



Lecture 2: Recap of Probability Theory

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Trustworthy AI

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Bibliography

Introduction

Discrete Random Variables

Continuous Random Variables

Moments

Bayes' Theorem

- Statistics Lab notes by Prof. Wolf
- Bishop - Chapter 1.2

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Bayes' Theorem

- A key concept in ML is uncertainty.
- Source of uncertainty are diverse and include the noise in the measurements (i.e., in the observed data) and the finite sample size from the underlying data distribution.
- Probability theory gives a theoretical framework to reason under uncertainty, i.e., to quantify and manipulate uncertainty.
- **Frequentist interpretation:** Probability as the frequency or propensity of some event, i.e.,

$$P(A) = \lim_{n \rightarrow \infty} \frac{n_A}{n},$$

where n_A is the number of times A happens in n trials (usually it is assumed that $n \rightarrow \infty$).

- **Bayesian interpretation:**
Probabilities as quantification of a belief or the uncertainty on unobserved quantities.

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Bayes' Theorem

- A random variable is used to represent the outcome of an experiment. When the number of possible outcomes is countable, then we encounter a **discrete random variable**.
- The set of all possible outcomes is called the **sample space**: $\Omega = \{\omega_1, \dots, \omega_n\}$ (e.g., in tossing a coin experiment, $\Omega = \{H, T\}$).
- **Elementary event** is a singleton $\{\omega_r\}$ of Ω , i.e., is an event which cannot be further divided into other events.
- **The set of all possible events** is the power set 2^Ω (for the coin: $\{\emptyset, \{H\}, \{T\}, \{H, T\}\}$).
- The **probability function** P maps events $A \in 2^\Omega$ into the probability of such an event, i.e., $P : 2^\Omega \rightarrow [0, 1]$, such that
 - $P(\emptyset) = 0$ and $P(\Omega) = 1$,
 - $\sum_{\omega_i \in \Omega} P(\{\omega_i\}) = 1$,
 - $A \in 2^\Omega \implies P(A) = \sum_{\omega_i \in A} P(\{\omega_i\})$.
- **Additive rule of probabilities:**
Let $A, B \in 2^\Omega$, then $P(A \cup B) = P(A) + P(B) - P(A \cap B)$.

- An experiment with two possible outcomes $Y \in \{0, 1\}$ is called **Bernoulli trial** (or binomial trial) and is defined by the “success” probability $p = P(Y = 1)$.
- The **binomial distribution** models n repeated Bernoulli trials where the outcomes are independent (e.g., in a coin toss experiment) and the random variable X accounts for the number of times we observe “success” $Y = 1$ (the order does not matter), i.e.,

$$P(X = k) = \binom{n}{k} p^k (1 - p)^{n-k},$$

with the binomial coefficient $\binom{n}{k} = \frac{n!}{k!(n-k)!}$.

- The sample space is thus $\Omega = \{0, 1, \dots, n\}$ and

$$P(\Omega) = \sum_{k=0}^n P(X = k) = \sum_{k=0}^n \binom{n}{k} p^k (1 - p)^{n-k} = (1 - p + p)^n = 1.$$

Example: Binomial distribution II

- Coin toss: $\Omega = \{H, T\}$, $P(H) = p$. Define $Y : \{H, T\} \rightarrow \{0, 1\}$ by

$$Y = \begin{cases} 1 & \text{if } H, \\ 0 & \text{if } T. \end{cases}$$

Y is a random variable with Bernoulli-distribution:

$$P_Y(Y = 1) = P(H) = p, \text{ and similarly } P_Y(Y = 0) = 1 - p.$$

- Repeat the coin toss independently n times and denote by X the number of times we observe head. Let Ω be the set of all sequences of n variables with the alphabet $\{H, T\}$, then $|\Omega| = 2^n$. X is a random variable $X : \Omega \rightarrow \mathbb{Z}$ with distribution

$$P_X(X = k) = P(X^{-1}(k)) = \binom{n}{k} p^k (1 - p)^{n-k}.$$

If $n = 3$, then $X^{-1}(2) = \{HHT, HTH, THH\}$.

- There are two fundamental rules of probability theory:

$$\textbf{Sum rule: } P(X) = \sum_Y P(X, Y) \quad (1)$$

$$\textbf{Product rule: } P(X, Y) = P(Y | X)P(X)(= P(X \cap Y)) \quad (2)$$

- Let X, Y be discrete random variables. X and Y are **independent** if,

$$P_{X \times Y}(X = i, Y = j) = P_X(i) P_Y(j), \quad \forall i, j \in \mathbb{Z}.$$

- The **conditional probability** $P(X = i | Y = j)$ of X given $Y = j$ is,

$$P(X = i | Y = j) = \frac{P_{X \times Y}(X = i, Y = j)}{P(Y = j)}, \quad \forall j \text{ with } P(Y = j) > 0.$$

Example: Oranges v.s Apples from Bishop

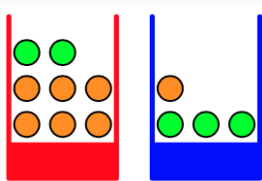


Figure 1: Figure 1.9 from Bishop

$$P(B = r) = 4/10$$

$$P(B = b) = 6/10$$

$$P(F = a|B = r) = 1/4$$

$$P(F = o|B = r) = 3/4$$

$$P(F = a|B = b) = 3/4$$

$$P(F = o|B = b) = 1/4$$

$$P(F = a) = P(F = a|B = r)P(B = r) + P(F = a|B = b)P(B = b)$$

$$= \frac{1}{4} \times \frac{4}{10} + \frac{3}{4} \times \frac{6}{10} = \frac{11}{20}$$

$$P(B = r|F = o) = \frac{P(F = o|B = r)P(B = r)}{P(F = o)} = \frac{3/4 \times 4/10}{9/20} = \frac{2}{3}$$

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- So far, random variables taking discrete values $X \in \{1, 2, 3, \dots\}$, thus Ω is a countable set.
- What if we consider continuous variables, e.g., $X \in \mathbb{R}$, and thus $\Omega = \mathbb{R}$ is uncountable?
How do we assign probabilities to all 2^Ω events?
- If all numbers are equally likely to occur, how do we ensure that $\sum_{\omega_i \in \Omega} P(\omega_i) = 1$?

Definition (σ -algebra)

A set $\mathcal{A} \subset 2^\Omega$ is called a σ -**algebra**:

1. If $\emptyset \in \mathcal{A}$ and $\Omega \in \mathcal{A}$,
2. If $A \in \mathcal{A}$, then also the complement A^c is contained in \mathcal{A} ,
3. If \mathcal{A} is closed under **countable** unions, that is if A_1, A_2, \dots is a sequence of events in \mathcal{A} , then $\bigcup_{i=1}^{\infty} A_i \in \mathcal{A}$.

Definition (Probability measure)

A **probability measure** defined on a σ -algebra \mathcal{A} of Ω is a function $P : \mathcal{A} \rightarrow [0, 1]$ that satisfies:

1. $P(\Omega) = 1$,
2. For every countable sequence $(A_n)_{n \geq 1}$ of elements of \mathcal{A} , pairwise disjoint (that is $A_m \cap A_n = \emptyset$ whenever $m \neq n$), one has

$$P\left(\bigcup_{n=1}^{\infty} A_n\right) = \sum_{n=1}^{\infty} P(A_n).$$

- Any discrete **probability space** $(\Omega, 2^{\Omega}, P)$ is a probability measure, since 2^{Ω} is a σ -algebra and P is a probability measure.

Let $C \subset 2^\Omega$. The σ -algebra generated by C is the smallest σ -algebra containing C .

Definition (Borel σ -algebra)

The **Borel σ -algebra** \mathcal{B} in \mathbb{R}^d is the σ -algebra generated by the open sets in \mathbb{R}^d .

Lebesgue Measure on \mathbb{R}^d

- The Lebesgue measure $\mu : \mathcal{B} \rightarrow \mathbb{R}_+$ is now just the usual measure of volume. For the one-dimensional case, we have

$$\mu([a, b[) = b - a,$$

- A set $A \in \mathcal{B}$ has **measure zero** if $\mu(A) = 0$. Any countable set of points has Lebesgue measure zero.

Warning: The Lebesgue measure works on its own (larger) σ -algebra but the difference is for our purposes negligible.

In the case $\Omega = \mathbb{R}^d$ we will work with measures which have a density with respect to the **Lebesgue measure**.

Let \mathcal{B} be the Borel σ -algebra in \mathbb{R}^d . A probability measure P on $(\mathbb{R}^d, \mathcal{B})$ has a **density** p if p is a non-negative (Borel measurable) function on \mathbb{R}^d satisfying for all $A \in \mathcal{B}$ that:

$$P(A) = \int_A p(x) dx = \int_A p(x_1, \dots, x_d) dx_1 \dots dx_d,$$

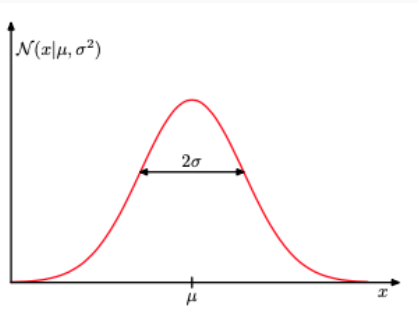
where $dx = dx_1 \dots dx_d$.

- This implies: $P(\mathbb{R}^d) = \int_{\mathbb{R}^d} p(x) dx = 1$.
- Observation: Not all probability measures on \mathbb{R}^d have a density.

Example of a probability measure with density

The **Gaussian distribution** or normal distribution on \mathbb{R} has two parameters μ (mean) and σ^2 (variance). The associated density function is denoted by $\mathcal{N}(\mu, \sigma^2)$ and defined as:

$$p(X = x) = \frac{1}{\sqrt{2\pi\sigma^2}} e^{-\frac{(x-\mu)^2}{2\sigma^2}}.$$



$$\mathbb{E}[x] = \int_{-\infty}^{\infty} \mathcal{N}(x | \mu, \sigma^2) x \, dx = \mu$$

$$\mathbb{E}[x^2] = \int_{-\infty}^{\infty} \mathcal{N}(x | \mu, \sigma^2) x^2 \, dx = \mu^2 + \sigma^2$$

$$\text{var}[x] = \mathbb{E}[x^2] - \mathbb{E}[x]^2 = \sigma^2$$

Figure 2: Figure 1.13 from Bishop

- **Multivariate Gaussian** $\mathcal{N}(\mu, \Sigma)$ is uniquely determined by the mean $\mu \in \mathbb{R}^d$ and the covariance matrix $\Sigma \in \mathbb{R}^{d \times d}$ (positive-definite) as

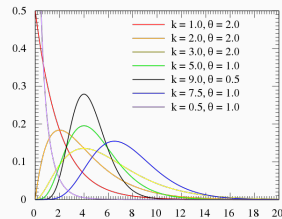
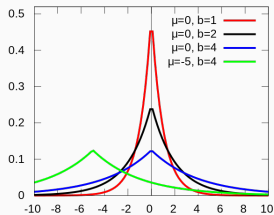
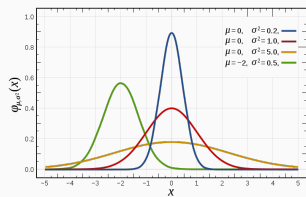
$$p(x) = \frac{1}{(2\pi)^{\frac{d}{2}} |\det \Sigma|^{\frac{1}{2}}} e^{-\frac{1}{2}(x-\mu)^T \Sigma^{-1}(x-\mu)}$$

- **Laplace distribution** $\text{Laplace}(\mu, b)$ is given by

$$p(x) = \frac{1}{2b} e^{-\frac{1}{b}|x-\mu|}$$

- **Gamma distribution** $\Gamma(\alpha, \beta)$ given by:

$$p(x) = \frac{x^{\alpha-1} \beta^\alpha e^{-\beta x}}{\Gamma(\alpha)}, \text{ where } \Gamma(\cdot) \text{ is the Gamma function.}$$



- The **(cumulative) distribution function** of a probability measure P on $(\mathbb{R}, \mathcal{B})$ is the function

$$F(x) = P(X \in (-\infty, x]) = P(X \leq x) = \int_{-\infty}^x p(t) dt.$$

If the distribution function F is sufficiently differentiable, then

$$p(x) = \left. \frac{\partial F}{\partial x} \right|_x.$$

- The distribution function of P on $(\mathbb{R}^d, \mathcal{B})$ is the function

$$F(x_1, \dots, x_d) = P(X_1 \leq x_1, \dots, X_d \leq x_d).$$

If the distribution function F is sufficiently differentiable, then

$$p(x_1, \dots, x_d) = \left. \frac{\partial^d F}{\partial x_1 \dots \partial x_d} \right|_{x_1, \dots, x_d}.$$

Quantiles: Quantiles are only defined for distributions on \mathbb{Z} and \mathbb{R} .

Definition

The α -**quantile** of a probability measure on \mathbb{Z} or \mathbb{R} is the real number q_α such that

$$F(q_\alpha) = P([-\infty, q_\alpha]) = \alpha.$$

The **median** is the $\frac{1}{2}$ -quantile.

- Median and mean agree if the distributions are symmetric (and unimodal).
- The median is more robust to changes of the probability measure.

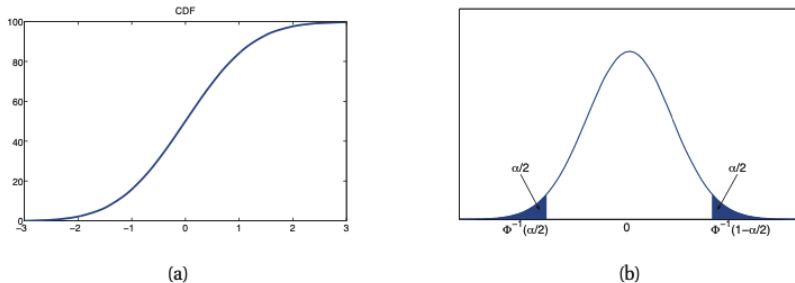


Figure 2.3 (a) Plot of the cdf for the standard normal, $\mathcal{N}(0, 1)$. (b) Corresponding pdf. The shaded regions each contain $\alpha/2$ of the probability mass. Therefore the nonshaded region contains $1 - \alpha$ of the probability mass. If the distribution is Gaussian $\mathcal{N}(0, 1)$, then the leftmost cutoff point is $\Phi^{-1}(\alpha/2)$, where Φ is the cdf of the Gaussian. By symmetry, the rightmost cutoff point is $\Phi^{-1}(1 - \alpha/2) = -\Phi^{-1}(\alpha/2)$. If $\alpha = 0.05$, the central interval is 95%, and the left cutoff is -1.96 and the right is 1.96. Figure generated by `quantileDemo`.

Let $X = (X_1, X_2)$ be a \mathbb{R}^2 -valued random variable with density p_X on \mathbb{R}^2 . Then the densities p_{X_1} of X_1 and p_{X_2} of X_2 are given as

$$p_{X_1}(x_1) = \int_{\mathbb{R}} p_X(x_1, x_2) dx_2, \quad p_{X_2}(x_2) = \int_{\mathbb{R}} p_X(x_1, x_2) dx_1.$$

- $p_X(x_1, x_2)$ denotes the **joint density**.
- p_{X_1} and p_{X_2} are called **marginal densities** of X and are associated to the probability measures of X_1 respectively X_2 .

Observation: The joint measure can in general not be reconstructed from the knowledge of the marginal densities (only if X_1 and X_2 are independent).

Let X, Y be \mathbb{R} -valued random variables with joint-density $p_{X \times Y}$ and marginal densities p_X and p_Y , then X and Y are **independent** if

$$p_{X \times Y}(x, y) = p_X(x) p_Y(y), \quad \forall x, y \in \mathbb{R}.$$

The **conditional density** $p(x|Y = y)$ of X given $Y = y$ is defined as,

$$p(x|y) = \frac{p(x, y)}{p(y)}, \quad \forall y \text{ with } p(y) > 0.$$

Example: Joint, marginals and conditionals

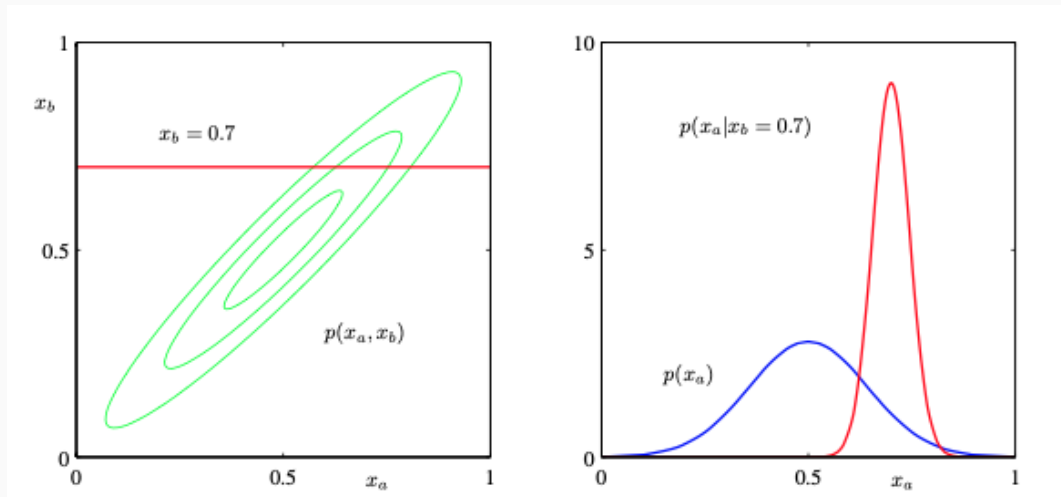


Figure 2.9 from Bishop

Theorem

Let $X = (X_1, \dots, X_d)$ have joint density p_X . Let $g : \mathbb{R}^d \rightarrow \mathbb{R}^d$ be continuously differentiable and injective, with non-vanishing Jacobian. Then $Y = g(X)$ has density

$$p_Y(y) = p_X(g^{-1}(y)) |\det J_{g^{-1}}(y)|$$

- The Jacobian $J_g(x)$ of a function $g : \mathbb{R}^d \rightarrow \mathbb{R}^d$ at value x is the $d \times d$ - matrix

$$J_g(x)_{ij} = \left. \frac{\partial g_i}{\partial x_j} \right|_x, \quad i, j = 1, \dots, d$$

- This result allows us to generate samples from complicated densities from simple ones.

Example: Sampling from an exponential distribution

$$p_{\lambda}(y) = \lambda \exp(-\lambda y), \text{ for } y \geq 0.$$

1. We can first sample from a uniform distribution on $[0, 1]$.
2. Apply a function $g : [0, 1] \rightarrow \mathbb{R}_+$ (resp. g^{-1}) such that

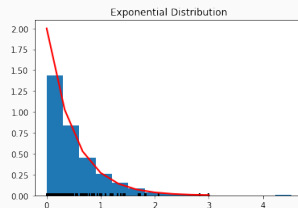
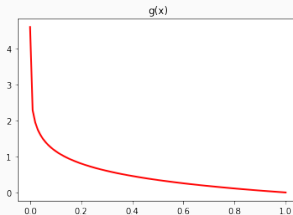
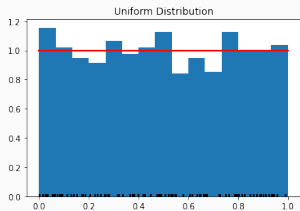
$$p_{\lambda}(y) = \lambda \exp(-\lambda y) = p_X(g^{-1}(y)) \left| \frac{\partial g^{-1}}{\partial y} \right| = \left| \frac{\partial g^{-1}}{\partial y} \right|.$$

General case: complicated differential equation.

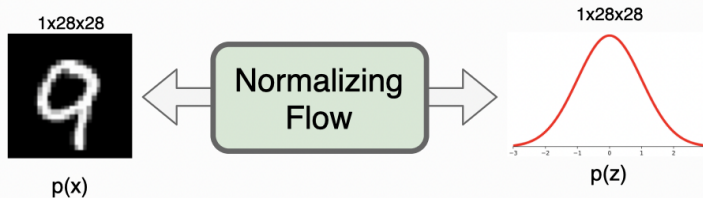
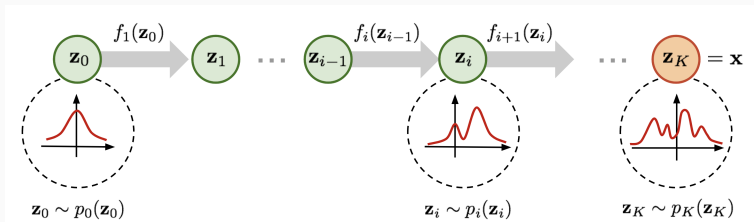
This case: $g^{-1}(y) = \exp(-\lambda y) \implies g(x) = -\frac{\log(x)}{\lambda}$

- X_i samples from the uniform distribution on $[0, 1]$,
- $Y_i = g(X_i) = -\frac{\log(X_i)}{\lambda}$ are samples from the exponential distribution.

Example: Sampling from an exponential distribution



Outlook: State of the Art Normalizing Flow Models



e.g. Kingma'18, Flow++, GLOW

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The **expected value** or **expectation** of a \mathbb{R}^d -valued random variable X is defined as

$$(\mathbb{E}[X])_i = \int_{\mathbb{R}^d} x_i p(x) dx = \int_{\mathbb{R}^d} x_i p(x_1, \dots, x_d) dx_1 \dots dx_d,$$

and for a discrete random variable X taking values in \mathbb{Z} it is defined as,

$$\mathbb{E}[X] = \sum_{n=-\infty}^{\infty} n P(X = n).$$

Expectation of functions of random variables

We can also define the expectation of functions of random variables.

$$\mathbb{E}[f(X)] = \int_{\mathbb{R}^d} f(x) p(x) dx = \int_{\mathbb{R}^d} f(x_1, \dots, x_d) p(x_1, \dots, x_d) dx_1 \dots dx_d.$$

The **variance** $\text{Var}[X]$ (also $\sigma^2(X)$) of an \mathbb{Z} - or \mathbb{R} -valued random variable X is defined as

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

The standard deviation of X is $\sigma(X) = \sqrt{\text{Var}[X]}$.

The covariance matrix Σ of an \mathbb{R}^d -valued random variable X is given as $\Sigma_{ij} = \text{Cov}(X_i, X_j)$ or in matrix form

$$\Sigma = \mathbb{E}[(X - \mathbb{E}[X])(X - \mathbb{E}[X])^T].$$

The **covariance** $\text{Cov}(X, Y)$ of two \mathbb{R} -valued random variables X and Y is defined as,

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

The **correlation** $\text{Corr}(X, Y)$ of two \mathbb{R} -valued random variables X and Y is then defined as,

$$\text{Corr}(X, Y) = \frac{\text{Cov}(X, Y)}{\sqrt{\text{Cov}(X, X) \text{Cov}(Y, Y)}} = \frac{\text{Cov}(X, Y)}{\sigma(X)\sigma(Y)}.$$

- The expectation and variance have the following properties $\forall a, b \in \mathbb{R}$,

$$\begin{aligned}\mathbb{E}[aX + b] &= a \mathbb{E}[X] + b, & \mathbb{E}[X + Y] &= \mathbb{E}[X] + \mathbb{E}[Y], \\ \text{Var}[aX + b] &= a^2 \text{Var}[X], \\ \text{Var}[X + Y] &= \text{Var}[X] + \text{Var}[Y] + 2 \text{Cov}(X, Y).\end{aligned}$$

- Correlation is a measure of **linear dependence**, and satisfies $-1 \leq \text{Corr}(X, Y) \leq 1$. If X and Y are linearly dependent, that is $Y = aX + b$ with $a, b \in \mathbb{R}$, then

$$\text{Corr}(X, Y) = \text{Corr}(X, aX + b) = \frac{a}{|a|} = \begin{cases} 1, & \text{if } a > 0, \\ 0, & \text{if } a = 0, \\ -1, & \text{if } a < 0. \end{cases}$$

In words, linearly dependent random variables achieve maximal correlation.

Let X, Y be two \mathbb{R} -valued random variables. The **conditional expectation** $\mathbb{E}[X|Y = y]$ of X given $Y = y$ is defined for y with $p(y) > 0$ as the quantity

$$\mathbb{E}[X|Y = y] = \int_{\mathbb{R}} x p(x|y) dx.$$

The **conditional expectation** $\mathbb{E}[X|Y]$ of X given Y is a random variable $h(Y)$ with values

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

Important properties of the conditional expectation are:

- $\mathbb{E}[X|Y] = \mathbb{E}[X]$, if X and Y are **independent**,
- $\mathbb{E}[\mathbb{E}[X|Y]] = \mathbb{E}[X]$,
- $\mathbb{E}[f(Y)|Y] = f(Y)$ and $\mathbb{E}[f(Y)g(X)|Y] = f(Y)\mathbb{E}[g(X)|Y]$.

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Bayes' Theorem

Assume that we have a finite or countably infinite number of events $\mathcal{A} = \{A_1, A_2, A_3, \dots\}$ and $\Omega = A_1 \cup A_2 \cup A_3 \cup \dots$

Definition

A collection of events $(A_n)_{n \geq 1}$ is called a **partition** of Ω if $A_n \in \mathcal{A}$ for each n , they are pairwise disjoint, $A_n \cap A_m = \emptyset$ for $m \neq n$, $P(A_n) > 0$ for each n , and $\cup_n A_n = \Omega$.

Theorem (Law of total probability)

Let $(A_n)_{n \geq 1}$ be a finite or countable partition of Ω . Then if $B \in \mathcal{A}$,

$$P(B) = \sum_n P(B|A_n)P(A_n).$$

Theorem (Bayes' theorem)

Let A, B be two events and $P(B) > 0$, then

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

- The above definition follows from the definition of conditional probability.
- Implication: Let $(A_n)_{n \geq 1}$ be a finite or countable partition of Ω , and suppose $P(B) > 0$.
Then

$$P(A_i|B) = \frac{P(B|A_i)P(A_i)}{\sum_n P(B|A_n)P(A_n)}.$$

$$P(A, B) = P(A, B)$$

$$P(A|B)P(B) = P(B|A)P(A)$$

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

What is the probability of having Covid given that a test is positive? $P(\text{covid}|\text{positive})$

- Sensitivity, e.g. 96.5% $\rightarrow P(\text{positive}|\text{covid}) = 0.965$
False-negative-rate $1 - \text{sensitivity} = 3.5\%$
- Specificity, e.g. 99.7% $\rightarrow P(\text{negative}|\text{healthy}) = 0.997$
False-positive-rate is $1 - \text{specificity} = 0.3\%$
- Prevalence, e.g. 0.25% $\rightarrow P(\text{covid}) = 0.0025$ (Note: we pick a **random** person here!)

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

$$P(\text{covid}|\text{positive}) = \frac{P(\text{positive}|\text{covid})P(\text{covid})}{P(\text{positive})}$$

$$P(\text{covid}|\text{positive}) = \frac{P(\text{positive}|\text{covid})P(\text{covid})}{P(\text{positive}|\text{covid})P(\text{covid}) + P(\text{positive}|\text{healthy})P(\text{healthy})}$$

$$P(\text{covid}|\text{positive}) = \frac{0.965 * 0.0025}{0.965 * 0.0025 + 0.003 * 0.9975} = 0.446$$



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