#Code

Artificial Intelligence and Machine Learning (AIML)

2023–24

- **Module so far**:
  - Symbolic AI
  - Logical reasoning
  - Machine Learning
    - Unsupervised technique (clustering)
    - Supervised techniques
      - Regression and classification
      - Neural networks and deep learning

- **This lecture**: statistical machine learning
  - Probability and probabilistic AI, probabilistic graphical models

Quantifying uncertainty in probabilistic AI and ML

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- Most of real-world problems need to handle **uncertainty**
  - Noise on measurements
  - Partial observability

- In these situations, the optimal decision will be taken under uncertainty and depends on both the relative importance of various goals and the likelihood that it can be achieved.
  - **Example:** uncertain logical reasoning: toothache diagnosis
    - toothache ⇒ cavity 口腔 ✗ *not all patients with toothaches have cavities*
    - toothache ⇒ (cavity) ∨ (gum problem) ∨ (abscess) ✗ *what is the size of the list?*
    - cavity ⇒ tootache 脓肿 ✗ *not all cavities cause pain*
    - Makes more sense to provide a **degree of belief** to a given proposition

Probability Theory

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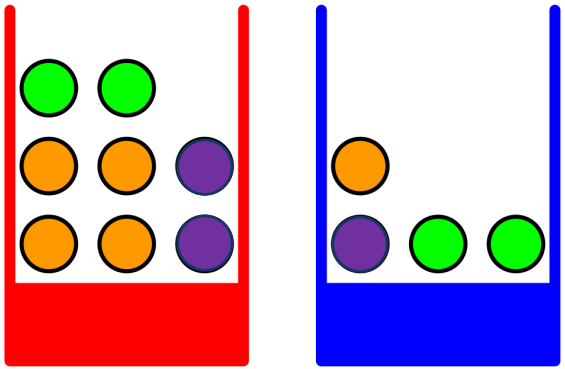
- Consistent framework for the quantification and manipulation of uncertainty
- Probability provides a calculus for **random events**, conveniently indexed using **random variables** (RVs)



Identity of the box is a random variable: B

Two possible values (outcomes): red ($B = r$) or blue ($B = b$)

Suppose we are presented with the red box 40% of the time:

$$P(B = r) = \frac{40}{100} = 0.4$$

If the two boxes are the only possibilities we have, what would be the chances of being presented with the blue box? 1-0.4=0.6

What would be the chances of being presented with either the red or the blue boxes? 1

Probability Theory

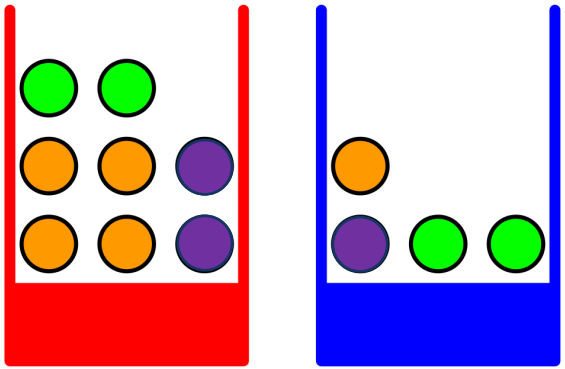
#Code

- **Rules (axioms) of probability**

(i) $P(A) \geq 0$

(ii) $P(A \cup B) = P(A) + P(B)$, if events are non-overlapping (i.e., $A \cap B = \emptyset$) ∅ = empty set

(iii) if Ω represents all possible events (e.g., $\Omega = \{A, B, \ldots, N\}$), then $P(\Omega) = 1$



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Probability distribution functions

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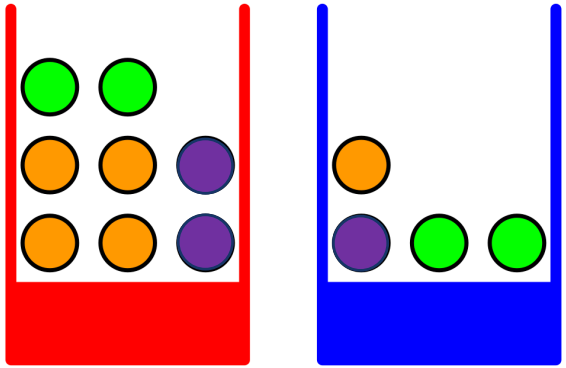
- Informs how are the “chances” of obtaining outcomes for a random variable, which can be **discrete** or **continuous**.

  - **Discrete probability mass function (PMF)** gives the probability that the RV X takes on the value x (i.e., $P(X = x)$)
    - Each possibility lies in the range $[0,1]$ and must have $\sum_{x \in \Omega} P(X = x) = 1$ (normalization).
  - **Continuous probability density function (PDF)** gives the amount of **probability per unit** (probability density)
    - must satisfy $p(x) \geq 0$ for all $x \in \Omega_X$;
    - volume under this function gives the probability of the event represented by that volume, $\int_A p(x)\, dx = \mathrm{P}(A)$, and it must be normalized, $\int_{\Omega X} p(x)\, dx = 1$.

The probability of every event x is greater or equal to 0

Probability distribution functions

#Code



Identity of the box is a random variable: B

Two possible values (outcomes): red ($B = r$) or blue ($B = b$)

$$P(B = r) = 0.4$$

$$P(B = b) = 0.6$$

Bernoulli Distribution

- Binary distribution
- **Sample space**: $\Omega = \{r,b\}$
- **Mass function (PMF)**:

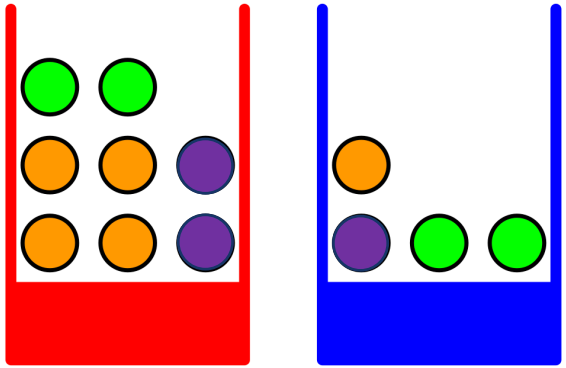
$$P(B = r) = p \qquad p \in [0,1]$$
$$P(B = b) = 1 - p$$

- **Normalization**:

$$\sum_{x \in \Omega} P(X = x) = P(X = r) + P(X = b)$$
$$= p + 1 - p = 1$$

Probability distribution functions

#Code



Colour of the ball as a random variable: C

Three possible values (outcomes):

- green ($C = g$)
- orange ($C = o$)
- purple ($C = p$)

Categorical Distribution

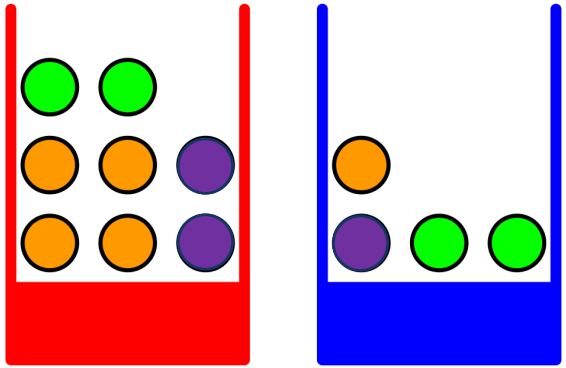
- Discrete distribution
- **Sample space**: $\Omega = \{1, 2, \ldots, N\}$
- **Mass function (PMF)**: each outcome can have a different probability, so $P(X = x) = p_x$ (i.e., parameter vector with each $p_x \in [0,1]$)
- **Normalization**:

$$\sum_{x \in \{1,2,\ldots,N\}} p_x = 1$$

The sum of the probability of each color category

Probability distribution functions

#Code



Colour of the ball as a random variable: C

Three possible values (outcomes):

- green ($C = g$)
- orange ($C = o$)
- purple ($C = p$)

Uniform Distribution

- Special case of the categorical distribution where each outcome is equally likely
- **Sample space**: $\Omega = \{1, 2, \ldots, N\}$
- **Mass function (PMF)**: each outcome can have a different probability, so

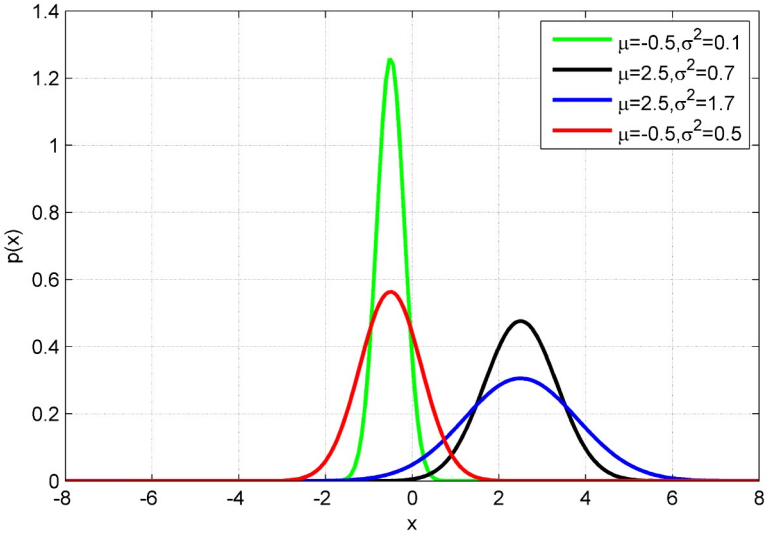
$$P(X = x) = p = \frac{1}{N}, \qquad p \in [0,1]$$

- **Normalization**:

$$\sum_{x \in \{1,2,\ldots,N\}} \frac{1}{N} = N \times \frac{1}{N} = 1$$

Probability distribution functions

#Code



Gaussian (Normal) distribution

- Most ubiquitous continuous distribution
- **Sample space**: $\Omega = \mathbb{R}$
- **Density function (PDF)**:

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

with **mean** $\mu \in \mathbb{R}$ and **variance** $\sigma^2 > 0$.

- **Notes:** μ is both **mean**, **median** and **mode** of the density

Other probabilities intuition

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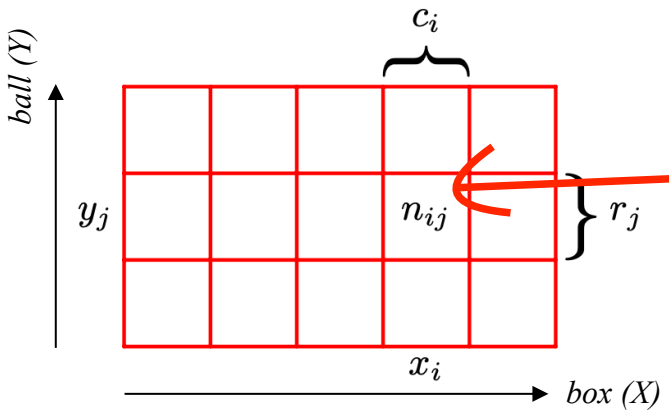
- Extension to *M* boxes and *L* colors for each ball



Consider *N* trials in which we sample a ball within a box.

What is the probability that we will take a box $X = x_i$ and ball $Y = y_i$?

Joint Probability

- Two or more events occurring simultaneously are represented by **joint RVs**, and corresponding **joint PMFs and/or PDFs**
- For this case, $P(X = x_i, Y = y_i) = \frac{n_{ij}}{N}$
- The joint probability should also be normalized. For the discrete case,

$$\sum_{x \in \Omega_X, y \in \Omega_Y} P(X = x, Y = y) = 1$$

- We often use the simplified notation $P(X, Y)$ to indicate $P(X = x, Y = y)$, where there is no ambiguity.

Other probabilities intuition

#Code

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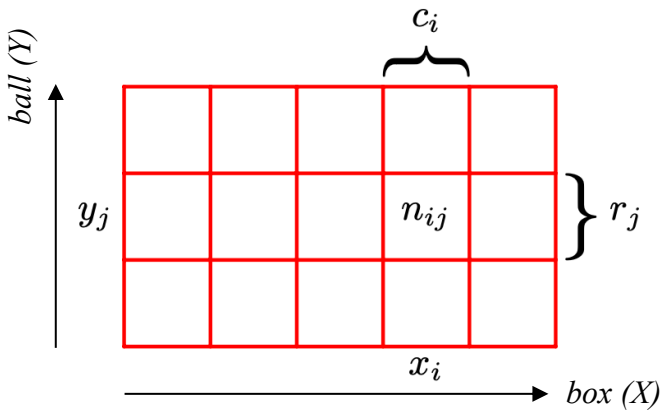


Consider *N* trials in which we sample a ball within a box.

What is the probability that we will take a box $X = x_i$, irrespective of the ball $Y = y_i$ we take?

Marginal Probability

- A joint distribution contains all information about the RVs; we can find the distribution of one of the RVs from the joint, by **marginalizing** (i.e., summing out) the other RVs
- For this case,

$$P(X = x_i) = \frac{c_i}{N}$$

- Since $c_i = \sum_j n_{ij}$, we can also write

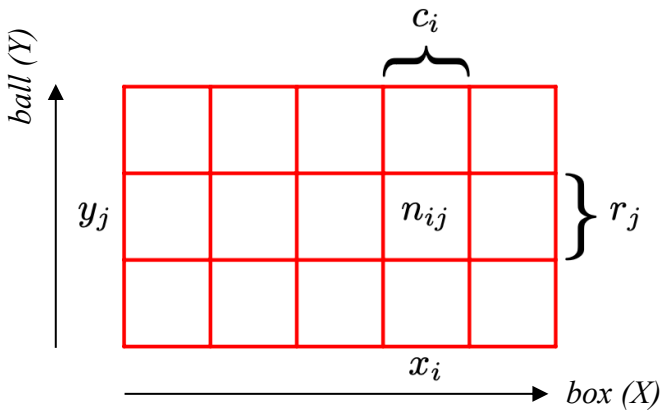
$$P(X = x) = \sum_{y \in \Omega_Y} P(X = x, Y = y)$$

$$P(Y = y) = \sum_{x \in \Omega_X} P(X = x, Y = y)$$

Other probabilities intuition

#Code

- Extension to *M* boxes and *L* colors for each ball



Consider *N* trials in which we sample a ball within a box.

What is the probability that we will take a ball $Y = y_i$, given we took box $X = x_i$ already?

Conditional Probability

- Properly normalized, fixing one variable allows the joint to behave as a new distribution called the **conditional**.
- For this case,

$$P(Y = y_i | X = x_i) = \frac{n_{ij}}{c_i}$$

- Since $p(X = x, Y = y) = \frac{n_{ij}}{N}$,

$$P(X = x, Y = y) = p(Y = y | X = x)p(X = x)$$

$$P(X, Y) = p(Y|X)p(X) \text{ or } P(X, Y) = p(X|Y)p(Y)$$

Marginals and conditionals: another example (Table 15.1)

#Code

Joint $P(X,Y)$	$y=0$	$y=1$
$x=0$	$\frac{3}{7}$	$\frac{1}{7}$
$x=1$	$\frac{3}{15}$	$\frac{8}{35}$

Marginal $P(X)$	
$x=0$	$P(X=0,Y=0)+P(X=0,Y=1)=\frac{4}{7}$
$x=1$	$P(X=1,Y=0)+P(X=1,Y=1)=\frac{3}{7}$

Marginal $P(Y)$	
$y=0$	$P(X=0,Y=0)+P(X=1,Y=0)=\frac{22}{35}$
$y=1$	$P(X=0,Y=1)+P(X=1,Y=1)=\frac{13}{35}$

Conditional $P(X\|Y)$	$y=0$	$y=1$
$x=0$	$\frac{P(X=0,Y=0)}{P(Y=0)}=\frac{15}{22}$	$\frac{P(X=0,Y=1)}{P(Y=1)}=\frac{5}{13}$
$x=1$	$\frac{P(X=1,Y=0)}{P(Y=0)}=\frac{7}{22}$	$\frac{P(X=1,Y=1)}{P(Y=1)}=\frac{8}{13}$

Conditional $P(Y\|X)$	$y=0$	$y=1$
$x=0$	$\frac{P(X=0,Y=0)}{P(X=0)}=\frac{3}{4}$	$\frac{P(X=0,Y=1)}{P(X=0)}=\frac{1}{4}$
$x=1$	$\frac{P(X=1,Y=0)}{P(X=1)}=\frac{7}{15}$	$\frac{P(X=1,Y=1)}{P(X=1)}=\frac{8}{15}$

Probabilistic graphical models

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- Given a probability distribution with multiple RVs, we can represent their mutual conditional dependence graphically using a **probabilistic graphical model** (PGM)
- Consider an arbitrary joint distribution over 3 RVs: X, Y, Z

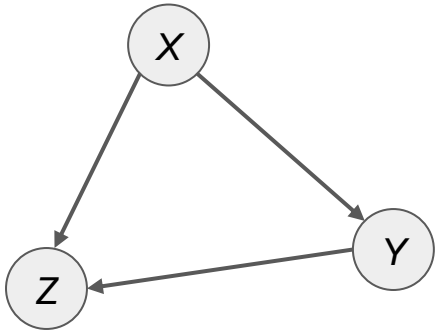
$$P(X, Y, Z) = P(Z|X, Y)P(X, Y)$$

- Applying the product rule again on $P(X, Y) = P(Y|X)P(X)$, we have

$$P(X, Y, Z) = P(Z|X, Y)P(Y|X)P(X)$$

- **Note:** While the left-hand side is symmetrical w.r.t. the 3 RVs, the right-hand side is not; we have chosen a particular ordering that yielded a specific decomposition.

There are as many different forms of the chain rule, as there are **permutations** of the variables



- One node for each RV
- Associate each node with the corresponding conditional distribution

- X is **parent** of Y, Z
- Y is **child** of X

AIML

Independence of RVs

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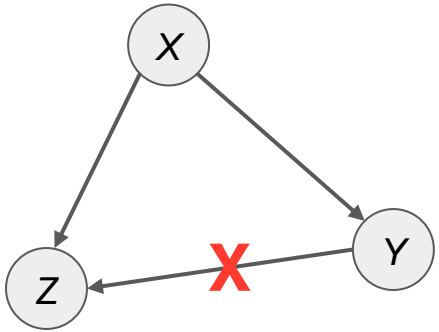
- Two RVs are **independent** if and only if their joint distribution factors into a product of marginals:

$$P(X = x, Y = y) = P(X = x)P(Y = y), \qquad \forall x \in \Omega_X, y \in \Omega_Y$$

- Since $P(X, Y) = p(Y|X)p(X)$, the condition above implies that

$$P(Y|X) = p(Y), \qquad \forall y \in \Omega_Y$$

- We can read the above as "X does NOT add any information about Y", or "knowing X does not change our belief in Y"



- If Z is **conditionally independent** on Y in the example before, then

$$P(Z|X, Y) = P(Z|X)$$

PGMs in Probabilistic AI and ML

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- Independence/conditional independence such as this, is critical important in probabilistic AI and ML, since it allows joint RVs to be modelled by subsets of the data; basis of **probabilistic graphical models**
    - Special graph structures for applications such as time or spatially ordered data
- The graph must have **no cycles** (loops), a **directed acyclic graph** (DAG)
- Every PGM has a corresponding **Markov factorization**, which is a form of the chain rule compatible with a **topological ordering** of the DAG, taking into account the conditional independencies due to the absence of edges

PGMs: Markov factorization

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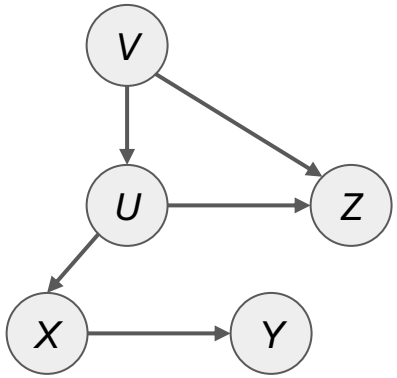
- Markov factorization of the PGM below, considering the specific topological order $[V, U, X, Y, Z]$



$$P(U,V,X,Y,Z) = P(Y|X,U,V,Z)P(X,U,V,Z)$$

$$P(U,V,X,Y,Z) = P(Y|X,U,V,Z)P(X|U,V,Z)P(U,V,Z)$$

$$P(U,V,X,Y,Z) = P(Y|X,U,V,Z)P(X|U,V,Z)P(Z|U,V)P(U,V)$$

$$P(U,V,X,Y,Z) = P(Y|X,U,V,Z)P(X|U,V,Z)P(Z|U,V)P(U|V)P(V)$$

Simplify using conditional independence:

$$P(U,V,X,Y,Z) = P(Y|X,U,V,Z)P(X|U,V,Z)P(Z|U,V)P(U|V)P(V)$$

$$P(U,V,X,Y,Z) = P(V)P(U|V)P(X|U)P(Y|X)P(Z|U,V)$$

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To recap

- We touched on key probabilistic concepts to build a **probabilistic graphical model (PGM)**
- Learned how to find a **Markov factorization** of a given PGM, considering a topological ordering

- **Next**: Bayesian Models and probabilistic classification using naïve Bayes

Further Reading

- **PRML**, Section 1.2, Section 8.1-8.2
- **MLSP**, Section 1.4, Section 1.6, Section 5.1-5.2
- **R&N**, Section 14.1-14.2