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$$

## Probabilistic Modeling

- Where does data come from?
- We might imagine that "Nature" generates it using some random (i.e., probabilistic) process.
- Maybe modeling this probabilistic process will suggest new ways of making predictions?


## Example: Flowers

- Suppose there are two species of flower.
- One species tends to have more petals.
- Goal: Given a new flower with $X=x$ petals predict its species, $Y$.



## Example: Flowers

- Idea: The number of petals, $X$, and the species, $Y$, are random variables.
- Assumption: When Nature generates a new flower, it picks $X$ and $Y$ from some probability distribution.
- Let's imagine (for now) that we know this distribution.


## The Joint Distribution

- The joint distribution $\mathbb{P}(X=x, Y=y)$ gives us full information.

|  | $Y=0$ | $Y=1$ |
| :--- | ---: | ---: |
| $X=0$ | $0 \%$ | $0 \%$ |
| $X=1$ | $5 \%$ | $0 \%$ |
| $X=2$ | $10 \%$ | $5 \%$ |
| $X=3$ | $15 \%$ | $15 \%$ |
| $X=4$ | $5 \%$ | $20 \%$ |
| $X=5$ | $0 \%$ | $15 \%$ |
| $X=6$ | $0 \%$ | $10 \%$ |

## Observation

- The entries of the joint distribution table sum to $100 \%$.
- Mathematically: $\sum_{x \in\{0,1, \ldots, 6\}} \sum_{y \in\{0,1\}} \mathbb{P}(X=x, Y=y)=1$.

|  | $Y=0$ | $Y=1$ |
| :--- | ---: | ---: |
| $X=0$ | $0 \%$ | $0 \%$ |
| $X=1$ | $5 \%$ | $0 \%$ |
| $X=2$ | $10 \%$ | $5 \%$ |
| $X=3$ | $15 \%$ | $15 \%$ |
| $X=4$ | $5 \%$ | $20 \%$ |
| $X=5$ | $0 \%$ | $15 \%$ |
| $X=6$ | $0 \%$ | $10 \%$ |

## Marginal Distributions

- What is the probability that a new flower has $X=4$ petals (regardless of species)?

|  | $Y=0$ | $Y=1$ |
| :--- | ---: | ---: |
| $X=0$ | $0 \%$ | $0 \%$ |
| $X=1$ | $5 \%$ | $0 \%$ |
| $X=2$ | $10 \%$ | $5 \%$ |
| $X=3$ | $15 \%$ | $15 \%$ |
| $X=4$ | $5 \%$ | $20 \%$ |
| $X=5$ | $0 \%$ | $15 \%$ |
| $X=6$ | $0 \%$ | $10 \%$ |

## Marginal Distributions

The marginal distribution for $X$ is found by summing over values of $Y$.
$\Rightarrow$ That is: $\mathbb{P}(X=x)=\sum_{y \in\{0,1\}} P(X=x, Y=y)$

|  | $Y=0$ | $Y=1$ |
| :--- | ---: | ---: |
| $X=0$ | $0 \%$ | $0 \%$ |
| $X=1$ | $5 \%$ | $0 \%$ |
| $X=2$ | $10 \%$ | $5 \%$ |
| $X=3$ | $15 \%$ | $15 \%$ |
| $X=4$ | $5 \%$ | $20 \%$ |
| $X=5$ | $0 \%$ | $15 \%$ |
| $X=6$ | $0 \%$ | $10 \%$ |


| $X=0$ | $0 \%$ |
| :--- | ---: |
| $X=1$ | $5 \%$ |
| $X=2$ | $15 \%$ |
| $X=3$ | $30 \%$ |
| $X=4$ | $25 \%$ |
| $X=5$ | $15 \%$ |
| $X=6$ | $10 \%$ |

joint

## Marginal Distributions

- What is the probability that a new flower is species 1 (regardless of number of petals)?

|  | $Y=0$ | $Y=1$ |
| :--- | ---: | ---: |
| $X=0$ | $0 \%$ | $0 \%$ |
| $X=1$ | $5 \%$ | $0 \%$ |
| $X=2$ | $10 \%$ | $5 \%$ |
| $X=3$ | $15 \%$ | $15 \%$ |
| $X=4$ | $5 \%$ | $20 \%$ |
| $X=5$ | $0 \%$ | $15 \%$ |
| $X=6$ | $0 \%$ | $10 \%$ |

## Marginal Distributions

$\Rightarrow$ The marginal distribution for $Y$ is found by summing over values of $X$.
$\Rightarrow$ That is: $\mathbb{P}(Y=y)=\sum_{x \in\{0, \ldots, 6\}} P(X=x, Y=y)$

|  | $Y=0$ | $Y=1$ |
| :--- | ---: | ---: |
| $X=0$ | $0 \%$ | $0 \%$ |
| $X=1$ | $5 \%$ | $0 \%$ |
| $X=2$ | $10 \%$ | $5 \%$ |
| $X=3$ | $15 \%$ | $15 \%$ |
| $X=4$ | $5 \%$ | $20 \%$ |
| $X=5$ | $0 \%$ | $15 \%$ |
| $X=6$ | $0 \%$ | $10 \%$ |

$$
\begin{array}{l|l}
Y=0 & 35 \% \\
Y=1 & 65 \% \\
\hline
\end{array}
$$

marginal in $Y$
joint

## Observation

The probabilities in the marginal distributions also sum to 1 .

## Exercise

Suppose flower A has 4 petals. What do you predict its species to be?

|  | $Y=0$ | $Y=1$ |
| :--- | ---: | ---: |
| $X=0$ | $0 \%$ | $0 \%$ |
| $X=1$ | $5 \%$ | $0 \%$ |
| $X=2$ | $10 \%$ | $5 \%$ |
| $X=3$ | $15 \%$ | $15 \%$ |
| $X=4$ | $5 \%$ | $20 \%$ |
| $X=5$ | $0 \%$ | $15 \%$ |
| $X=6$ | $0 \%$ | $10 \%$ |

## Intuition

- It seems more likely that a petal with 4 flowers is from species 1 .

|  | $Y=0$ | $Y=1$ |
| :--- | ---: | ---: |
| $X=0$ | $0 \%$ | $0 \%$ |
| $X=1$ | $5 \%$ | $0 \%$ |
| $X=2$ | $10 \%$ | $5 \%$ |
| $X=3$ | $15 \%$ | $15 \%$ |
| $X=4$ | $5 \%$ | $20 \%$ |
| $X=5$ | $0 \%$ | $15 \%$ |
| $X=6$ | $0 \%$ | $10 \%$ |

## Conditional Probabilities

- This is captured by the conditional probability

$$
\mathbb{P}(Y=y \mid X=x)=\mathbb{P}(X=x, Y=y) / \mathbb{P}(X=x) .
$$

| $\mid$ |  | $Y=0$ |
| :--- | ---: | ---: |
|  | $Y=1$ |  |
| $X=0$ | $0 \%$ | $0 \%$ |
| $X=1$ | $5 \%$ | $0 \%$ |
| $X=2$ | $10 \%$ | $5 \%$ |
| $X=3$ | $15 \%$ | $15 \%$ |
| $X=4$ | $5 \%$ | $20 \%$ |
| $X=5$ | $0 \%$ | $15 \%$ |
| $X=6$ | $0 \%$ | $10 \%$ |

joint

| $\mathbb{P}(Y=y \mid X=1)$ |  |
| :--- | ---: |
| $Y=0$ | $100 \%$ |
| $Y=1$ | $0 \%$ |

$$
\begin{array}{c|c}
\mathbb{P}(Y=y \mid X=2) \\
\hline Y=0 & 66.5 \% \\
Y=1 & 33.3 \% \\
\hline
\end{array}
$$

$$
\begin{array}{l|l}
\mathbb{P}(Y=y \mid X=4) \\
\hline Y=0 & 20 \% \\
Y=1 & 80 \%
\end{array}
$$

## Conditional Probabilities

- The conditional probability

$$
\mathbb{P}(X=x \mid Y=y)=\mathbb{P}(X=x, Y=y) / \mathbb{P}(Y=y) .
$$

|  | $Y=0$ | $Y=1$ |
| :--- | ---: | ---: |
| $X=0$ | $0 \%$ | $0 \%$ |
| $X=1$ | $5 \%$ | $0 \%$ |
| $X=2$ | $10 \%$ | $5 \%$ |
| $X=3$ | $15 \%$ | $15 \%$ |
| $X=4$ | $5 \%$ | $20 \%$ |
| $X=5$ | $0 \%$ | $15 \%$ |
| $X=6$ | $0 \%$ | $10 \%$ |


| $\mathbb{P}(X=x \mid Y=0)$ |  |
| :--- | ---: |
| $X=0$ | $0 \%$ |
| $X=1$ | $14.2 \%$ |
| $X=2$ | $28.5 \%$ |
| $X=3$ | $42.8 \%$ |
| $X=4$ | $14.2 \%$ |
| $X=5$ | $0 \%$ |
| $X=6$ | $0 \%$ |

joint

## Observation

- Conditional probabilities sum to 1 as well.
- For any fixed $x$ :

$$
\sum_{y} \mathbb{P}(Y=y \mid X=x)=1
$$

- For any fixed $y$ :

$$
\sum_{x} \mathbb{P}(X=x \mid Y=y)=1
$$

## Five Distributions

- We've seen five distributions:
$>$ Joint: $\mathbb{P}(X=x, Y=y)$
- Marginal in $X: \mathbb{P}(X=x)$
> Marginal in $Y: \mathbb{P}(Y=y)$
- Conditional on $X: \mathbb{P}(Y=y \mid X=x)$
- Conditional on $Y: \mathbb{P}(X=x \mid Y=y)$
- If we know the joint distribution, we can compute any of the others.


## Bayes' Theorem

Bayes' Theorem relates conditional probabilities and provides another way of computing them:

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

Bayes' Theorem
Derivation:

$$
\begin{gathered}
P(Y=y \mid X=x) P(X=x)=P(X=x, Y=y) \\
P(X=x \mid Y=y) P(Y=y)=P(X=x, Y=y) \\
P(Y=y \mid X=x)=\frac{P(X=x \mid Y=y) P(Y=y)}{P(X=x)}
\end{gathered}
$$

## Bayes Decision Theory

- Goal: Given a new flower with $X=x$ petals, predict its species, $Y$.
- Idea: Predict species 1 if $\mathbb{P}(Y=1 \mid X=x)>\mathbb{P}(Y=0 \mid X=x)$; otherwise predict species 0 .
- That is, pick whichever species is more likely.


## Bayes Classification Rule

$\downarrow$ This is the Bayes classification rule:

- Predict class 1 if $\mathbb{P}(Y=1 \mid X=x)>\mathbb{P}(Y=0 \mid X=x)$;
- Otherwise, predict class 0 .


## Bayes Decision Theory

- Using Bayes' rule,

$$
\mathbb{P}(Y=y \mid X=x)=\mathbb{P}(X=x \mid Y=y) \mathbb{P}(Y=y) / \mathbb{P}(X=x)
$$

- Bayes classification rule (original form):
$\Rightarrow$ Predict class 1 if $\mathbb{P}(Y=1 \mid X=x)>\mathbb{P}(Y=0 \mid X=x)$;
- Otherwise, predict class 0.
- Bayes classification rule (alternative form):
- Predict class 1 if

$$
\mathbb{P}(X=x \mid Y=1) \mathbb{P}(Y=1)>\mathbb{P}(X=x \mid Y=0) \mathbb{P}(Y=0)
$$

- Otherwise, predict class 0 .


## Main Idea

If we know the conditional probability of the label $Y$ given feature $X$, the Bayes classification rule is a natural way to make predictions.

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## Example: Penguins

- Suppose there are two species of penguin.
- One species tends to have longer flippers.
- Goal: given a new penguin with flipper length $X=x$, predict its species, $Y$.


## Five Distributions

- In this situation, what do the five distributions look like?
$\Rightarrow$ Joint distribution of $X$ and $Y$
- Marginal distribution in $X$
- Marginal distribution in $Y$
- Conditional on $X$
- Conditional on $Y$


## Marginal in $Y$

- What is the probability that Nature generates a penguin from species $Y$ ?
- Marginal distribution: $\mathbb{P}(Y=y)$.
- This is a discrete distribution, as before.
- Example:

$$
\begin{array}{l|l}
Y=0 & 30 \% \\
Y=1 & 70 \% \\
\hline
\end{array}
$$

## Marginal in $X$

- What is the probability that Nature generates a flipper length of $x$, without regard to species?
- Flipper length is a continuous random variable.
- Distribution is described by a probability density function (pdf), $p: \mathbb{R} \rightarrow \mathbb{R}^{+}$.


## Recall: Density Functions

- A probability density function (pdf) for a random variable $X$ is a function $p: \mathbb{R} \rightarrow \mathbb{R}^{+}$satisfying:

$$
\mathbb{P}(a<X<b)=\int_{a}^{b} p_{X}(x) d x
$$

- That is, the pdf $p$ describes how likely it is to get a value of $X$ in any interval $[a, b]$.
- Note: $\int_{-\infty}^{\infty} p_{\chi}(x) d x=1$, but $p(x)$ can be larger than one.


## Marginal in $X$

- The distribution of flipper lengths is described by a density function, $p_{x}(x)$.



## Exercise

What is the probability that Nature generates a penguin with flipper length equal to 10 cm ?


## Solution

- Zero!
$p_{X}(x)$ is not the probability that $X=x$.

Instead, $\mathbb{P}(X=x)=\mathbb{P}(x<X<x)=\int_{x}^{x} p_{X}(x) d x=0$

- The probability of a continuous random variable being exactly a certain value is zero.


## Example

- What is the probability that Nature generates a penguin whose flipper length is between 7.5 and 10 cm ?


$$
\mathbb{P}(7.5<X<10)=\int_{7.5}^{10} p_{x}(x) d x
$$

## Conditional on $Y$

- What is the probability of a certain flipper length, given that the species is $y$ ?
- Also a continuous distribution, described by conditional density $p(x \mid Y=y)$.
- Two conditional density functions: one for $Y=0$ and one for $Y=1$.
$\Rightarrow$ Each integrates to one.


## Conditional on $Y$



## Conditional on $X$

- What is the probability that the species is $y$ given a flipper length of $x$ ?
- The conditional distribution of $Y$ given $X$.


## Exercise

Is this distribution continuous or discrete?

## Conditional on $X$

- Answer: discrete, because $Y$ is discrete.
- One distribution $P(Y=y \mid X=x)$ for each possible value of $X$ (infinitely many).


## Conditional on $X$

- Although for any fixed $x, \mathbb{P}(Y=y \mid X=x)$ is discrete, we can plot the functions $f_{0}(x)=\mathbb{P}(Y=0 \mid X=x)$ and $f_{1}(x)=\mathbb{P}(Y=1 \mid X=x)$



## Bayes' Rule

- Bayes' Rule applies to densities, too:

$$
\mathbb{P}(Y=y \mid X=x)=\frac{p(x \mid Y=y) \mathbb{P}(Y=y)}{p_{X}(x)}
$$

## Bayes Decision Theory

- Bayes classification rule:
$>$ Predict class 1 if $\mathbb{P}(Y=1 \mid X=x)>\mathbb{P}(Y=0 \mid X=x)$;
- Otherwise, predict class 0.
- Bayes classification rule (alternative form):
- Predict class 1 if

$$
p(x \mid Y=1) \mathbb{P}(Y=1)>p(X=x \mid Y=0) \mathbb{P}(Y=0)
$$

$\Rightarrow$ Otherwise, predict class 0.

## Exercise

Penguins with flippers of length $\frac{1}{0}, \frac{0}{3}$, and $\frac{1}{12}$ are observed. What are their predicted species according to the Bayes' classification rule?


## Joint <br> $\mathbb{P}(x=x, y=y)$

- The joint distribution in this case is neither totally continuous nor totally discrete.
- From Bayes' rule:

$$
\begin{aligned}
& p(x, 0)=p(x \mid Y=0) \mathbb{P}(Y=0) \\
& p(x, 1)=p(x \mid Y=1) \mathbb{P}(Y=1)
\end{aligned}
$$

## $P(y=1 \mid x=x)>P\left(y=0 D_{X=x}\right.$ Distribution

$P(Y=1)=70 \%$
$P(\varphi=0)=30 \%$


## Exercise

Where does the Bayes decision rule make a prediction for class 1?


- Predict class 1 if $p(x \mid Y=1) \mathbb{P}(Y=$ 1) $>p(X=x \mid Y=0) \mathbb{P}(Y=0)$
- Otherwise, predict class 0 .


## Multivariate Distributions

- In binary classification, $y \in\{0,1\}$.
- But we usually deal with feature vectors, $\vec{x}$.
- The previous applies with straightforward changes.


## Example: Penguins

- Again consider penguins of two species, but now consider both flipper length and body mass.
- Each penguin's measurements are a random vector: $\vec{x}$.
- Densities are now functions of a vector.
- E.g., marginal: $p_{x}(\vec{x}): \mathbb{R}^{2} \rightarrow \mathbb{R}^{+}$



## Conditional on $Y$

$$
\begin{aligned}
& p(\vec{x} \mid \psi=0) \\
& p(\vec{x} \mid \psi=1)
\end{aligned}
$$



Conditional on $X$

$$
\begin{aligned}
& P(y=1 \mid \vec{x}=\vec{x}) \\
& P(y=0 \mid \vec{x}=\vec{x})
\end{aligned}
$$

$$
(1,1)
$$



$$
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$$

$P(Y=1 \mid X=x)$
$P(Y=0 \mid X=x)$ Bayes Error

- If we know the joint distribution, the Bayes classification rule is a natural approach to making predictions.
- It is also the best you can do, in a sense.

Intuition


## Error Probability

- In binary classification, there are two kinds of errors:
- Predicted 0 , but the right answer is 1 (Case 1).
- Predicted 1, but the right answer is 0 (Case 2).
- The probability of an error is:

$$
\mathbb{P}(\text { error })=\mathbb{P}(\text { Case } 1)+\mathbb{P}(\text { Case } 2)
$$

## Example

- Case 1: Predicted 0, but the right answer is 1.
- Case 2: Predicted 1, but the right answer is 0.



## Example

- Case 1: Predicted 0, but the right answer is 1.
- Case 2: Predicted 1, but the right answer is 0.



## Optimality

- The Bayes decision rule achieves the minimum possible error probability.
- Sometimes called the Bayes classifier.
- In most cases, the minimum possible error probability is $>0$.


## $p(p=1 \mid x=x)$

## What's next?

- The Bayes classifier is optimal.
- But it requires knowing the joint distribution; we almost never know this.
> Next time: estimating probability distributions from data.

