Machine Learning: Probability Theory

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Probabilities

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- convenience: declaring all conditions, exceptions, assumptions would be too complicated.
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  Example: weather forcasting
- intrinsic randomness: non-deterministic processes.
  Example: appearance of photons in a physical process

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

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

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  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 occuring at same time: $P(A, B)$
  example:
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- 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:

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- with the above, we also have

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

- example: $P\big($“caries”$\big|$“toothaches”$\big) = 0.8$
  $P\big($“toothaches”$\big|$“caries”$\big) = 0.3$

Joint events (cont.)

- a contigency table makes clear the relationship between joint probabilities and conditional probabilities:

	B	$\neg B$		
A	$P(A,B)$	$P(A,\neg B)$	$P(A)$	marginals
$\neg A$	$P(\neg A,B)$	$P(\neg A,\neg B)$	$P(\neg A)$	
	$P(B)$	$P(\neg B)$		

joint prob.

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

- example $\longrightarrow$ blackboard (cars: colors and drivers)

Marginalisation

- Let $B_1, ...B_n$ disjoint events with $\cup_i B_i = \Omega$. Then
  $P(A) = \sum_i P(A, B_i)$
  This process is called marginalisation.

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- repeated application: chainrule:

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

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

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- causality and conditionals:

  causality typically causes conditional probabilities close to 1:

  $P(\text{“wet”}|\text{“taking a shower”}) = 1$, 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:

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

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- example:

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

Bayes rule (cont)

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

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- 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'
  $\longrightarrow$ contingency table at blackboard

Random variables

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- 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

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- cumulative distribution functions (cdf):
  A function $F : \mathbb{R} \longrightarrow [0, 1]$ 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, $\lim_{x \to -\infty} F(x) = 0$, $\lim_{x \to \infty} F(x) = 1$

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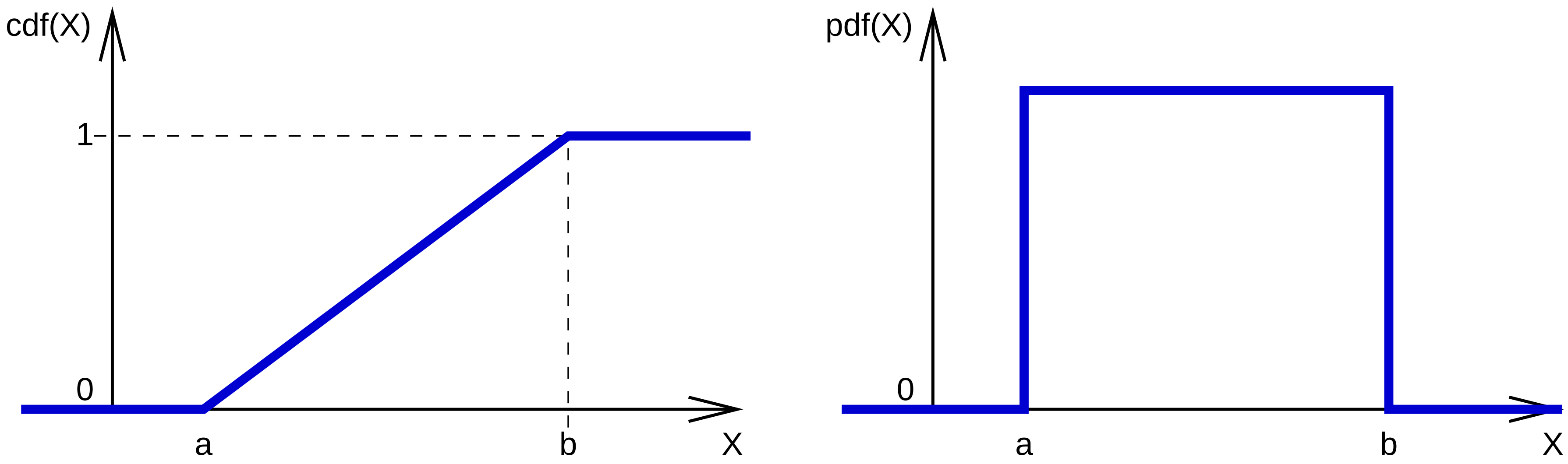
- F is monotonically increasing, $\lim_{x \to -\infty} F(x) = 0$, $\lim_{x \to \infty} F(x) = 1$
- if exists, the derivative of F is called a probability density function (pdf). It yields large values in the areas of large probability and small values in the areas with small probability. But: the value 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):

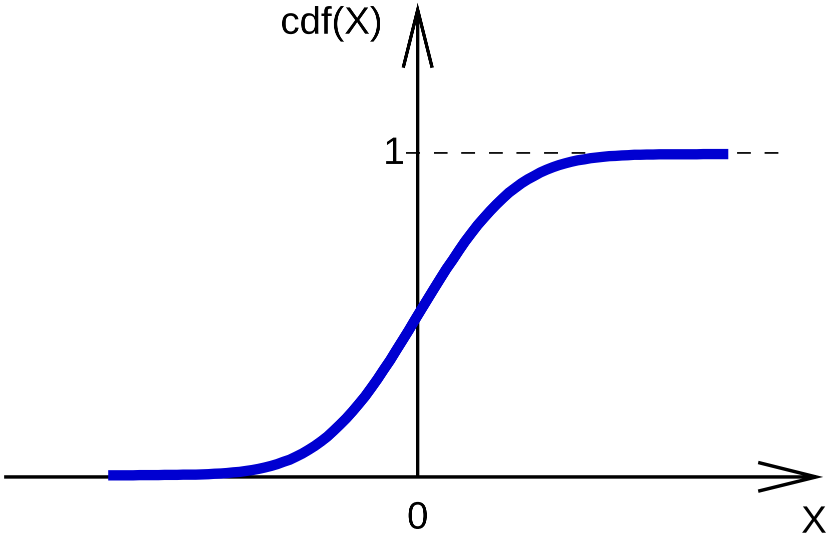


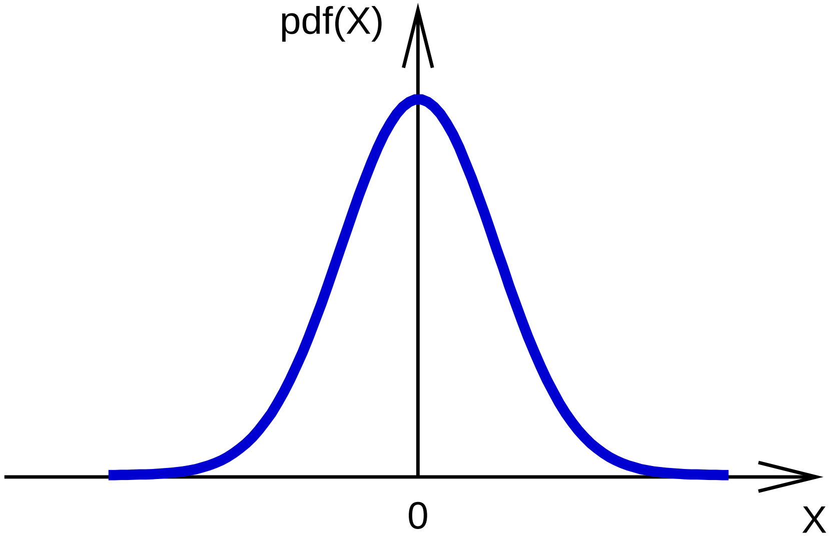
Gaussian distribution

- 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





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- adapt a generic probability distribution to the data. example:
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- maximum-likelihood approach:

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

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  You observe k times ’head’ and n times ’number’
  Probabilisitic model: ’head’ occurs with (unknown) probability p, ’number’ with probability $1 - p$
- maximize the likelihood, e.g. for the above sample:

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

Statistical inference (cont.)

- simplification:

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

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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

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  assume independence of the observed data:

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

replacing probability by density:

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

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performing $\log$ transformation:

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

Statistical inference (cont.)

- minimizing negative log likelihood instead of maximizing log likelihood:

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

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- transforming into:

$$\underset{\mu,\sigma^2}{minimize} \; \frac{p}{2}\log(\sigma^2) + \frac{p}{2}\log(2\pi) + \frac{1}{\sigma^2}\Big(\frac{1}{2}\sum_{i=1}^{p}(x^{(i)}-\mu)^2\Big)$$

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- 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

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- 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:

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

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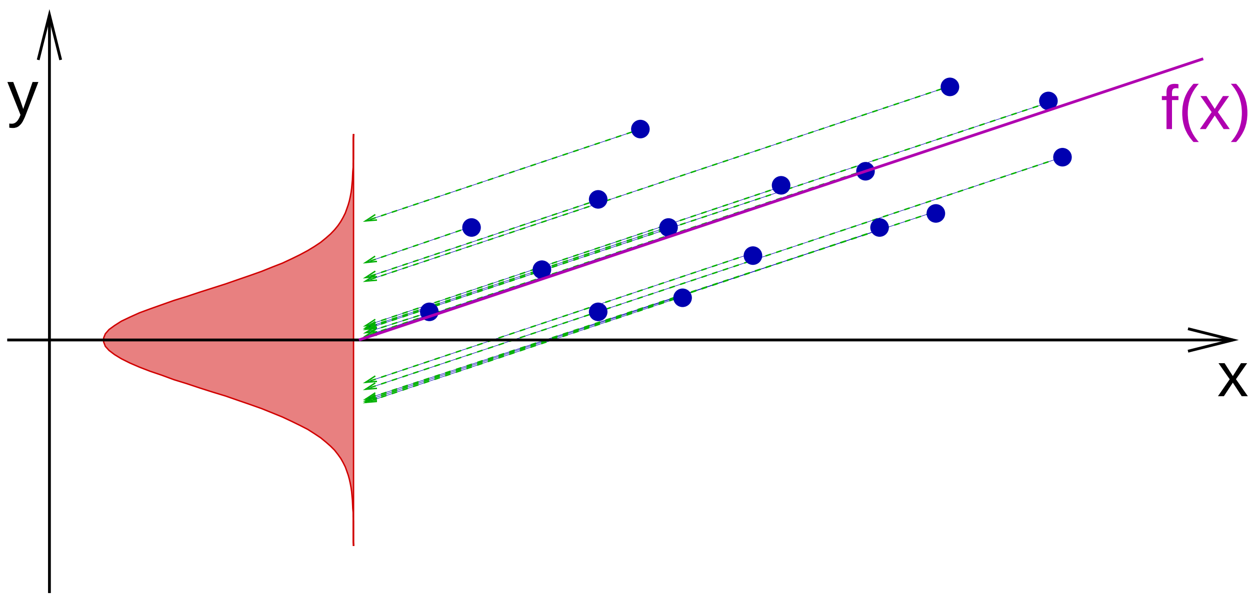
- f could be, e.g., a linear function or a multi layer perceptron



- minimizing the squared error term can be interpreted as maximizing the data

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 $P(\text{class}\mid\text{input pattern})$
regression	predicting the output from input pattern	estimating $P(\text{output}\mid\text{input pattern})$

- 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

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- Chris Bishop: Neural Networks for Pattern Recognition