DDA3020 Machine Learning
Lecture 02 Probability Theory

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Outline

Definition and branches of machine learning

Basic concepts, learning process

Random experiment, sample space, event

- Random experiment: we describe a random experiment by its **procedure** and observations of its **outcomes**. For example, we toss a coin 2 times, and observe which side is up after each toss.
- Sample space: All possible outcomes of the random experiment form a sample space S. For the above coin toss example, we define

$$S = \{(Head, Head), (Head, Tail), (Tail, Head), (Tail, Tail)\}.$$

- Event: A **subset** of sample space S, denoted as A, can be called as an event in a random experiment, *i.e.*, $A \subset S$. In the above example, we define an event A as *at least one head up*, then it can be represented by

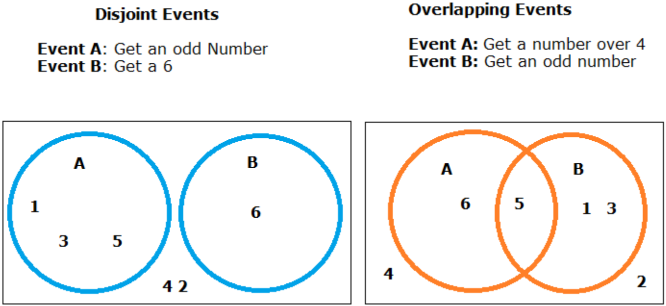
$$A = \{(Head, Head), (Head, Tail), (Tail, Head)\} \subset S.$$

.

Probability of events

Assuming events $A \subset S$ and $B \subset S$, the probabilities of events related with and must satisfy,

- $P(A) \geq 0$
- $P(S) = 1$
- If $A \cap B = \emptyset$, then $P(A \cup B) = P(A) + P(B)$; otherwise, $P(A \cup B) = P(A) + P(B) - P(A \cap B)$



Random variables

- A random variable is a real valued function from the sample space S to a real space $\mathbb{R}$, as follows:

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

- Still take the 2-times coin toss as example, if we define the random variable as the number of tails, then we have

$$X((H,H)) = 0, X((H,T)) = 1, X((T,H)) = 1, X((T,T)) = 2.$$

  Then, the output space of X is denoted as $\{0, 1, 2\}$, also called state space $\mathcal{X}$.

- There are two types of random variables:
  - **Discrete**: $\mathcal{X}$ is discrete
  - **Continuous**: $\mathcal{X}$ is continuous

Exercises of Random variables

- `Exercise 1`: For the random experiment of throwing a pair of dice, please write down its sample space, and the event *at least one number 3 on two dice* as well as its probability.

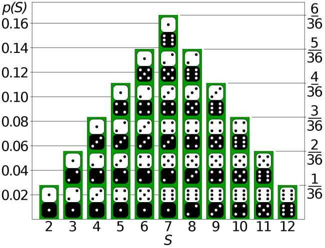
- `Exercise 2`: For the above random experiment, we define the random variable as *the number summation of two dice*, please write down its state space.

Probability of discrete random variables

- Probability of discrete random variable describes the chance of each state x in $\mathcal{X}$ for random variable X in a random experiment, denoted as

$$P(X = x), x \in \mathcal{X}.$$

- `Exercise 1`: If we assume the coin is fair in the random experiment of 2-times coin toss, *i.e.*, $P(Head) = P(Tail) = \frac{1}{2}$ for toss, please compute the probability of different number of tails.
- `Exercise 2`: For the random experiment of throwing a pair of dice, please compute the probability of the state of 3 (*i.e.*, the number summation of two dice equals to 3).



Joint, marginal, conditional probability

- Probability of a union of two events: Given two events A and B, we define the probability of A or B as follows:

$$\begin{aligned} P(A \cup B) &= P(A) + P(B) - P(A \cap B), \\ &= P(A) + P(B) \text{ if } A \text{ and } B \text{ are } \textbf{mutually exclusive}. \end{aligned} \tag{1}$$

- Joint probabilities: The probability of the joint event A and B is defined as follows:

$$P(A, B) = P(A \cap B) = P(A|B)P(B) = P(B|A)P(A), \tag{2}$$

  It is called the **product rule**.

- Marginal distribution: Given the above joint distribution, we can define the **marginal distribution** as follows:

$$P(A) = \sum_b P(A, B) = \sum_b P(A|B = b)P(B = b), \tag{3}$$

  which sums over all possible states of B. It is called the **sum rule**.

Conditional probability and Bayes rule

- Conditional probability: Recalculating probability of event A after someone tells you that event B happened, as follows:

$$P(A|B) = \frac{P(A \cap B)}{P(B)} \tag{4}$$

$$P(A \cap B) = P(A|B)P(B) \tag{5}$$

- Bayes Rule: Combining the definition of conditional probability with the product and sum rules yields Bayes rule, as follows:

$$P(B|A) = \frac{P(A|B)P(B)}{P(A)}, \tag{6}$$

$$P(X = x|Y = y) = \frac{P(X = x, Y = y)}{P(Y = y)} = \frac{P(X = x)P(Y = y|X = x)}{\sum_{x' \in \mathcal{X}} P(X = x')P(Y = y|X = x')} \tag{7}$$

Application of Bayes rule: medical diagnosis

- Suppose that you do a medical test for breast cancer, the test result could be *positive* or *negative*. We denote $x = 1$ as the event of positive test, while $x = 0$ as the event of negative test. We denote $y = 1$ as the event of having breast cancer, while $y = 0$ as the event of no breast cancer.
- Suppose that if one has breast cancer, the test will be positive with the probability 0.8, *i.e.*,

$$P(x = 1|y = 1) = 0.8. \tag{8}$$

- Then, if one gets a positive test result, what is the probability of having breast cancer? $P(y = 1|x = 1) = 0.8?$

Application of Bayes rule: medical diagnosis

- It is WRONG! It ignores the prior probability of having breast cancer.
- According to statistics, the average risk of a woman in the United States developing breast cancer sometime in her life is about 13%, *i.e.*,

$$P(y = 1) = 0.13. \tag{9}$$

- We also need to take into account the fact that the test may be a **false positive** or **false alarm**. Unfortunately, such false positives are quite likely (with current screening technology):

$$P(x = 1|y = 0) = 0.1. \tag{10}$$

- Combining all above probabilities using Bayes rule, we can compute

$$\begin{aligned} P(y = 1|x = 1) &= \frac{P(x = 1|y = 1)P(y = 1)}{P(x = 1|y = 1)P(y = 1) + P(x = 1|y = 0)P(y = 0)} \\ &= \frac{0.8 \times 0.13}{0.8 \times 0.13 + 0.1 \times 0.87} = 0.5445. \end{aligned} \tag{11}$$

It tells that if you test positive, you have have about a 54% chance of really having breast cancer!

Independent random variables

- Independent: If X and Y are independent, denoted as $X \perp Y$, then the joint probability can be represented as the product of two marginals, *i.e.*,

$$X \perp Y \Longleftrightarrow P(X, Y) = P(X)P(Y). \tag{12}$$

- Given the above independence, we can use fewer parameters to define a joint probability. Suppose that X has 3 states, Y has 4 states, then we need $3 - 1 = 2$ and $4 - 1 = 3$ free parameters to define $P(X)$ and $P(Y)$, respectively.
- If without the independence, how many free parameters do we need to define the joint probability $P(X, Y)$? $(3 \times 4) - 1 = 11$.
- If given the independence, *i.e.*, $P(X, Y) = P(X)P(Y)$, how many free parameters do we need? $(3 - 1) + (4 - 1) = 5$.

Expectation and variance of discrete random variables

- Expectation (or mean): $E(X) = \sum_{x \in \mathcal{X}} x P(X = x)$
- Expectation of a function: $E(f(X)) = \sum_{x \in \mathcal{X}} f(x) P(X = x)$
- Moments: expectation of power of X: $M_k = E(X^k)$
- Variance: Average (squared) fluctuation from the mean

$$\mathrm{Var}(X) = E((X - E(X))^2) = E(X^2) - E(X)^2 = M_2 - M_1^2. \tag{13}$$

- Standard deviation: Square root of variance, *i.e.*,

$$\mathrm{Std} = \sqrt{\mathrm{Var}(X)}. \tag{14}$$

- `Exercise` : For the random variable of the number of tails in the random experiment of 2-times coin toss, please compute the above values.

Continuous random variables

- A random variable X is continuous if its state space $\mathcal{X}$ is uncountable.
- In this case, $P(X = x) = 0$ for each x.
- If $p_X(x)$ is a probability density function (PDF) for X, then

$$P(a < X < b) = \int_a^b p(x)dx \tag{15}$$

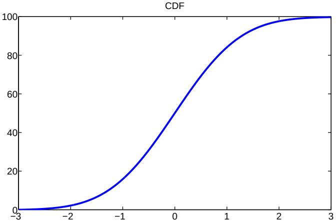
$$P(a < X < a + dx) \approx p(a) \cdot dx \tag{16}$$

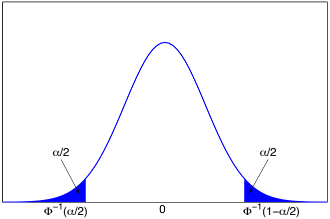
- The cumulative distribution function (CDF) is $F_X(x) = P(X < x)$. We have that $p_X(x) = F'(x)$, and $F(x) = \int_{-\infty}^{x} p(s)ds$.

Bivariate continuous distributions: Marginalization, Conditioning and Independence

- $p_{X,Y}(x, y)$, joint probablity density function of X and Y
- $\int_x \int_y p(x, y) dx dy = 1$
- Marginal distribution: $p(x) = \int_{-\infty}^{\infty} p(x, y) dy$
- Conditional distribution: $p(x|y) = \frac{p(x,y)}{p(y)}$
- Note: $P(Y = y) = 0$! Formally, conditional probability in the continuous case can be derived using infinitesimal events.
- Independence: X and Y are independent if $p_{X,Y}(x, y) = p_X(x) p_Y(y)$

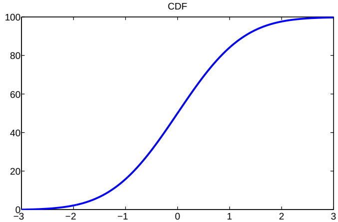
Quantiles

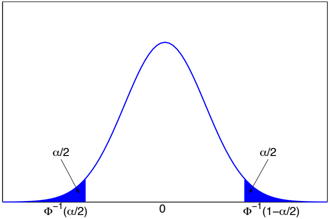




- Since the CDF $F(\cdot)$ is a monotonically increasing function, it has an inverse; let us denote this by $F^{-1}(\cdot)$.
- If $F(x)$ is the CDF of X, then $F^{-1}(\alpha)$ is the value of x_α such that $P(X \leq x_\alpha) = \alpha$; this is called the a quantile of F. The value $F^{-1}(0.5)$ is the median of the distribution, with half of the probability mass on the left, and half on the right. The values $F^{-1}(0.25)$ and $F^{-1}(0.75)$ are the **lower** and **upper quartiles**.

Quantiles





- We can also use the inverse CDF to compute tail area probabilities.
- For example, if Φ is the CDF of the Gaussian distribution $\mathcal{N}(0, 1)$, then points to the left of $\Phi^{-1}(\alpha/2)$ contain $\alpha/2$ probability mass. By symmetry, points to the right of $\Phi^{-1}(1 - \alpha/2)$ also contain $\alpha/2$ probability mass.
- Hence, the central interval $(\Phi^{-1}(\alpha/2), \Phi^{-1}(1 - \alpha/2))$ contains $1 - \alpha$ of the mass. If we set $\alpha = 0.05$, the central 95% interval is covered by the range

$$(\Phi^{-1}(0.025), \Phi^{-1}(0.975)) = (-1.96, 1.96). \tag{17}$$

  For a Gaussian distribution $\mathcal{N}(\mu, \sigma^2)$, the central 95% interval is $(\mu - 1.96\sigma, \mu + 1.96\sigma)$.

Expectation and variance of continuous random variables

Similar to that of discrete random variables, only change the summation $\sum$ to the integral $\int$.

- Expectation (or mean): $\mu = E(X) = \int_{\mathcal{X}} x \cdot p(x)dx$
- Moments: expectation of power of X: $M_k = E(X^k) = \int_{\mathcal{X}} x^k \cdot p(x)dx$
- Variance: Average (squared) fluctuation from the mean

$$\text{Var}(X) = E((X - E(X))^2) = E(X^2) - E(X)^2 = M_2 - M_1^2. \tag{18}$$

- Standard deviation: Square root of variance, *i.e.*,

$$\text{Std} = \sqrt{\text{Var}(X)}. \tag{19}$$

Binary variables (discrete r.v.)

- We firstly consider the probability of a binary random variable $x \in \{0, 1\}$. Suppose that you toss a coin, and $x = 1$ denotes the event of 'heads', while $x = 0$ indicates the event of 'tails'.
- The probability of $x = 1$ is described by a parameter μ,

$$p(x = 1|\mu) = \mu, \tag{20}$$

  where $\mu \in [0, 1]$, and we can obtain that $p(x = 0|\mu) = 1 - \mu$.
- The probability distribution over x can therefore be written in the form

$$\text{Bern}(x|\mu) = \mu^x (1 - \mu)^{1-x}, \tag{21}$$

  which is called Bernoulli distribution.
- Its mean and variance are

$$\mathbb{E}[x] = \sum_x x\text{Bern}(x|\mu) = \mu, \tag{22}$$

$$\text{var}[x] = \mathbb{E}[(x - \mu)^2] = \mu(1 - \mu). \tag{23}$$

Binomial variables

- Imagine that you toss the coin N times, and each tossing follows the Bernoulli distribution $p(x|\mu)$. We denote the variable m as the numbers of heads, then its distribution is formulated as follows:

$$\text{Bin}(m|N,\mu) = \binom{N}{m} \mu^m (1-\mu)^{N-m}, \tag{24}$$

which is called Binomial distribution, where

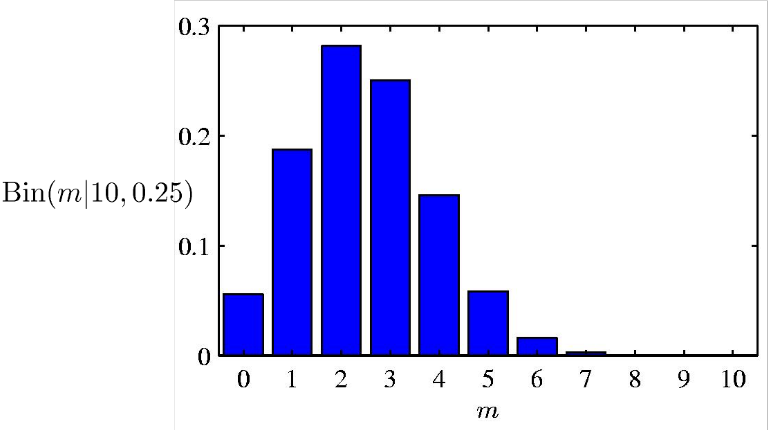
$$\binom{N}{m} = \frac{N!}{(N-m)!m!}. \tag{25}$$

- Its mean and variance are

$$\mathbb{E}[m] = \sum_{m=0}^{N} m\text{Bin}(m|N,\mu) = N\mu, \tag{26}$$

$$\text{var}[m] = \mathbb{E}[(m-N\mu)^2] = N\mu(1-\mu). \tag{27}$$

Binomial distribution



Gaussian distribution (continuous r.v.)

- The Gaussian, also known as the **normal** distribution, is a widely used model for the distribution of **continuous** variables. In the case of a single variable x, the Gaussian distribution can be written in the form

$$\mathcal{N}(x|\mu,\sigma) = \frac{1}{(2\pi\sigma^2)^{\frac{1}{2}}} \exp\left(-\frac{(x-\mu)^2}{2\sigma^2}\right), \tag{28}$$

  where μ is the **mean** and σ^2 is the **variance**.

- For a D-dimensional vector $\boldsymbol{x}$, the multivariate Gaussian distribution takes the form

$$\mathcal{N}(\boldsymbol{x}|\boldsymbol{\mu},\boldsymbol{\Sigma}) = \frac{1}{(2\pi)^{\frac{D}{2}}|\boldsymbol{\Sigma}|^{\frac{1}{2}}} \exp\left(-\frac{(\boldsymbol{x}-\boldsymbol{\mu})^\top\boldsymbol{\Sigma}^{-1}(\boldsymbol{x}-\boldsymbol{\mu})}{2}\right), \tag{29}$$

  where $\boldsymbol{\mu}$ is a D-dimensional **mean vector**, and $\boldsymbol{\Sigma}$ is a $D \times D$ **covariance matrix**, and $|\boldsymbol{\Sigma}|$ denotes the determinant of $\boldsymbol{\Sigma}$.

What is information

- To know what is information, we need to know a bit who is Claude Shannon and his information theory (let's see a video).
- Shannon defined the measure that quantifies the uncertainty of an event with given probability - a bit.
- For a discrete random variable (a source) with finite alphabet, as follows

$$\mathcal{X} = \{x_0, \cdots, x_k, \cdots x_S\},$$

  where the probability of each symbol is given by $P(X = x_k) = p_k$.
- We define the information as

$$I(x_k) = \log \frac{1}{p_k} = -\log(p_k).$$

  If logarithm is base 2, information is given in bits.
- Note that $I(x_k) \geq 0$, *i.e.*, non-negative. The equality only holds when $p_k = 1$, which means there is **no uncertainty**, then **no information**.

What is information

- It represents the *surprise* of seeing the outcome (a highly probable outcome is not surprising).

event	probability	surprise
one equals one	1	0 bits
wrong guess on a 4-choice question	3/4	0.415 bits
correct guess on true-false question	1/2	1 bit
correct guess on a 4-choice question	1/4	2 bits
seven on a pair of dice	6/36	2.58 bits
win any prize at Euromilhões	1/24	4.585 bits
win Euromilhões Jackpot	$\approx$ 1/76 million	$\approx$ 26 bits
gamma ray burst mass extinction today	$< 2.7 \cdot 10^{-12}$	$>$ 38 bits

Larger surprise/uncertainty, more information/bits.

Entropy

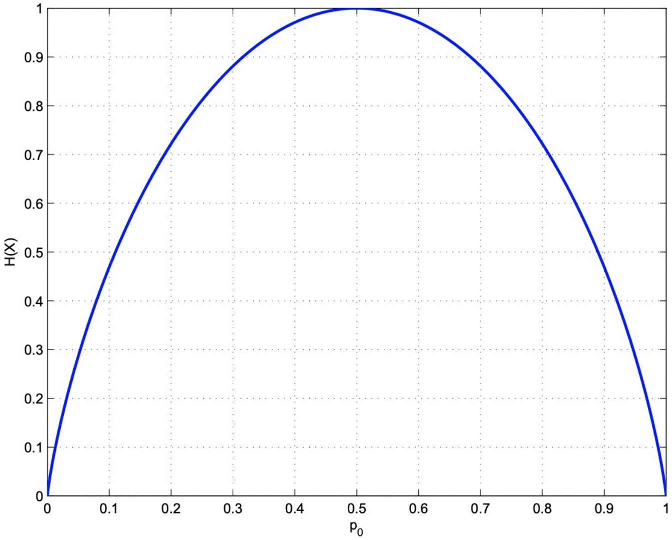
- Entropy is defined as the **expected value of information** from a source,

$$
\begin{aligned}
H_P(\mathcal{X}) &= E[I(x_k)] \\
&= \sum_{x_k \in \mathcal{X}} p_k \cdot I(x_k) \\
&= -\sum_{x_k \in \mathcal{X}} p_k \cdot \log(p_k).
\end{aligned}
$$

- Let $\mathcal{X} = \{0, 1\}$ be a binary source with p_0 and p_1 being the probability of symbols $x_0 = 0$ and $x_1 = 1$, respectively, we have

$$
\begin{aligned}
H_P(\mathcal{X}) &= E[I(x_k)] \\
&= -p_0 \log p_0 - p_1 \log p_1 \\
&= -p_0 \log p_0 - (1 - p_0) \log (1 - p_0)
\end{aligned}
$$

Entropy of binary source



Cross Entropy

- Cross-entropy builds upon the idea of entropy. It calculates the number of bits required to represent or transmit an average event from one distribution $P(X)$, compared to another distribution $Q(X)$,

$$H_{P,Q}(\mathcal{X}) = -\sum_{x_k \in \mathcal{X}} P(X = x_k) \cdot \log(Q(X = x_k)),$$

  where $P(X = x_k)$ is the probability of the event x_k in $P(X)$, $Q(X = x_k)$ is the probability of event x_k in $Q(X)$.

- Let $\mathcal{X} = \{0, 1\}$ be a binary source with p_0 and p_1 being the probability of symbols $x_0 = 0$ and $x_1 = 1$, respectively, then we have

$$\begin{aligned} H_{P,Q}(\mathcal{X}) &= -p_0 \log q_0 - p_1 \log q_1 \\ &= -p_0 \log q_0 - (1 - p_0) \log (1 - q_0). \end{aligned}$$

Cross Entropy

There are two properties of cross-entropy:

- It is a **non-negative**, *i.e.*, $H_{P,Q}(\mathcal{X}) \geq 0$
- Cross-entropy is not smaller than entropy, *i.e.*, $H_{P,Q}(\mathcal{X}) \geq H_P(\mathcal{X})$, and the equality holds only when $P = Q$.

`Exercise: Prove the above two properties`
`(hint: Jensen inequality and` $\log(\cdot)$ `is concave)`

Reference: `https://machinelearningmastery.com/cross-entropy-for-machine-learning/`

Relative entropy: Kullback-Leibler divergence

- The relative entropy between two continuous probability density functions $p_X(x)$ and $q_X(x)$ is defined as follows

$$D_{P,Q}(\mathcal{X}) = \int_{x \in \mathcal{X}} p_X(x) \log \frac{p_X(x)}{q_X(x)}.$$

- It is also called KL divergence, which measures the distance between two distributions.

Relative entropy: Kullback-Leibler divergence

- Exercise 1: What is a KL divergence for a discrete r.v. ?
- There are two properties of KL divergence:
  - **Non-negativity**: $D_{P,Q}(\mathcal{X}) \geq 0$
  - **Asymmetry**: $D_{P,Q}(\mathcal{X}) \neq D_{Q,P}(\mathcal{X})$
- Exercise 2: Prove the above two properties (hint: Jensen inequal and $\log(\cdot)$ is concave)
- The cross-entropy $H_{P,Q}(\mathcal{X})$ is the entropy of the distribution $H_P(\mathcal{X})$ plus the additional KL divergence $D_{P,Q}(\mathcal{X})$.

$$H_{P,Q}(\mathcal{X}) = H_P(\mathcal{X}) + D_{P,Q}(\mathcal{X})$$

- Exercise 3: Can you prove the equality of the equation?

Reference:
https://machinelearningmastery.com/cross-entropy-for-machine-learning/
https://stats.stackexchange.com/questions/335197/why-kl-divergence-is-non-negative