FYS-2021 Machine Learning

Bayes Rule and Classification (Part 1)

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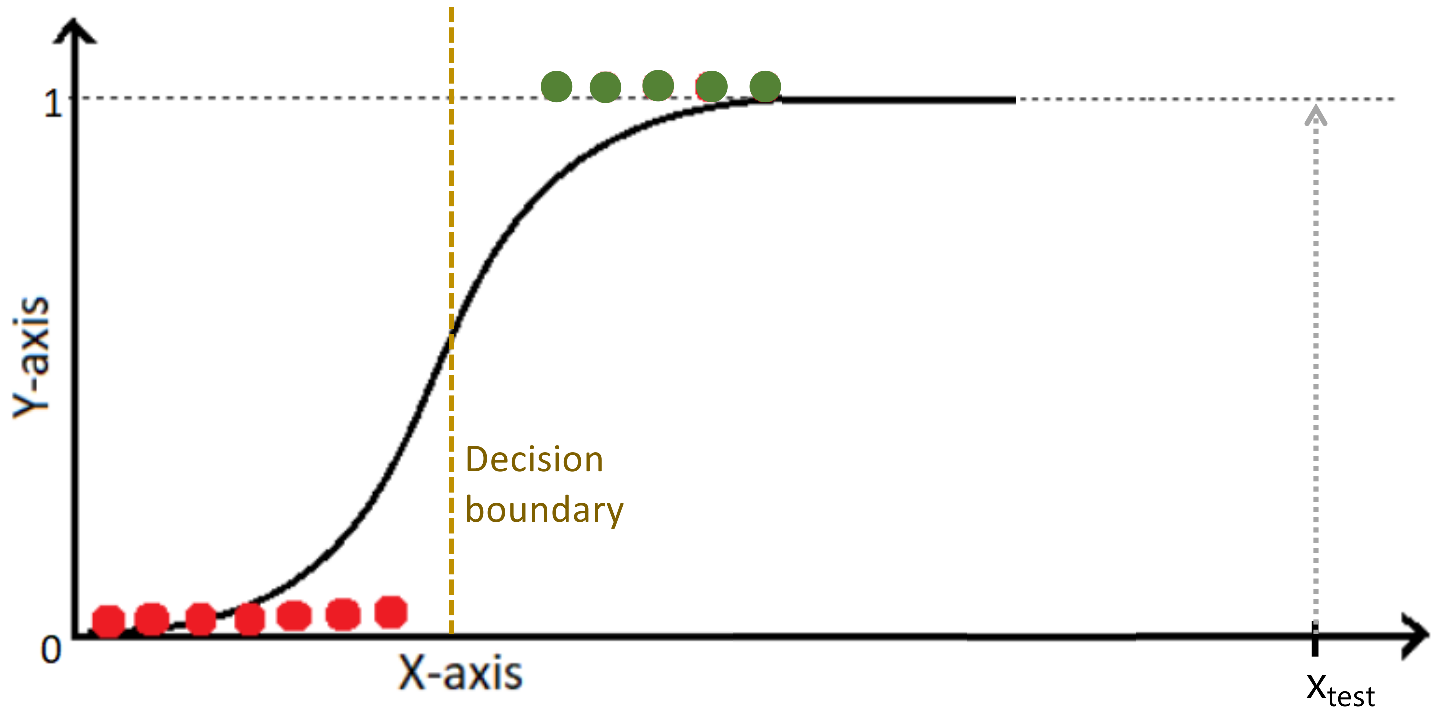
Roadmap

1. Probabilistic thinking and random variables
2. Intuition of the Bayes classifier
3. Bayes rule
4. Bayes decision rule

   Break

5. Training a Bayes Classifier
6. Maximum likelihood
7. The univariate Gaussian Bayes classifier
8. Practical connection

Why probabilistic machine learning?



$\hat{y}_{test} \approx 1$

Desirable to return a probability!

Modelling uncertainty

The real world is uncertain.

Probability is used to quantify uncertainty.

In the Bayes classifier:

- Features and class labels are treated as random variables
- Dependencies between random variables are encoded in probability distributions

Probabilistic thinking

A random variable is a function that assigns a value to each outcome of a random experiment.

A probability distribution describes how the probabilities are distributed over the possible values of a random variable.

Probabilistic thinking: Discrete random variables

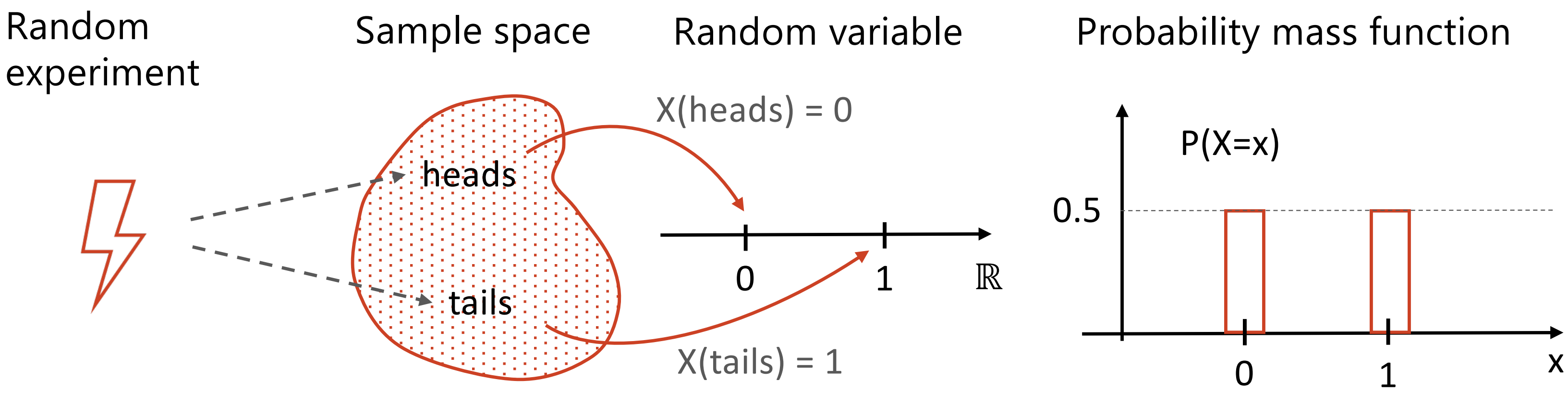
$X=\begin{cases}0 \text{ if heads} \\ 1 \text{ if tails}\end{cases}$

A random variable is a function that assigns a value to each outcome of a random experiment.

coin toss

pmf

A probability distribution describes how the probabilities are distributed over the possible values of a random variable.



Probabilistic thinking: Continuous random variables

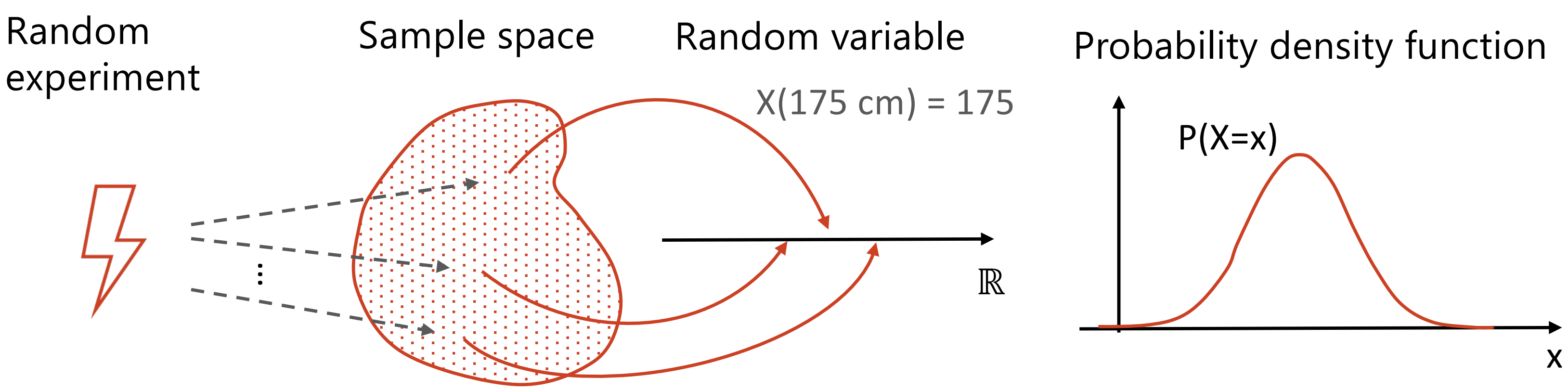
$X \in \mathbb{R}^+$

A random variable is a function that assigns a value to each outcome of a random experiment.

Measure the height of individuals

pdf

A probability distribution describes how the probabilities are distributed over the possible values of a random variable.



Probability theory

Sum rule is defined as

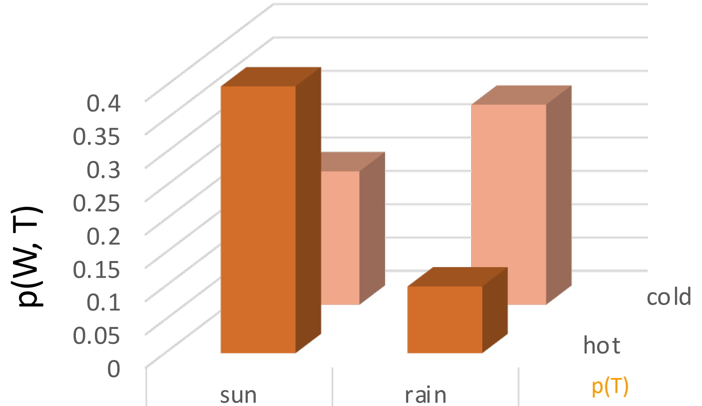
$p(X) = \sum_Y p(X,Y)$ joint distribution

Product rule is defined as

marginal distribution

$p(X,Y) = p(Y|X)p(X) = p(X|Y)p(Y)$

conditional distribution



	sun	rain	p(T)
hot	0.4	0.1	0.5
cold	0.2	0.3	0.5
p(W)	0.6	0.4	

Marginal distributions are obtained through the sum rule

$p(W) = \sum_T p(W,T)$ and $p(T) = \sum_W p(W,T)$

Conditional probabilities are computed as

$$p(W|T) = \frac{p(W,T)}{p(T)}$$

W	P(W|T=hot)
sun	0.4/0.5 = 0.8
rain	0.1/0.5 = 0.2

W	P(W|T=cold)
sun	0.2/0.5 = 0.4
rain	0.3/0.5 = 0.6

Notation

Description	Notation
Random variable	X
Realization of random variable	x
Set of N realizations	$\{x^1, x^2, \ldots, x^N\}$
Class i	C_i
Model parameters	θ

The intuition behind the Bayes classifier

height Basketball player or not

Example: Classify a realization of a random variable $X = x$ into one of two classes C_1 and C_2.

Bayes Classifier: "Assign the sample to the **most probable class, given the data**"

Decision rule:

$$x \rightarrow C_1 \quad if \quad p(C_1|X = x) > p(C_2|X = x)$$

Need to compute these conditional probabilities!

How to compute $p(C_i|X = x)$?

Use Bayes' Rule!

$$\underbrace{p(C_i|x)}_{\text{Posterior}} = \frac{\overbrace{p(x|C_i)}^{\text{Likelihood}}\ \overbrace{p(C_i)}^{\text{Prior}}}{\underbrace{p(x)}_{\text{Evidence}}}$$

Normalizing constant!

$$p(x) = \underbrace{\sum_{C_i} p(x, C_i)}_{\text{sum rule}} = \underbrace{\sum_{C_i} p(x|C_i)p(C_i)}_{\text{product rule}}$$

$$p(x|C_i)p(C_i) \underbrace{=}_{\text{product rule}} p(x, C_i) \underbrace{=}_{\text{product rule}} p(C_i|x)p(x)$$

How to compute $p(C_i|X = x)$?

Example: Compute the probability of having a disease given a positive test.

$C = \{\text{disease}, \text{not disease}\}$
$X \in \{1, 0\}$ (positive/negative test) discrete random variable

Want to compute

$$\underset{\text{Posterior}}{p(C_i|x)} = \frac{\overset{\text{Likelihood}}{p(x|C_i)}\ \overset{\text{Prior}}{p(C_i)}}{\underset{\text{Evidence}}{p(x)}}$$

$$p(x) = \underbrace{\sum_{C_i} p(x, C_i)}_{\text{sum rule}} = \underbrace{\sum_{C_i} p(x|C_i)p(C_i)}_{\text{product rule}}$$

Posterior $\mathrm{p}(\text{disease}|x = 1) = \frac{p(x=1|\text{disease})p(\text{disease})}{p(x=1)} = \frac{0.8 * 0.004}{0.004 * 0.8 + 0.996 * 0.1} = 0.031$ ← If the test is positive, the chance of disease is 3 %

Likelihood $p(x = 1|\text{disease}) = 0.8$ (sensitivity of test is known to be 80 %)

Prior $p(\text{disease}) = 0.004$ (0.4 % of the population gets the disease)

Evidence $p(x = 1) = p(\text{disease})p(x = 1|\text{disease}) + p(\text{not disease})p(x = 1|\text{not disease})$
$= 0.004 * 0.8 + 0.996 * 0.1$
(FP rate of test is known to be 10 %)

Example from: Murphy, K. P. (2012). Machine learning: a probabilistic perspective. MIT press.

Bayes Classifier: Decision rule

$$p(C_i|x) = \frac{\overset{\text{Likelihood}}{p(x|C_i)}\ \overset{\text{Prior}}{p(C_i)}}{\underset{\text{Evidence}}{p(x)}}$$

$$x \to C_1 \quad if \qquad p(C_1|x) > p(C_2|x)$$

$$\frac{p(x|C_1)\,p(C_1)}{p(x)} > \frac{p(x|C_2)\,p(C_2)}{p(x)}$$

$$p(x|C_1)\,p(C_1) > p(x|C_2)\,p(C_2)$$

$$\boxed{x \to C_i \quad if \quad p(x|C_i)\,p(C_i) > p(x|C_j)\,p(C_j)\ \forall\, j \neq i}$$

Bayes classifier

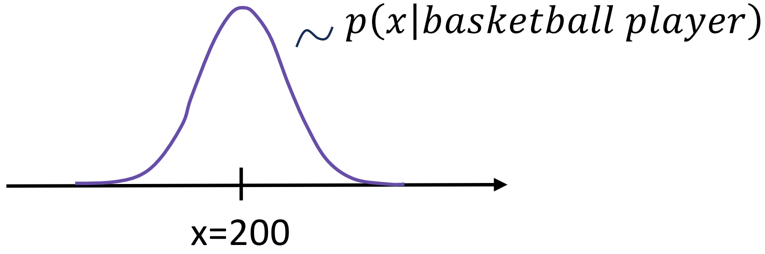
Example: Classify whether a person is a basketball player based on height.

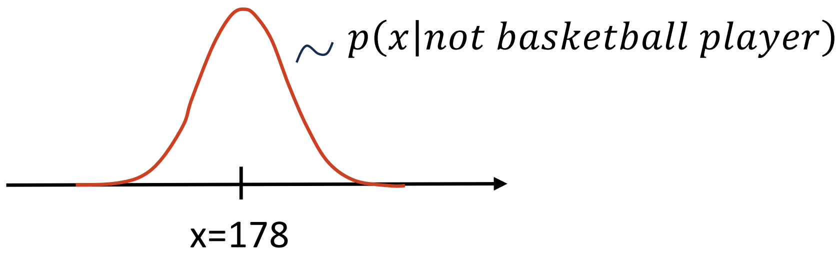
C = {basketball player, not basketball player}
$X \in \mathbb{R}$ (height in cm) continuous random variable

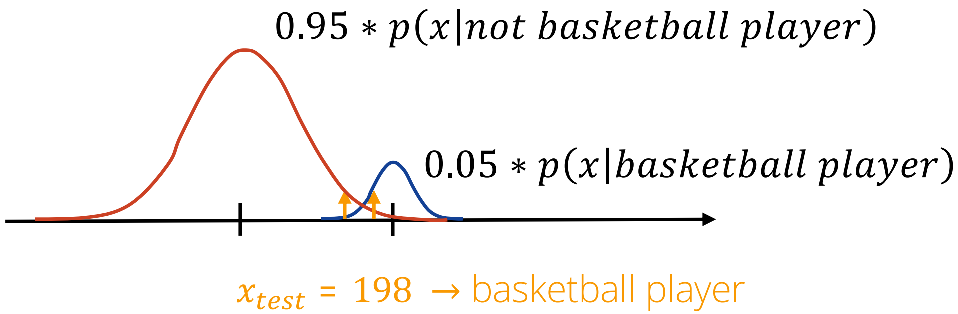
- Estimate likelihoods, $p(x|C_i)$
- Estimate priors, $p(C_i)$

$$p(basketball\ player) = 0.05$$

$$p(not\ basketball\ player) = 0.95$$





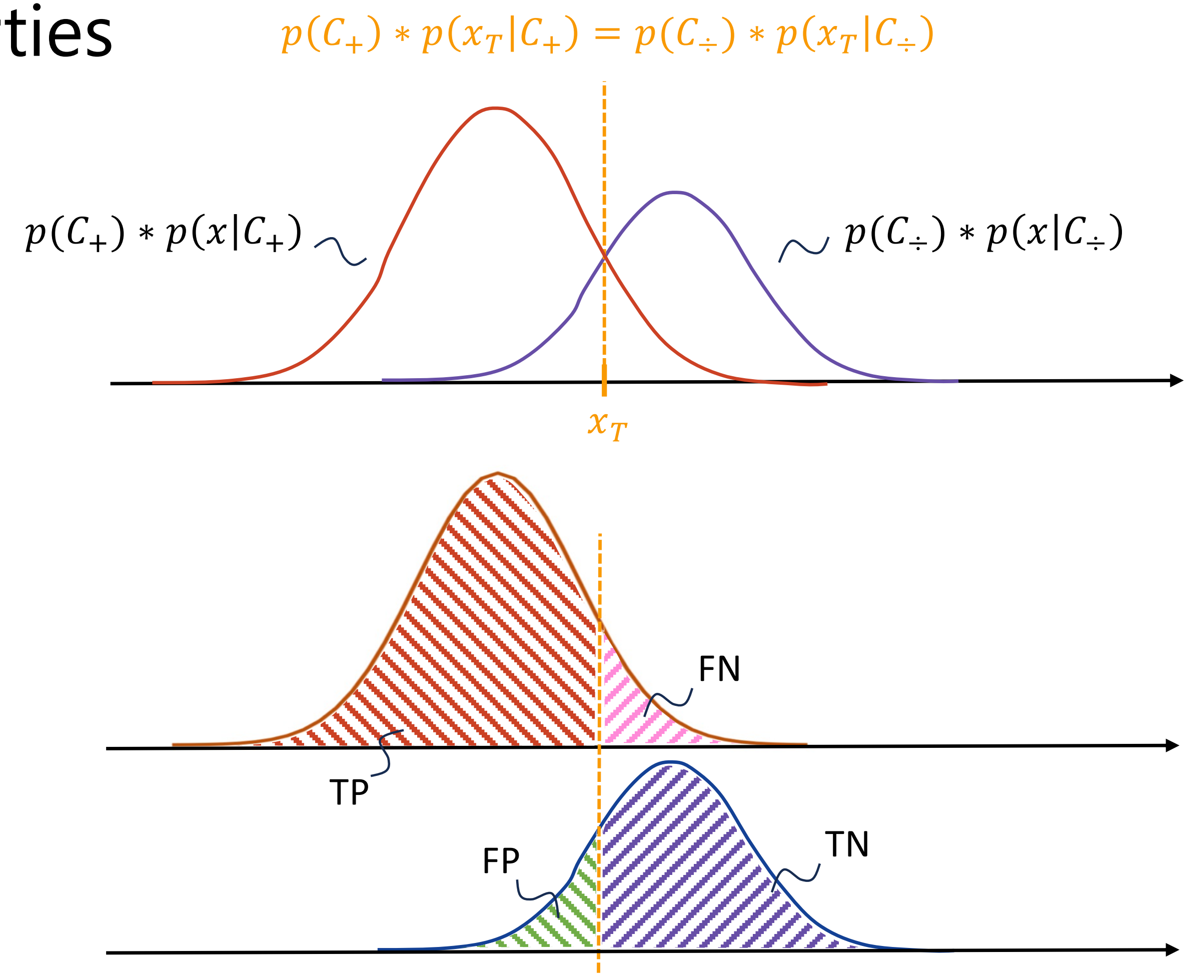


Bayes classifier: Properties

- Threshold where $p(C_+|x) = p(C_\div|x)$

- $p(error) = \int_{x_T}^{\infty} p(C_+) * p(x|C_+)dx + \int_{-\infty}^{x_T} p(C_\div) * p(x|C_\div)dx$

- Probability of errors is minimized if we have the true $p(x|C_i)$ and $p(C_i)$!



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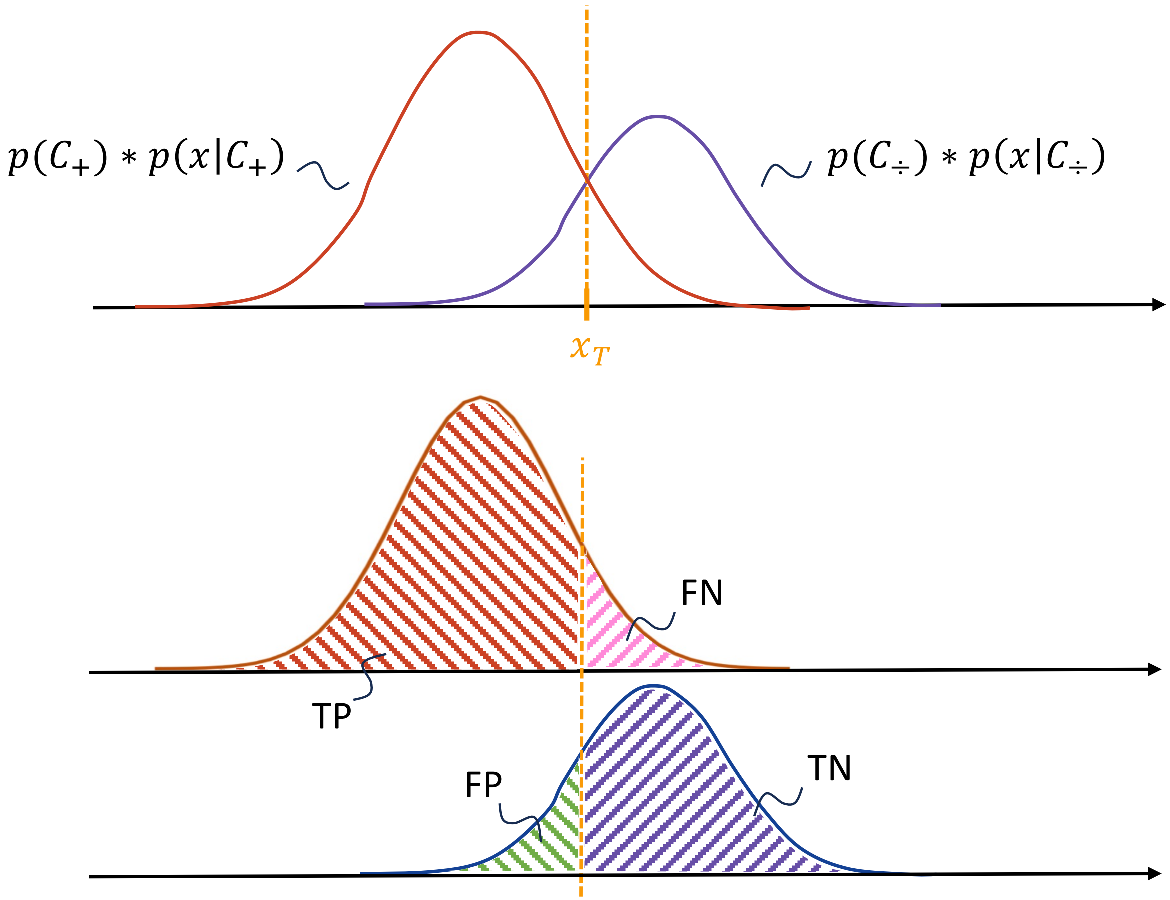
$p(C_+) * p(x_T|C_+) = p(C_\div) * p(x_T|C_\div)$



Need to estimate $p(C_i)$ and $p(x|C_i)$ from data

To train a Bayes classification model = To estimate $p(C_i)$ and $p(x|C_i)$ from training data $\mathcal{D} = \{(x^i, y^i)\}_{i=1}^N$!

Scaling Shape/position

Prior class probabilities, $p(C_i)$

are estimated as the frequency of class C_i in the training data:

$$p(C_i) = \frac{\#\mathcal{D}\{y^i = C_i\}}{N}$$

Number of training samples belonging to class C_i

Likelihood terms, $p(x|C_i)$

are estimated via **maximum likelihood**!

Maximum likelihood estimation (MLE)

Estimating the parameter values θ of a statistical model that maximize the likelihood of the observed data

In practice:

1. Assume some parameterized distribution $p_\theta(x|C_i)$
   can be Gaussian, Laplacian, Bernoulli, etc. depending on the type of features

2. Estimate the distribution's parameter(s) as

$$\hat{\theta}_{MLE} = arg\max_\theta \ell(\theta|\mathcal{D}) \equiv arg\max_\theta p_\theta(x^1, \dots, x^N|C_i)$$

iid

$$= arg\max_\theta \prod_{j=1}^{N} p_\theta(x^j|\, C_i)$$

Ind. variables: P(A, B) = P(A)*P(B)

$$= arg\max_\theta \underbrace{\sum_{j=1}^{N} \log p_\theta(x^j|C_i)}_{\text{log likelihood, } L(\theta|\mathcal{D})}$$

log(a*b) = log(a) + log(b)

Maximum likelihood estimation (MLE)

log likelihood, $L(\theta|\mathcal{D})$

$$\hat{\theta}_{MLE} = \underset{\theta}{argmax} \sum_{j=1}^{N} \log p_\theta(x^j|C_i) \quad \rightarrow \text{solve:} \qquad \frac{\partial}{\partial\theta} L(\theta|\mathcal{D}) = 0$$

Example: Univariate gaussian distribution, $p_\theta(x|C_i) \sim \mathcal{N}(\mu, \sigma)$ Here: θ=[μ, σ]

Assuming we have N_i observed samples from class C_i, $\{x^1, x^2, \dots, x^{N_i}\}$

$$L(\theta|\mathcal{D}) = \sum_{j=1}^{N_i} \log p_\theta(x^j|C_i)$$

$$= \sum_{j=1}^{N_i} \log\left[\frac{1}{\sqrt{2\pi}\sigma} e^{-\frac{1}{2}\left(\frac{x^j-\mu}{\sigma}\right)^2}\right]$$

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

$$\frac{\partial}{\partial\mu} L(\theta|\mathcal{D}) = 0 \quad \rightarrow \quad \hat{\mu}_{MLE} = \frac{1}{N_i}\sum_{j=1}^{N_i} x^j$$

$$\frac{\partial}{\partial\sigma} L(\theta|\mathcal{D}) = 0 \quad \rightarrow \quad \hat{\sigma}^2_{MLE} = \frac{1}{N_i}\sum_{j=1}^{N_i}\left(x^j - \mu\right)^2$$

(Univariate) Gaussian Bayes classifier

Putting it all together

Assuming we have N training samples from class C_+, $\{x^1, x^2, \ldots, x^N\}$, and M training samples from class $C_\div$, $\{x^1, x^2, \ldots, x^M\}$, and that $p(x|C_i) \sim \mathcal{N}(\mu_i, \sigma_i)$, $\; i = \{+, \div\}$.

Training:

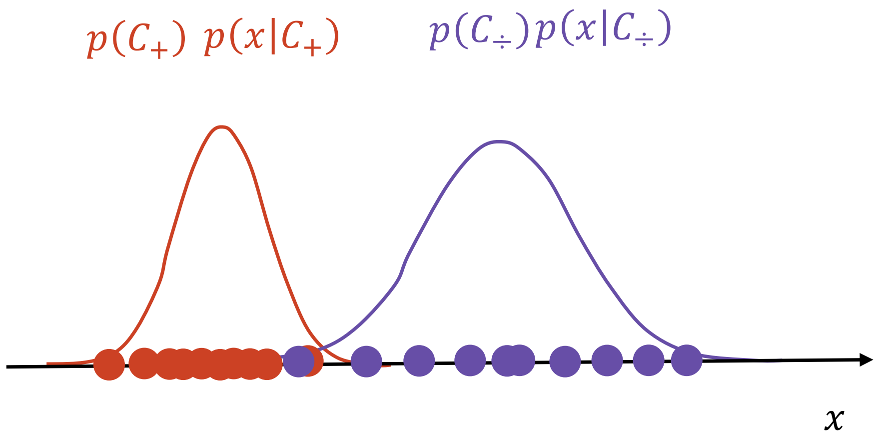
MLEs for likelihood terms are given by

$$\hat{\mu}_+ = \frac{1}{N}\sum_{j=1}^{N} x^j \qquad \hat{\mu}_\div = \frac{1}{M}\sum_{j=1}^{M} x^j$$

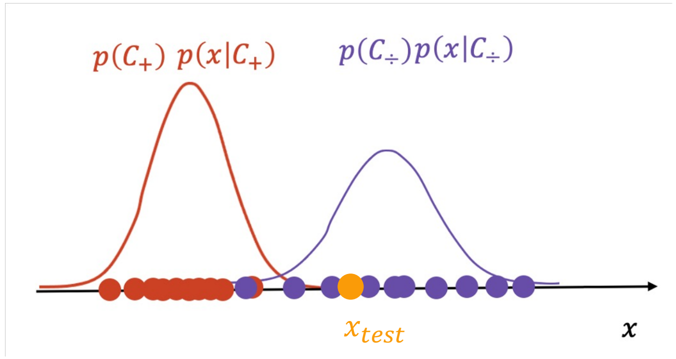
$$\hat{\sigma}_+^2 = \frac{1}{N}\sum_{j=1}^{N}\left(x^j - \mu\right)^2 \qquad \hat{\sigma}_\div^2 = \frac{1}{M}\sum_{j=1}^{M}\left(x^j - \mu\right)^2$$

Prior class probability estimates are given by

$$\hat{p}(C_+) = \frac{N}{N+M} \qquad \hat{p}(C_\div) = \frac{M}{N+M}$$



(Univariate) Gaussian Bayes classifier



Test time (inference)

$$\boxed{\begin{array}{c} x \ \rightarrow C_i \quad if \\ p(x|C_i)\, p(C_i) > p(x|C_j)\, p(C_j)\ \forall\, j \neq i \end{array}}$$

Decision rule

When we have some test sample x_{test} that we want to classify, we need to evaluate

$$g_i(x_{test}) = \ p(x_{test}|C_i)\, p(C_i)$$

(discriminant function)

for all i. Then chose class C_i if

$$g_i(x_{test}) = \ \max_k g_k(x_{test})$$

$$g_+(x_{test}) = \left(\frac{1}{\sqrt{2\pi}\,\hat{\sigma}_+} e^{-\frac{1}{2}\left(\frac{x_{test}-\hat{\mu}_+}{\hat{\sigma}_+}\right)^2}\right)\left(\frac{N}{N+M}\right)$$

$$g_-(x_{test}) = \left(\frac{1}{\sqrt{2\pi}\,\hat{\sigma}_\div} e^{-\frac{1}{2}\left(\frac{x_{test}-\hat{\mu}_\div}{\hat{\sigma}_\div}\right)^2}\right)\left(\frac{M}{N+M}\right)$$

Quiz: Training a Bayes classifier

Assume a three-class classification problem where the likelihoods are Gaussians. How many parameters do you have to estimate to train the univariate Bayes classifier?

A: 3 parameters

B: 6 parameters

C: 9 parameters

D: It depends on the dataset

Answer: 3 classes * (prior + mean + std) = 9 parameters

Practical connection

0. [If not done] Split data into train/test

On training data:

1. Sort samples according to labels (class)
2. For each class: Compute estimates for class prior as class frequency
3. For each class: Assume distribution of likelihood and compute corresponding $\hat{\theta}_{MLE}$

On test data:

1. For each class: Compute discriminant function
2. Assign samples to class with maximum discriminant function
3. Compare predictions to labels and compute your confusion matrix

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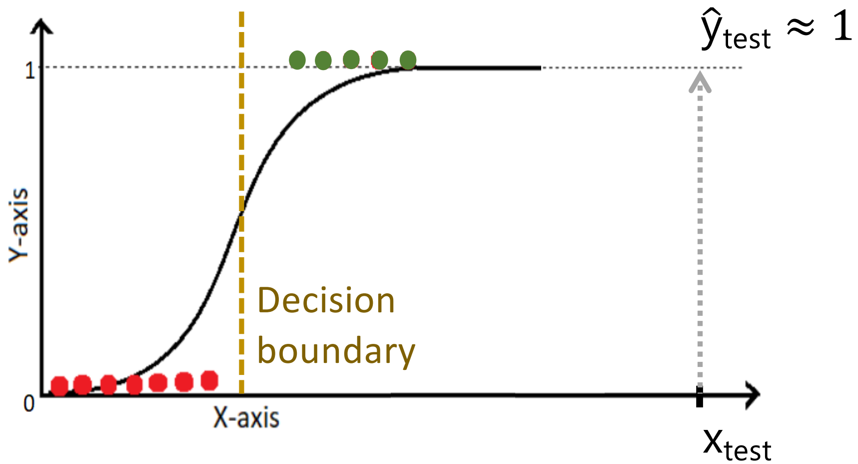
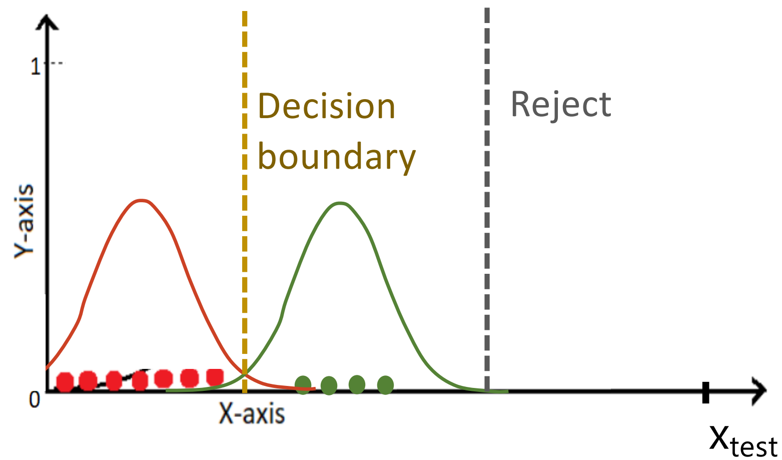
Reject option

Logistic regression



Bayes classifier w/ reject option



$$x \rightarrow C_i \quad if \quad p(C_i|x) > p(C_j|x) \forall\, j \neq i$$

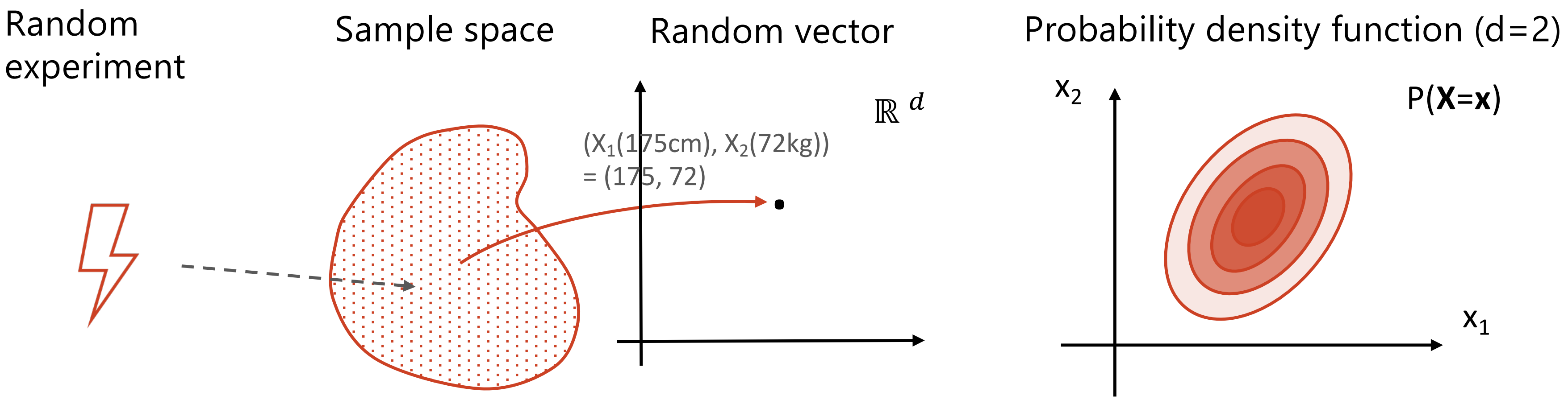
$$\text{and } p(C_i|x) > 1 - \lambda$$

reject otherwise

Conclusion

- Supervised classification model
- Bayes classifier for univariate data
  - Assume distribution for the likelihoods
  - Learn class priors and MLE parameters for each class
- Closed form solutions to MLE (no iterative optimization)
- Possible to reject samples during inference

Thursday: From univariate to multivariate data



Video by 3Blue1Brown

- https://www.youtube.com/watch?v=HZGCoVF3YvM