

PROBABILITY THEORY



Dr. Joschka Boedecker
AG Maschinelles Lernen
Albert-Ludwigs-Universität Freiburg

jboedeck@informatik.uni-freiburg.de

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Probabilities

probabilistic statements subsume different effects due to:

- ▶ **convenience**: declaring all conditions, exceptions, assumptions would be too complicated.
Example: "I will be in lecture if I go to bed early enough the day before and I do not become ill and my car does not have a breakdown and ..."
or simply: I will be in lecture with probability of 0.87
- ▶ **lack of information**: relevant information is missing for a precise statement.
Example: weather forecasting
- ▶ **intrinsic randomness**: non-deterministic processes.
Example: appearance of photons in a physical process

Probabilities (cont.)

- ▶ intuitively, probabilities give the expected relative frequency of an event
- ▶ mathematically, probabilities are defined by axioms (Kolmogorov axioms). We assume a set of possible outcomes Ω . An event A is a subset of Ω
 - ▶ the probability of an event A , $P(A)$ is a welldefined non-negative number:
 $P(A) \geq 0$
 - ▶ the certain event Ω has probability 1: $P(\Omega) = 1$
 - ▶ for two disjoint events A and B : $P(A \cup B) = P(A) + P(B)$

P is called **probability distribution**

- ▶ important conclusions (can be derived from the above axioms):

$$P(\emptyset) = 0$$

$$P(\neg A) = 1 - P(A)$$

if $A \subseteq B$ follows $P(A) \leq P(B)$

$$P(A \cup B) = P(A) + P(B) - P(A \cap B)$$

Probabilities (cont.)

- ▶ example: rolling the dice $\Omega = \{1, 2, 3, 4, 5, 6\}$

Probability distribution (optimal dice):

$$P(1) = P(2) = P(3) = P(4) = P(5) = P(6) = \frac{1}{6}$$

probabilities of events, e.g.:

$$P(\{1\}) = \frac{1}{6}$$

$$P(\{1, 2\}) = P(\{1\}) + P(\{2\}) = \frac{1}{3}$$

$P(\{1, 2\} \cup \{2, 3\}) = \frac{1}{2}$ Probability distribution (manipulated dice):

$$P(1) = P(2) = P(3) = 0.13, P(4) = P(5) = 0.17, P(6) = 0.27$$

- ▶ typically, the actual probability distribution is not known in advance, it has to be **estimated**

Joint events

- ▶ for pairs of events A, B , the **joint probability** expresses the probability of both events occurring at same time: $P(A, B)$

example:

$$P(\text{"Bayern München is losing"}, \text{"Werder Bremen is winning"}) = 0.3$$

- ▶ Definition: for two events the **conditional probability** of $A|B$ is defined as the probability of event A if we consider only cases in which event B occurs. In formulas:

$$P(A|B) = \frac{P(A, B)}{P(B)}, P(B) \neq 0$$

- ▶ with the above, we also have

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

- ▶ example: $P(\text{"caries"} | \text{"toothaches"}) = 0.8$
 $P(\text{"toothaches"} | \text{"caries"}) = 0.3$

Joint events (cont.)

- ▶ a **contingency table** makes clear the relationship between joint probabilities and conditional probabilities:

| | B | $\neg B$ | |
|----------|----------------|---------------------|-------------|
| A | $P(A, B)$ | $P(A, \neg B)$ | $P(A)$ |
| $\neg A$ | $P(\neg A, B)$ | $P(\neg A, \neg B)$ | $P(\neg A)$ |
| | $P(B)$ | $P(\neg B)$ | |

marginals

joint prob

$$\text{with } P(A) = P(A, B) + P(A, \neg B),$$

$$P(\neg A) = P(\neg A, B) + P(\neg A, \neg B),$$

$$P(B) = P(A, B) + P(\neg A, B),$$

$$P(\neg B) = P(A, \neg B) + P(\neg A, \neg B)$$

conditional probability = joint probability / marginal probability

Joint events (Example)

- ▶ example of a **contingency table**: cars and drivers

| | <i>red</i> | <i>blue</i> | <i>other</i> | |
|---------------|------------|-------------|--------------|------|
| <i>male</i> | 0.05 | 0.15 | 0.35 | 0.55 |
| <i>female</i> | 0.2 | 0.05 | 0.2 | 0.45 |
| | 0.25 | 0.2 | 0.55 | 1 |

marginals

joint prob

e.g: I observed a blue car. How likely is the driver female?

How to express that in probabilistic terms?

$$P('female' | 'blue') = \frac{P('female', 'blue')}{P('blue')}$$

How to access these values?

$P('female', 'blue')$: from table

$$P('blue') = P('blue', 'male') + P('blue', 'female') = 0.2 \text{ ('Marginalisation')}$$

$$\text{Therefore, } P('female' | 'blue') = \frac{0.05}{0.2} = 0.25$$

⇒ joint probability table allows to answer arbitrary questions about domain.

Marginalisation

- ▶ Let B_1, \dots, B_n disjoint events with $\cup_i B_i = \Omega$. Then
$$P(A) = \sum_i P(A, B_i)$$

This process is called marginalisation.

Productrule and chainrule

- ▶ from definition of conditional probability:

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

- ▶ repeated application: chainrule:

$$\begin{aligned} & P(A_1, \dots, A_n) = P(A_n, \dots, A_1) \\ = & P(A_n | A_{n-1}, \dots, A_1) P(A_{n-1}, \dots, A_1) \\ = & P(A_n | A_{n-1}, \dots, A_1) P(A_{n-1} | A_{n-2}, \dots, A_1) P(A_{n-2}, \dots, A_1) \\ = & \dots \\ = & \prod_{i=1}^n P(A_i | A_1, \dots, A_{i-1}) \end{aligned}$$

Conditional Probabilities

- ▶ conditionals:

Example: if someone is taking a shower, he gets wet (by causality)

$$P(\text{"wet"} | \text{"taking a shower"}) = 1$$

while:

$$P(\text{"taking a shower"} | \text{"wet"}) = 0.4$$

because a person also gets wet if it is raining

- ▶ causality and conditionals:

causality typically causes conditional probabilities close to 1:

$$P(\text{"wet"} | \text{"taking a shower"}) = 1, \text{ e.g.}$$

$P(\text{"score a goal"} | \text{"shoot strong"}) = 0.92$ ('vague causality': if you shoot strong, you very likely score a goal').

Offers the possibility to express vagueness in reasoning.

you cannot conclude causality from large conditional probabilities:

$$P(\text{"being rich"} | \text{"owning an airplane"}) \approx 1$$

but: owning an airplane is not the reason for being rich

Bayes rule

- ▶ from the definition of conditional distributions:

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

Hence:

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

is known as **Bayes rule**.

- ▶ example:

$$P(\text{"taking a shower"} | \text{"wet"}) = P(\text{"wet"} | \text{"taking a shower"}) \frac{P(\text{"taking a shower"})}{P(\text{"wet"})}$$

$$P(\text{reason} | \text{observation}) = P(\text{observation} | \text{reason}) \frac{P(\text{reason})}{P(\text{observation})}$$

Bayes rule (cont)

- ▶ often this is useful in diagnosis situations, since $P(\text{observation}|\text{reason})$ might be easily determined.
- ▶ often delivers surprising results

Bayes rule - Example

- ▶ if patient has meningitis, then very often a stiff neck is observed
 $P(S|M) = 0.8$ (can be easily determined by counting)
- ▶ observation: 'I have a stiff neck! Do I have meningitis?' (is it reasonable to be afraid?)
 $P(M|S) = ?$

- ▶ we need to now: $P(M) = 0.0001$ (one of 10000 people has meningitis) and $P(S) = 0.1$ (one out of 10 people has a stiff neck).

- ▶ then:

$$P(M|S) = \frac{P(S|M)P(M)}{P(S)} = \frac{0.8 \times 0.0001}{0.1} = 0.0008$$

- ▶ Keep cool. Not very likely

Independence

- ▶ two events A and B are called **independent**, if

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

- ▶ independence means: we cannot make conclusions about A if we know B and vice versa. Follows: $P(A|B) = P(A)$, $P(B|A) = P(B)$
- ▶ example of independent events: roll-outs of two dices
- ▶ example of dependent events: $A =$ 'car is blue', $B =$ 'driver is male'
→ (from example)
 $P('blue') P('male') = 0.2 \cdot 0.55 = 0.11 \neq P('blue', 'male') = 0.15$

Random variables

- ▶ **random variables** describe the outcome of a random experiment in terms of a (real) number
- ▶ a **random experiment** is a experiment that can (in principle) be repeated several times under the same conditions
- ▶ discrete and continuous random variables
- ▶ probability distributions for discrete random variables can be represented in tables:

Example: random variable X (rolling a dice):

| | | | | | | |
|--------|---------------|---------------|---------------|---------------|---------------|---------------|
| X | 1 | 2 | 3 | 4 | 5 | 6 |
| $P(X)$ | $\frac{1}{6}$ | $\frac{1}{6}$ | $\frac{1}{6}$ | $\frac{1}{6}$ | $\frac{1}{6}$ | $\frac{1}{6}$ |

- ▶ probability distributions for continuous random variables need another form of representation

Continuous random variables

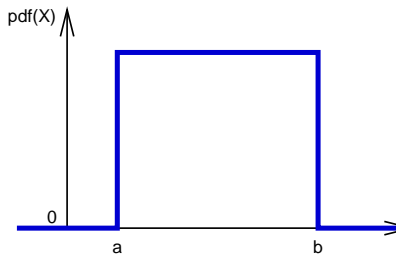
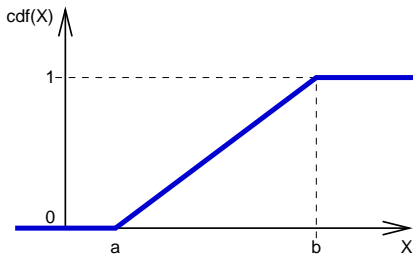
- ▶ problem: infinitely many outcomes
- ▶ considering intervals instead of single real numbers: $P(a < X \leq b)$
- ▶ cumulative distribution functions (cdf):
A function $F : \mathbb{R} \rightarrow [0, 1]$ is called **cumulative distribution function** of a random variable X if for all $c \in \mathbb{R}$ hold:

$$P(X \leq c) = F(c)$$

- ▶ Knowing F , we can calculate $P(a < X \leq b)$ for all intervals from a to b
- ▶ F is monotonically increasing, $\lim_{x \rightarrow -\infty} F(x) = 0$, $\lim_{x \rightarrow \infty} F(x) = 1$
- ▶ if exists, the derivative of F is called a **probability density function** (pdf). It yields large values in the areas of large probability and small values in the areas with small probability. But: the value of a pdf cannot be interpreted as a probability!

Continuous random variables (cont.)

- ▶ example: a continuous random variable that can take any value between a and b and does not prefer any value over another one (uniform distribution):



Gaussian distribution

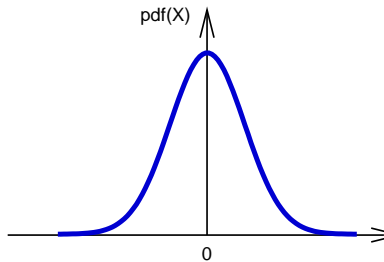
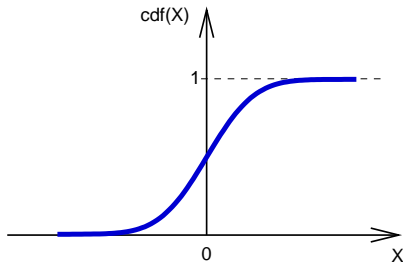
- ▶ the **Gaussian/Normal distribution** is a very important probability distribution. Its pdf is:

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

$\mu \in \mathbb{R}$ and $\sigma^2 > 0$ are parameters of the distribution.

The cdf exists but cannot be expressed in a simple form

μ controls the position of the distribution, σ^2 the spread of the distribution



Statistical inference

- ▶ determining the probability distribution of a random variable (estimation)
- ▶ collecting outcome of repeated random experiments (data sample)
- ▶ adapt a generic probability distribution to the data. example:
 - ▶ Bernoulli-distribution (possible outcomes: 1 or 0) with success parameter p (=probability of outcome '1')
 - ▶ Gaussian distribution with parameters μ and σ^2
 - ▶ uniform distribution with parameters a and b
- ▶ maximum-likelihood approach:

$$\underset{\text{parameters}}{\text{maximize}} P(\text{data sample}|\text{distribution})$$

Statistical inference (cont.)

- ▶ maximum likelihood with Bernoulli-distribution:
- ▶ assume: coin toss with a twisted coin. How likely is it to observe head?
- ▶ repeat several experiments, to get a sample of observations, e.g.: 'head', 'head', 'number', 'head', 'number', 'head', 'head', 'head', 'number', 'number', ...

You observe k times 'head' and n times 'number' Probabilistic model:
'head' occurs with (unknown) probability p , 'number' with probability $1 - p$

- ▶ maximize the likelihood, e.g. for the above sample:

$$\underset{p}{\text{maximize}} p \cdot p \cdot (1 - p) \cdot p \cdot (1 - p) \cdot p \cdot p \cdot p \cdot (1 - p) \cdot (1 - p) \cdots = p^k (1 - p)^n$$

Statistical inference (cont.)

$$\underset{p}{\text{maximize}} \ p \cdot p \cdot (1-p) \cdot p \cdot (1-p) \cdot p \cdot p \cdot p \cdot (1-p) \cdot (1-p) \cdot \dots = p^k (1-p)^n$$

Trick 1: Taking logarithm of function does not change position of minima
rules: $\log(a \cdot b) = \log(a) + \log(b)$, $\log(a^b) = b \log(a)$

Trick 2: Minimizing $-\log()$ instead of maximizing $\log()$

This yields:

$$\underset{p}{\text{minimize}} \ -\log(p^k (1-p)^n) = -k \log p - n \log(1-p)$$

calculating partial derivatives w.r.t p and zeroing: $p = \frac{k}{k+n}$

⇒ The relative frequency of observations is used as estimator for p

Statistical inference (cont.)

- ▶ maximum likelihood with Gaussian distribution:

- ▶ given: data sample $\{x^{(1)}, \dots, x^{(p)}\}$

- ▶ task: determine optimal values for μ and σ^2

assume independence of the observed data:

$$P(\text{data sample}|\text{distribution}) = P(x^{(1)}|\text{distribution}) \cdots P(x^{(p)}|\text{distribution})$$

replacing probability by density:

$$P(\text{data sample}|\text{distribution}) \propto \frac{1}{\sqrt{2\pi\sigma^2}} e^{-\frac{1}{2} \frac{(x^{(1)} - \mu)^2}{\sigma^2}} \cdots \frac{1}{\sqrt{2\pi\sigma^2}} e^{-\frac{1}{2} \frac{(x^{(p)} - \mu)^2}{\sigma^2}}$$

performing log transformation:

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

Statistical inference (cont.)

- ▶ minimizing negative log likelihood instead of maximizing log likelihood:

$$\underset{\mu, \sigma^2}{\text{minimize}} - \sum_{i=1}^p \left(\log \frac{1}{\sqrt{2\pi\sigma^2}} - \frac{1}{2} \frac{(x^{(i)} - \mu)^2}{\sigma^2} \right)$$

- ▶ transforming into:

$$\underset{\mu, \sigma^2}{\text{minimize}} \frac{p}{2} \log(\sigma^2) + \frac{p}{2} \log(2\pi) + \frac{1}{\sigma^2} \left(\frac{1}{2} \sum_{i=1}^p (x^{(i)} - \mu)^2 \right) \underbrace{\left(\frac{1}{2} \sum_{i=1}^p (x^{(i)} - \mu)^2 \right)}_{\text{sq. error term}}$$

- ▶ observation: maximizing likelihood w.r.t. μ is equivalent to minimizing squared error term w.r.t. μ

Statistical inference (cont.)

- ▶ extension: regression case, μ depends on input pattern and some parameters
- ▶ given: pairs of input patterns and target values $(\vec{x}^{(1)}, d^{(1)}), \dots, (\vec{x}^{(p)}, d^{(p)})$, a parameterized function f depending on some parameters \vec{w}
- ▶ task: estimate \vec{w} and σ^2 so that $d^{(i)} - f(\vec{x}^{(i)}; \vec{w})$ fits a Gaussian distribution in best way
- ▶ maximum likelihood principle:

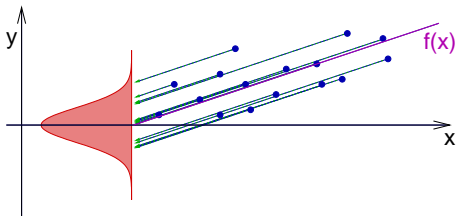
$$\underset{\vec{w}, \sigma^2}{\text{maximize}} \frac{1}{\sqrt{2\pi\sigma^2}} e^{-\frac{1}{2} \frac{(d^{(1)} - f(\vec{x}^{(1)}; \vec{w}))^2}{\sigma^2}} \dots \frac{1}{\sqrt{2\pi\sigma^2}} e^{-\frac{1}{2} \frac{(d^{(p)} - f(\vec{x}^{(p)}; \vec{w}))^2}{\sigma^2}}$$

Statistical inference (cont.)

- ▶ minimizing negative log likelihood:

$$\underset{\vec{w}, \sigma^2}{\text{minimize}} \frac{P}{2} \log(\sigma^2) + \frac{P}{2} \log(2\pi) + \frac{1}{\sigma^2} \left(\frac{1}{2} \sum_{i=1}^P (d^{(i)} - f(\vec{x}^{(i)}; \vec{w}))^2 \right) \underbrace{\left(\frac{1}{2} \sum_{i=1}^P (d^{(i)} - f(\vec{x}^{(i)}; \vec{w}))^2 \right)}_{\text{sq. error term}}$$

- ▶ f could be, e.g., a linear function or a multi layer perceptron



- ▶ minimizing the squared error term can be interpreted as maximizing the data likelihood $P(\text{training data} | \text{model parameters})$

Probability and machine learning

| | machine learning | statistics |
|-----------------------|--|--|
| unsupervised learning | we want to create a model of observed patterns | estimating the probability distribution $P(\text{patterns})$ |
| classification | guessing the class from an input pattern | estimating $P(\text{class} \text{input pattern})$ |
| regression | predicting the output from input pattern | estimating $P(\text{output} \text{input pattern})$ |

- ▶ probabilities allow to precisely describe the relationships in a certain domain, e.g. distribution of the input data, distribution of outputs conditioned on inputs, ...
- ▶ ML principles like minimizing squared error can be interpreted in a stochastic sense

References

- ▶ Norbert Henze: Stochastik für Einsteiger
- ▶ Chris Bishop: Neural Networks for Pattern Recognition