Machine Learning CSE2510 – Lecture 1.2: Probability theory / Bayes

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Welcome to week 1 - lecture 2

- Administrative questions?
- Recap previous lecture
- Probability theory: Introduction
- Bayes' Rule
- Decision theory
- Bayes error
- Misclassification costs

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Administrative questions?

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Recap of the previous lecture

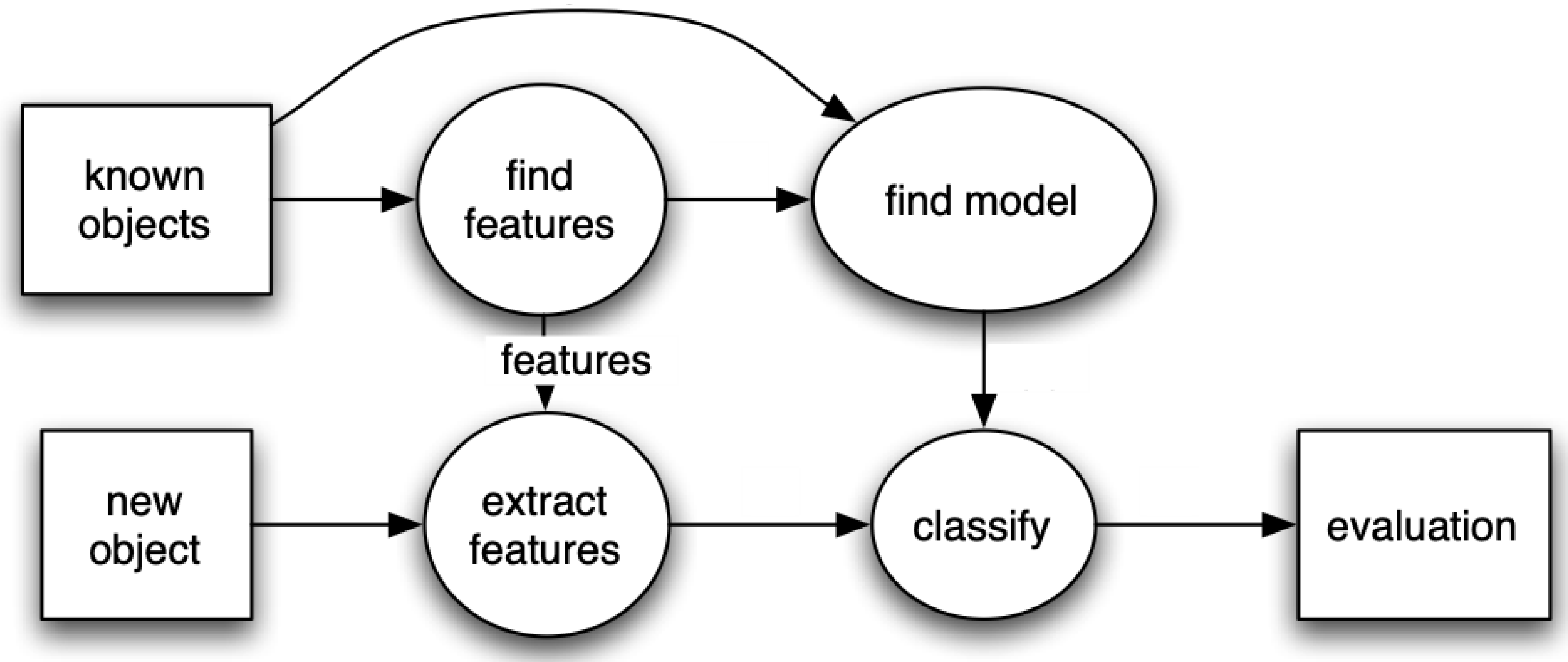
A(nother) definition of ML

- The learning of patterns or regularities in data by computer algorithms in order for these computer algorithms to carry out a specific task without using explicit instructions, but instead relying on these patterns and inference

[Wikipedia]

ML pipeline

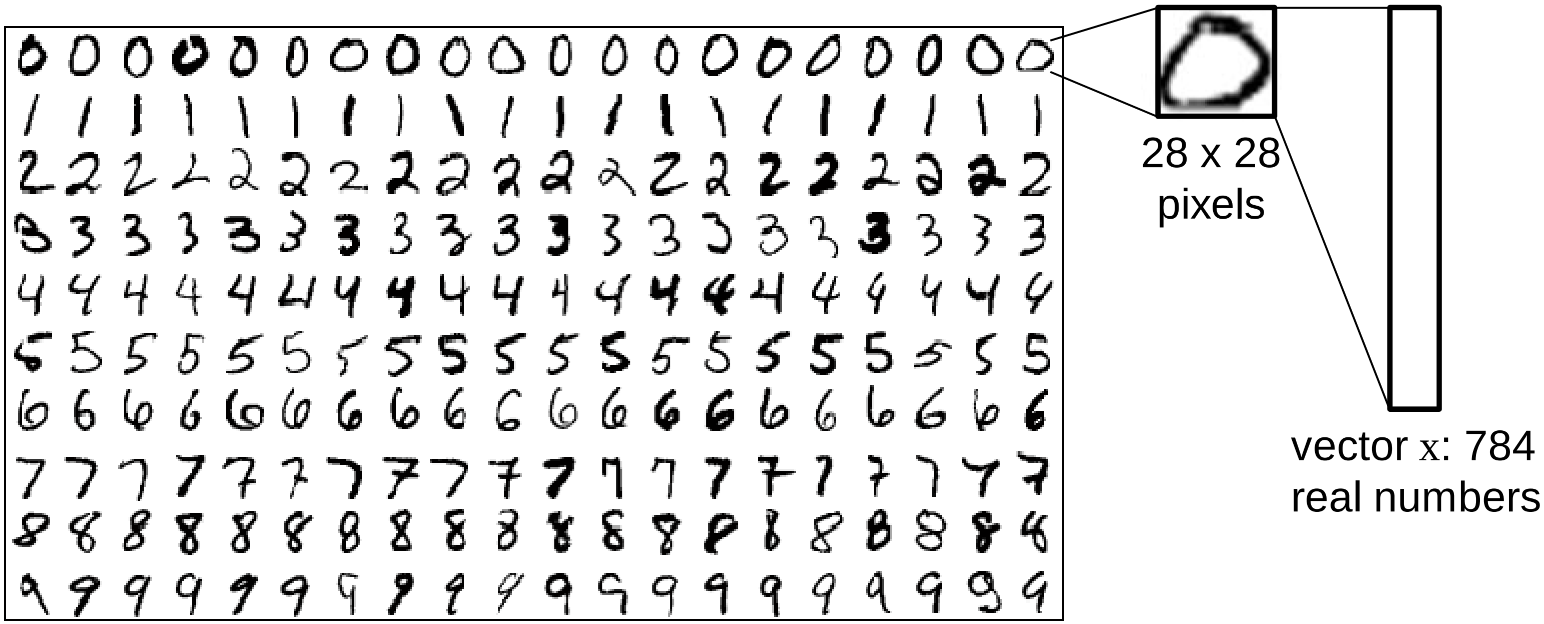
applying, generalisation



testing

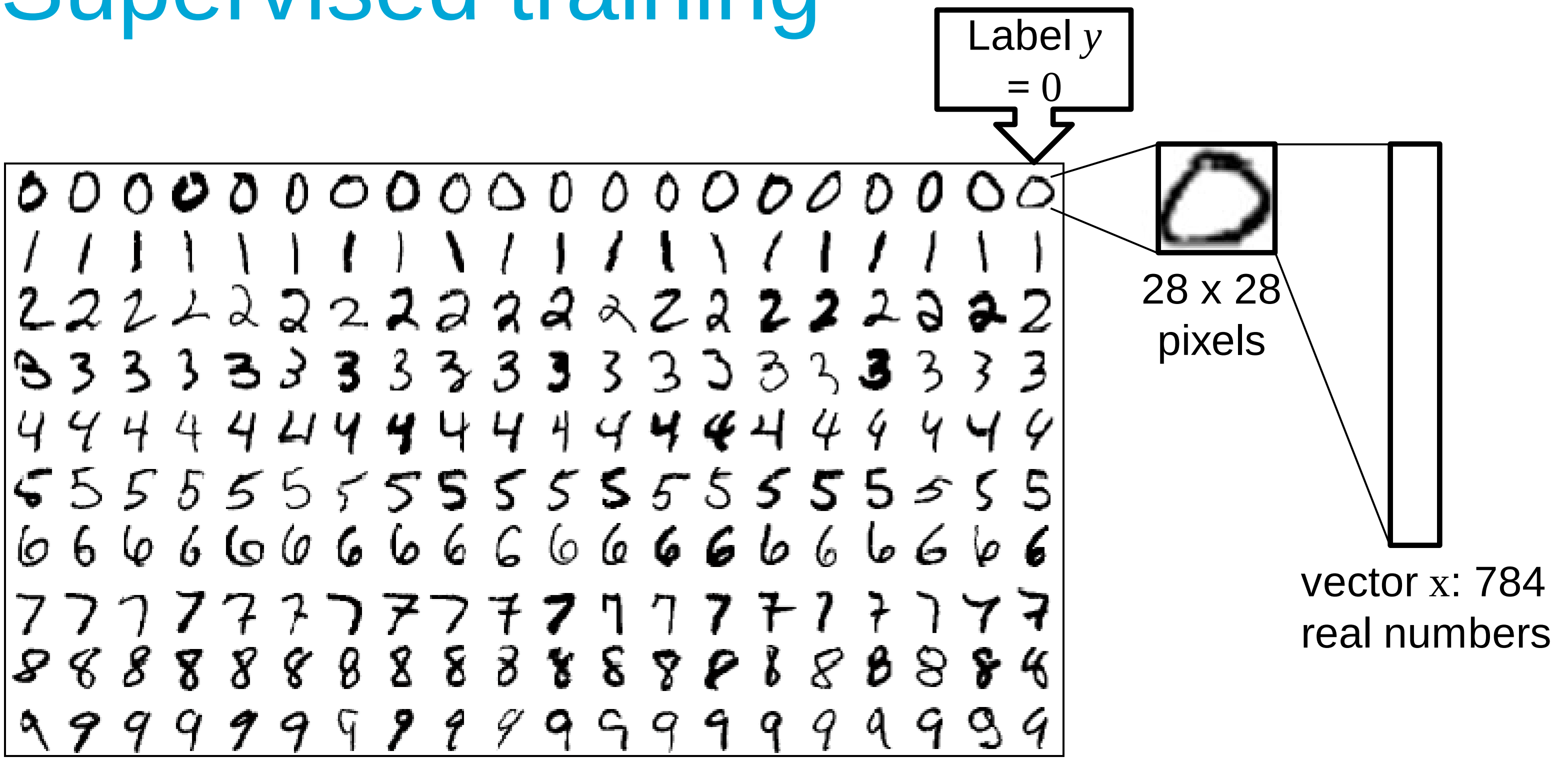
Slide adapted from Dr. David Tax

Example: handwritten digit recognition



Goal: build machine that takes a new input x and outputs the identity of the digit $0 \,..\, 9$

Supervised training



Training set: N digits $\{\mathrm{x}_1, .., \mathrm{x}_N\}$

with for each digit: label y (= target)

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Train/test performance

1. Train on training data

- Performance is measured on the training set to guide the learning process

➔ Optimisation error

2. Evaluate the model

- Test model on *independent* test set for an unbiased estimate of the generalisability
  - No overlap with examples in training set
  - Similar to training data

➔ Test or generalisation error

Different ML tasks

- Supervised learning:
  - Classification: categorization into a prespecified number of discrete categories
  - Regression: predicting a continous value
  - Clustering: split the data into a number of groups with similar examples

Irrespective of the task; underlying it all $p(y|x)$:

Probability theory ➔ Today!

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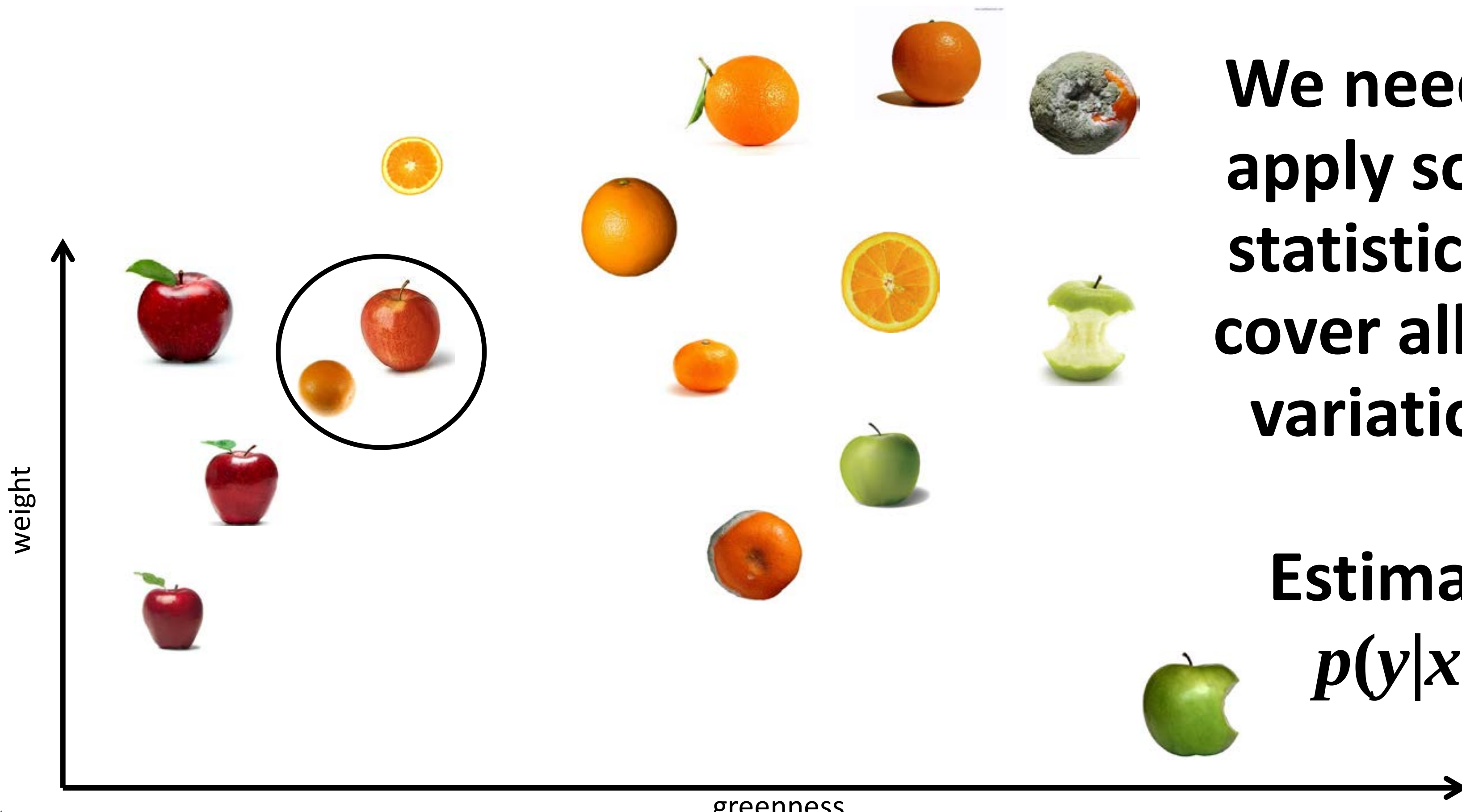
ML techniques are based on measurements

Slide adapted from Dr. Marco Loog

Noise in the measurements



We need to apply some statistics to cover all the variations

Estimate
$$p(y|x)$$

Probabilistic classifiers

- Tuesday: “Hard” classification
  - Assign a sample to a class
  - Output the class label

- In the ideal world: “Probabilistic” classification
  - Estimate the probability distribution over a set of classes
  - Estimate the probability that sample belongs to a class
  - “Hard” classification: give sample label of the most likely class

  ➔ Probabilistic classifiers are a generalisation of the first type of classifiers

Today’s learning objectives

After practicing with the concepts of this week you are able to:

- Explain the basic ideas of probability theory, decision theory, and Bayes Rule and their application in Machine Learning

Introduction to Probability Theory

ML: design classifiers that classify an unknown object in the most likely class

→ Our task: how do we determine what is "most likely"?

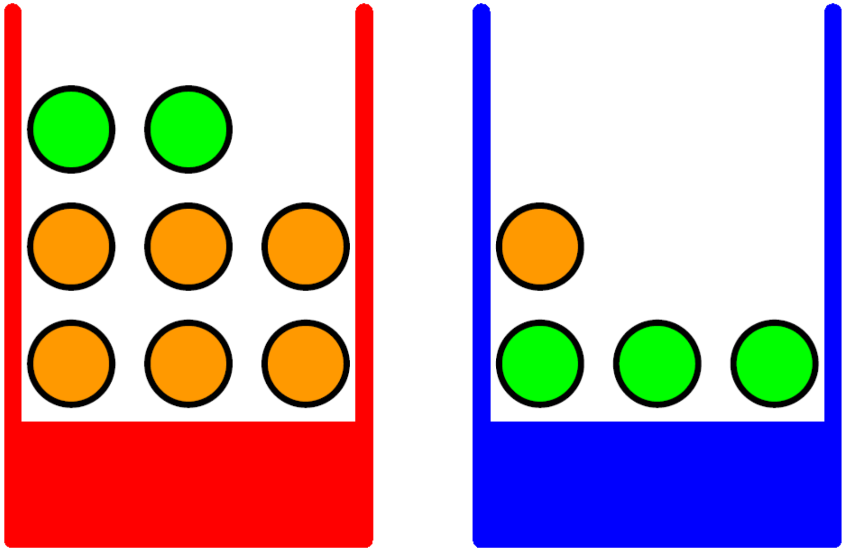
→ Estimate $p(y|x) = p(class|object)$

$$p(label|feature\ vector)$$

Probability theory: The discrete case

- Prob of selecting the red box $= p(B = \mathrm{r})$: $\frac{4}{10}$
- Prob of selecting the blue box $= p(B = \mathrm{b})$: $\frac{6}{10}$

Mutually exclusive?
Probability must sum to 1



$\frac{4}{10}$ $\frac{6}{10}$

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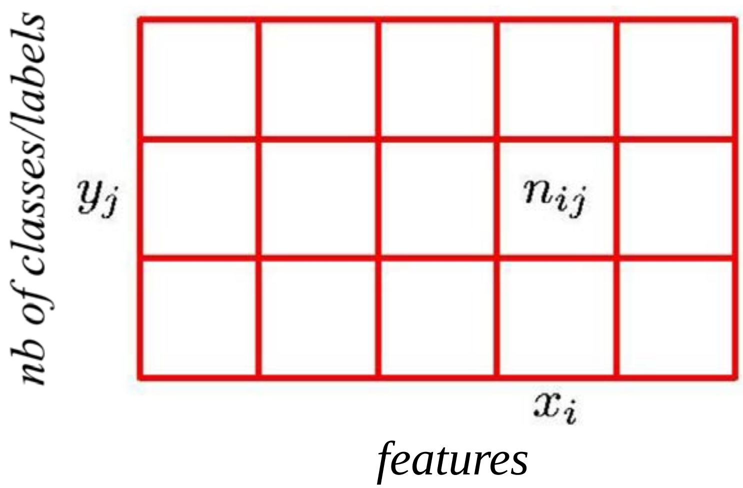
Joint probability: The discrete case

- Probability that $X = x_i$ (feature, F) and $Y = y_j$ (label, B): $p(X = x_i, Y = y_j)$
- E.g., probability that F=o (x) and B=r (y)



Joint Probability

$$p(X = x_i, Y = y_j) = \frac{n_{ij}}{N}$$

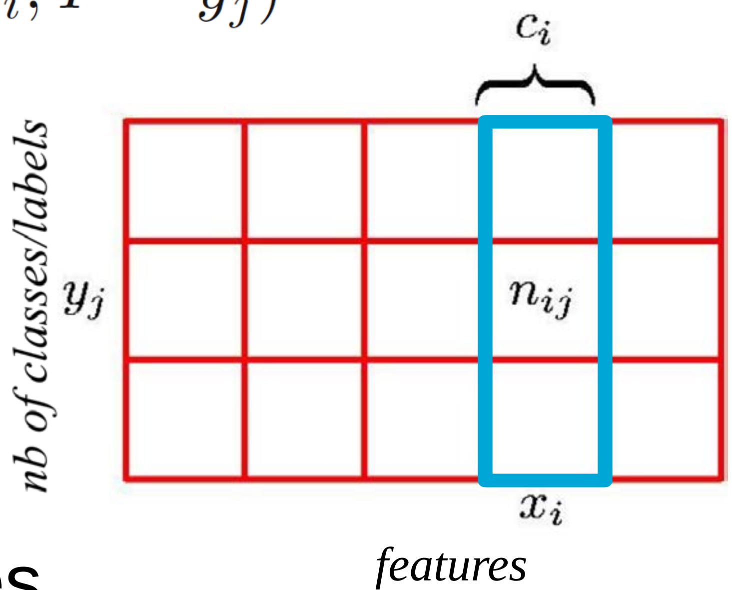
Sum rule of probability

- Probability that $X = x_i$ irrespective of Y: $p(X = x_i)$

$$p(X = x_i) = \sum_{j=1}^{L} p(X = x_i, Y = y_j)$$

c_i: nb of trials that $X = x_i$ irrespective of Y

L: total number of classes



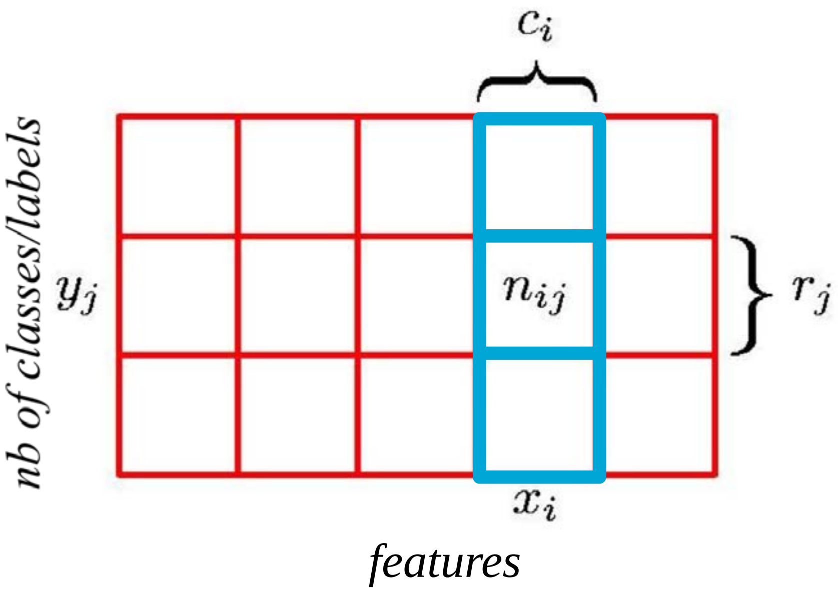
Marginal Probability

$$p(X = x_i) = \frac{c_i}{N}.$$

Conditional probability: $p(y|x)$

- Probability $Y = y_j$ given that $X = x_i$: $p(Y = y_j \mid X = x_i)$
- E.g., probability that $B = r$ given that $F = o$

$$p(Y = y_j | X = x_i) = \frac{n_{ij}}{\boxed{c_i}}$$



- Q: What is the difference between the conditional and the joint probability?

Fundamental rules of probability

- $p(X,Y)$: joint probability = probability of X **and** Y
- $p(Y|X)$: conditional probability = probability of Y **given** X
- $p(X)$: marginal probability of X

- $p(X,Y) = p(Y,X)$: symmetry property
- $p(X,Y) = p(Y|X)\, p(X)$: product rule

Bayes' Rule

With labeled examples of the classes → estimate a probability density per class

$$p(Y|X) = \frac{p(X|Y)p(Y)}{p(X)}$$

Difficult to estimate for continuous variables

→ Central role in machine learning

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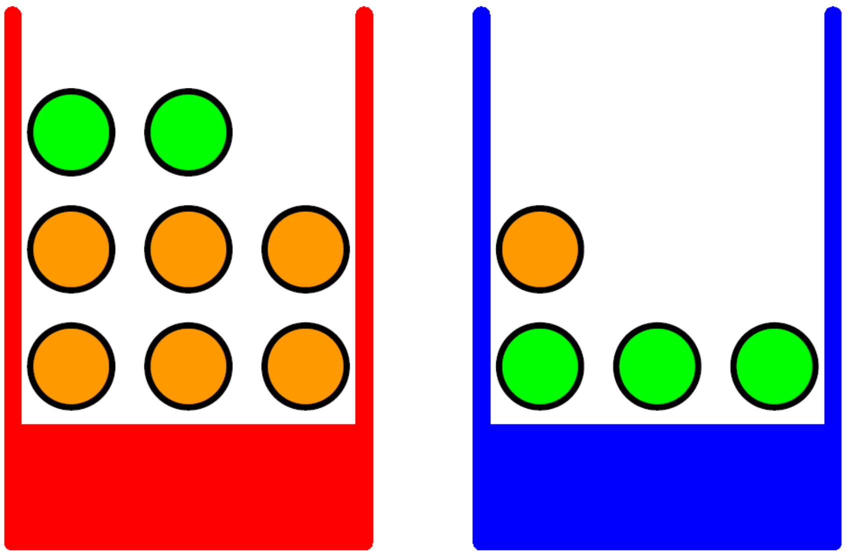
An exercise

- Probability of picking an apple? = $p(F{=}a)$

$$
\begin{aligned}
p(F=a) &= p(F=a|B=r)p(B=r) + p(F=a|B=b)p(B=b) \\
&= \frac{1}{4} \times \frac{4}{10} + \frac{3}{4} \times \frac{6}{10} = \frac{11}{20}
\end{aligned}
$$

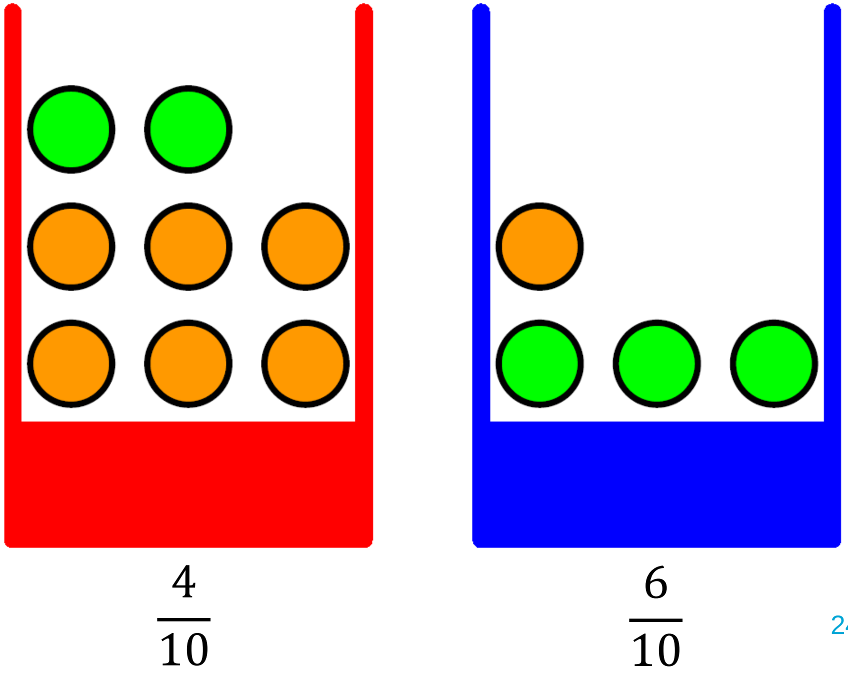


$\frac{4}{10}$ $\frac{6}{10}$

Another exercise

- Probability of picking an orange? = $p(F=o)$

➔ Sum rule: $p(F=o) = 1 - 11/20 = 9/20$



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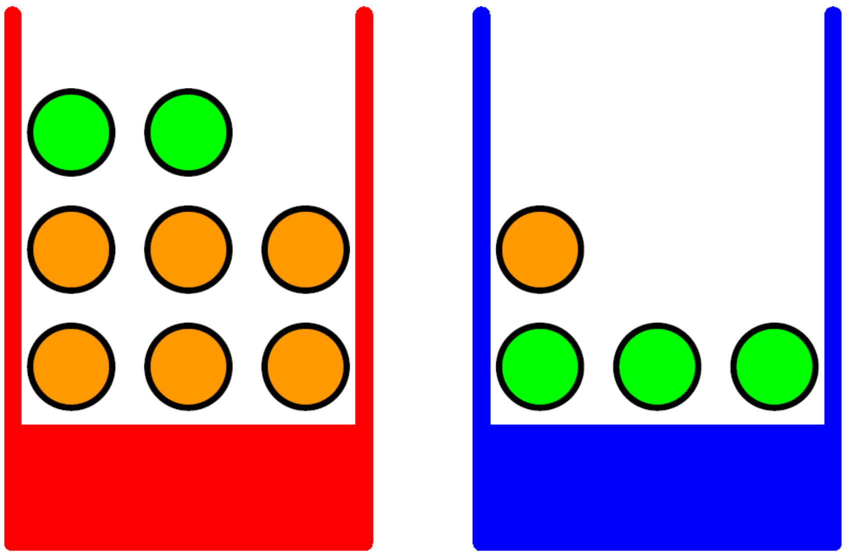
Conditional probability: $p(y|x)$

- Q: Probability of B=r given that F=o?

$$p(B=r|F=o) = \frac{p(F=o|B=r)p(B=r)}{p(F=o)} = \frac{3}{4} \times \frac{4}{10} \times \frac{20}{9} = \frac{2}{3}$$

$$p(Y|X) = \frac{p(X|Y)p(Y)}{p(X)}$$



$\frac{4}{10}$ $\frac{6}{10}$

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Bayes' Rule

Prior probability

Posterior probability

$$p(Y|X) = \frac{p(X|Y)p(Y)}{p(X)}$$

Prior prob of selecting the red box (Y), i.e., *before* observing an orange: $p(B{=}\mathrm{r})$: $\frac{4}{10}$

Posterior prob of selecting the red box (Y), i.e., *after* observing an orange: $p(B{=}\mathrm{r} \mid F{=}\mathrm{o})$: $\frac{2}{3}$

Classification

- Training: Estimate the probability distribution over a set of classes

- Testing: Estimate the probability that sample belongs to a class

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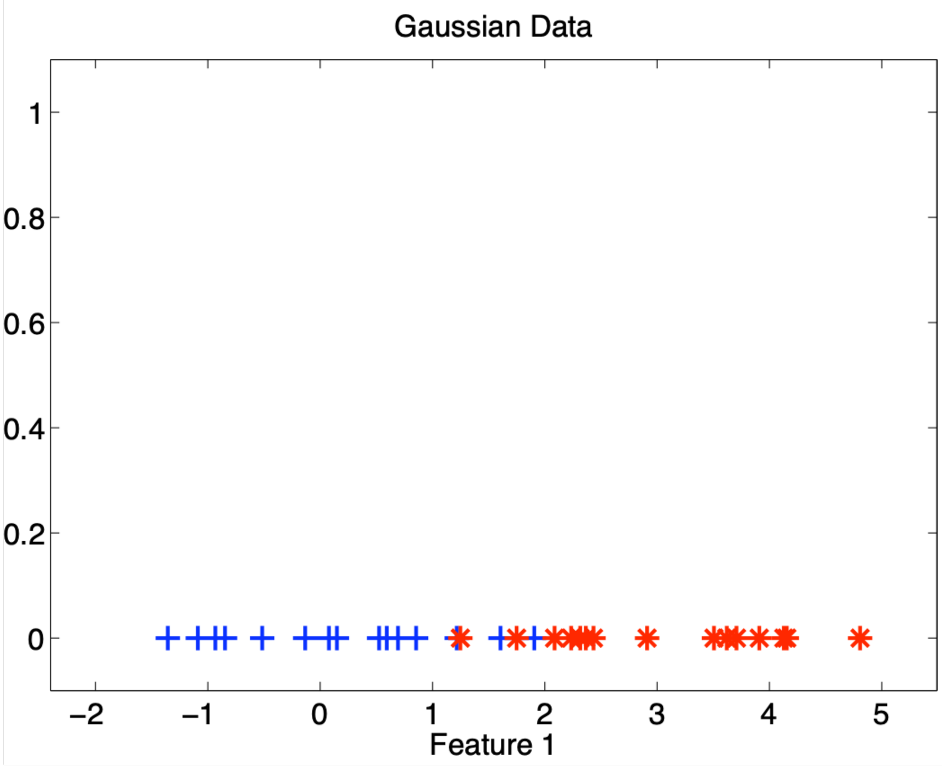
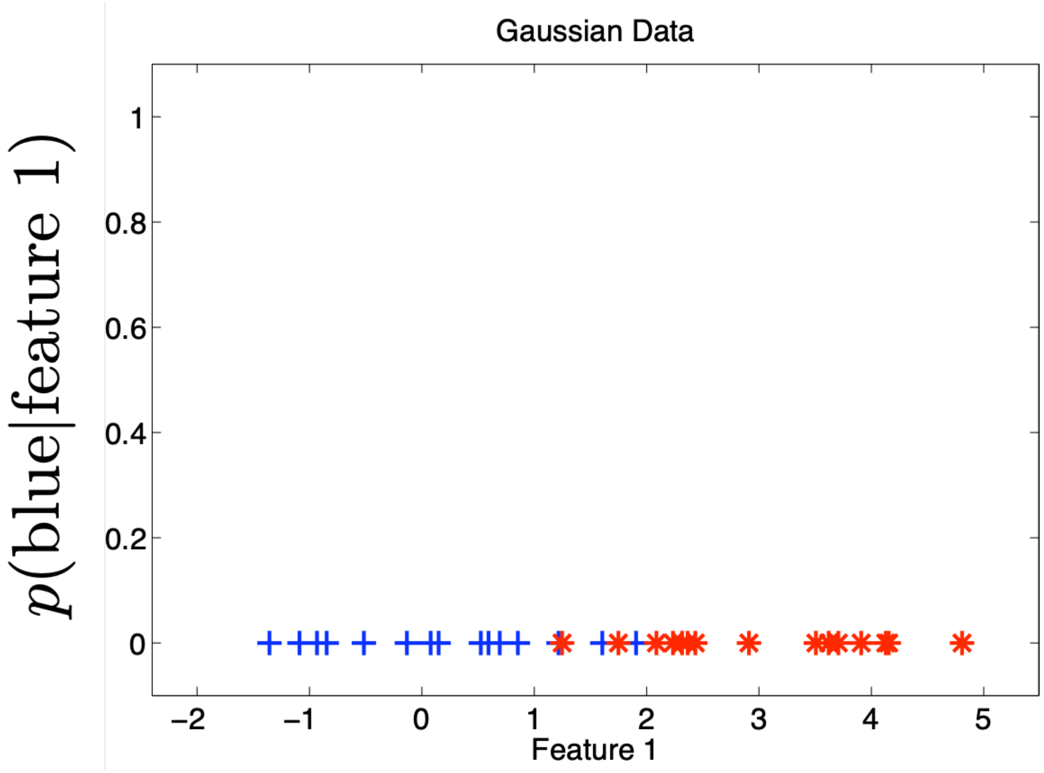
Estimating the probability distribution over a set of classes: The continuous case

- Given a feature, and a training set, where is the blue (e.g., apples) class?



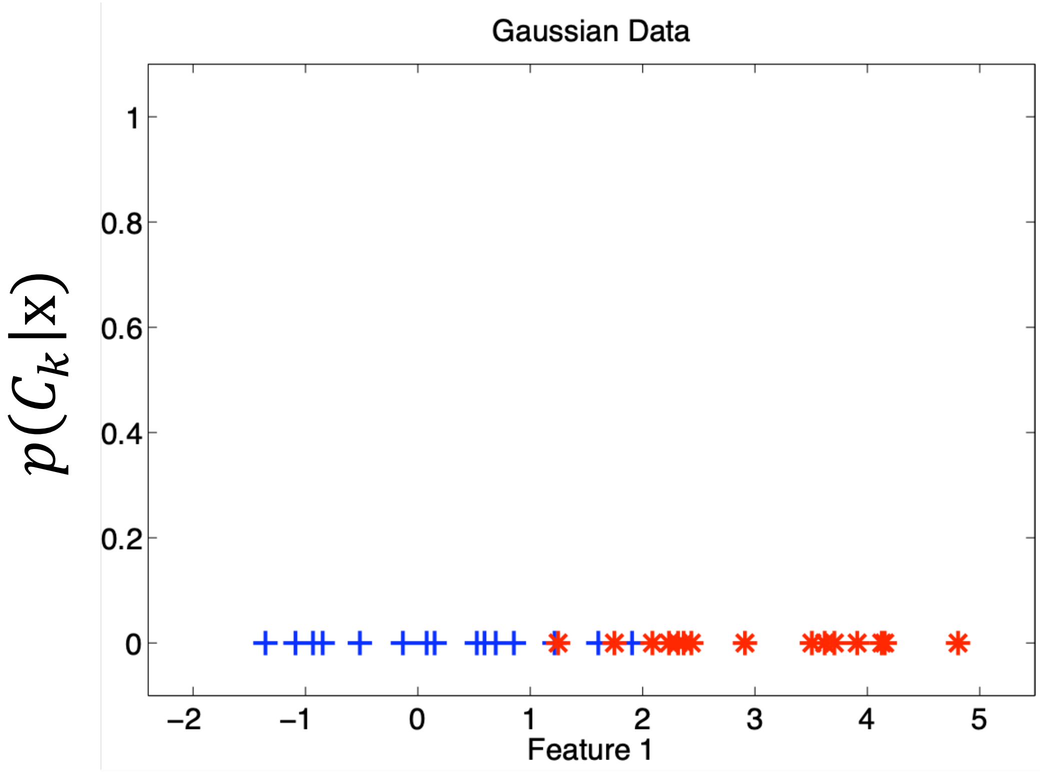
Estimating the probability distribution over a set of classes: The continuous case

- For each object we want to estimate $p(\text{blue}|\text{feature } 1)$



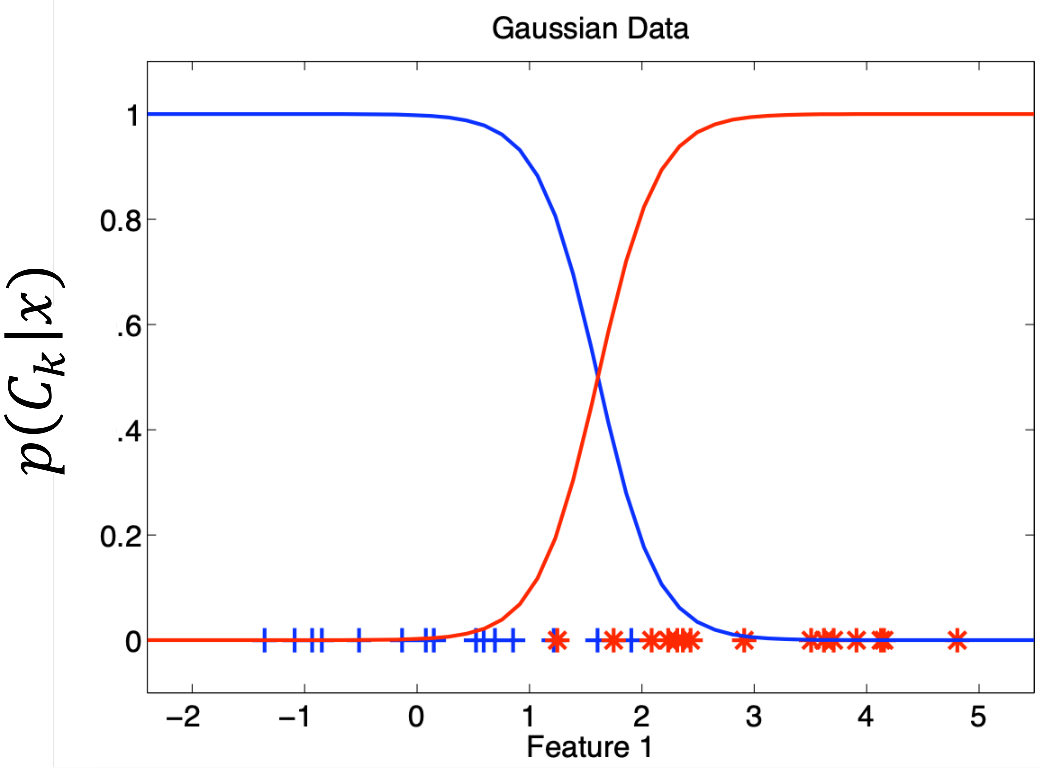
Class conditional probability

- For each object we want to estimate $p(C_k|x)$



Probability distribution over the classes

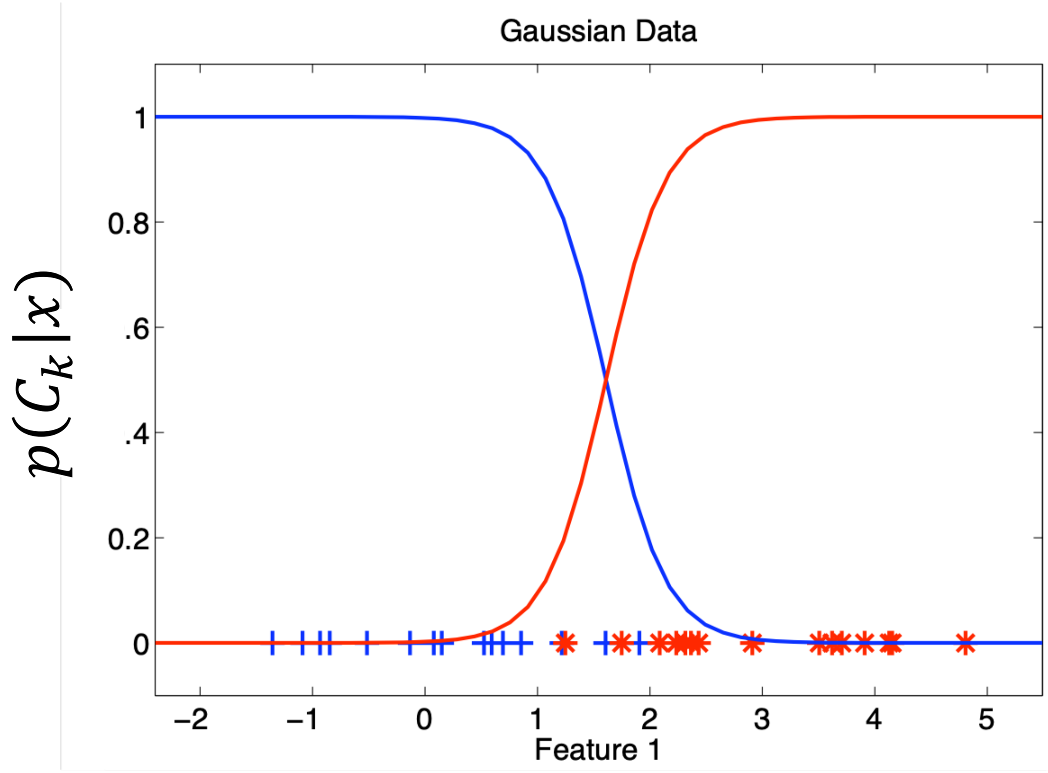
- For each object we have to estimate $p(C_k|x)$



$$\sum_k p(C_k|x) = 1$$

In order to classify a new x

- Estimate the posterior probability $p(C_k|x)$

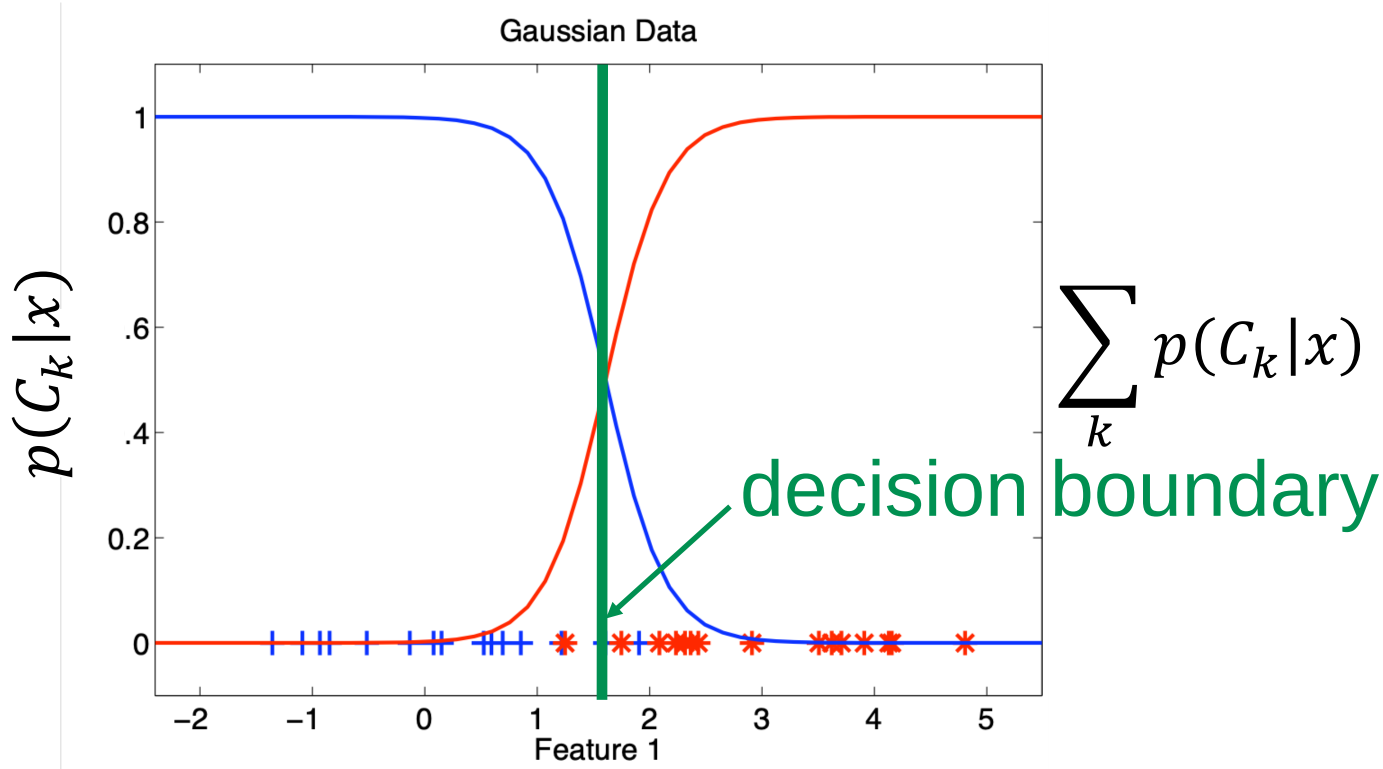


$$\sum_k p(C_k|x) = 1$$

Slide adapted from Dr. David Tax

In order to classify a new x

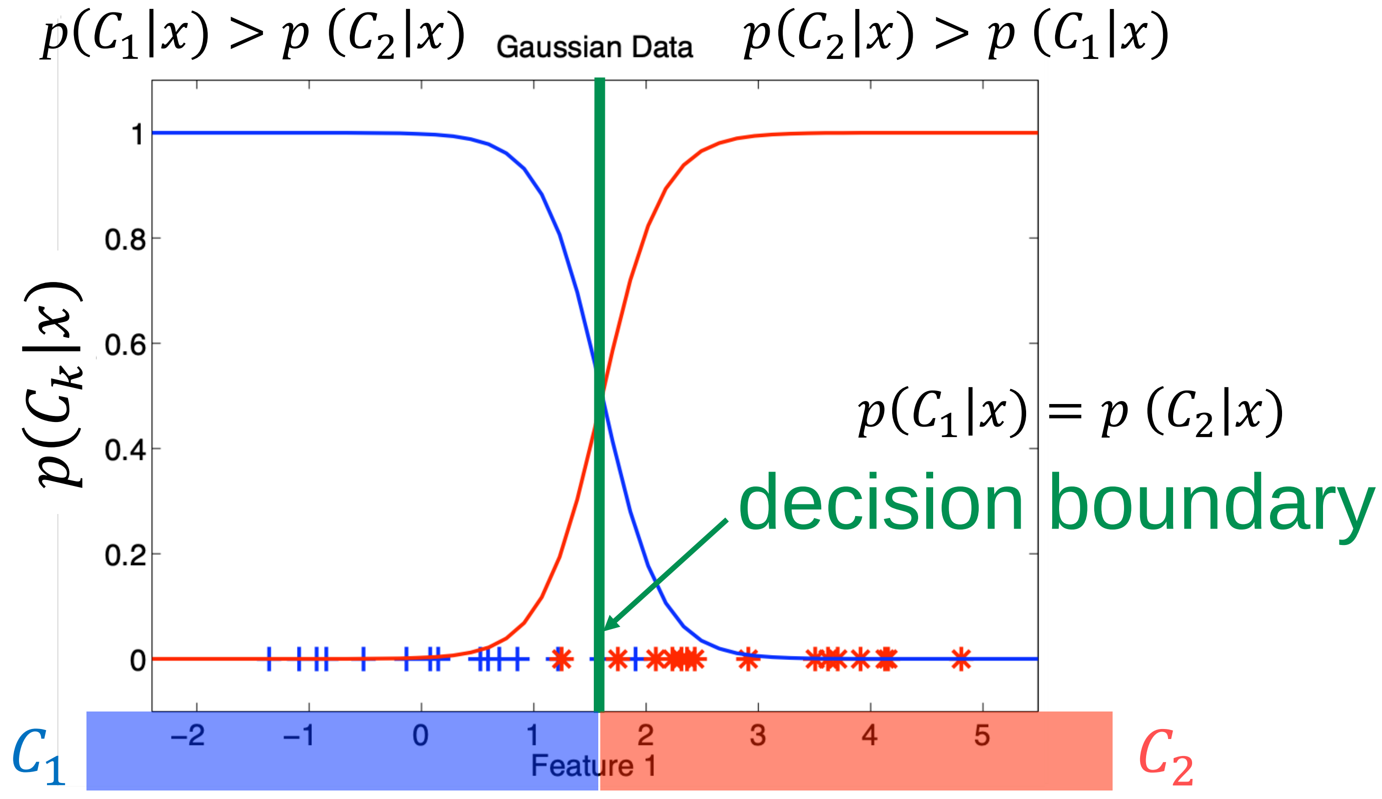
- Estimate the posterior probability $p(C_k|x)$



$$\sum_k p(C_k|x) = 1$$

"Hard" classification of the new object x

- Assign the label of the class with the largest posterior probability



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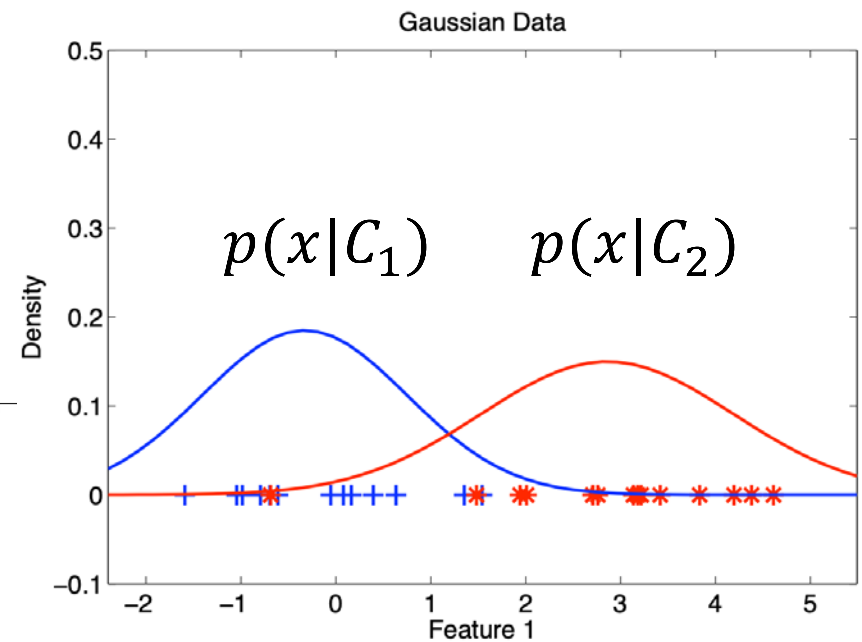
Description of a classifier: Decision theory

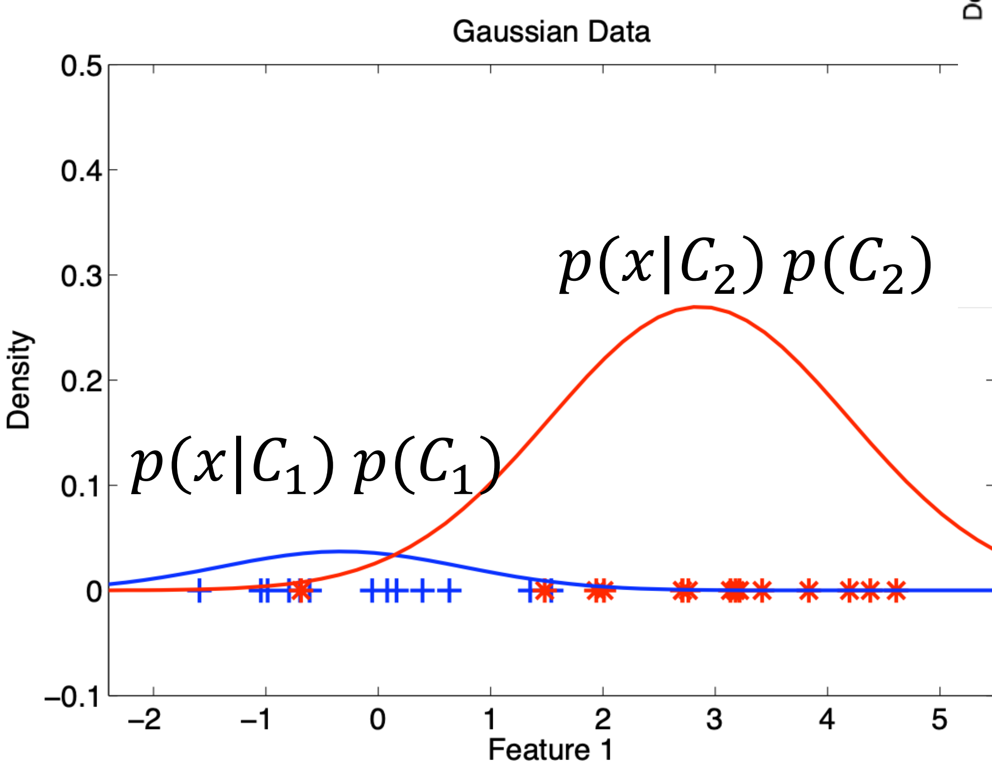
There are several ways to describe a classifier:

- if $p(C_1|\mathrm{x}) > p\,(C_2|\mathrm{x})$ then assign to C_1
  otherwise C_2
- if $p(C_1|\mathrm{x}) - p(C_2|\mathrm{x}) > 0$ then assign to C_1
- or $\frac{p(C_1|\mathrm{x})}{p(C_2|\mathrm{x})} > 1$ then assign to C_1
- or …

How do we calculate the posterior probabilities?

➔ Bayes' Rule





1. Estimate the class probabilities

2. Multiply with the class priors

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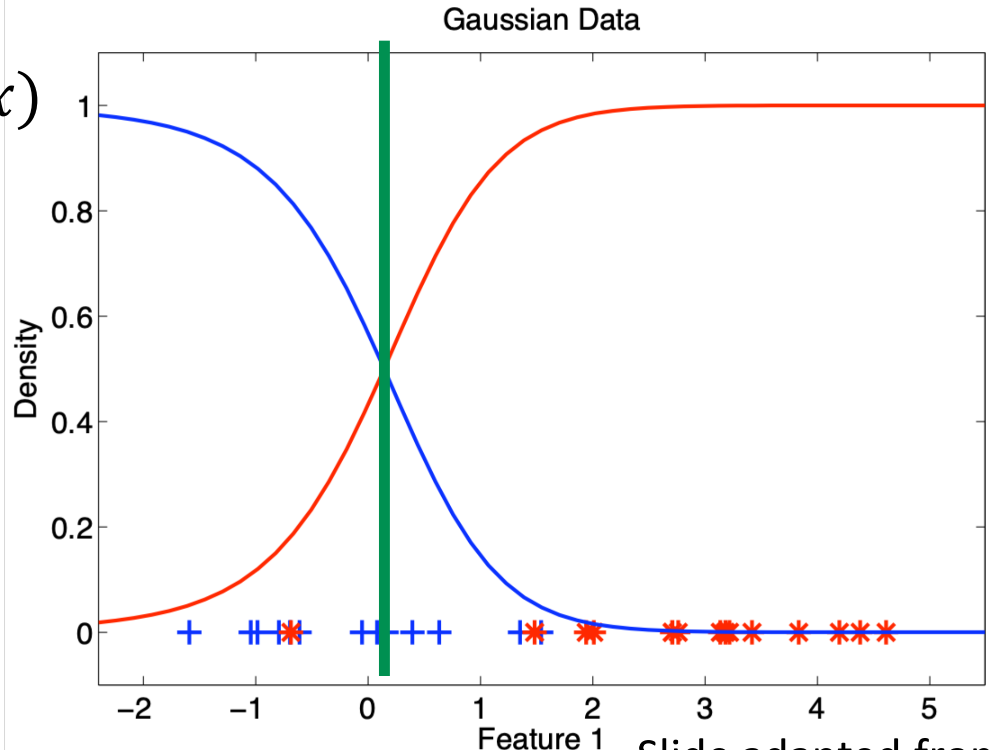
Bayes' Rule

3. Compute the class posterior probabilities
4. Assign objects to the class with the highest posterior probability

$p(C_1|x)$



$p(C_2|x)$

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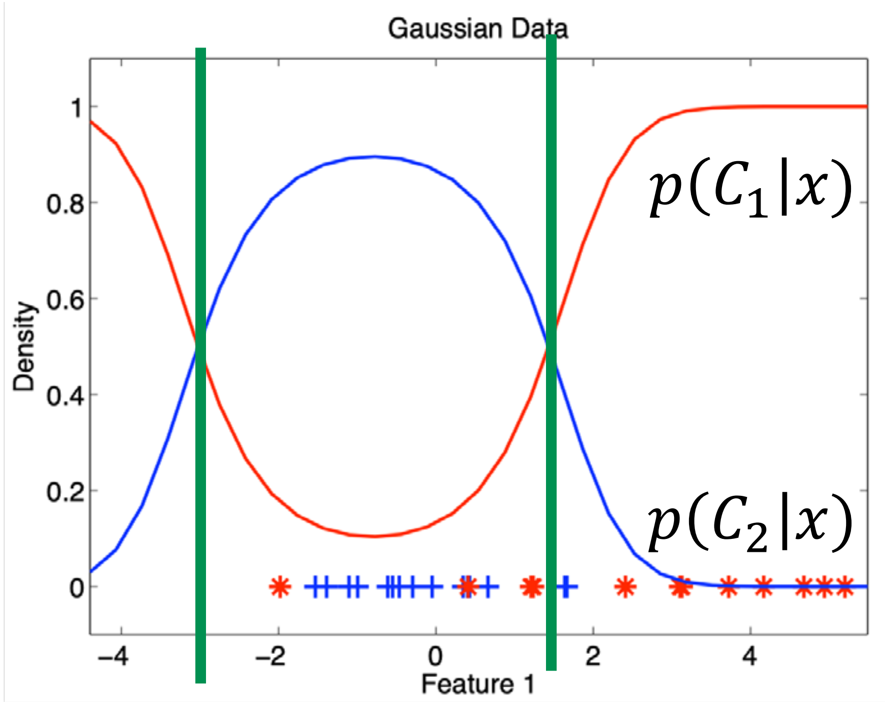
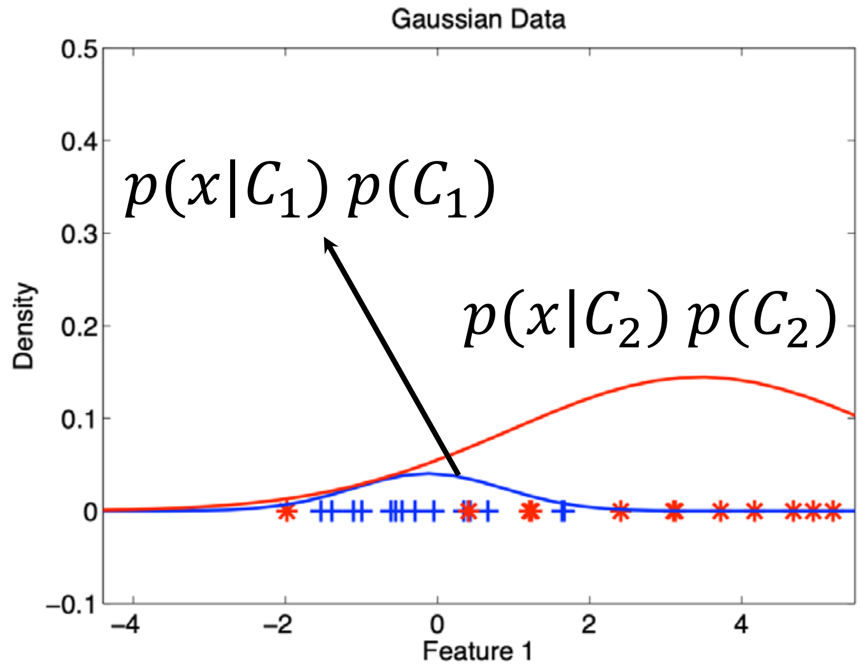
Complicated decision boundary



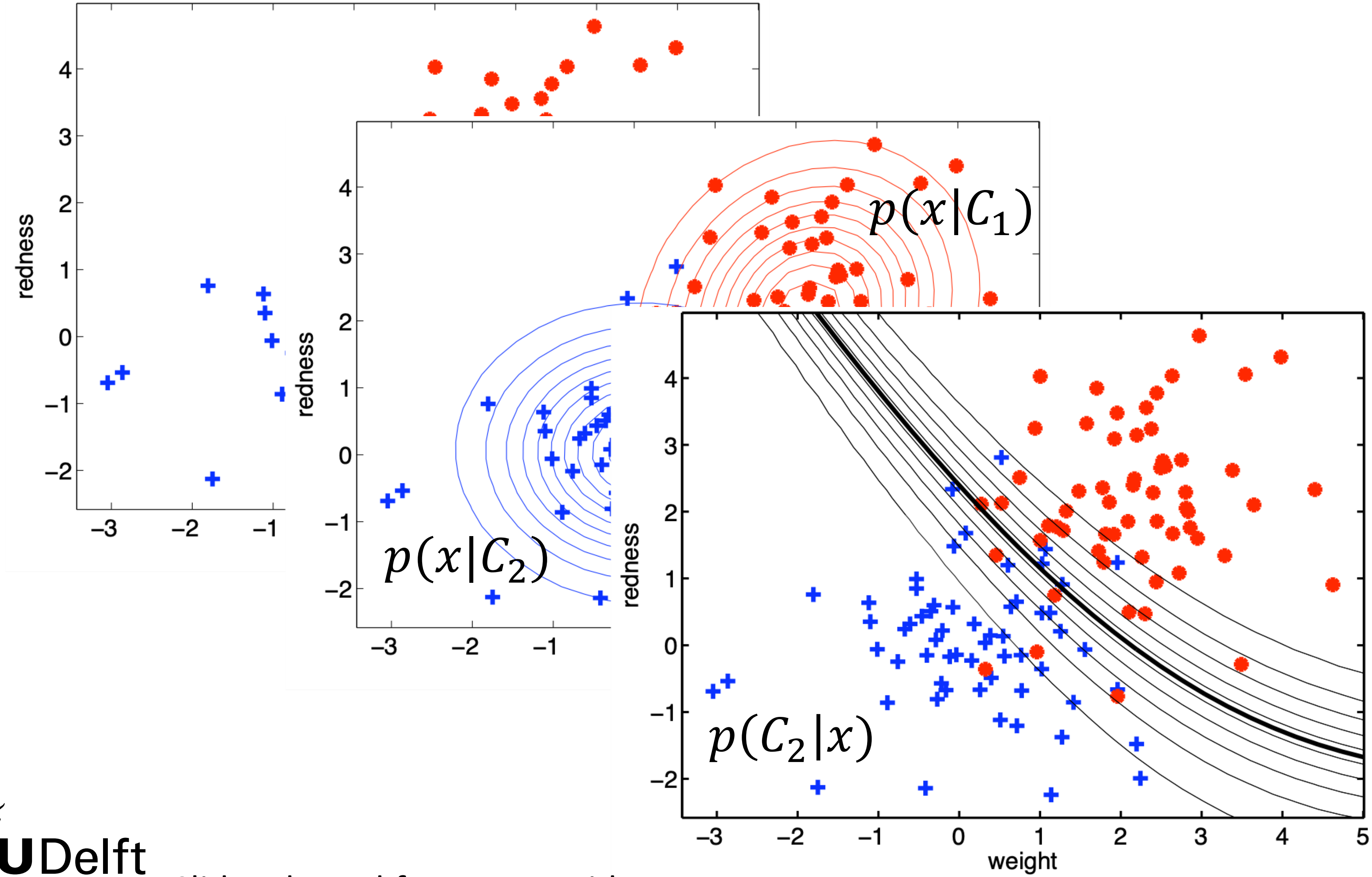
- Depending on the class conditional probability densities, complicated decision boundaries can appear

Missing decision boundary

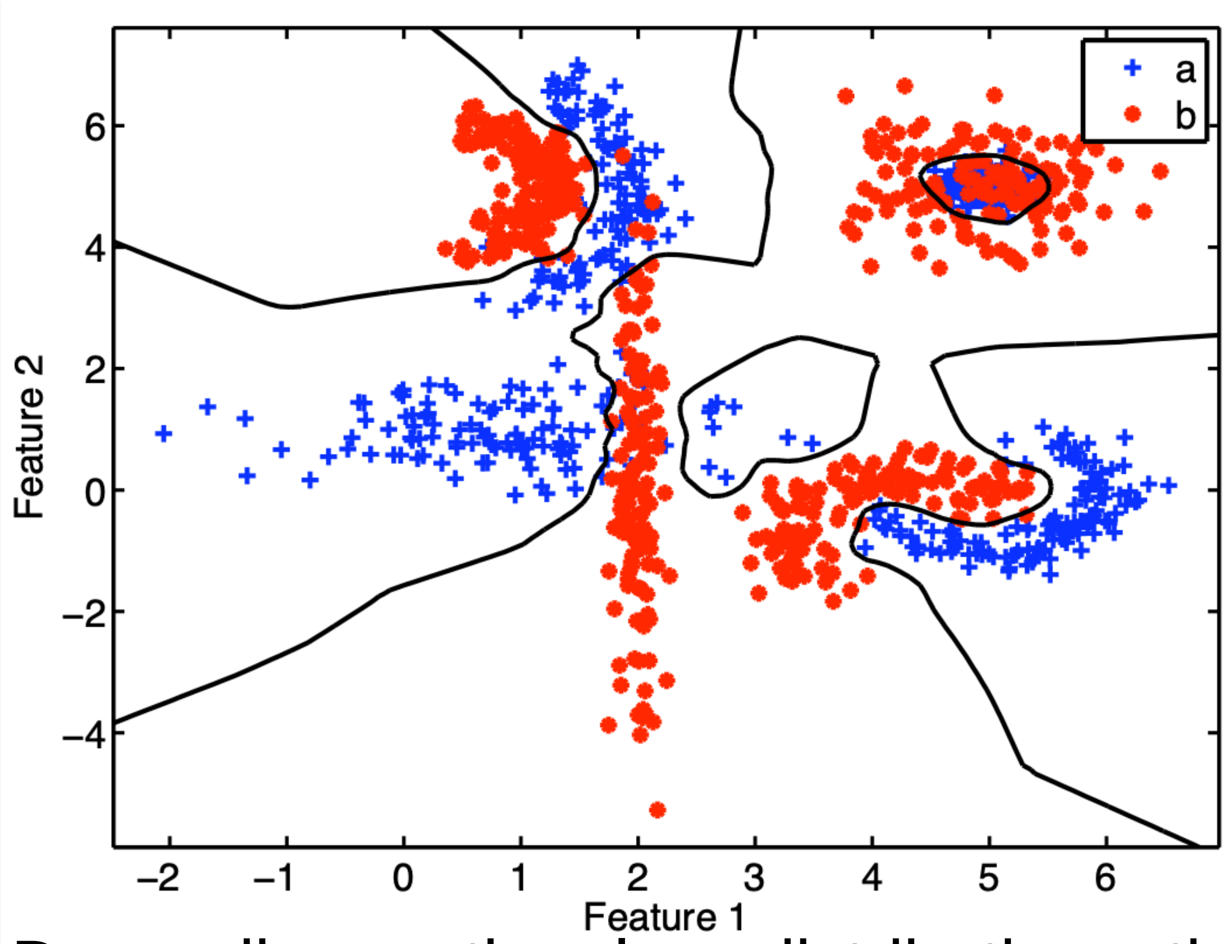


- A class can be too small (class prior is low) or too dispersed, that no objects are assigned to that class

Higher (2)-dimensional feature space



Multi-modal distributions



- Depending on the class distributions, the decision boundary can have arbitrary shapes

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The class conditional probabilities

- How do we obtain the class conditional probabilities $p(x|C_k)$?
- We need a model
- During training, estimate the model parameters such that the example objects fit well: maximum likelihood estimators
- This will be the topic for the coming weeks

Bayes Error

- Even if $p(x, y)$ is perfectly known (true distribution), errors predicting y from x will occur because the posteriors $p(y|x)$ are often not exactly 0 or 1

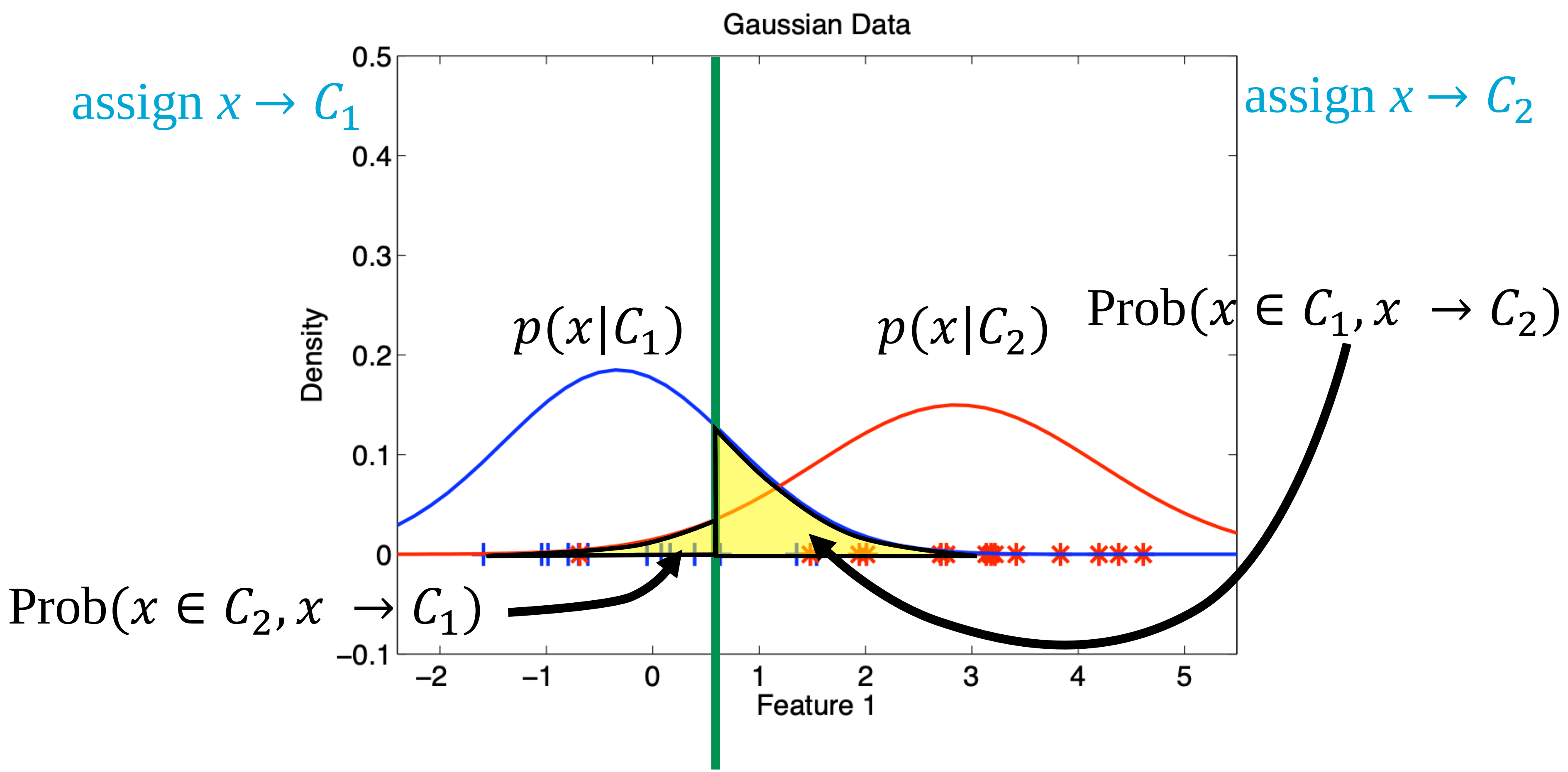
➔ lowest possible prediction error

== Bayes' error

== irreducible error

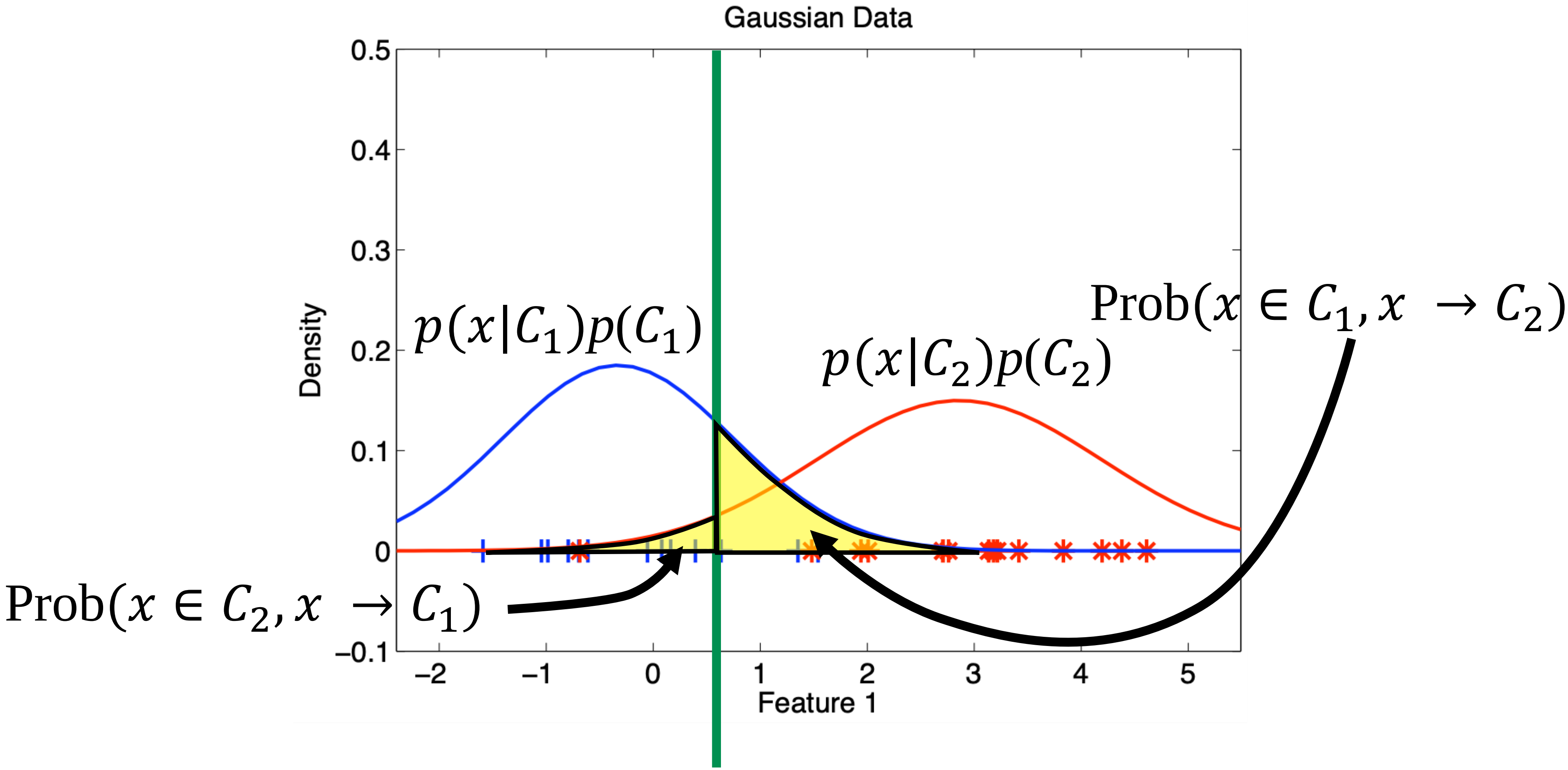
How good is the classifier?

- The error of the green decision boundary:



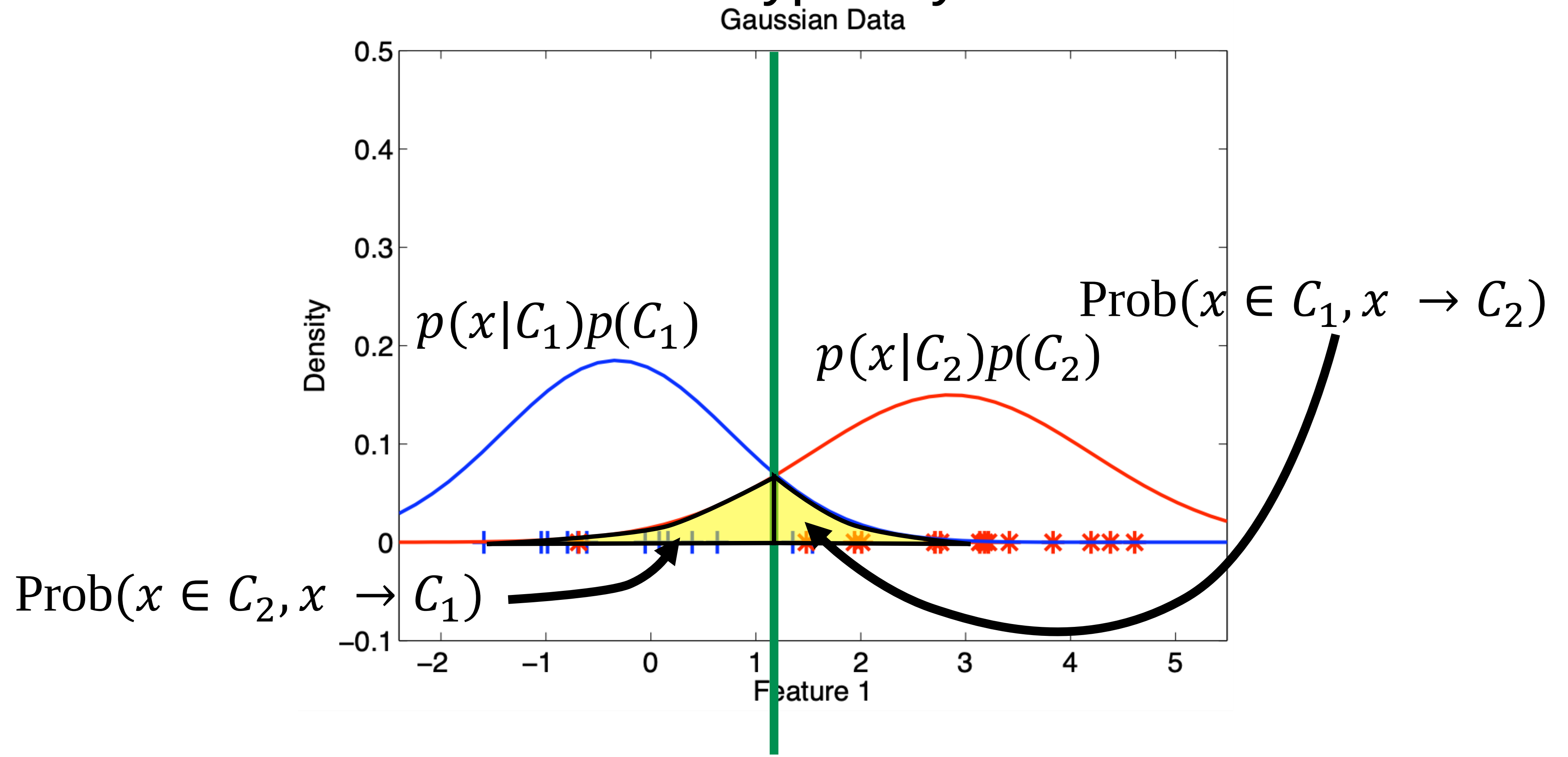
Classification error

- The error: $P(error) = \sum_{i=1}^{C} P(error|C_i)P(C_i)$



Bayes Error ε^*

- The **minimum** error: typically > 0!



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Bayes Error

- Bayes error is the **minimum** attainable ε^* error
- In practice, we do not have the true distributions, and we cannot obtain them
- The Bayes' error does not depend on the classification rule that you apply, but on the distribution of the data
- In general you cannot compute the Bayes' error:
  - You don't know the true class conditional probabilities
  - The (high) dimensional integrals are very complicated

Misclassification costs

- We want to make as few errors as possible with the assignment of x to class C
- Error: x is assigned to C_1 but should have been assigned to C_2 and vv.

Misclassification costs

- Sometimes: misclassification of class A to class B is much more dangerous than misclassification of class B to class A

misclassification:

classify ‘healthy’ as ‘ill’

misclassification:

classify ‘ill’ as ‘healthy’

Misclassification cost

- Introduce a loss that measures the cost of assigning an object that came from class C_j to class C_i : λ_{ji}

misclassification:

$\lambda_{healthy,ill} = 1$

misclassification:

$\lambda_{ill,healthy} = 1000$

Misclassification cost

- Preferably fewer $\lambda_{ill,healthy}$ misclassifications than $\lambda_{healthy,\,ill}$ misclassifications
- Even if that means an increase in $\lambda_{healthy,\,ill}$ misclassifications

→ Loss function balances these wishes

- Measure of loss incurred in taking any of the available decisions or actions

→ Minimise the loss function

Solving decision problems

1. Generative models (week 2 & 3)
2. Discriminative models (week 4 & 6)

Generative vs discriminative models

- Generative models (week 2 & 3):
  - Model the actual distribution of each class
  - Learn the class conditional probability $p(X|Y)$
  - Allows you to *generate* new samples from all classes
  - Predict the posterior probability using Bayes' Rule

- Discriminative models (week 4 & 6):
  - Directly estimate $p(Y|X)$ which *discriminates* between classes
  - No $p(X|Y)$ → no generation of new data from classes

Conclusions

- ML is "probabilistic" classification:
  - Estimate the posterior conditional probability using

Bayes' Rule: $$p(Y|X) = \frac{p(X|Y)p(Y)}{p(X)}$$

- "Hard classification" is done using decision theory