Lecture 4: Probability Theory and Probabilistic Modeling

COMP90049
Introduction to Machine Learning

Semester 1, 2024

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Roadmap

Last time... Concepts and KNN classification

- data, features, classes
- K Nearest Neighbors algorithm
- Application to classification

Today... Probability

- basics / refresher
- distributions and parameterizations
- why probability in ML?

Estimating confidence in different possible outcomes

Probability Theory

"The calculus of probability theory provides us with a **formal framework** for considering multiple possible **outcomes** and their **likelihood**. It defines a set of **mutually exclusive** and **exhaustive** possibilities, and associates each of them with a probability — **a number between 0 and 1**, so that the **total probability of all possibilities is 1**. This framework allows us to consider options that are **unlikely, yet not impossible**, without reducing our conclusions to content-free lists of every possibility."

From Probabilistic Graphical Models: Principles and Techniques (2009; Koller and Friedman) `http://pgm.stanford.edu/intro.pdf`

(Very) Basics of Probability Theory

P(A): **the probability of A** the fraction of times the event A is true in independent trials

$$0 <= P(A) <= 1$$

$$P(True) = 1$$

$$P(False) = 0$$

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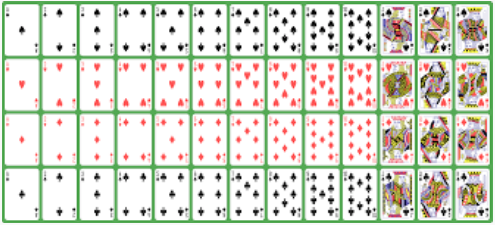
Given a deck of 52 cards

- 13 ranks (ace, 2-10, jack, queen, king)
- of each of four suits (clubs, spades = black; hearts, diamonds = red)
- A is a random variable denoting the value of a randomly selected card. We denote the probability of A taking on a specific value *a* as P(A=a).



https://commons.wikimedia.org/wiki/File:English_pattern_playing_cards_deck.svg

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$$P(\mathtt{A} = \mathtt{queen}) \;= ?\; \frac{1}{13} \qquad P(A = \mathtt{red}) \;= ?\; \frac{1}{2}$$

$$P(\mathtt{A} = \mathtt{heart}) \;= ?\; \frac{1}{4}$$

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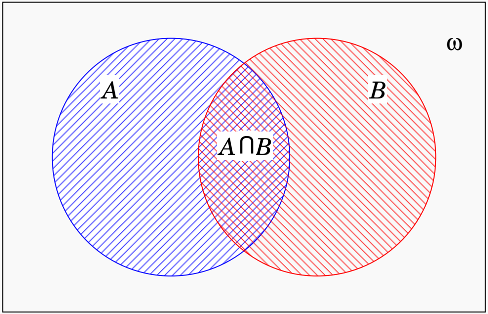

$$P(A = \texttt{ace}, B = \texttt{heart}) = ?$$

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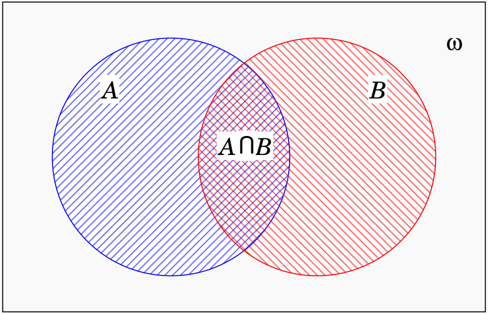

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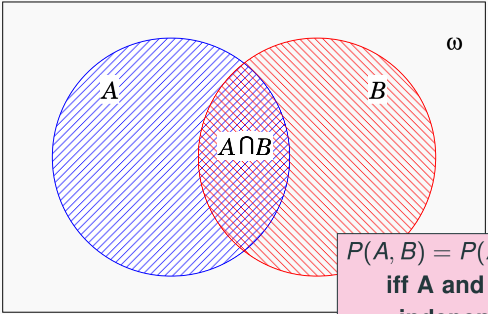

$P(A, B) = P(A) * P(B)$
iff A and B are independent

$$P(A = \texttt{ace}, B = \texttt{heart}) = \frac{1}{52}$$

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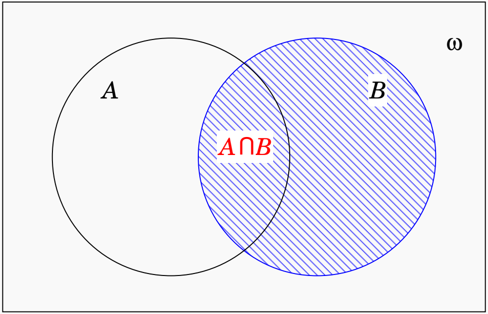
Conditional Probability

P(A|B): **conditional probability** the probability of $A{=}a$ given the observation $B{=}b = \frac{P(A \cap B)}{P(B)}$



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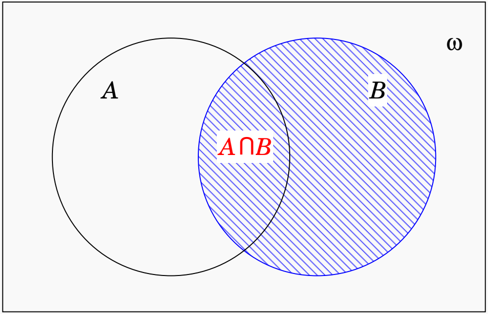


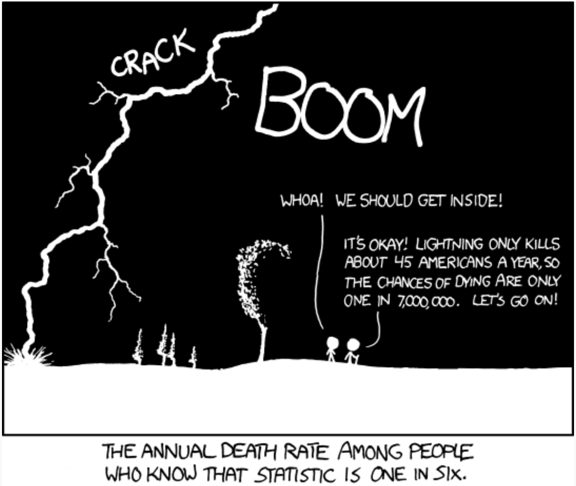
$$P(A = \texttt{ace} | B = \texttt{heart}) = \frac{1}{52} / \frac{1}{4} = \frac{1}{13}$$

$$P(A = \texttt{heart} | B = \texttt{red}) = \frac{1}{4} / \frac{1}{2} = \frac{1}{2}$$

Notation

1. $P(A = x)$ probability that random variable A takes on value x
2. $P(A)$ probability distribution over random variable A
3. $P(x)$ I'll often use this as a short-hand for 1. if clear from the context

What type of probability?



https://imgs.xkcd.com/comics/conditional_risk.png

Rules of Probability I

- **Independence:** A and B are independent iff $P(A \cap B) = P(A)P(B)$

- **Disjoint events:** The probability of two disjoint events, such that $A \cap B = \emptyset$, is $P(A \text{ or } B) = P(A) + P(B)$

- **Product rule**: $P(A \cap B) = P(A|B)P(B) = P(B|A)P(A)$

- **Chain rule**: $P(A_1 \cap ... \cap A_n) = P(A_1)P(A_2|A_1)P(A_3|A_2 \cap A_1) \ ... \ P(A_n| \cap_{i=1}^{n-1} A_i)$

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  again, we can choose the factorization, e.g., :

$$P(July, 5^\circ C, sick) = P(July) \times P(5^\circ C|July) \times P(sick|5^\circ C, July)$$

makes sense

$$= P(5^\circ C) \times P(sick|5^\circ C) \times P(July|5^\circ C, sick)$$

???

Rules of Probability II

Bayes Rule

$$P(A|B) = \frac{P(A)P(B|A)}{P(B)} \qquad \left(\text{cf., } P(A|B) = \frac{P(A \cap B)}{P(B)}\right)$$

Basic rule of probability

- Bayes' Rule allows us to compute $P(A|B)$ given knowledge of the 'inverse' probability $P(B|A)$.

More philosophically,

- Bayes' Rule allows us to update prior belief with empirical evidence

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Posterior Probability $P(A|B)$

- the degree of belief having accounted for B.

Prior Probability $P(A)$

- the initial degree of belief in A.
- the probability of A occurring, given no additional knowledge about A

Likelihood $P(B|A)$

- the support B provides for A

Normalizing constant ('Evidence') $P(B) = \sum_A P(B|A)P(A)$

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Example

Estimate the probability of a student **being smart** given that (s)he **achieved H1** score, $P(smart|H1)$ from the following information:

$P(Smart) = 0.3$	prior rate of smart students
$P(H1|Smart) = 0.6$	empirically measured $H1|smart$
$P(H1) = 0.2$	emprirically measured

(What if $P(H1) = 0.4$?)

Binomial Distributions

- A **binomial distribution** results from a
  series of independent trials with only two outcomes (aka **Bernoulli trials**)
  e.g. multiple coin tosses ($\langle H, T, H, H, ..., T \rangle$)

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$$P(m, n, p) \quad = \quad \binom{n}{m} p^m (1-p)^{n-m}$$

$$P(m, n, p) \quad = \quad \underbrace{\frac{n!}{m!(n-m)!}}_{\substack{\text{possible distributions} \\ \text{of } m \text{ successes} \\ \text{over } n \text{ trials}}} \; \underbrace{p^m}_{m \text{ successes}} \; \underbrace{(1-p)^{n-m}}_{n-m \text{ failures}}$$

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What is the probability of getting times 2 heads out of 3 tosses of a fair coin?

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Binomial Example: Coin Toss

Go through solution:

Binomial Example: Coin Toss

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$$P\left(2, 3, \frac{1}{2}\right) = \frac{3!}{2!(3-2)!} \left(\frac{1}{2}\right)^2 \left(\frac{1}{2}\right)^{3-2} = 3\left(\frac{1}{4}\right)\left(\frac{1}{2}\right)$$

Multinomial Distributions

- A **multinomial distribution** models the probability of **counts** of different events from a series of independent trials with **more than two possible outcomes**, e.g.,

  - a fair 6-sided dice is rolled 5 times
  - what is the probability of observing exactly 3 ’ones’ and 2 ’fives’?
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- The probability of events $X_1, X_2, ..., X_n$ with probabilities $\mathbf{p} = p_1, p_2, ..., p_n$ occurring exactly $x_1, x_2, ..., x_n$ times, respectively, is given by

$$
\begin{aligned}
P(X_1 = x_1, X_2 = x_2, ..., X_n = x_n; \mathbf{p}) &= \frac{(\sum_i x_i)!}{x_1! \dots x_n!} p_1^{x_1} \times p_2^{x_2} \times \cdots \times p_n^{x_n} \\
&= \frac{(\sum_i x_i)!}{x_1! \dots x_n!} \prod_i p_i^{x_i}
\end{aligned}
$$

Categorical Distributions

- The **categorical distribution** models the probability of **events** resulting from a single trial with **more than two possible outcomes**, e.g.,

  - we roll a fair-sided dice once
  - what is the probability of observing a 'five'?

- Events $X_1 \dots X_n$ have associated probabilities $\mathbf{p} = p_1, ..., p_n$.
- The probability of a single event is given by

$$P(X_i = 1|\mathbf{p}) = p_i$$

- Equivalently, let's represent the one observation as a one-hot vector $X_1 = x_1, X_2 = x_1, ..., X_n = x_n$ where exactly one of the x_i is 1 and the others are 0. We can write probability of the observation

$$\begin{aligned} P(X_1 = x_1, X_2 = x_2, ..., X_n = x_n; \mathbf{p}) &= p_1^{x_1} \times p_2^{x_2} \times \cdots \times p_n^{x_n} \\ &= \prod_i p_i^{x_i} \end{aligned}$$

Now the relation to the Multinomial distribution is more explicit.

Marginalization

Intuition

We want to know the probability of an event A *irrespective of* the outcome of another event B. We can obtain it, by summing over all possible outcomes $\mathcal{B}$ of B.

- Take an event B. The set of *all* possible *individual* outcomes of B, $\mathcal{B}$ is the **partition** of the outcome space
- E.g., $\mathcal{B}=$\{head, tail\} for a coin flip; $\mathcal{B}=$\{king, heart, diamond, spades\} for card suits
- We can **marginalize** over the set of outcomes of B as follows

$$P(A) = \sum_{b \in \mathcal{B}} P(A, B = b)$$

or equivalently (remember the product rule?)

$$P(A) = \sum_{b \in \mathcal{B}} P(A|B = b)P(B = b)$$

and even for conditional probabilities

$$P(A|C) = \sum_{b \in \mathcal{B}} P(A|C, B = b)P(B = b|C)$$

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Marginalization

Example

We want to know the probability of success of movies of a specific genre ($\mathcal{A} = \{comedy, thriller, romance\}$). But we only have data on movie success probabilities in a specific market, namely ($\mathcal{B} = \{EU, NA, AUS\}$).

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romance	NA	0.1
romance	AUS	0.3
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thriller	AUS	0.1
comedy	EU	0.1
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$\sum$ $\sum$ $\sum$

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	1.0

Quiz!

Please go to

`https://pollev.com/iml2021`

for a quick quiz on probabilities!

Probability and Machine Learning

We probably all agree that probabilities are useful for thinking about card games or coin flips

... but why should we care in machine learning?

Consider typical classification problems

- document $\rightarrow$ {spam, no spam}
- hand-written digit $\rightarrow$ {0,1,2,3,4,5,6,7,8,9}
- purchase history $\rightarrow$ recommend {book a, book b, book c, ...}

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- **uncertainty**, due to few observations, noisy data, ...
- model features as following certain **probability distributions**
- **soft predictions** ("we are 60% confident that Bob will like *Harry Potter* given his purchase history")
- ...

"All models are wrong, but some are useful."
(George Box, Statistician)

Probabilistic Models

- allow to reason about random events in a **principled** way.
- allow to formalize hypotheses as different types of probability distributions, and use the laws of probability to derive predictions

Example: Spam classification

- An email is a random event with two possible outcomes: `spam`, `not spam`
- The probability of observing a spam email $P(spam) = \theta$, and trivially $P(not\ spam) = 1 - \theta$.
- We might care about a random variable X as the number of spam emails in an inbox of 100 emails. X is distributed according to the **binomial distribution**, and depends on the **parameters** θ and $N = 100$

$$X \sim Binomial(\theta, N = 100)$$

Learning Probabilistic Models I

X is distributed according to the **binomial distribution**, and depends on the **parameters** θ and $N = 100$

$$X \sim Binomial(\theta, N = 100)$$

- In order to make predictions of X we need to know the parameters θ. **How do we learn them?**
- Typically, θ is unknown, but if we have **data** available we can **estimate** θ
- One common choice is to pick θ that maximizes the probability of the observed data

  $$\hat{\theta} = \underset{\theta}{\operatorname{argmax}}\, P(X; \theta, N)$$

  That is the **maximum likelihood estimate (MLE)** of θ.
- Once we have estimated θ we can use it to **predict** values for unseen data

The **maximum likelihood principle**

$$\hat{\theta} = \underset{\theta}{\operatorname{argmax}}\, P(X; \theta, N) \tag{1}$$

- Consider a **data set** consisting of 100 emails, 20 of which are spam.
- Following from the binomial distribution

$$\mathcal{L}(\theta) = P(X; \theta, N) = \binom{n}{m} \theta^x (1-\theta)^{N-x}$$

the **likelihood of the data**[1] is $\propto \ \theta^{20}(1-\theta)^{100-20}$

- What do you think would be a good value for $\theta = p(spam = 1)$? Why?
- Next lecture, we will see how to derive this value in a principled way

[1] $\propto$ means 'proportional to'. $\binom{n}{m}$ can be ignored because it is independent of θ.

Maximum likelihood is only one choice of estimator among many

- Consider a data set of one inbox with no spam email. MLE: $\theta = 1$, and hence $P(\textit{not spam}) = \theta = 1$ and $P(\textit{spam}) = 1 - \theta = 0$.
  $\rightarrow$ "spam emails don't exist"
- We could modify this estimate with our **prior belief**. E.g., we might believe that about 80 of 100 emails are not spam. We 'nudge' θ from $\theta = 1$ towards $\theta = 0.80$
- We can combine our prior belief with the estimate from the data to arrive at a **posterior probability distribution** over θ: $P(\theta)$.

$$P(\theta|x) = \frac{P(\theta)P(x|\theta)}{P(x)} \propto P(\theta)P(x|\theta) \qquad \text{(looks familiar)?}$$

- The **maximum a posteriori estimate** is then

$$\hat{\theta} = \underset{\theta}{\operatorname{argmax}}\, P(\theta)P(x|\theta)$$

Summary

Probability underlies many modern knowledge technologies

- estimate the (conditional, joint) probability of observations
- Bayes rule
- Expectations and marginalization
- Probabilistic models
- Maximum likelihood estimation (taster)
- Maximum aposteriori estimation (taster)

Next Lecture(s):

- Optimization
- Naive Bayes Classification

References

Chris Bishop. Pattern Recognition and Machine Learning. Chapters: 1.2 (intro), 1.2.3, 2 (intro), 2.1 (up to 2.1.1), 2.2 (up to 2.2.1)

Optional / If time permits: Expectations

The **expectation** of a function (like a probability distribution) is the **weighted average** of all possible outcomes, weighted by their respective probability.

- For functions with discrete outputs

$$E[f(x)] = \sum_{x \in \mathcal{X}} f(x)P(x)$$

- For functions with continuous outputs

$$E[f(x)] = \int_{\mathcal{X}} f(x)P(x)dx$$

Optional / If time permits: Expectations

The **expectation** of a function (like a probability distribution) is the **weighted average** of all possible outcomes, weighted by their respective probability.

- On sunny days Bob watches 1 movie
- On rainy days Bob watches 3 movies
- Bob lives in Melbourne, it rains on 70% of all days
- What is the expected number of movies Bob watches per day?

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$$1 * 0.3 + 3 * 0.7 = 2.4$$