captures correlation between random variables...can be viewed as set of ellipses...



Positive  
Correlation



Uncorrelated



Uncorrelated and  
same variance  
(isotropic / spherical)

# Covariance Matrix

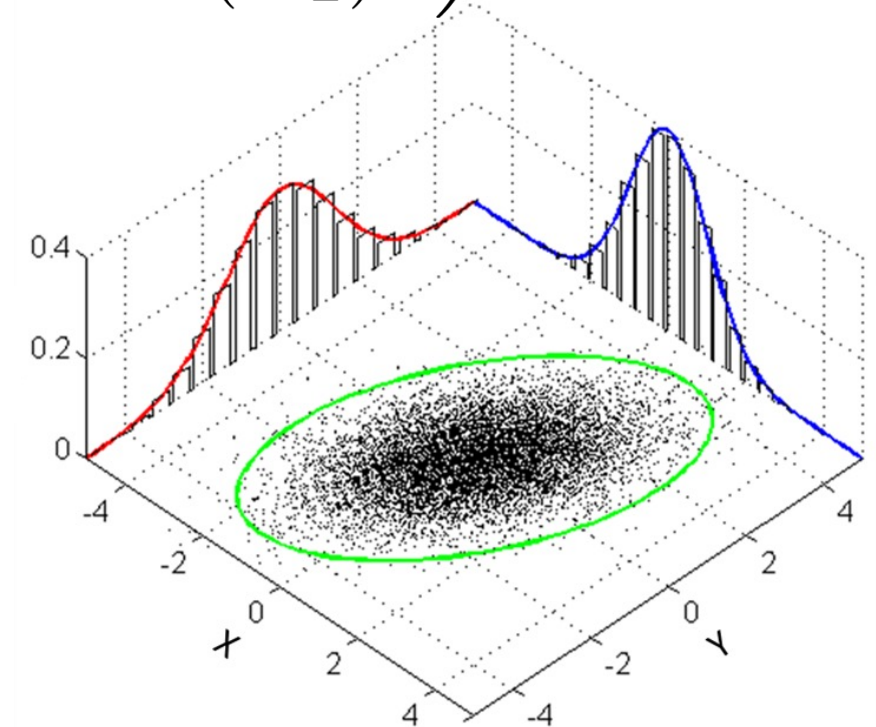
$$\Sigma = \text{Cov}(X) = \begin{pmatrix} \text{Var}(X_1) & \rho\sigma_{X_1}\sigma_{X_2} \\ \rho\sigma_{X_1}\sigma_{X_2} & \text{Var}(X_2) \end{pmatrix}$$

# Covariance Matrix

**Marginal variance of  
just the RV  $X_1$**

$$\Sigma = \text{Cov}(X) = \begin{pmatrix} \text{Var}(X_1) & \rho\sigma_{X_1}\sigma_{X_2} \\ \rho\sigma_{X_1}\sigma_{X_2} & \text{Var}(X_2) \end{pmatrix}$$

**i.e. How “spread out” is the distribution  
in the  $X_1$  dimension...**



# Covariance Matrix

Correlation between  
 $X_1$  and  $X_2$

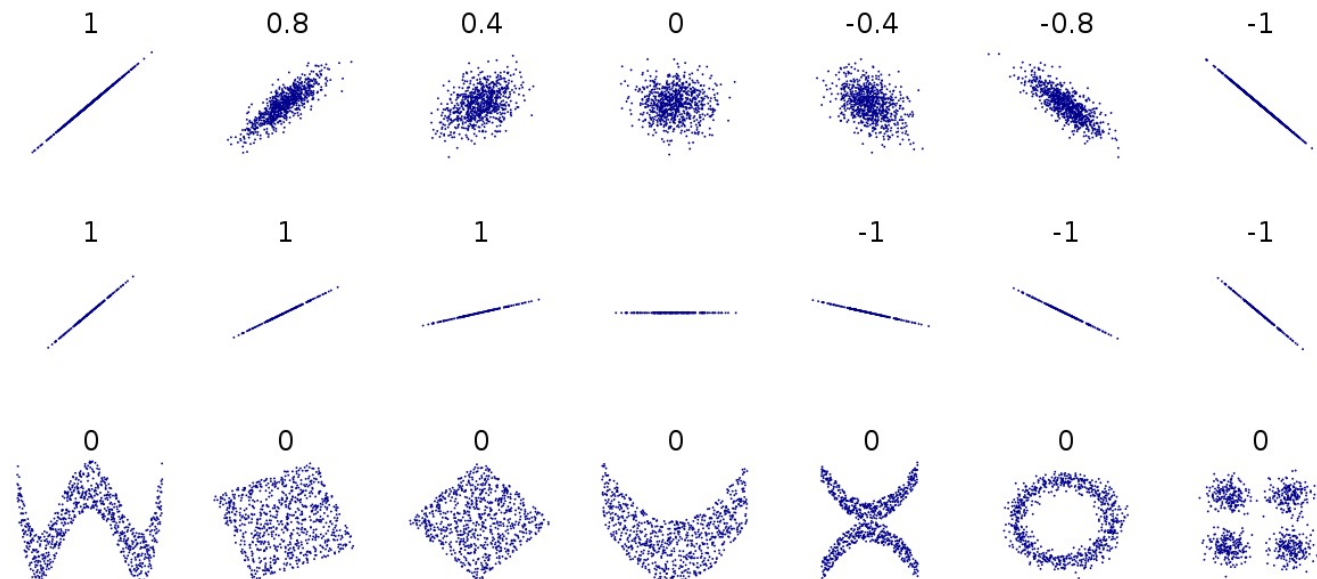


$$\Sigma = \text{Cov}(X) = \begin{pmatrix} \text{Var}(X_1) & \rho\sigma_{X_1}\sigma_{X_2} \\ \rho\sigma_{X_1}\sigma_{X_2} & \text{Var}(X_2) \end{pmatrix}$$

Recall, correlation is given by:

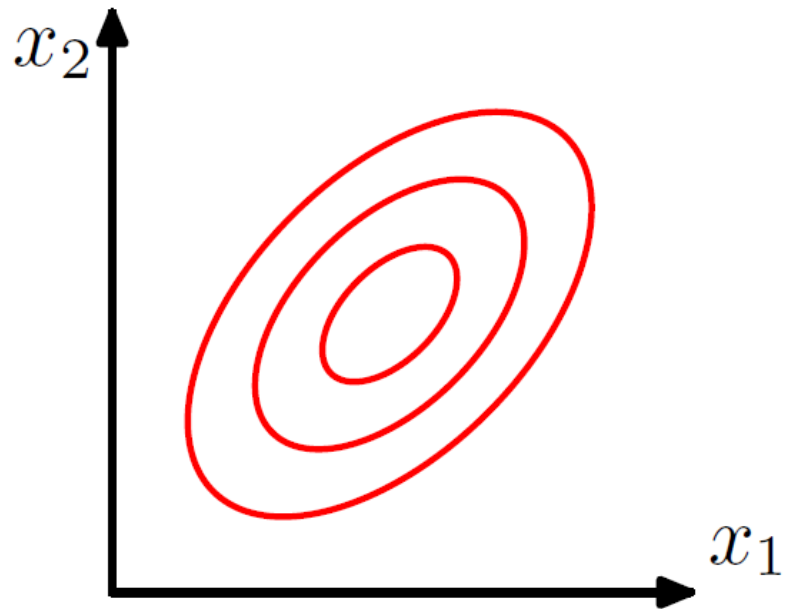
$$\rho = \frac{\text{Cov}(X_1, X_2)}{\sigma_{X_1}\sigma_{X_2}}$$

Captures *linear* dependence of RVs



# Covariance

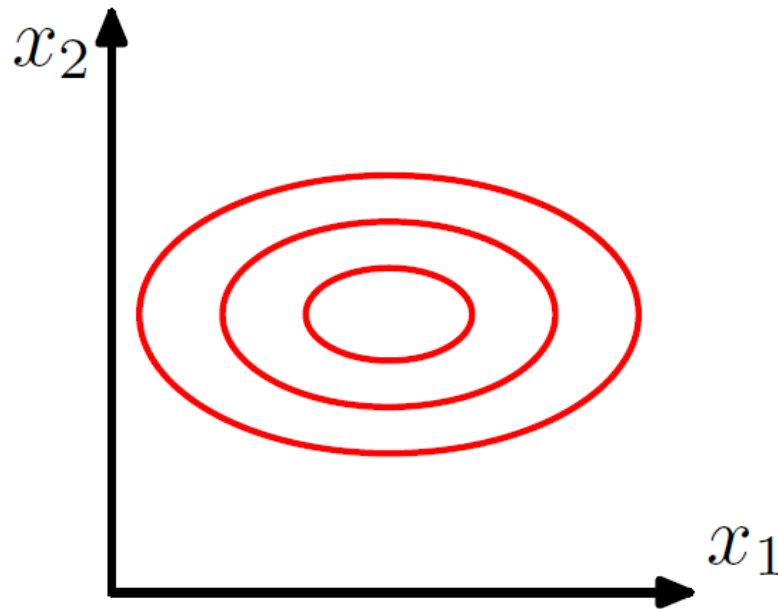
Captures correlation between random variables...can be viewed as set of ellipses...



Positive Correlation

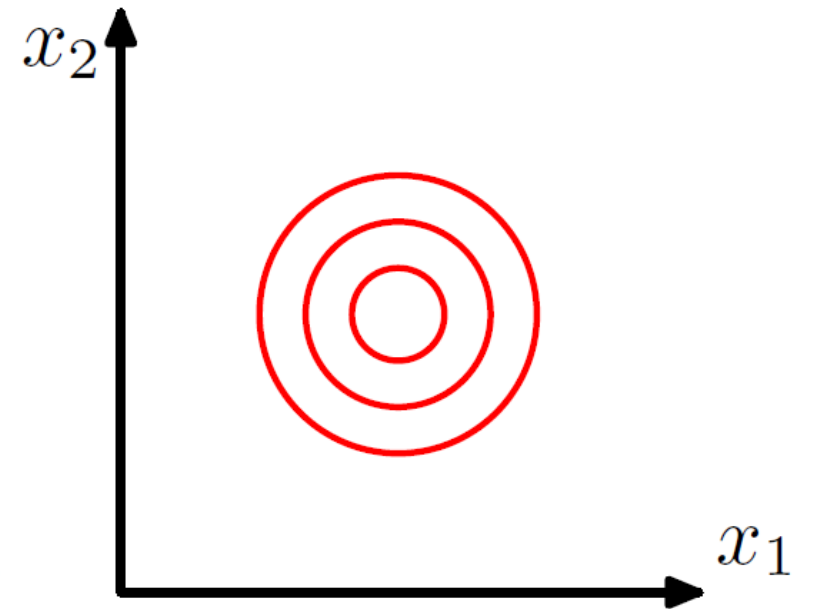
$$\rho > 0$$

Full matrix  $\Sigma$



Uncorrelated

$$\Sigma = \begin{pmatrix} \sigma_{X_1}^2 & 0 \\ 0 & \sigma_{X_2}^2 \end{pmatrix}$$



Isotropic / Spherical

$$\Sigma = \begin{pmatrix} \sigma^2 & 0 \\ 0 & \sigma^2 \end{pmatrix} = \sigma^2 I$$



# Outline

- Random Variables and Discrete Probability
- Fundamental Rules of Probability
- Expected Value and Moments
- Continuous Probability
- **Bayesian Inference**

# What is Probability?

*What does it mean that the probability of heads is  $\frac{1}{2}$  ?*



*Two schools of thought...*

## **Frequentist Perspective**

Proportion of successes (heads) in repeated trials (coin tosses)

## **Bayesian Perspective**

Belief of outcomes based on assumptions about nature and the physics of coin flips

*Neither is better/worse, but we can compare interpretations...*

# Frequentist & Bayesian Modeling

*We will use the following notation throughout:*

$\theta$  - Unknown (e.g. coin bias)

$y$  - Data

## Frequentist

(Conditional Model)

$$p(y; \theta)$$

- $\theta$  is a non-random unknown parameter
- $p(y; \theta)$  is the *sampling / data generating distribution*

## Bayesian

(Generative Model)

Prior Belief  $\rightarrow p(\theta)p(y | \theta) \leftarrow$  Likelihood

- $\theta$  is a random variable (latent)
- Requires specifying  $p(\theta)$  the prior belief

# Bayes' Rule

*Posterior represents all uncertainty after observing data...*

The diagram shows the Bayes' Rule equation with four labels and arrows pointing to its components:

- prior** probability: points to  $p(\theta)$
- likelihood** function for the parameters: points to  $p(y | \theta)$
- posterior** probability: points to  $p(\theta | y)$
- marginal likelihood** or: **evidence** or: **partition function** or: **normalizer**: points to  $p(y)$

$$p(\theta | y) = \frac{p(\theta)p(y | \theta)}{p(y)}$$

# Bayes' Rule : Marginal Likelihood

$$p(\theta | y) = \frac{p(\theta)p(y | \theta)}{p(y)} \propto \underbrace{p(\theta)p(y | \theta)}$$

**Often hard to calculate**

**Often know this (the model)**

Marginal likelihood integrates (marginalizes) over unknown  $\theta$  :

$$p(y) = \int p(\theta)p(y | \theta) d\theta$$

**Marginal likelihood is less problematic in discrete models (not always)**

This integral often lacks a closed form and cannot be computed...

# Bayesian Inference Example

About **29%** of American adults have high blood pressure (BP). Home test has **30% false positive** rate and **no false negative error**.



A recent home test states that you have high BP. Should you start medication?

An Assessment of the Accuracy of Home Blood Pressure Monitors When Used in Device Owners

Jennifer S. Ringrose,<sup>1</sup> Gina Polley,<sup>1</sup> Donna McLean,<sup>2-4</sup> Ann Thompson,<sup>1,5</sup> Fraulein Morales,<sup>1</sup> and Raj Padwal<sup>1,4,6</sup>

# Bayesian Inference Example

About **29%** of American adults have high blood pressure (BP). Home test has **30% false positive** rate and **no false negative error**.



- Latent quantity of interest is hypertension:  $\theta \in \{true, false\}$
- Measurement of hypertension:  $y \in \{true, false\}$
- Prior:  $p(\theta = true) = 0.29$
- Likelihood:  $p(y = true \mid \theta = false) = 0.30$   
 $p(y = true \mid \theta = true) = 1.00$

# Bayesian Inference Example

About **29%** of American adults have high blood pressure (BP). Home test has **30% false positive** rate and **no false negative error**.



Suppose we get a positive measurement, then posterior is:

$$\begin{aligned} p(\theta = \text{true} \mid y = \text{true}) &= \frac{p(\theta = \text{true})p(y = \text{true} \mid \theta = \text{true})}{p(y = \text{true})} \\ &= \frac{0.29 * 1.00}{0.29 * 1.00 + 0.71 * 0.30} \approx 0.58 \end{aligned}$$

**What conclusions can be drawn from this calculation?**



# Aside : Proportionality

Recall PMF / PDF must sum / integrate to 1,

$$\begin{array}{cc} \text{PMF} & \text{PDF} \\ \sum_x p(x) = 1 & \int p(x) dx = 1 \end{array}$$

May only know distribution constant that does not depend on RV  $x$ ,

$$\int \tilde{p}(x) dx = \mathcal{Z} \quad \text{so} \quad p(x) \propto \tilde{p}(x)$$

Properly normalized distribution by dividing our normalization constant:

$$\int p(x) dx = \int \frac{1}{\mathcal{Z}} \tilde{p}(x) dx = \frac{1}{\int \tilde{p}(x) dx} \int \tilde{p}(x) dx = 1$$

# Aside : Proportionality

**Example** Let  $X$  be a Bernoulli RV (coinflip) with probabilities *proportional to*:

$$\tilde{p}(X = 0) = 0.5$$

$$\tilde{p}(X = 1) = 1.5$$

Greater than 1, but  
It is an *unnormalized*  
probability

Compute normalization constant,

$$\mathcal{Z} = \tilde{p}(X = 0) + \tilde{p}(X = 1) = 2.0$$

Normalize probability distribution,

$$p(X) = \frac{1}{\mathcal{Z}} \tilde{p}(X) = \begin{pmatrix} 1/4 \\ 3/4 \end{pmatrix}$$

Sums to 1

# Frequentist vs. Bayesian Inference

We have data  $X_1, \dots, X_N$  and want to infer unknown parameter  $\theta$

## Frequentist Inference

The data *uniquely determines*  $\theta$ , e.g. by the likelihood:

**Not a distribution on parameter**       $p(X_1, \dots, X_N; \theta)$       **How well it explains the data**

## Bayesian Inference

The data *updates our belief* about  $\theta$ , which is random:

$$p(\theta \mid X_1, \dots, X_N) \propto p(\theta \mid X_1, \dots, X_{N-1})p(X_N \mid \theta)$$

**Our belief changes with more data**

# Minimum Mean Squared Error (MMSE)

Posterior mean minimizes squared error,

$$\hat{\theta}^{\text{MMSE}} = \arg \min \mathbb{E}[(\hat{\theta} - \theta)^2 \mid y] = E[\theta \mid y]$$

- Minimizes error conditioned on observed data
- MMSE is an **unbiased estimator**
- MMSE is **asymptotically unbiased** and **asymptotically normal**,

$$\sqrt{N}(\hat{\theta}^{\text{MMSE}} - \theta) \rightarrow \mathcal{N}(0, \sigma^2)$$

# Bayes Estimators

Minimizes expected loss function,

$$\hat{\theta} = \arg \min_{\hat{\theta}} \mathbf{E} \left[ L(\theta, \hat{\theta}) \mid y \right]$$

Expected loss referred to as *Bayes risk*.

**MMSE** minimizes squared-error loss  $L(\theta, \hat{\theta}) = (\theta - \hat{\theta})^2$

**Minimum absolute error (MAE)** is posterior *median*,

$$\arg \min \mathbf{E}[|\hat{\theta} - \theta| \mid y] = \text{median}(\theta \mid y)$$

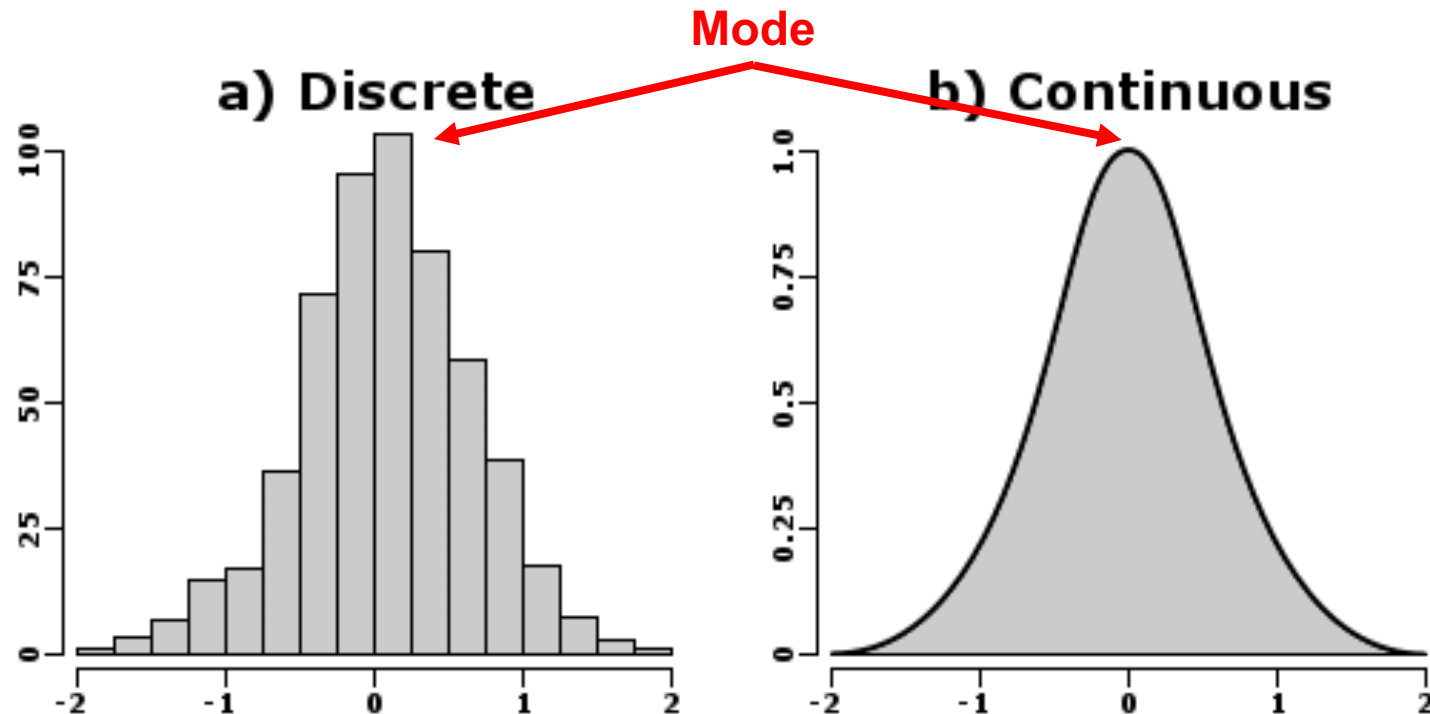
Note: Same answer for linear function:  $L(\theta, \hat{\theta}) = c|\hat{\theta} - \theta|$

# Maximum a Posteriori (MAP)

Very common to produce maximum probability estimates,

$$\hat{\theta}^{\text{MAP}} = \arg \max p(\theta | y)$$

*MAP is the **mode** ( highest probability outcome ) of the posterior*



# Maximum a Posteriori (MAP)

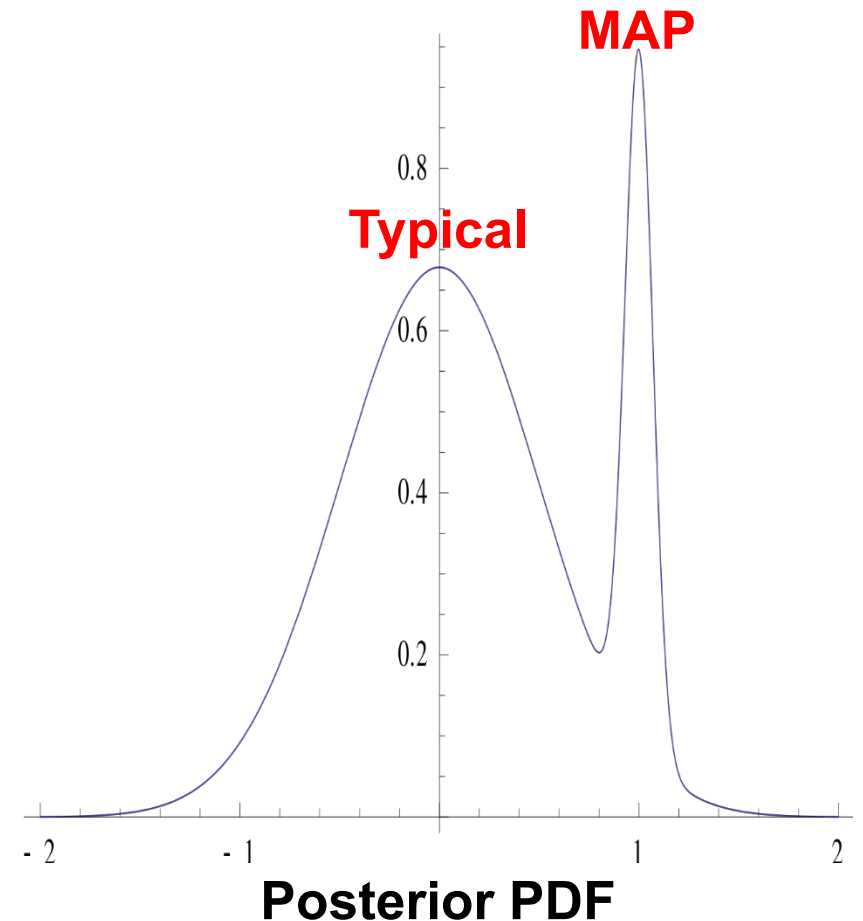
*MAP (mode) may not be representative of typical outcomes*

Also, not a Bayes estimator (unless discrete),

$$\lim_{c \rightarrow 0} L(\theta, \hat{\theta}) = \begin{cases} 0, & \text{if } |\hat{\theta} - \theta| < c \\ 1, & \text{otherwise} \end{cases}$$

**Degenerate loss function**

Despite its issues, MAP is frequently used in “Bayesian” inference and estimation



# Example: Beta-Bernoulli MAP

Let  $X_1, \dots, X_N \sim \text{Bernoulli}(\pi)$  and  $\pi \sim \text{Beta}(\alpha, \beta)$  then posterior is,

$$p(\pi | X_1^N) = \text{Beta}(\alpha + \underbrace{\text{number of heads}}_{N_H}, \beta + \text{number of tails})$$

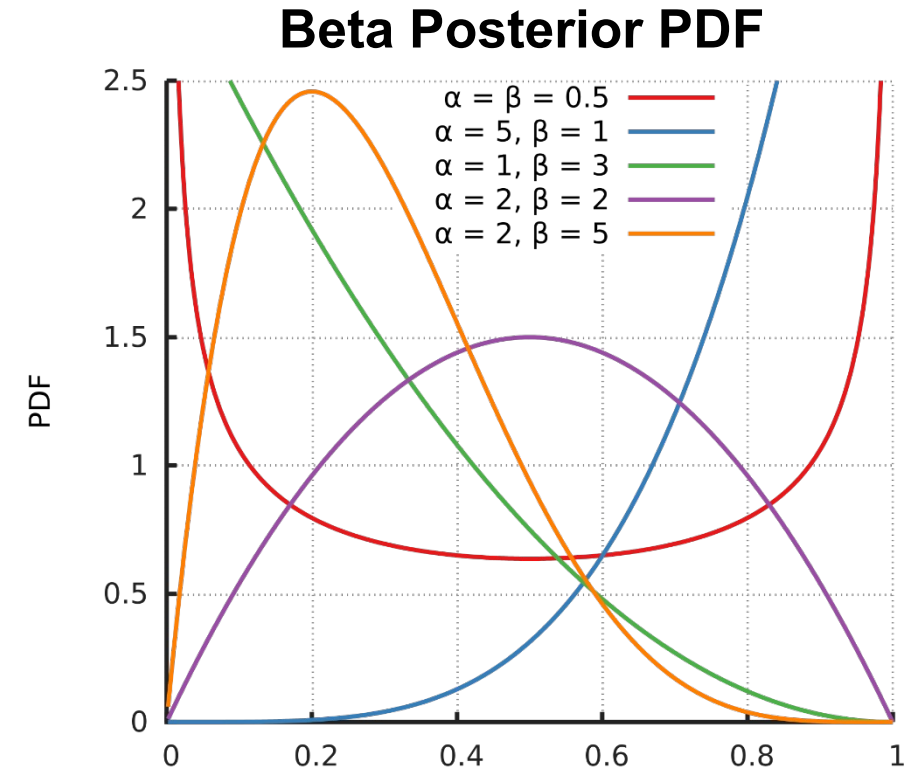
Highest probability (mode) of Beta given by,

Take derivative,  
set to zero, solve.

$$\hat{\pi}^{\text{MAP}} = \frac{\alpha + N_H - 1}{\alpha + \beta + N - 2}$$

Beta distribution is not always convex!

- MAP is any value for  $\alpha = \beta = 1$
- Two modes (bimodal) for  $\alpha, \beta < 1$





# Maximum a Posteriori (MAP)

Equivalent to maximizing joint probability,

$$\arg \max_{\theta} p(\theta | y) = \arg \max_{\theta} \frac{p(\theta, y)}{p(y)} = \arg \max_{\theta} p(\theta, y)$$

**Constant**

For iid  $y_1, \dots, y_N$  solve in log-domain (like *maximum likelihood est.*),

$$\hat{\theta}^{\text{MAP}} = \arg \max_{\theta} \log p(\theta, y_1, \dots, y_N) = \underbrace{\sum_i \log p(y_i | \theta)}_{\text{Log-Likelihood (how well it fits data)}} + \underbrace{\log p(\theta)}_{\text{Log-Prior (how well it agrees with prior)}}$$

***Intuition*** MAP is like MLE but with a “penalty” term (log-prior)

# Prediction

Can make predictions of unobserved  $\tilde{y}$  before seeing any data,

$$p(\tilde{y}) = \sum_k p(\theta = k)p(\tilde{y} | \theta = k)$$

**Similar calculation to marginal likelihood**

*This is the **prior predictive** distribution*

For continuous parameters sum turns into integral,

$$p(\tilde{y}) = \int p(\theta)p(\tilde{y} | \theta) d\theta$$

*This is a prediction based on **no observed data***

# Prediction

When we observe  $y$  we can predict future observations  $\tilde{y}$ ,

$$p(\tilde{y} | y) = \sum_k \underbrace{p(\theta = k | y)}_{\text{This is now the posterior}} p(\tilde{y} | \theta = k)$$

This is now the posterior

*This is the **posterior predictive distribution***

Again, for continuous parameters sum turns into integral,

$$p(\tilde{y} | y) = \int p(\theta | y) p(\tilde{y} | \theta) d\theta$$

# Prediction Example

About **29%** of American adults have high blood pressure (BP). Home test has **30% false positive** rate and no false negative error.



What is the likelihood of *another* positive measurement?

$$p(\tilde{y} = true \mid y = true) = \sum_{\theta \in \{true, false\}} p(\theta \mid y = true) p(\tilde{y} = true \mid \theta)$$

$$= 0.42 * 0.30 + 0.58 * 1.00 \approx 0.71$$

**What conclusions can be drawn from this calculation?**

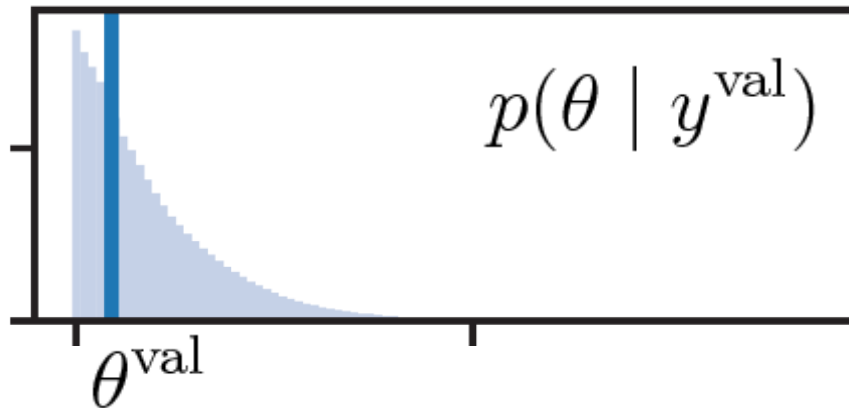
# Model Validation

*How do we know if the model  $p(\theta, y)$  is good?*

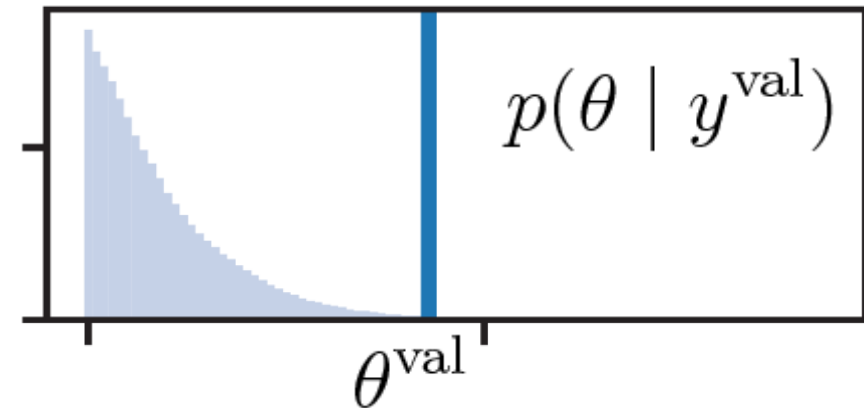
## Supervised Learning

Validation set  $\{(\theta^{\text{val}}, y^{\text{val}})\}$  consists of known  $\theta^{\text{val}}$ . Are true values typically preferred under the posterior?

Good (maybe lucky)



Not Good (maybe unlucky)



Repeat trials over validation set for more certainty

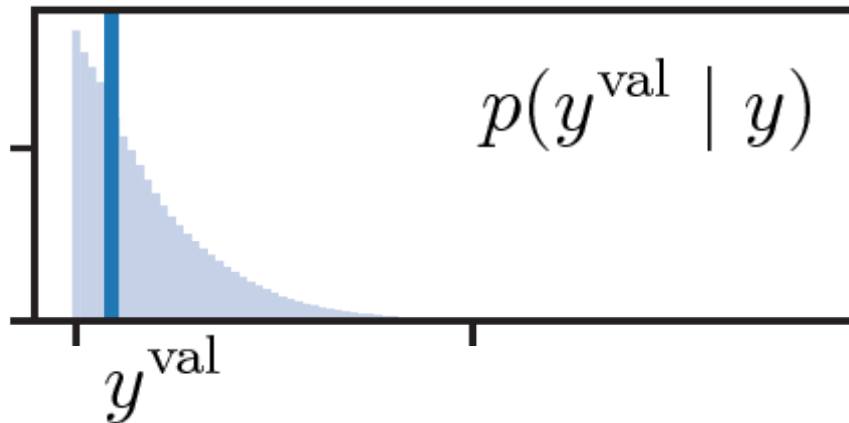
# Model Validation

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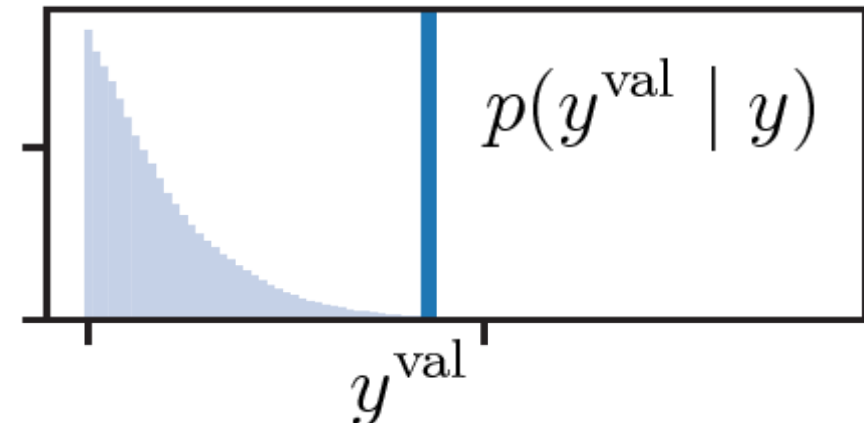
## Unsupervised Learning

Validation set  $\{y^{\text{val}}\}$  only contains observable data. Check validation data against posterior-predictive distribution.

Good (maybe lucky)



Not Good (maybe unlucky)



Repeat trials over validation set for more certainty

# Likelihood and Odds Ratios

Which parameter value  $\theta_1$  or  $\theta_2$  is more likely to have generated the observed data  $y$ ?

The **posterior odds ratio** is:

$$\frac{p(\theta_1 | y)}{p(\theta_2 | y)} = \frac{p(\theta_1) p(y | \theta_1) \cancel{p(y)}}{p(\theta_2) p(y | \theta_2) \cancel{p(y)}}$$

Prior Odds  
Ratio

Likelihood  
Ratio

**Observe:** the marginal likelihood  $p(y)$  cancels!

# Posterior Summarization

*Ideally we would report the full posterior distribution as the result of inference...but this is not always possible*

## **Summary of Posterior Location:**

Point estimates: mean (MMSE), mode, median (min. absolute error)

## **Summary of Posterior Uncertainty:**

Credible intervals / regions, posterior entropy, variance

**Bayesian analysis should report uncertainty when possible**



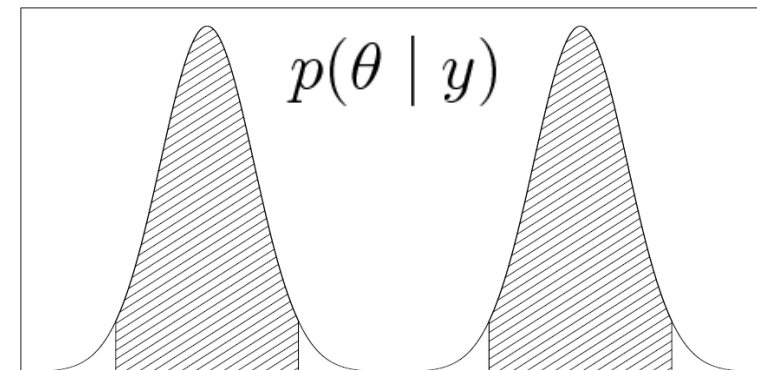
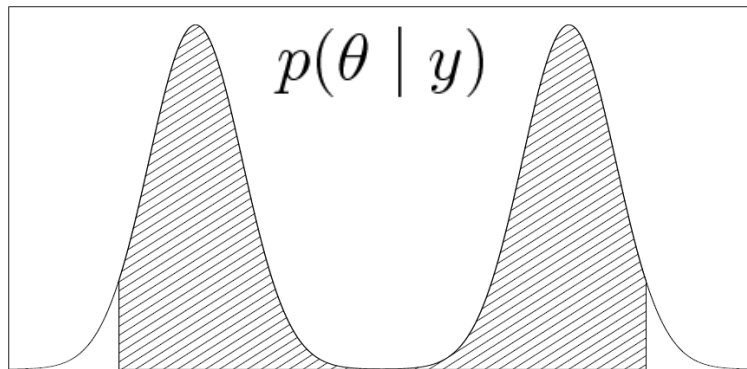
# Credible Interval

**Def.** For parameter  $0 < \alpha < 1$  the  $100(1 - \alpha)\%$  credible interval  $(L(y), U(y))$  satisfies,

$$p(L(y) < \theta < U(y) \mid y) = \int_{L(y)}^{U(y)} p(\theta \mid y) = 1 - \alpha$$

**Interval containing fixed percentage of posterior probability density.**

**Note:** This is not unique -- consider the 95% intervals below:



# Summary

- Bayesian statistics interprets probability differently than classical stats
  - Frequentist: Probability  $\rightarrow$  Long run odds in repeated trials
  - Bayesian: Probability  $\rightarrow$  Belief of outcome that captures all uncertainty
- Bayesian models treat unknown parameter as random, with a prior
- Bayesian inference via the *posterior distribution* using Bayes' rule

$$p(\theta | y) = \frac{p(\theta)p(y | \theta)}{p(y)}$$

- Bayesian estimators minimize expected risk (e.g. MMSE)
- Maximum a posteriori (MAP) estimate maximizes posterior probability

