Probabilistic Classification

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Here *probably* means that out of my extensive catalogue of four kinds of birds that I am able to recognize, "blackbird" gets the highest degree of belief based on *features* of this particular bird.

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The degree of belief (Bayesians), or the relative frequency (frequentists) is the *probability*.

Basic Discrete Probability Theory

- A finite or countably infinite set Ω of *possible outcomes*, Ω is called *sample space*.

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- Each element ω of Ω is assigned a "probability" value $f(\omega)$, here f must satisfy
  - $f(\omega) \in [0, 1]$ for all $\omega \in \Omega$,
  - $\sum_{\omega \in \Omega} f(\omega) = 1$.

  If the dice is fair, then $f(\omega) = \frac{1}{6}$ for all $\omega \in \{1, \ldots, 6\}$.

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  If the dice is fair, then $f(\omega) = \frac{1}{6}$ for all $\omega \in \{1, \ldots, 6\}$.
- An *event* is any subset E of Ω.
- The *probability* of a given event $E \subseteq \Omega$ is defined as

$$P(E) = \sum_{\omega \in E} f(\omega)$$

  Let E be the event that an odd number is rolled, i.e., $E = \{1, 3, 5\}$. Then $P(E) = \frac{1}{2}$.

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  Let E be the event that an odd number is rolled, i.e., $E = \{1, 3, 5\}$. Then $P(E) = \frac{1}{2}$.
- Basic laws: $P(\Omega) = 1$, $P(\emptyset) = 0$, given disjoint sets A, B we have $P(A \cup B) = P(A) + P(B)$, $P(\Omega \setminus A) = 1 - P(A)$.

Conditional Probability and Independence

- $P(A \mid B)$ is the probability of A given B (assume $P(B) > 0$) defined by

  $$P(A \mid B) = P(A \cap B)/P(B)$$

  (We assume that B is all and only information known.)

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  A fair dice: what is the probability that 3 is rolled assuming that an odd number is rolled? ... and assuming that an even number is rolled?

- A and B are independent if $P(A \cap B) = P(A) \cdot P(B)$.

  It is easy to show that if $P(B) > 0$, then

  $$A, B \text{ are independent iff } P(A \mid B) = P(A).$$

Random Variables and Random Vectors

- A *random variable* X is a function $X : \Omega \to \mathbb{R}$.
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- A *random vector* is a function $X : \Omega \to \mathbb{R}^d$.
  We use $X = (X_1, \ldots, X_d)$ where X_i is a random variable returning the i-th component of X.
- Consider random variables X_1, X_2 and Y. The variables X_1, X_2 are *conditionally independent given Y* if for all x_1, x_2 and y we have that

$$P(X_1 = x_1, X_2 = x_2 \mid Y = y) = P(X_1 = x_1 \mid Y = y) \cdot P(X_2 = x_2 \mid Y = y)$$

Random Vectors – Example

Let Ω be a space of colored geometric shapes that are divided into two categories ($\mathbf{1}$ and $\mathbf{0}$).

Assume a random vector $X = (X_{color}, X_{shape}, X_{cat})$ where

- $X_{color} : \Omega \rightarrow \{red, blue\}$,
- $X_{shape} : \Omega \rightarrow \{circle, square\}$,
- $X_{cat} : \Omega \rightarrow \{\mathbf{1}, \mathbf{0}\}$.

Probability distribution of values is given by the following tables:

category $\mathbf{1}$:

	circle	square
red	0.2	0.02
blue	0.02	0.01

category $\mathbf{0}$:

	circle	square
red	0.05	0.3
blue	0.2	0.2

Random Vectors – Example

Example:

$P(red, circle, \mathbf{1}) = P(X_{color} = red, X_{shape} = circle, X_{cat} = \mathbf{1}) = 0.2$

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"Summing over" all possible values of some variable(s) gives the distribution of the rest:

$$\begin{aligned} P(red, circle) &= P(X_{color} = red, X_{shape} = circle) \\ &= P(red, circle, \mathbf{1}) + P(red, circle, \mathbf{0}) \\ &= 0.2 + 0.05 = 0.25 \end{aligned}$$

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$$P(red) = 0.2 + 0.02 + 0.05 + 0.3 = 0.57$$

Thus also all conditional probabilities can be computed:

$$P(\mathbf{1} \mid red, circle) = \frac{P(red, circle, \mathbf{1})}{P(red, circle)} = \frac{0.2}{0.25} = 0.8$$

Bayesian Classification

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- Let X be the random vector describing n features of a given instance, i.e., $X = (X_1, \dots, X_n)$
  - Denote by $\vec{x} \in \mathbb{R}^n$ values of X,
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Bayes classifier: Given a vector of feature values $\vec{x}$,

$$C^{Bayes}(\vec{x}) := \begin{cases} \mathbf{1} & \text{if } P(Y = \mathbf{1} \mid X = \vec{x}) \geq P(Y = \mathbf{0} \mid X = \vec{x}) \\ \mathbf{0} & \text{otherwise.} \end{cases}$$

Intuitively, C^{Bayes} assigns to $\vec{x}$ the most probable category it might be in.

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The Bayes classifier compares $P(Y = \mathbf{1} \mid X = (40g, 5cm))$ with $P(Y = \mathbf{0} \mid X = (40g, 5cm))$ and selects the more probable category given the features.

Crucial question: Is such a classifier good?

There are other classifiers, e.g., one which compares the weight divided by 10 with the diameter and decides based on the answer, or maybe a classifier which sums the weight and the diameter and compares the result with a constant, etc.

Bayes Classifier

Let C be an arbitrary *classifier*, that is a function that to every feature vector $\vec{x} \in \mathbb{R}^n$ assigns a class from $\{\mathbf{0}, \mathbf{1}\}$.

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Define the error of the classifier C by

$$E_C = P(Y \neq C)$$

(Here we slightly abuse notation and apply C to samples, technically we apply the composition $C \circ X$ of C and X which first determines the features using X and then classifies according to C).

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Theorem

The Bayes classifier C^{Bayes} minimizes E_C, that is

$$E_{C^{Bayes}} = \min_{C \text{ is a classifier}} E_C$$

Practical Use of Bayes Classifier

The crucial problem: The probability P is not known!
In particular, where to get $P(Y = \mathbf{1} \mid X = \vec{x})$?
Note that $P(Y = \mathbf{0} \mid X = \vec{x}) = 1 - P(Y = \mathbf{1} \mid X = \vec{x})$

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Where to get these probabilities?

In some cases the probabilities might come from the knowledge of the solved problem (e.g., applications in physics might be supported by a theory giving the probabilities).

In most cases, however, P is estimated from sampled data by

$$\bar{P}(Y = \mathbf{1} \mid X = \vec{x}) = \frac{\text{number of samples with } Y = \mathbf{1} \text{ and } X = \vec{x}}{\text{number of samples with } X = \vec{x}}$$

(We use $\bar{P}$ to denote an estimate of P from data.)

Estimating P

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All data with $X_1 = 1$, $X_2 = 0$, $X_3 = 1$:

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The probability table and hence also the necessary data are typically too large!

Concretely, if all $X_1, \ldots, X_n$ are binary, there are 2^n probabilities $P(Y = \mathbf{1} \mid X = \vec{x})$, one for each possible $\vec{x} \in \{0, 1\}^n$.

Let's Look at It the Other Way Round

Theorem (Bayes,1764)

$$P(A \mid B) = \frac{P(B \mid A) \cdot P(A)}{P(B)}$$

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Proof.

$$P(A \mid B) = \frac{P(A \cap B)}{P(B)} = \frac{\frac{P(A \cap B)}{P(A)} \cdot P(A)}{P(B)} = \frac{P(B \mid A) \cdot P(A)}{P(B)}$$

$\square$

Bayesian Classification

Determine the category for $\vec{x}$ by computing

$$P(Y = y \mid X = \vec{x}) = \frac{P(Y = y) \cdot P(X = \vec{x} \mid Y = y)}{P(X = \vec{x})}$$

for both $y \in \{\mathbf{0}, \mathbf{1}\}$ and deciding whether or not the following holds:

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So in order to make the classifier we need to compute:

- The prior $P(Y = \mathbf{1})$ (then $P(Y = \mathbf{0}) = 1 - P(Y = \mathbf{1})$)
- The conditionals $P(X = \vec{x} \mid Y = y)$ for $y \in \{\mathbf{0}, \mathbf{1}\}$ and for every $\vec{x}$

Estimating the Prior and Conditionals

- $P(Y = \mathbf{1})$ can be easily estimated from data by

$$\bar{P}(Y = \mathbf{1}) = \frac{\text{number of samples with } Y = \mathbf{1}}{\text{number of all samples}}$$

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- If the dimension of features is small, $P(X = \vec{x} \mid Y = y)$ can be estimated from data similarly as $P(Y = \mathbf{1} \mid X = \vec{x})$ by

$$\bar{P}(X = \vec{x} \mid Y = y) = \frac{\text{number of samples with } Y = y \text{ and } X = \vec{x}}{\text{number of samples with } Y = y}$$

Unfortunately, for higher dimensional data too many samples are needed to estimate all $P(X = \vec{x} \mid Y = y)$ (there are too many $\vec{x}$'s).

So where is the advantage of using the Bayes thm.??

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So where is the advantage of using the Bayes thm.??

We introduce *independence assumptions* about the features!

Naive Bayes

- We assume that features are (conditionally) independent *given the category*. That is for all $\vec{x} = (x_1, \ldots, x_n)$ and $y \in \{\mathbf{0}, \mathbf{1}\}$ we **assume**:

$$
\begin{aligned}
P(X = x \mid Y = y) &= P(X_1 = x_1, \cdots, X_n = x_n \mid Y) \\
&= \prod_{i=1}^{n} P(X_i = x_i \mid Y = y)
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- Therefore, we only need to specify $P(X_i = x_i \mid Y = y)$ for each possible pair of a feature-value x_i and $y \in \{\mathbf{0}, \mathbf{1}\}$.

  Note that if all X_i are binary (values in $\{0, 1\}$), this requires specifying only $2n$ parameters:

$$P(X_i = 1 \mid Y = \mathbf{1}) \text{ and } P(X_i = 1 \mid Y = \mathbf{0}) \text{ for each } X_i$$

  as $P(X_i = 0 \mid Y = y) = 1 - P(X_i = 1 \mid Y = y)$ for $y \in \{\mathbf{0}, \mathbf{1}\}$.

Compared to specifying 2^n parameters without any independence assumption.

Estimating the marginal probabilities

Estimate the probabilities $P(X_i = x_i \mid Y = y)$ by

$$\bar{P}(X_i = x_i \mid Y = y) = \frac{\text{number of samples with } X_i = x_i \text{ and } Y = y}{\text{number of samples with } Y = y}$$

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Example: Consider a problem with $X = (X_1, X_2, X_3)$ where each X_i returns either 0 or 1. The data is

Y	X_1	X_2	X_3
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$\bar{P}(X_1 = 1 \mid Y = \mathbf{1}) = 1/3$ $\quad$ $\bar{P}(X_1 = 1 \mid Y = \mathbf{0}) = 2/3$
$\bar{P}(X_2 = 1 \mid Y = \mathbf{1}) = 1/3$ $\quad$ $\bar{P}(X_2 = 1 \mid Y = \mathbf{0}) = 1/3$
$\bar{P}(X_3 = 1 \mid Y = \mathbf{1}) = 2/3$ $\quad$ $\bar{P}(X_3 = 1 \mid Y = \mathbf{0}) = 1$

Naive Bayes – Example

Consider classification of geometric shapes:

$X_1 \in \{small, medium, large\}$

$X_2 \in \{red, blue, green\}$

$X_3 \in \{square, triangle, circle\}$

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We have already estimated the following probabilities:

	$Y = \mathbf{1}$	$Y = \mathbf{0}$
$\bar{P}(Y)$	0.5	0.5
$\bar{P}(small \mid Y)$	0.4	0.4
$\bar{P}(medium \mid Y)$	0.1	0.2
$\bar{P}(large \mid Y)$	0.5	0.4
$\bar{P}(red \mid Y)$	0.9	0.3
$\bar{P}(blue \mid Y)$	0.05	0.3
$\bar{P}(green \mid Y)$	0.05	0.4
$\bar{P}(square \mid Y)$	0.05	0.4
$\bar{P}(triangle \mid Y)$	0.05	0.3
$\bar{P}(circle \mid Y)$	0.9	0.3

Does $(medium, red, circle)$ belong to the category $\mathbf{1}$?

	$Y = \mathbf{1}$	$Y = \mathbf{0}$
$\bar{P}(Y)$	0.5	0.5
$\bar{P}(medium \mid Y)$	0.1	0.2
$\bar{P}(red \mid Y)$	0.9	0.3
$\bar{P}(circle \mid Y)$	0.9	0.3

Denote $\vec{x} = (medium, red, circle)$.

	$Y=\mathbf{1}$	$Y=\mathbf{0}$
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Denote $\vec{x} = (medium, red, circle)$.

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&P(Y=\mathbf{1} \mid X=\vec{x}) = \\
&\qquad = P(\mathbf{1}) \cdot P(medium \mid \mathbf{1}) \cdot P(red \mid \mathbf{1}) \cdot P(circle \mid \mathbf{1}) \,/\, P(X=\vec{x}) \\
&\qquad \doteq 0.5 \cdot 0.1 \cdot 0.9 \cdot 0.9 \,/\, P(X=\vec{x}) = 0.0405/P(X=\vec{x})
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(Note that we used the estimates $\bar{P}$ of P to finish the computation above.)

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Apparently,

$$P(Y = \mathbf{1} \mid X = \vec{x}) \doteq 0.0405/P(X = \vec{x}) > 0.009/P(X = \vec{x}) \doteq P(\mathbf{0} \mid X = \vec{x})$$

So we classify $\vec{x}$ to the category $\mathbf{1}$.

Estimating Probabilities in Practice

We already know that $P(X_i = x_i \mid Y = y)$ can be estimated by

$$\bar{P}(X_i = x_i \mid Y = y) = \ell_{y,x_i} \,/\, \ell_y$$

where

- ℓ_{y,x_i} = number of samples with $Y = y$ and $X_i = x_i$
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Problem: If, by chance, a rare value x_i of a feature X_i never occurs in the training data, we get

$$\bar{P}(X_i = x_i \mid Y = y) = 0 \quad \text{for both } y \in \{\mathbf{0}, \mathbf{1}\}$$

But then $\bar{P}(X = x) = 0$ for x containing the value x_i for X_i, and thus $\bar{P}(Y = y \mid X = x)$ is not well defined.
Moreover, $\bar{P}(Y = y) \cdot \bar{P}(X = x \mid Y = y) = 0$ (for $y \in \{\mathbf{0}, \mathbf{1}\}$) so even this cannot be used for classification.

Probability Estimation Example

Training data:

Size	Color	Shape	Class
small	red	circle	**1**
large	red	circle	**1**
small	red	triangle	**0**
large	blue	circle	**0**

Estimated probabilities:

	$Y = \mathbf{1}$	$Y = \mathbf{0}$
$\bar{P}(Y)$	0.5	0.5
$\bar{P}(small \mid Y)$	0.5	0.5
$\bar{P}(medium \mid Y)$	0	0
$\bar{P}(large \mid Y)$	0.5	0.5
$\bar{P}(red \mid Y)$	1	0.5
$\bar{P}(blue \mid Y)$	0	0.5
$\bar{P}(green \mid Y)$	0	0
$\bar{P}(square \mid Y)$	0	0
$\bar{P}(triangle \mid Y)$	0	0.5
$\bar{P}(circle \mid Y)$	1	0.5

Note that $\bar{P}(medium \mid \mathbf{1}) = P(medium \mid \mathbf{0}) = 0$ and thus also $\bar{P}(medium, red, circle) = 0$.

So what is $\bar{P}(\mathbf{1} \mid medium, red, circle)$?

Smoothing

- To account for estimation from small samples, probability estimates are adjusted or *smoothed*.

Smoothing

- To account for estimation from small samples, probability estimates are adjusted or *smoothed*.
- *Laplace smoothing* adds one to every count of feature values

$$\tilde{P}(X_i = x_i \mid Y = y) = \frac{\ell_{y,x_i} + 1}{\ell_y + v_i}$$

where

  - ℓ_y = number of training samples with $Y = y$,
  - ℓ_{y,x_i} = number of training samples with $Y = y$ and $X_i = x_i$,
  - v_i is the number of all distinct values of the variable X_i.

To understand note that

$$\ell_y = \sum_{x_i \text{ is a value of } X_i} \ell_{y,x_i}$$

and thus

$$\bar{P}(X_i = x_i \mid Y = y) = \ell_{y,x_i} \,/ \sum_{x_i \text{ is a value of } X_i} \ell_{y,x_i}$$

$$\tilde{P}(X_i = x_i \mid Y = y) = (\ell_{y,x_i} + 1) \,/ \sum_{x_i \text{ is a value of } X_i} (\ell_{y,x_i} + 1)$$

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- Assume training set contains 10 samples of category **1**:
  - 4 small
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- Assume training set contains 10 samples of category **1**:
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- Estimate parameters as follows
  - $\tilde{P}(small \mid \mathbf{1}) = (4+1)/(10+3) = 0.384$
  - $\tilde{P}(medium \mid \mathbf{1}) = (0+1)/(10+3) = 0.0769$
  - $\tilde{P}(large \mid \mathbf{1}) = (6+1)/(10+3) = 0.538$

Continuous Features

Ω may be (potentially) continuous, X_i may assign a continuum of values in $\mathbb{R}$.

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- The probabilities are computed using *probability density* $p : \mathbb{R} \to \mathbb{R}^+$.
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  Usually, $P(X_i \mid Y = y)$ is used to denote the *density* of X_i conditioned on $Y = y$.
- The densities $P(X_i \mid Y = y)$ are usually estimated using Gaussian densities as follows:
  - Estimate the mean μ_{iy} and the standard deviation σ_{iy} based on training data.
  - Then put
  $$\bar{P}(X_i \mid Y = y) = \frac{1}{\sigma_{iy}\sqrt{2\pi}} \exp\left(\frac{-(X_i - \mu_{iy})^2}{2\sigma_{iy}^2}\right)$$

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  Even if the probabilities are not accurately estimated, it often picks the correct maximum probability category.
- Directly constructs a hypothesis from parameter estimates that are calculated from the training data.
- Typically handles outliers and noise well.
- Missing values are easy to deal with (simply average over all missing values in feature vectors).

Bayesian Networks (Basic Information)

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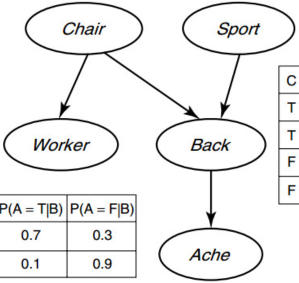
(But now in a well-defined sense.)

Bayesian networks are a graphical model that uses a directed acyclic graph to specify dependencies among variables.

Bayesian Networks – Example

P(C = T)	P(C = F)
0.8	0.2

P(S = T)	P(S = F)
0.02	0.98



C	P(W = T|C)	P(W = F|C)
T	0.9	0.1
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C	S	P(B = T|C,S)	P(B = F|C,S)
T	T	0.9	0.1
T	F	0.2	0.8
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B	P(A = T|B)	P(A = F|B)
T	0.7	0.3
F	0.1	0.9

Now, e.g.,

$$P(C, S, W, B, A) = P(C) \cdot P(S) \cdot P(W \mid C) \cdot P(B \mid C, S) \cdot P(A \mid B)$$

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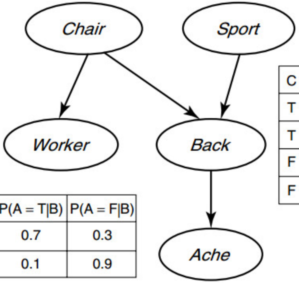

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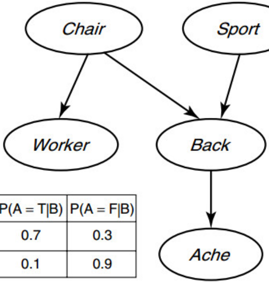

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Now we may, e.g., infer what is the probability $P(C = T \mid A = T)$ that we sit in a bad chair assuming that our back aches.

We have to store only 10 numbers as opposed to $2^5 - 1$ possible probabilities for all vectors of values of C, S, W, B, A.

Bayesian Networks – Learning & Naive Bayes

Many algorithms have been developed for learning:

- the structure of the graph of the network,
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Automatic procedures are usually combined with expert knowledge.

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Can you express the naive Bayes for $Y, X_1, \ldots, X_n$ using a Bayesian network?