## Lecture 4: Probability Theory and Probabilistic Modeling

COMP90049 Introduction to Machine Learning

Semester 1, 2021

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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



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

$$0 \le P(A) \le 1$$
  $P(True) = 1$   $P(False) = 0$ 

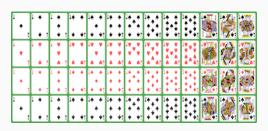


**P(A)**: **the probability of A** the fraction of times the event A is true in independent trials

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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)





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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)

$$P(\text{queen}) = ?$$
  $P(\text{red}) = ?$   $P(\text{heart}) = ?$ 



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

$$0 <= P(A) <= 1$$
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#### Given a deck of 52 cards

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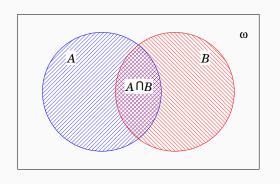
$$P(\text{queen}) = \frac{1}{13}$$
  $P(\text{red}) = \frac{1}{2}$   $P(\text{heart}) = \frac{1}{4}$ 



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# **Basics of Probability Theory**

**P(A, B)**: **joint probability of** the probability of both *A* and **A and B** B occurring =  $P(A \cap B)$ 



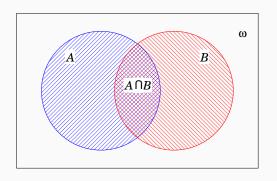
$$P(\text{heart}, \text{red}) = ?$$



# **Basics of Probability Theory**

P(A,B): joint probability of A and B

the probability of both A and B occurring =  $P(A \cap B)$ 



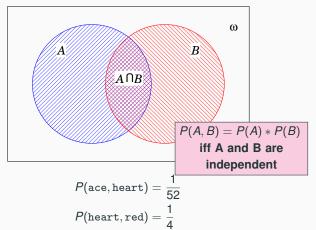
$$P(\text{ace}, \text{heart}) = \frac{1}{52}$$
  
 $P(\text{heart}, \text{red}) = \frac{1}{4}$ 



## **Basics of Probability Theory**

P(A, B): joint probability of A and B

the probability of both A and B occurring =  $P(A \cap B)$ 

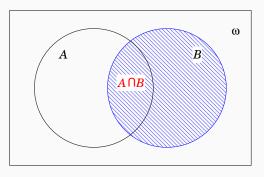




# **Conditional Probability**

 $P(A|B) \colon \quad conditional \ probability$ 

the probability of A given the occurrence of  $B = \frac{P(A \cap B)}{P(B)}$ 



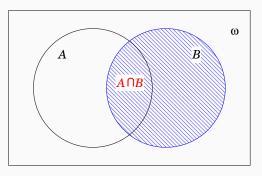
$$P(\text{heart}|\text{red}) = ?$$



# **Conditional Probability**

P(A|B): conditional probability

the probability of A given the occurrence of  $B = \frac{P(A \cap B)}{P(B)}$ 



$$P(\text{ace}|\text{heart}) = \frac{1}{52} / \frac{1}{4} = \frac{1}{13}$$
  
 $P(\text{heart}|\text{red}) = \frac{1}{4} / \frac{1}{2} = \frac{1}{2}$ 



# What type of probability?



THE ANNUAL DEATH RATE AMONG PEOPLE WHO KNOW THAT STATISTIC IS ONE IN SIX.



### 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 or B) = P(A) + P(B)
- Multiplication rule:  $P(A \cap B) = P(A|B)P(B) = P(B|A)P(A)$
- · Chain rule:

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



### 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  $P(A \text{ or } B) = P(A) + \emptyset$  e.g., draw an ace or a king:  $A = \emptyset$  draw an ace;  $B = \emptyset$  draw a king.
- Multiplication 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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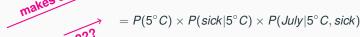
$$P(A_1 \cap ... \cap A_n) = P(A_1)P(A_2|A_1)P(A_3|A_2 \cap A_1) ... P(A_n|\cap_{i=1}^{n-1} A_i)$$

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

 $P(F^{\circ}C) \times P(sick|F^{\circ}C) \times P(sick|F^{\circ}C, sick)$ 





### Rules of Probability II

#### **Bayes Rule**

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

#### 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



### Rules of Probability II

#### **Bayes Rule**

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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')  $P(B) = \sum_{A} P(B|A)P(A)$ 



### Rules of Probability II

#### **Bayes Rule**

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

#### **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 ((H, T, H, H, ..., T))



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

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



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- 2. number of possible outcomes e from 3 coin flips:

$$2 * 2 * 2 = 2^3 = 8$$
 each with  $P(e) = \frac{1}{8}$ 



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3. Choose 2 out of 3:  $C(3,2) = \frac{3!}{2!1!} = 3$ 



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- 3. Choose 2 out of 3:  $C(3,2) = \frac{3!}{2!1!} = 3$
- 4. 3 possible outcomes,  $\frac{1}{8}$  for each:  $P(X=2) = \frac{3}{8}$



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

- 1. m = 2 successes (heads) when flipping coin n = 3 times; P(X = 2)
- 2. number of possible outcomes e from 3 coin flips:

$$2*2*2=2^3=8$$
 each with  $P(e)=\frac{1}{8}$ 

3. Choose 
$$P(m, n, p) = \frac{n!}{m!(n-m)!} p^m (1-p)^{n-m}$$

4. 3 possible outcomes,  $\frac{1}{8}$  for each:  $P(X = 2) = \frac{3}{8}$ 

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



#### **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'?
  - what is the probability of observing 5 'threes'?



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  - what is the probability of observing exactly 3 'ones' and 2 'fives'?
  - what is the probability of observing 5 'threes'?
- 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

$$P(X_{1} = x_{1}, X_{2} = x_{2}, ..., X_{n} = x_{n}; \mathbf{p}) = \frac{(\sum_{i} x_{i})!}{x_{1}! ... x_{n}!} p_{1}^{x_{1}} \times p_{2}^{x_{2}} \times \cdots \times p_{n}^{x_{n}}$$

$$= \frac{(\sum_{i} x_{i})!}{x_{1}! ... x_{n}!} \prod_{i} p_{i}^{x_{i}}$$



### **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'?
- 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

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



#### 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} = \{\text{head, tail}\}\$ for a coin flip;  $\mathcal{B} = \{\text{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 multiplication rule?)

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

and even for conditional probabilities

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



#### Example

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

Α	В	P(A, B)
romance	EU	0.05
romance	NA	0.1
romance	AUS	0.3
thriller	EU	0.1
thriller	NA	0.2
thriller	AUS	0.1
comedy	EU	0.1
comedy	NA	0.025
comedy	AUS	0.025
		4.0



#### Example

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thriller	NA	0.2		
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·		1.0		



# Marginalization

### Example

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

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# Marginalization

### **Example**

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thriller	NA	0.2		
thriller	AUS	0.1		
comedy	EU	0.1	comedy	0.15
comedy	NA	0.025		
comedy	AUS	0.025		
		1.0		1.0



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### 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 → {0,1,2,3,4,5,6,7,8,9}
- purchase history  $\rightarrow$  recommend {book a, book b, book c, ...}



# **Probability and Machine Learning**

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- hand-written digit → {0,1,2,3,4,5,6,7,8,9}
- purchase history  $\rightarrow$  recommend {book a, book b, book c, ...}
- 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")





### **Probabilistic Models**

"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**  $\theta$  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,  $\theta$  is unknown, but if we have **data** available we can **estimate**  $\theta$
- One common choice is to pick  $\theta$  that maximizes the probability of the observed data

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

That is the **maximum likelihood estimate (MLE)** of  $\theta$ .

- Once we have estimated  $\theta$  we can use it to  $\mathbf{predict}$  values for unseen data



# Learning Probabilistic Models II

### 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<sup>1</sup> 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



 $<sup>^{1}\</sup>infty$  means 'proportional to'.  $\binom{n}{m}$  can be ignored because it is independent of  $\theta$ .

# Learning Probabilistic Models III

### Maximum likelihood is only one choice of estimator among many

- Consider a data set of one inbox with no spam email. MLE: θ = 1, and hence P(not spam) = θ = 1 and P(spam) = 1 − θ = 0.
   → "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'  $\theta$  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(θ).

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

The maximum a posteriori estimate is then

$$\hat{\theta} = \operatorname*{argmax}_{\theta} P(\theta) P(x|\theta)$$



### **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?



# 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?

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

