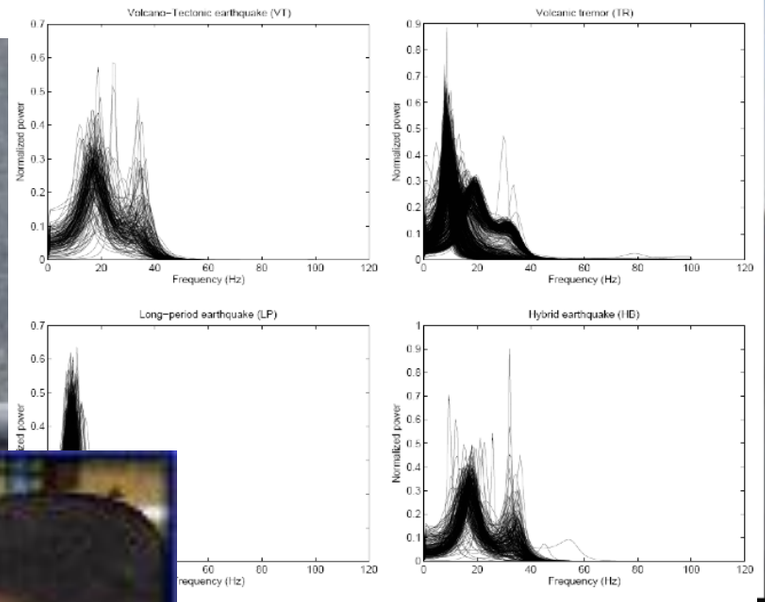
Machine Learning: the basics

- Learning from examples



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Outline of this lecture

- Objects, features, measurements,
- ... datasets and feature space
- Traditional pattern recognition: classification
- Class posterior probabilities and Bayes' rule
- Bayes' classifier and Bayes' error
- Misclassification costs

Learning from Examples

- Given some **examples**, we may perform:
  - clustering
  - outlier detection
  - classification
  - regression
  - …

  on new objects.

- We assume that no complete physical model is known!

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Generalization

We don't want to just describe the data...

We want to predict for new, unseen data!

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Generalization

- **Training set**:
  All examples are labeled
  This set is used to train/develop our system

- **Test set**:
  These examples cannot be used to train our system
  The examples do not have to be labeled
  When labels are available, we can objectively evaluate our system

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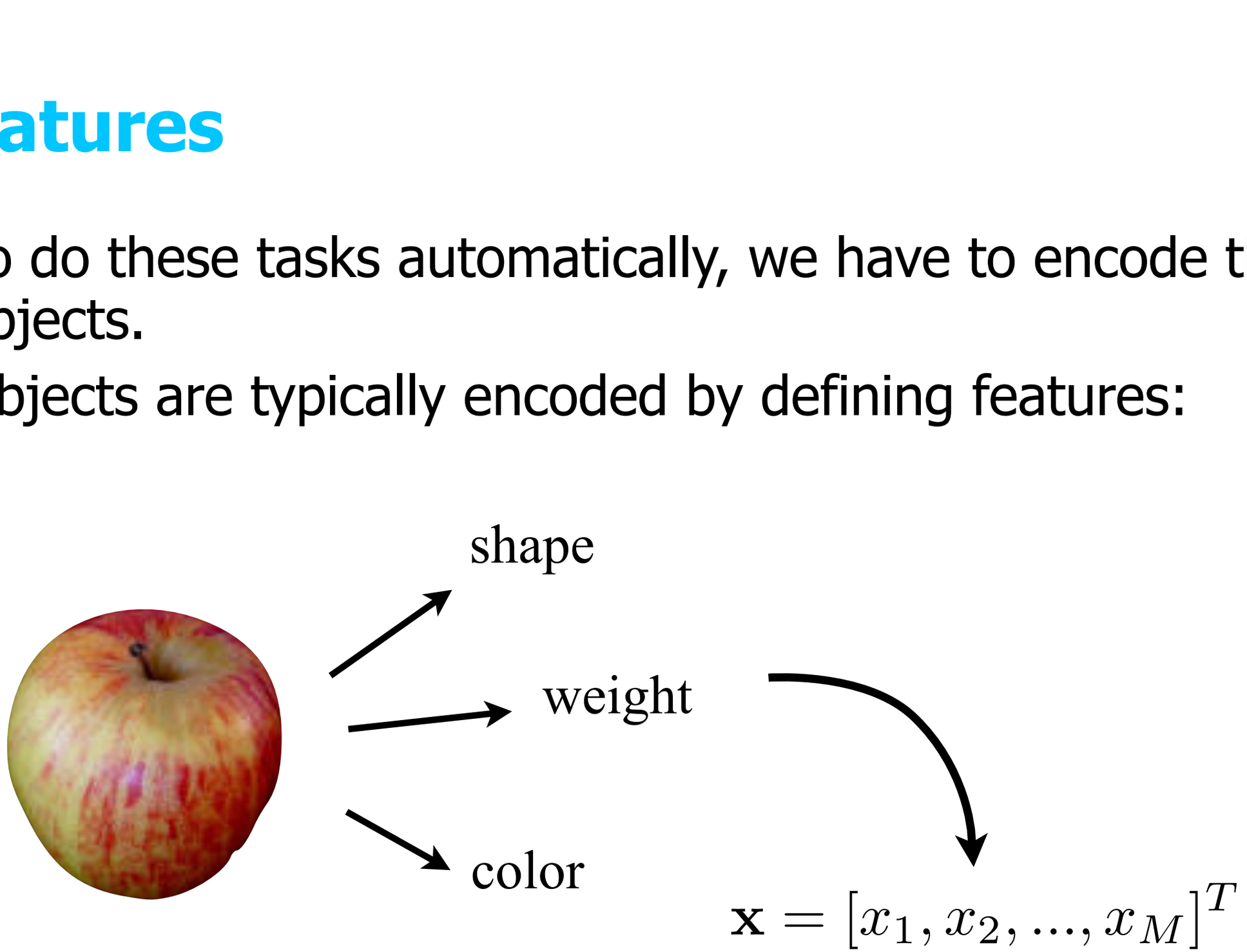
Features

- To do these tasks automatically, we have to encode the objects.
- Objects are typically encoded by defining features:



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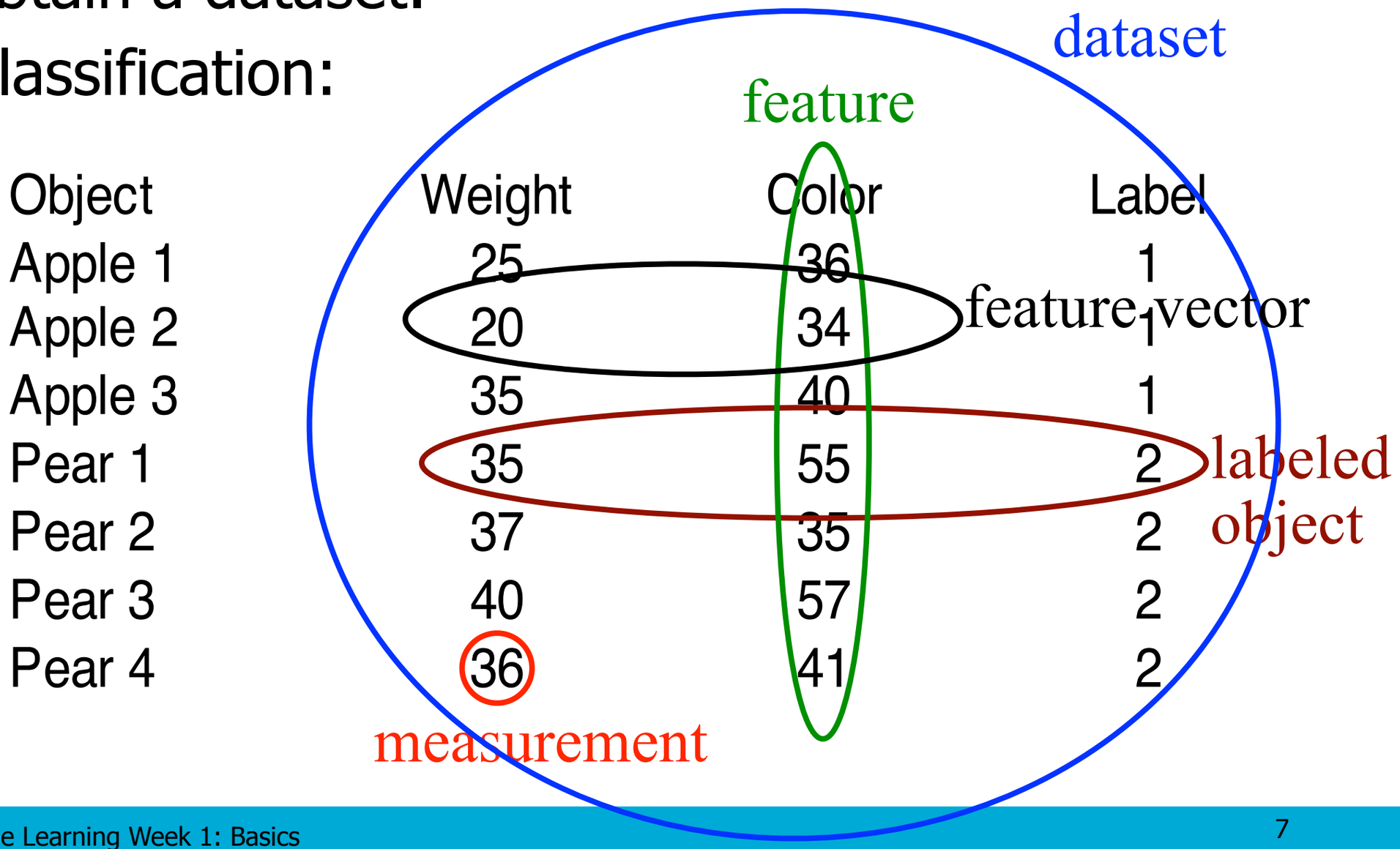
Datasets

- When we measure the features of many objects: we obtain a dataset.
- For classification:



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How to define features?

- Note that features reduce, and give a specific view of the objects: YOU (the user) is responsible for it
- Good features allow for pattern recognition, bad features allow for nothing
- Other (than feature vector) approaches of defining objects are:
  - Dissimilarity approach
  - Structural pattern recognition (graphs)

- Feature approach is very well developed, other approaches are still more research.

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Noise in the measurements

- The measurements will never be perfect
- Objects within a class will vary

We need to apply some statistics to cover all the variations

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Measurements

- Task: distinguish between 3 types of Iris flowers:

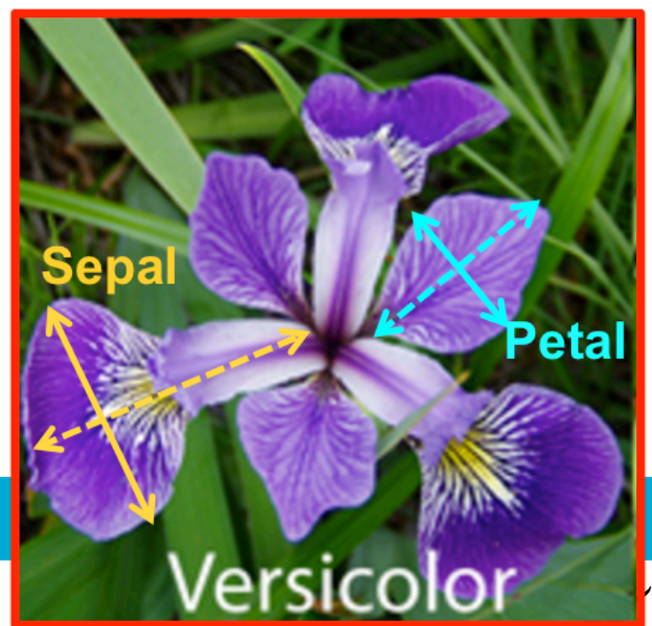
(Images from Wikipedia)

Iris Setosa

Iris Versicolor

Iris Virginica

- Measurements:
  sepal width, sepal length,
  petal width, petal length.



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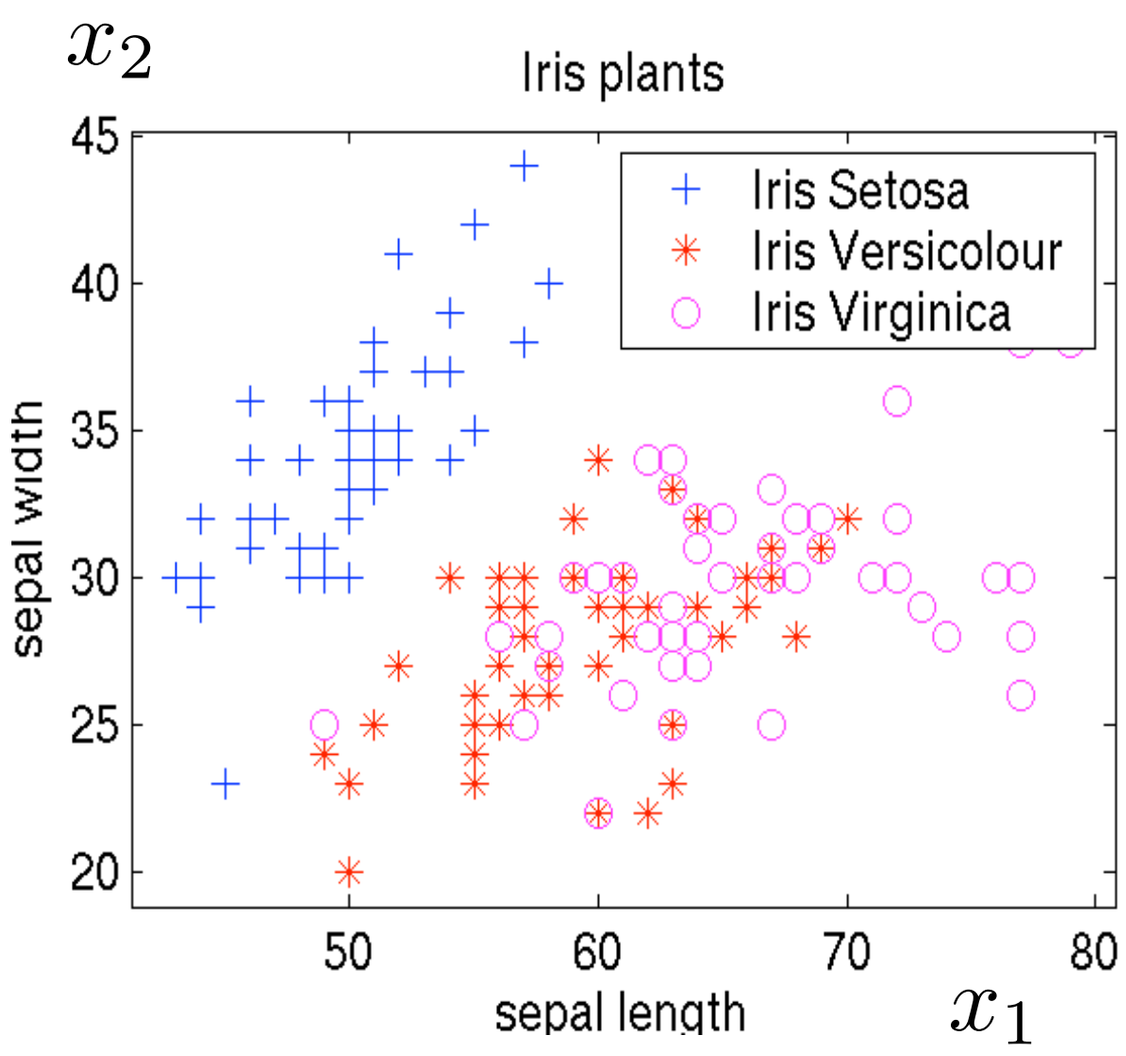
Objects in feature space

- We can interpret the measurements as a vector in a vector space:

$$\mathbf{x} = [x_1, x_2, ..., x_M]^T$$

- This originates in principle from a probability density over the whole feature space

$$p(\mathbf{x}, y)$$



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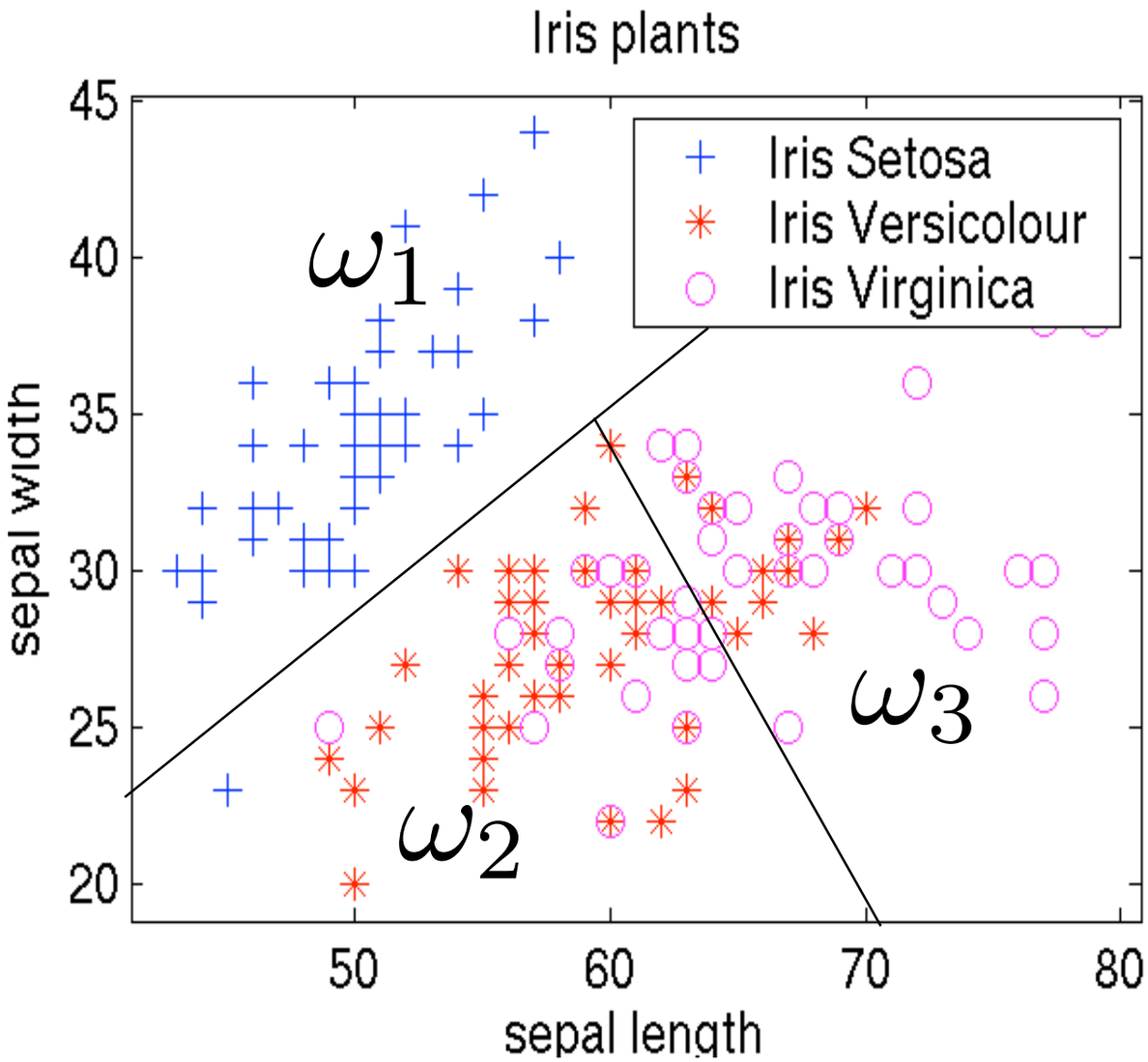
Classification

- Given labeled data: $\mathbf{x}$
- Assign to each object a class label ω
- In effect splits the feature space in separate regions



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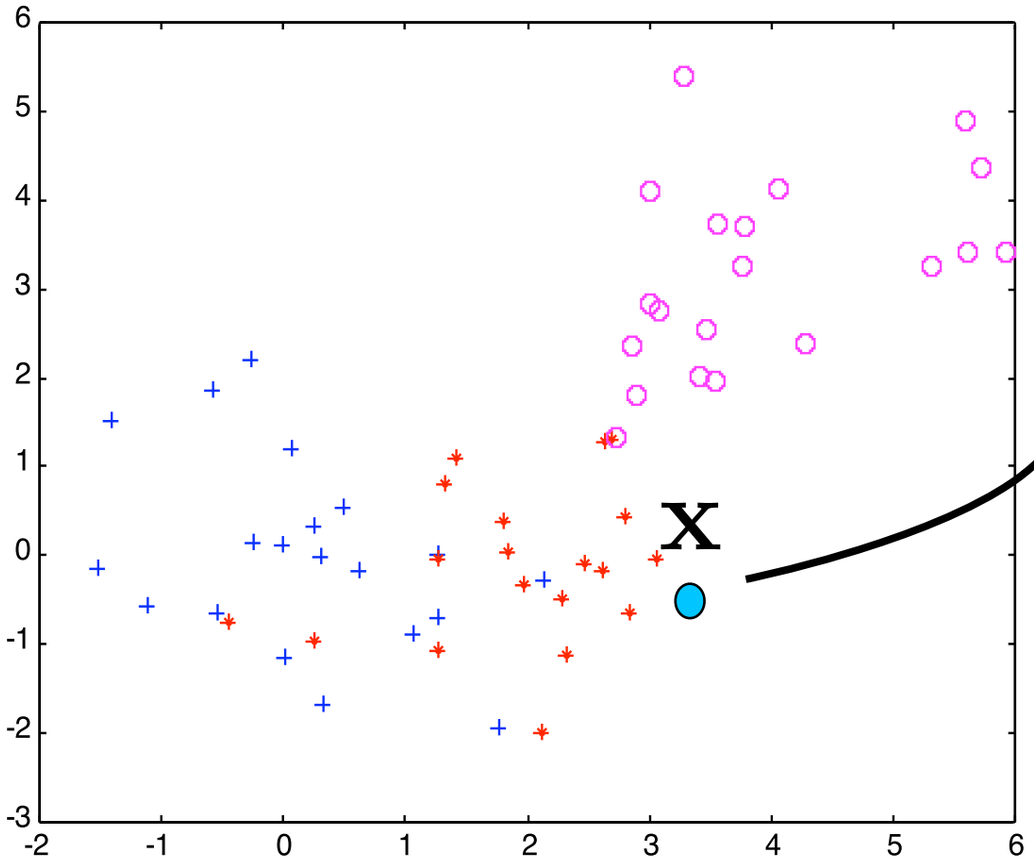
The general model



Function f should give the predicted output.

$f(\mathbf{x})$ → ω

$p(\omega|\mathbf{x})$

and... model should be fitted to the data!

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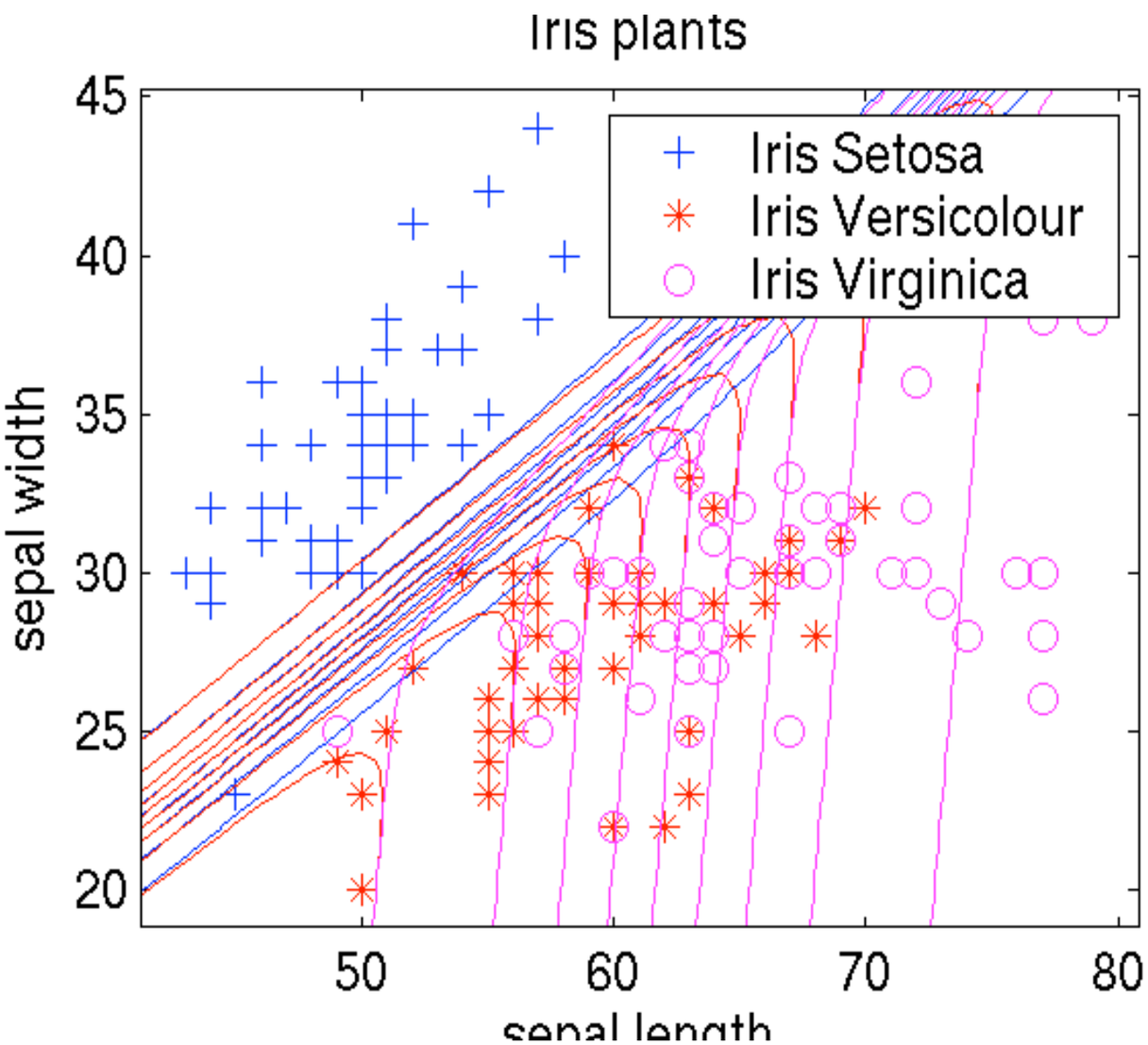
Output of the model



- For each object in the feature space, we should estimate:

$$p(\omega|\mathbf{x})$$

- In practice we fit a function:

$$f(\mathbf{x})$$

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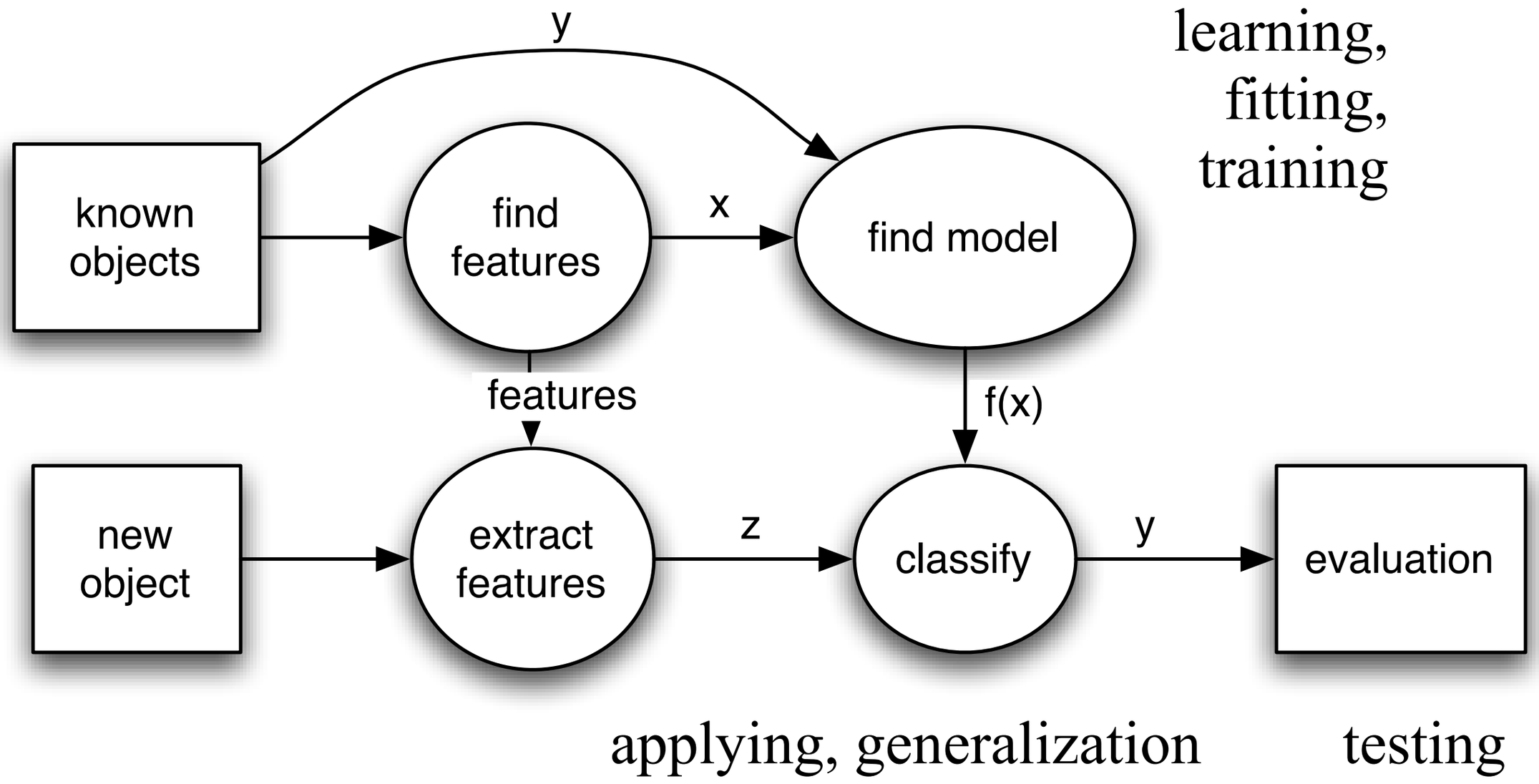
Pattern Recognition pipeline



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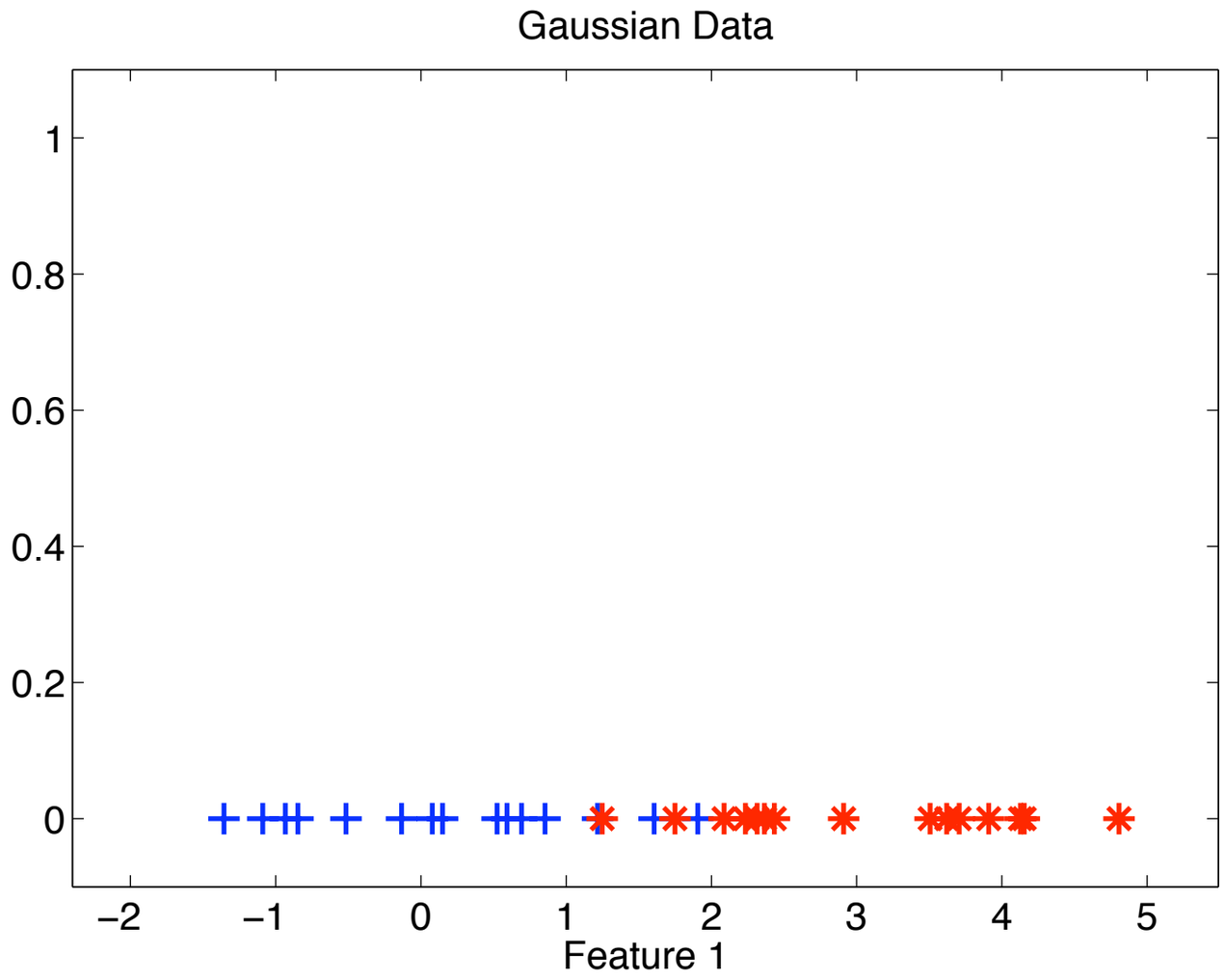
Classification, how to do it?

- Given a feature, and a training set, where is the blue class?



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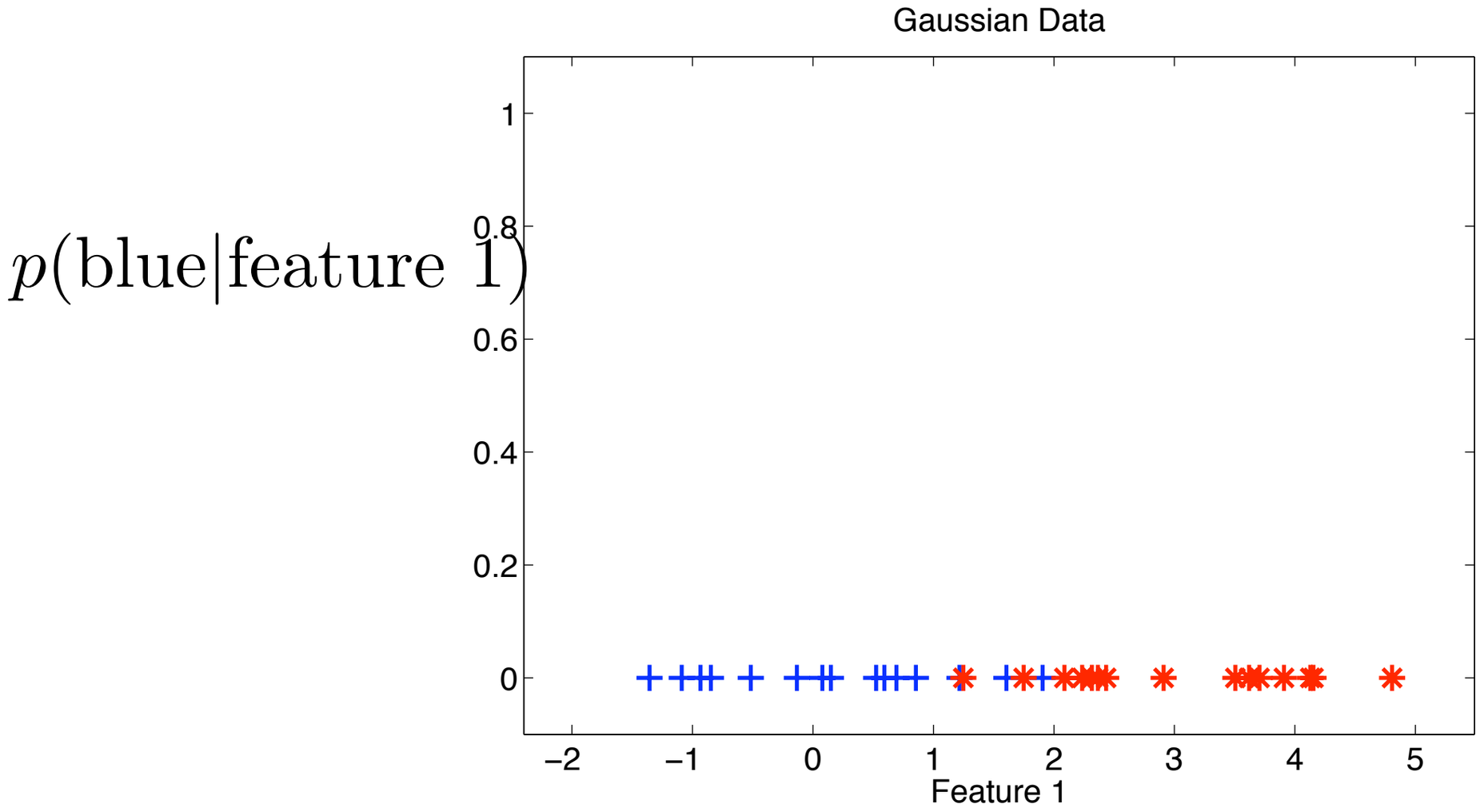
Class posterior probability

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



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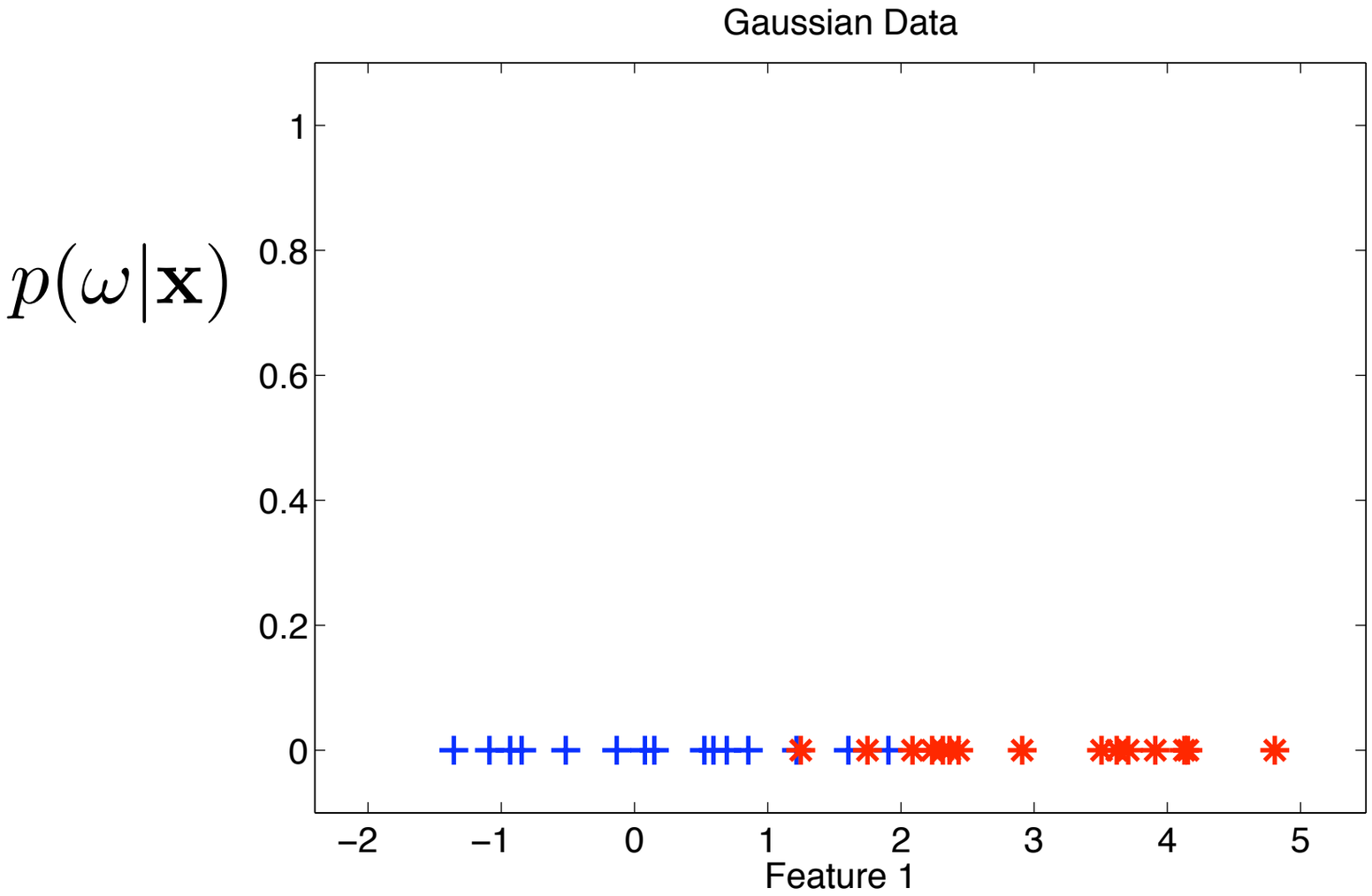
Class posterior probability

- For each object we want to estimate $p(\omega|\mathbf{x})$



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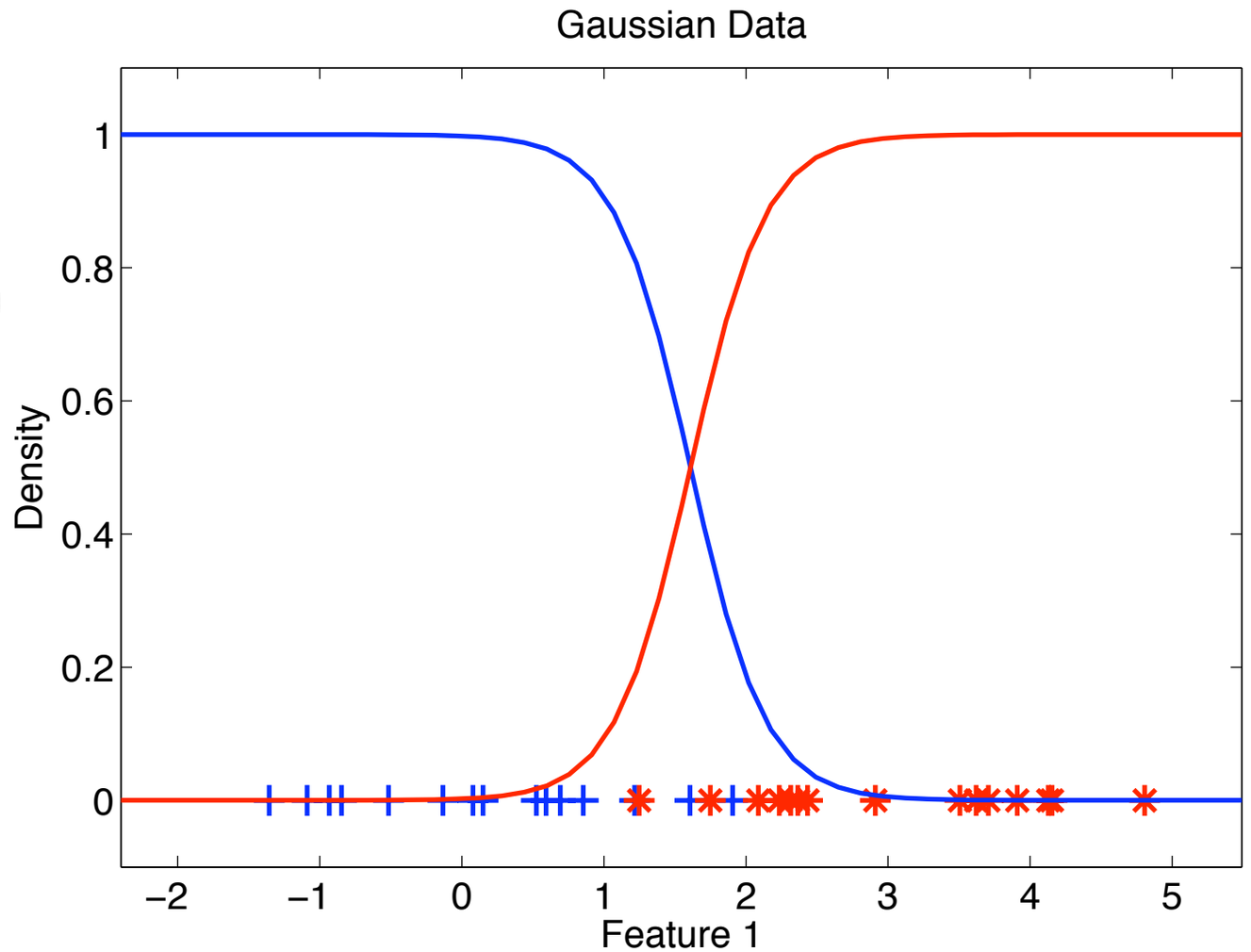
Class posterior probability

- For each object we have to estimate $p(\omega|\mathbf{x})$

$p(\omega|\mathbf{x})$



$$\sum_i p(\omega_i|\mathbf{x}) = 1$$

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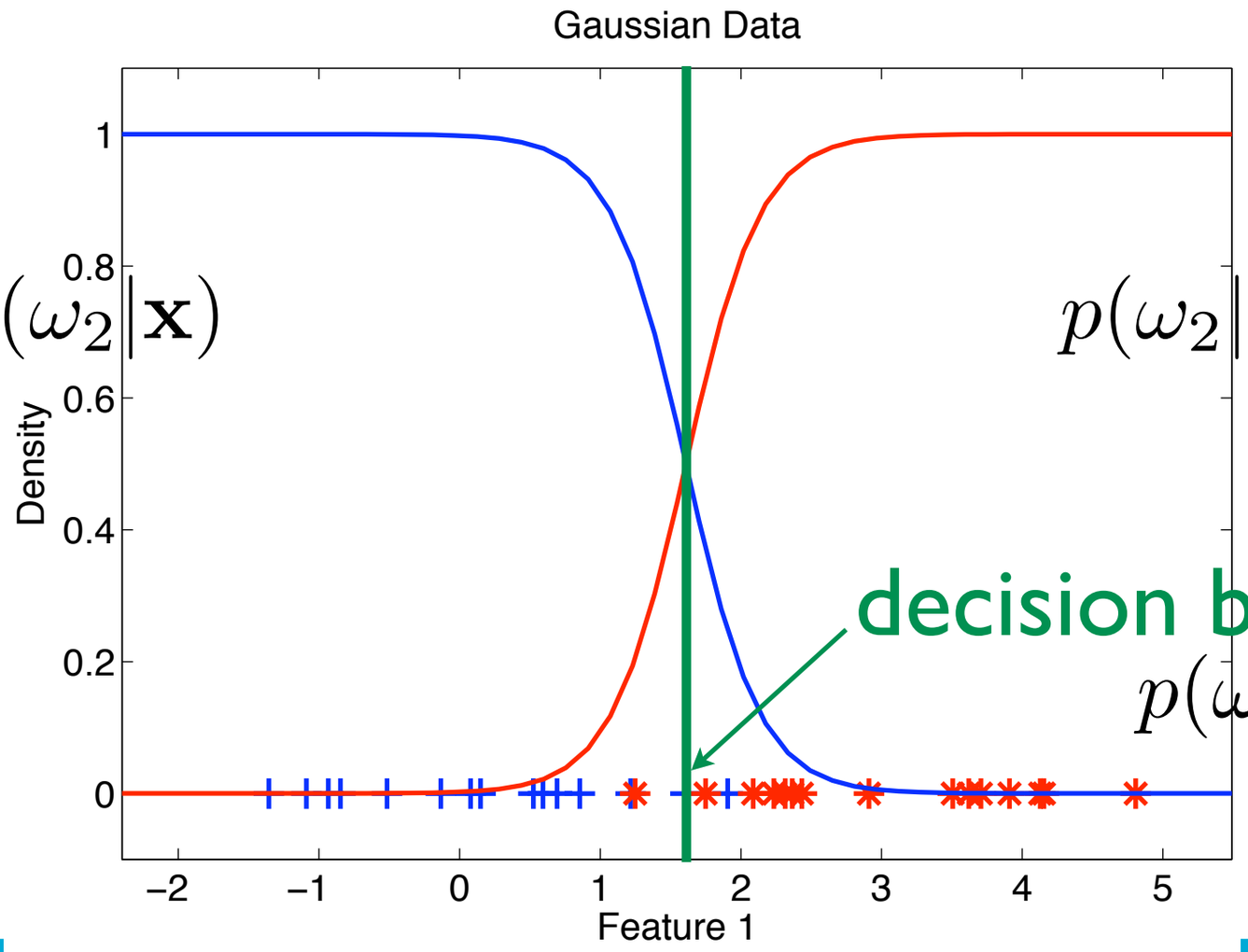
Classify new objects

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

$$p(\omega_1|\mathbf{x}) > p(\omega_2|\mathbf{x})$$



$$p(\omega_2|\mathbf{x}) > p(\omega_1|\mathbf{x})$$

$$p(\omega_2|\mathbf{x}) = p(\omega_1|\mathbf{x})$$

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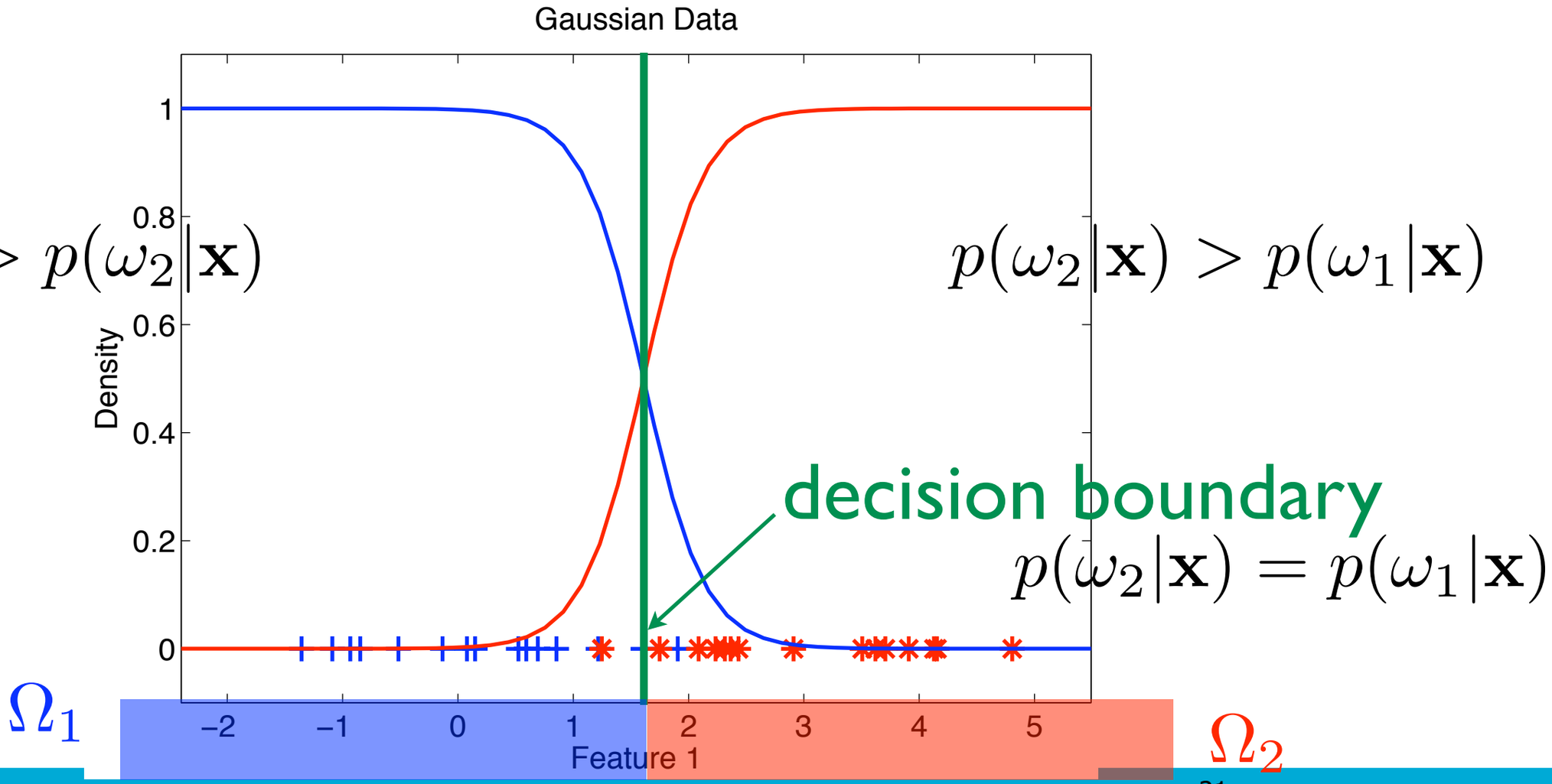
Classify new objects

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

$$p(\omega_1|\mathbf{x}) > p(\omega_2|\mathbf{x})$$

$$p(\omega_2|\mathbf{x}) > p(\omega_1|\mathbf{x})$$



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Description of a classifier

There are several ways to describe a classifier:

- if $p(\omega_1|\mathbf{x}) > p(\omega_2|\mathbf{x})$ then assign to ω_1
  otherwise ω_2

- if $p(\omega_1|\mathbf{x}) - p(\omega_2|\mathbf{x}) > 0$ then assign to ω_1

- or $\dfrac{p(\omega_1|\mathbf{x})}{p(\omega_2|\mathbf{x})} > 1$

- or $\ln(p(\omega_1|\mathbf{x})) - \ln(p(\omega_2|\mathbf{x})) > 0$

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Bayes' theorem

- In many cases the posterior is hard to estimate
- Often a functional form of the class distributions can be assumed
- Use Bayes' theorem to rewrite one into the other:

$$p(\omega|\mathbf{x}) = \frac{p(\mathbf{x}|\omega)p(\omega)}{p(\mathbf{x})}$$

class (conditional) distribution $p(\mathbf{x}|\omega)$
class prior $p(\omega)$
(unconditional) data distribution $p(\mathbf{x})$
posterior probability $p(\omega|\mathbf{x})$

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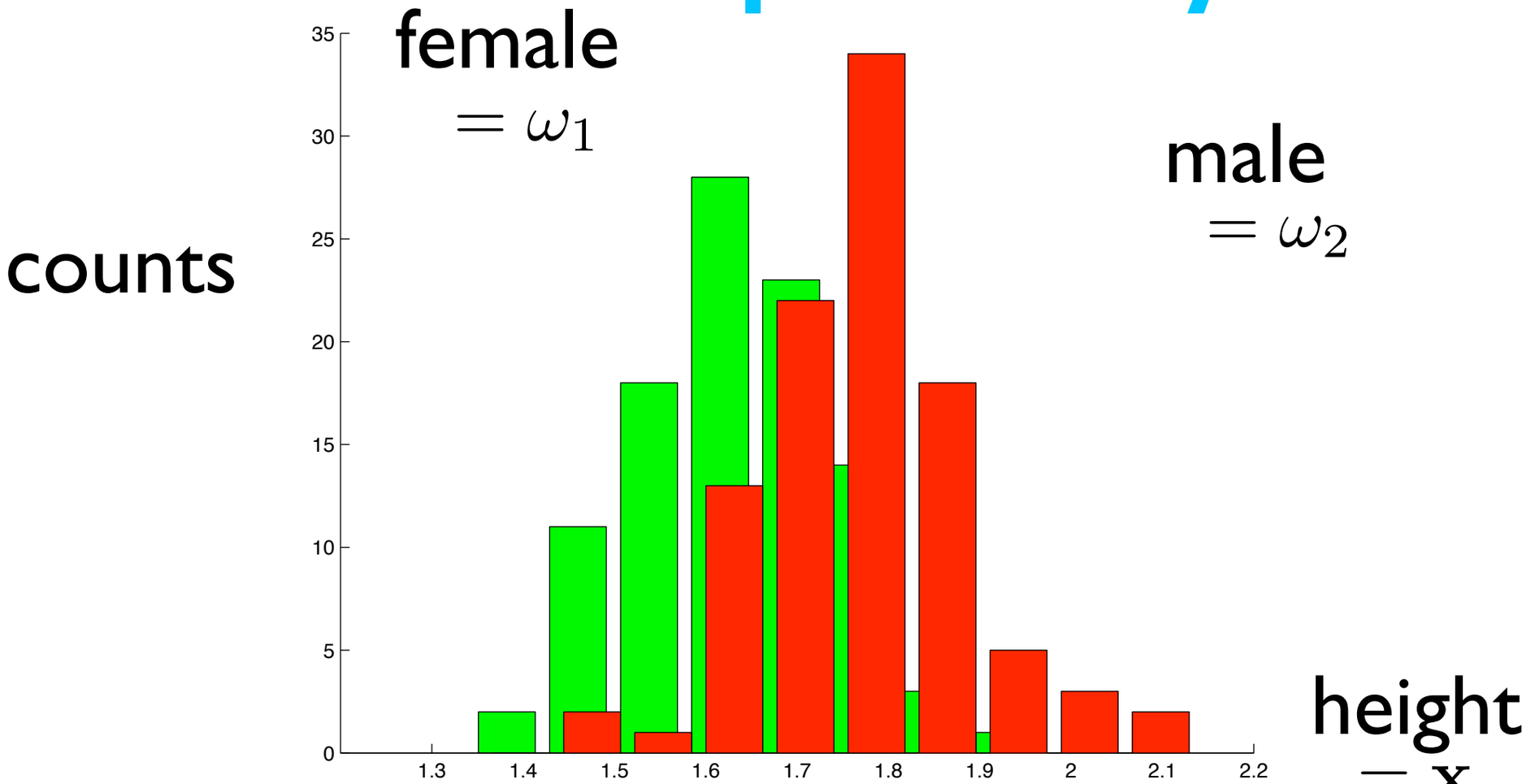
Class conditional probability



- Class conditional probabilities:
  - The distribution of the females $p(\mathbf{x}|\omega_1)$
  - The distribution of the males $p(\mathbf{x}|\omega_2)$

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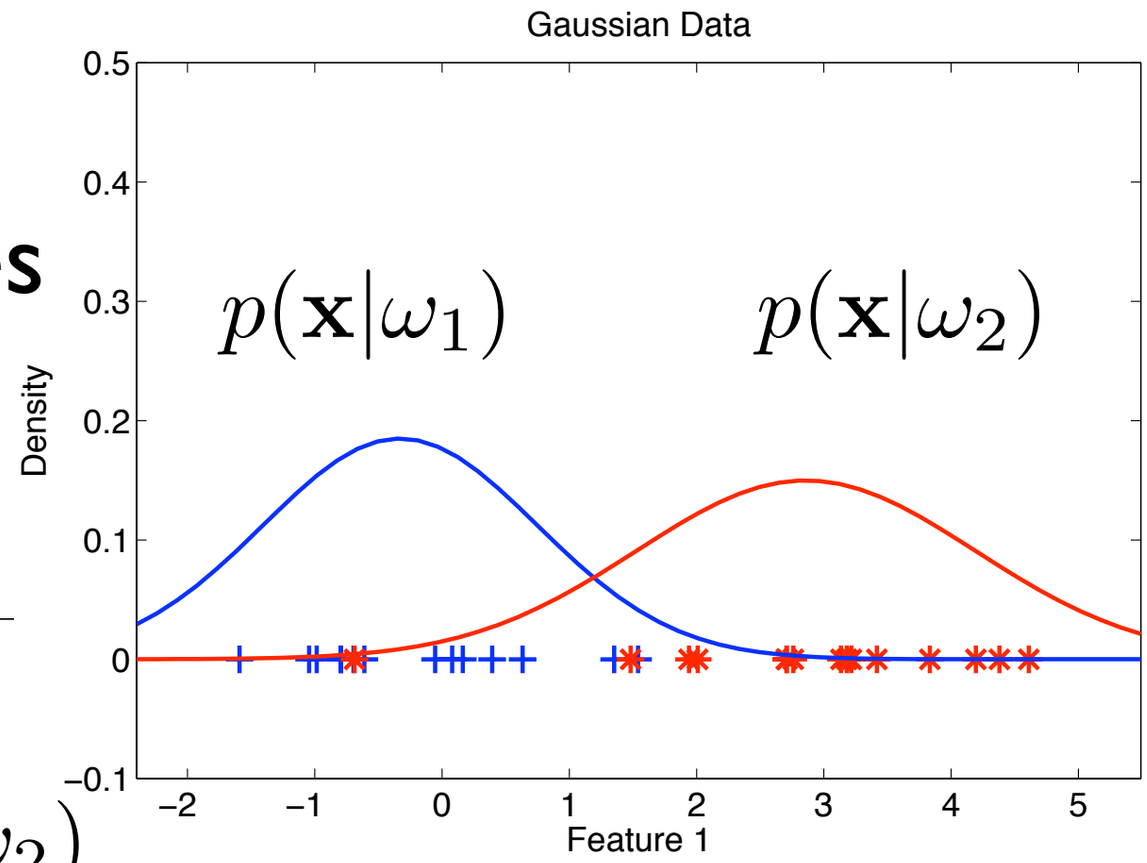
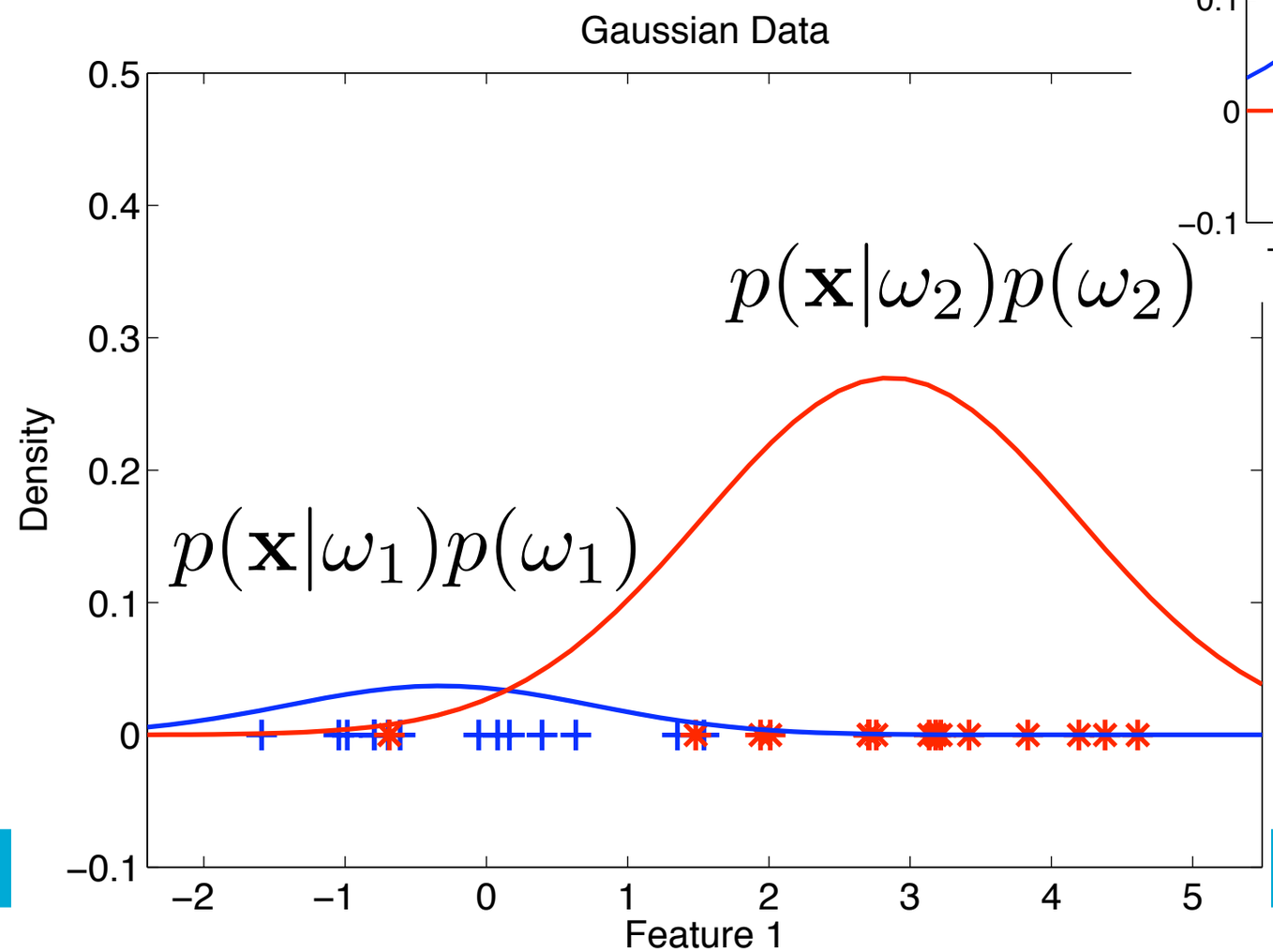
Bayes' rule

1. Estimate the class conditional probabilities





2. Multiply with the class priors

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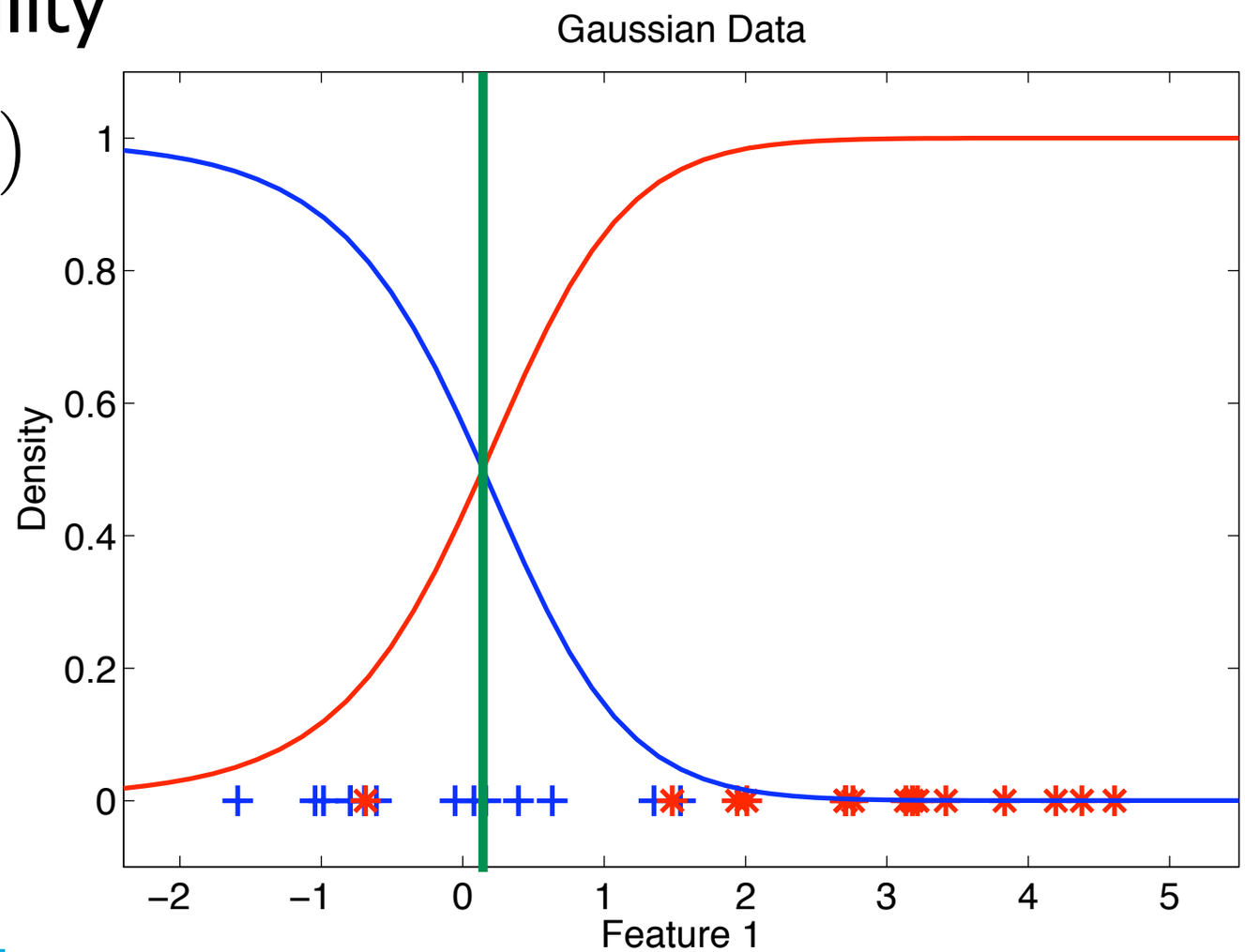
Bayes' rule

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

$p(\omega_1|\mathbf{x})$



$p(\omega_2|\mathbf{x})$

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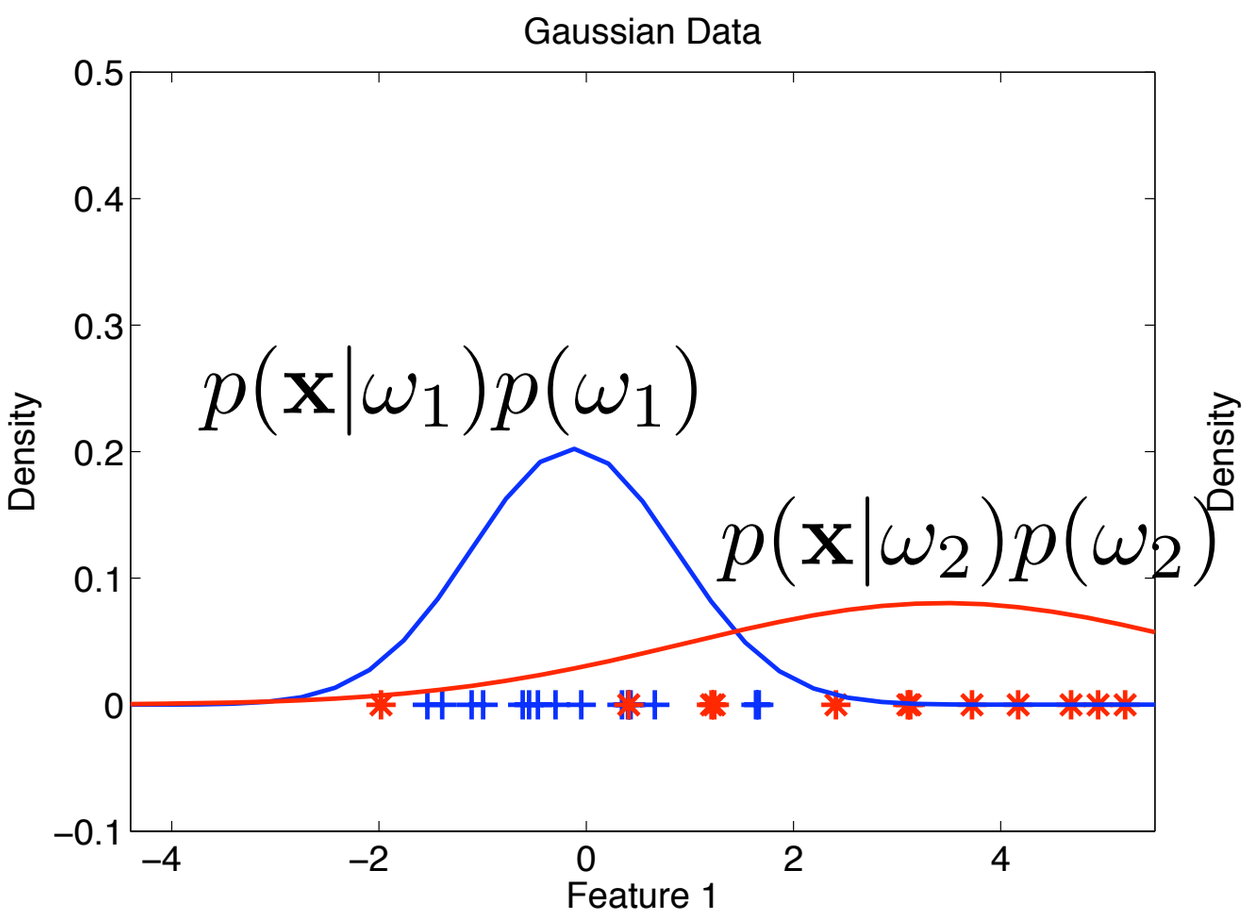
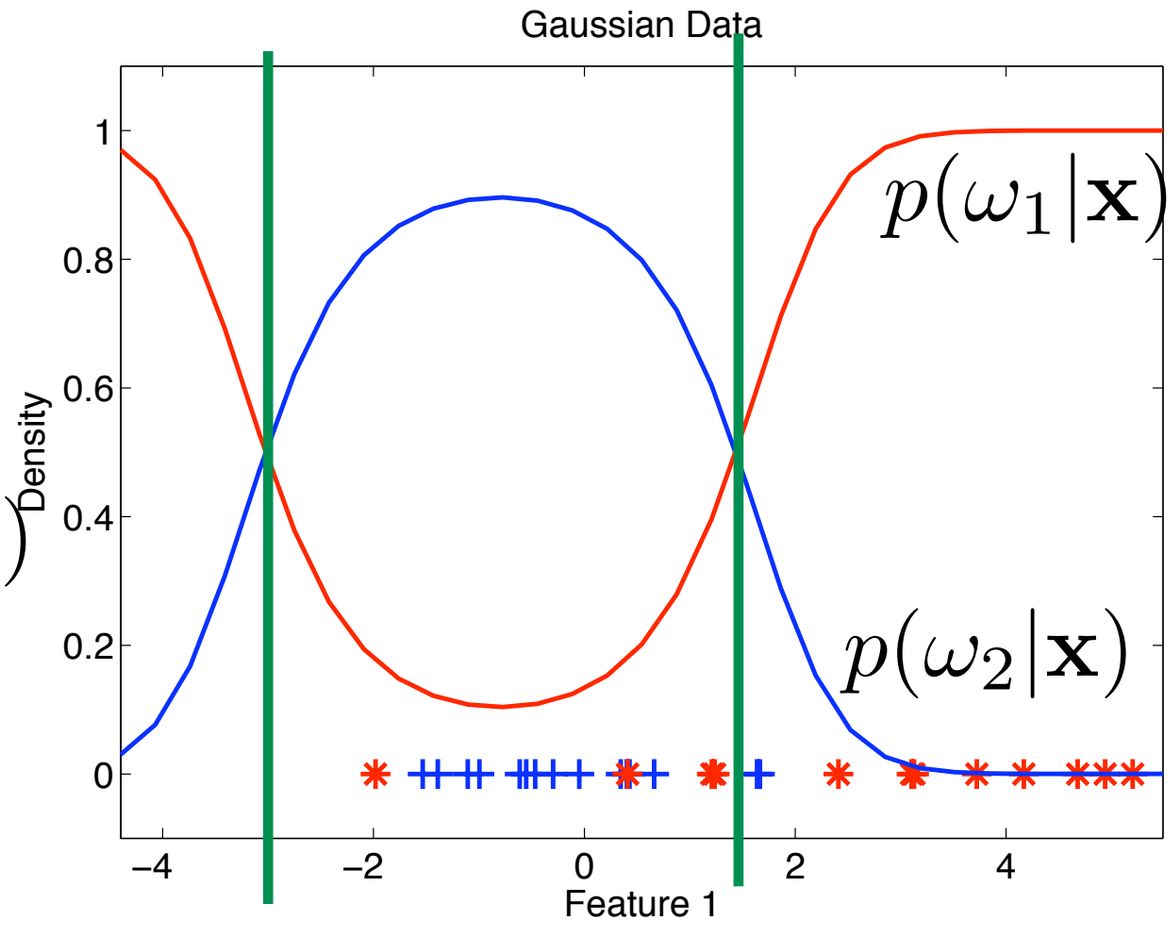
Complicated decision boundary





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

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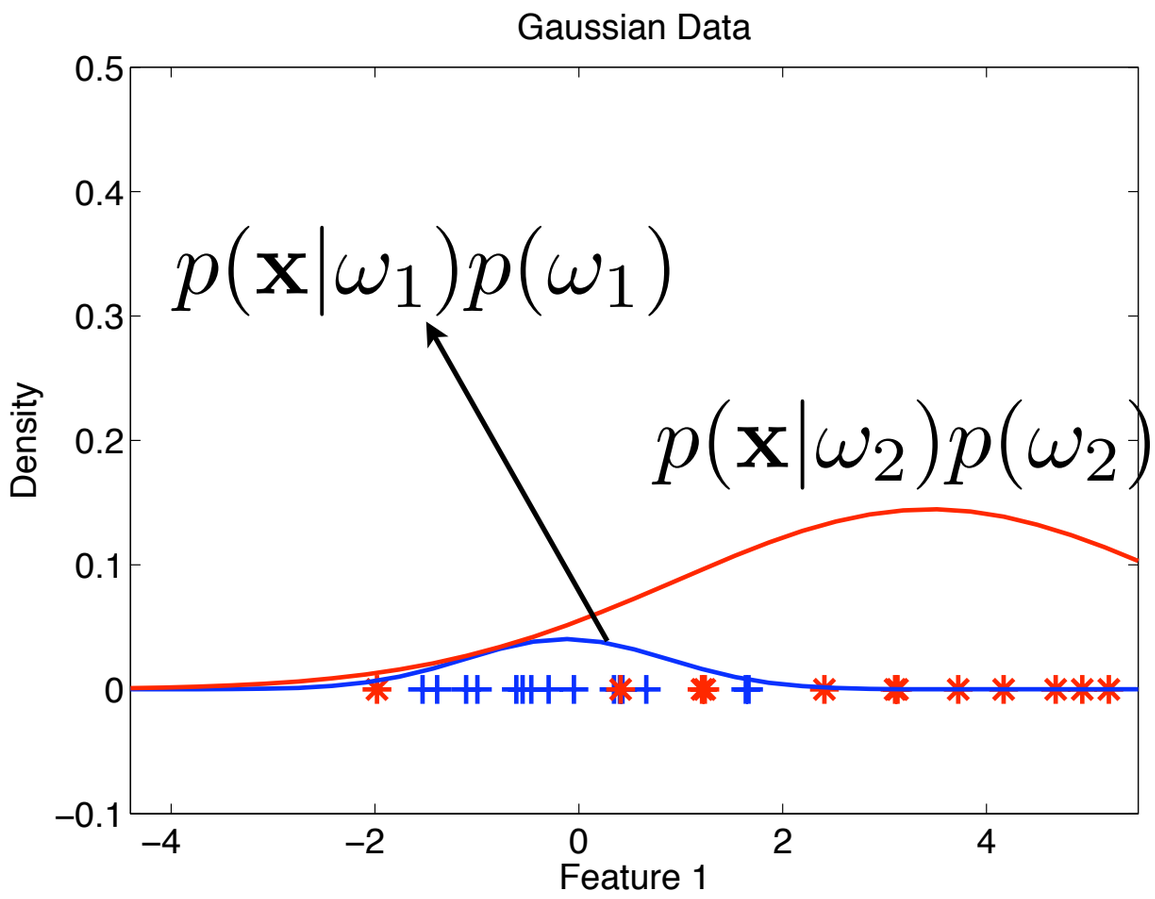
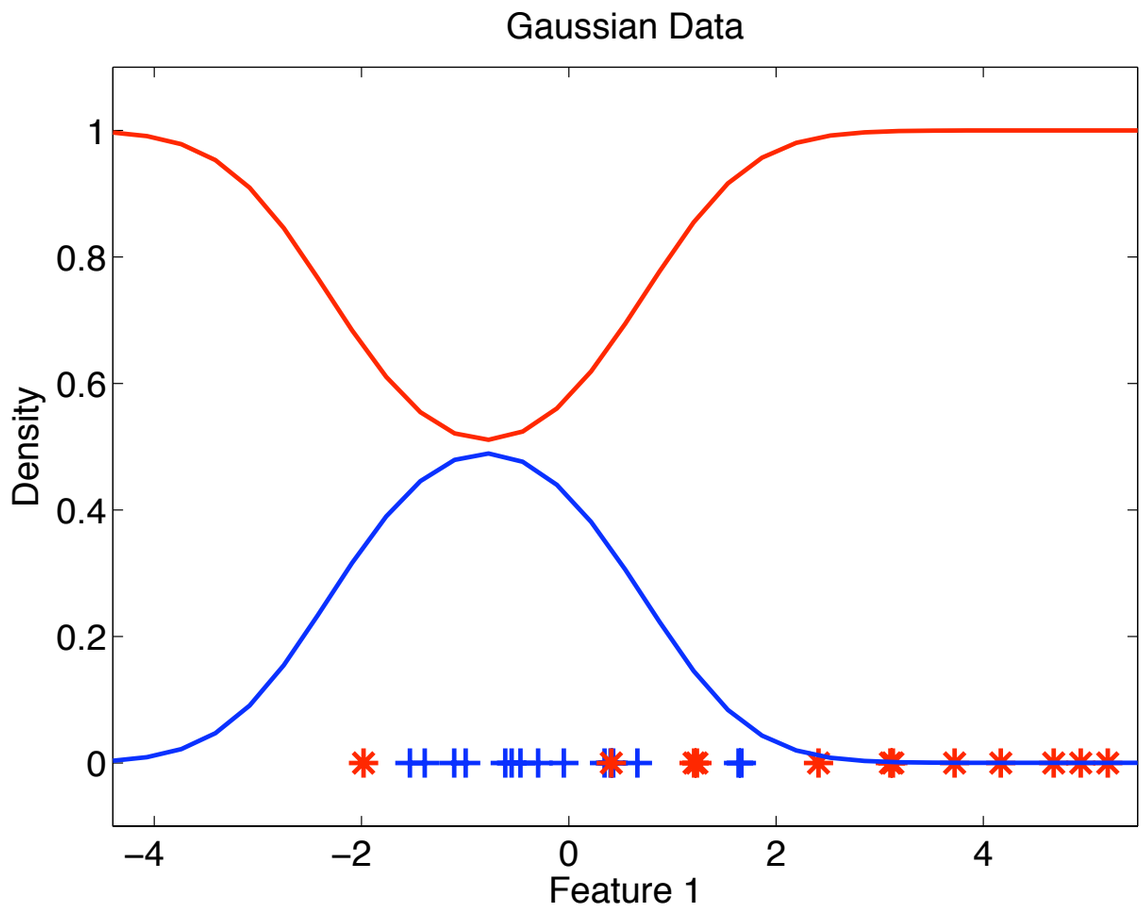
Missing decision boundary





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

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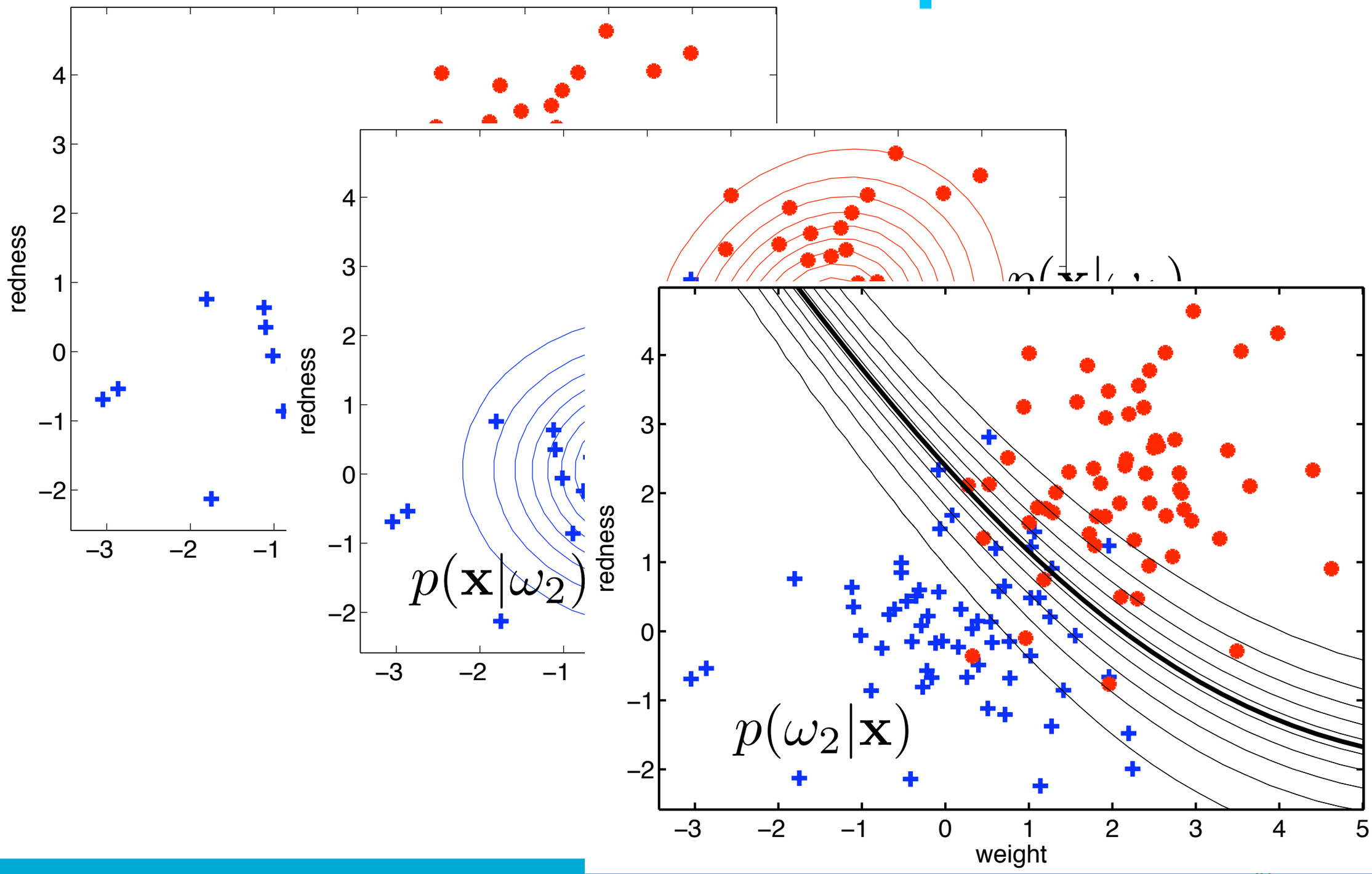
2-dimensional feature space



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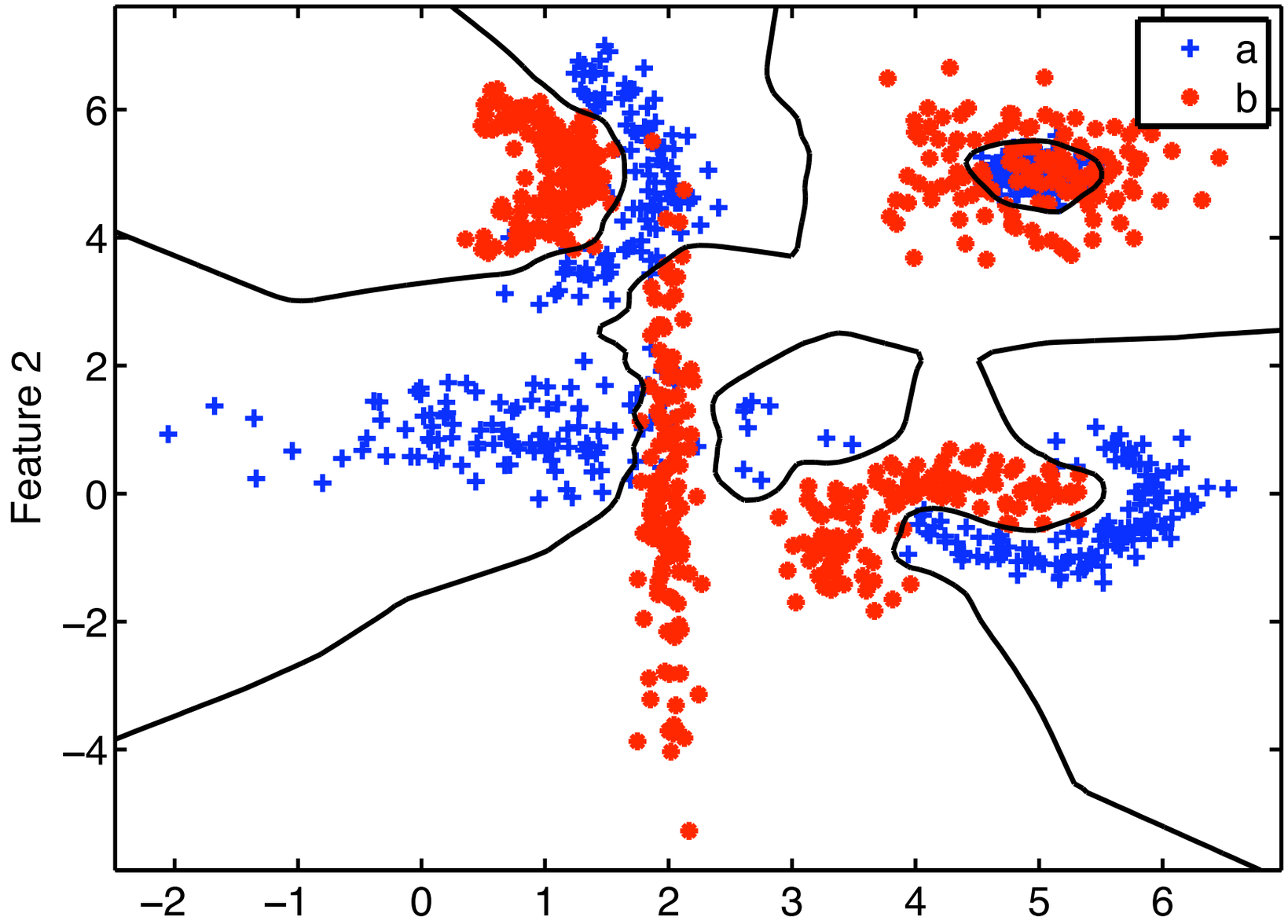
Multi-modal distributions



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

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The class conditional probabilities

- But, how do we obtain the class conditional probabilities $p(\mathbf{x}|\omega_i)$?
- Typically, you need to assume a model
- Estimate the model parameters such that the example objects fit well:
  maximum likelihood estimators
- This will be the topic for the coming weeks

- Note: other approaches than Bayes' rule are possible. We discuss it later…

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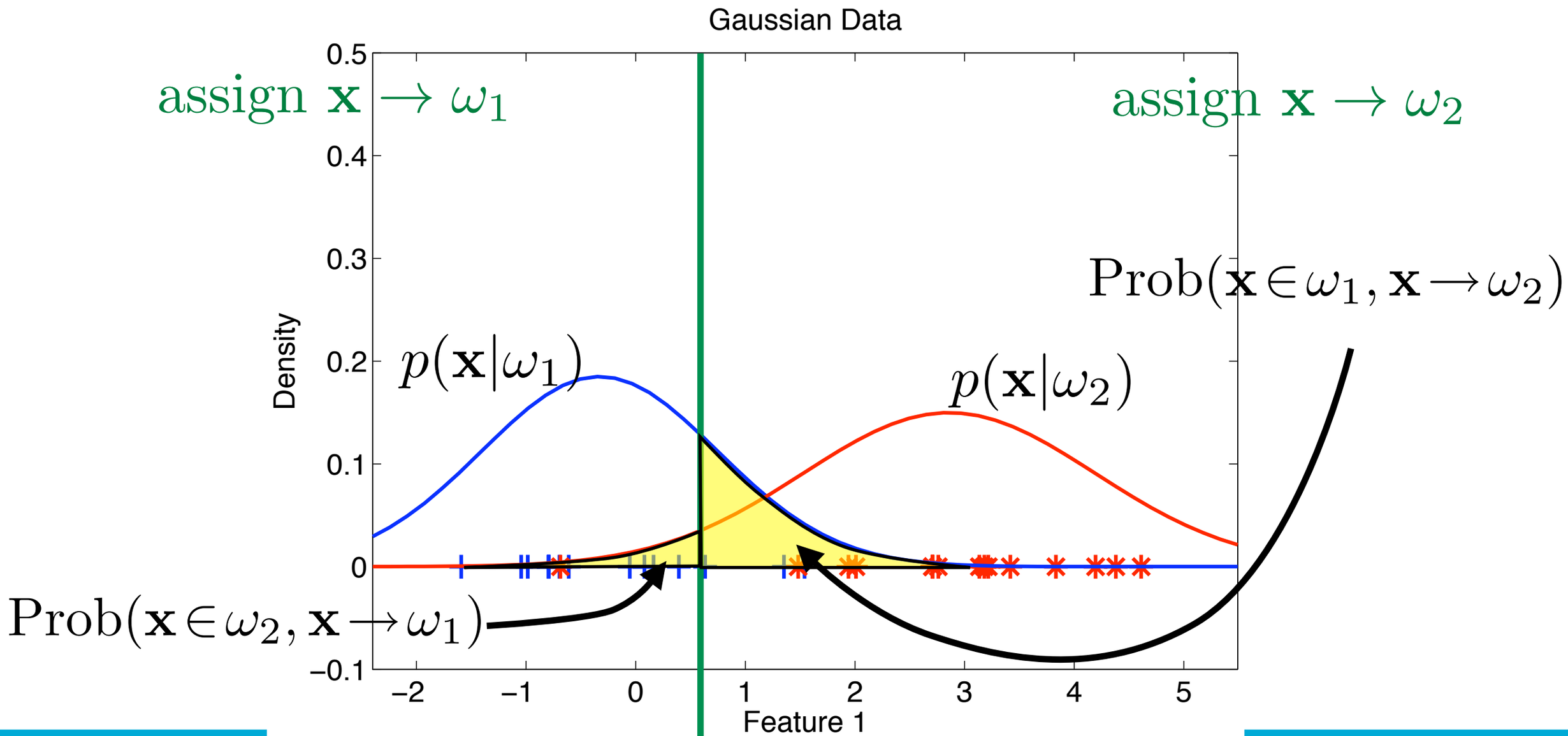
How good is it?

- The error of the green decision boundary:



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Error of type I and II

- For a two-class classification problem, the following two errors are defined:

- Type I error: $$\varepsilon_1 = \int_{\Omega_2} p(\mathbf{x}|\omega_1)d\mathbf{x}$$

- Type II error: $$\varepsilon_2 = \int_{\Omega_1} p(\mathbf{x}|\omega_2)d\mathbf{x}$$

- When we call ω_1 the positive class, and ω_2 the negative class, then ε_1 is the false negative fraction, and ε_2 is the false positive fraction.

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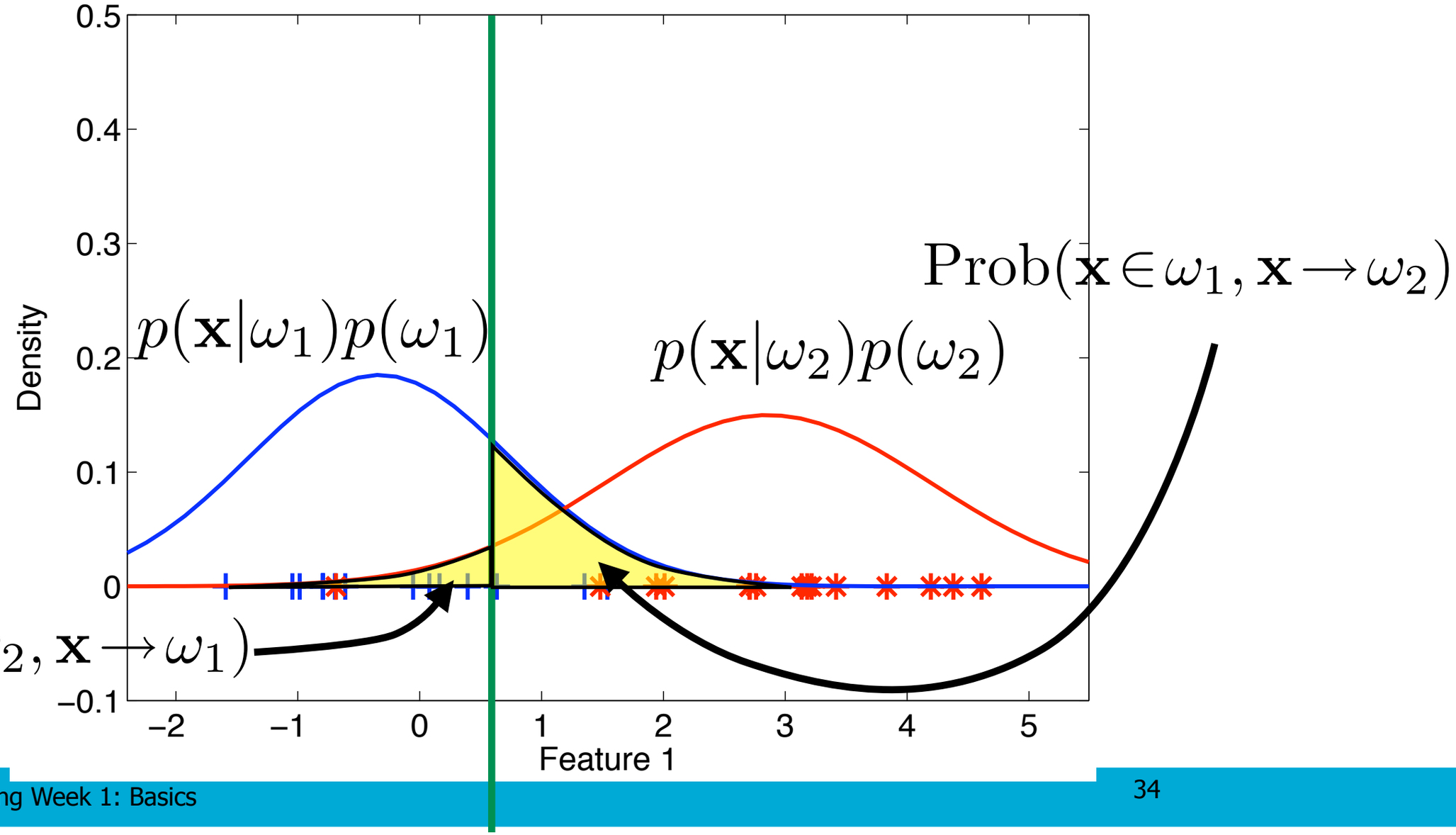
Classification error

- The error: $p(\text{error}) = \sum_{i=1}^{C} p(\text{error}|\omega_i)p(\omega_i)$



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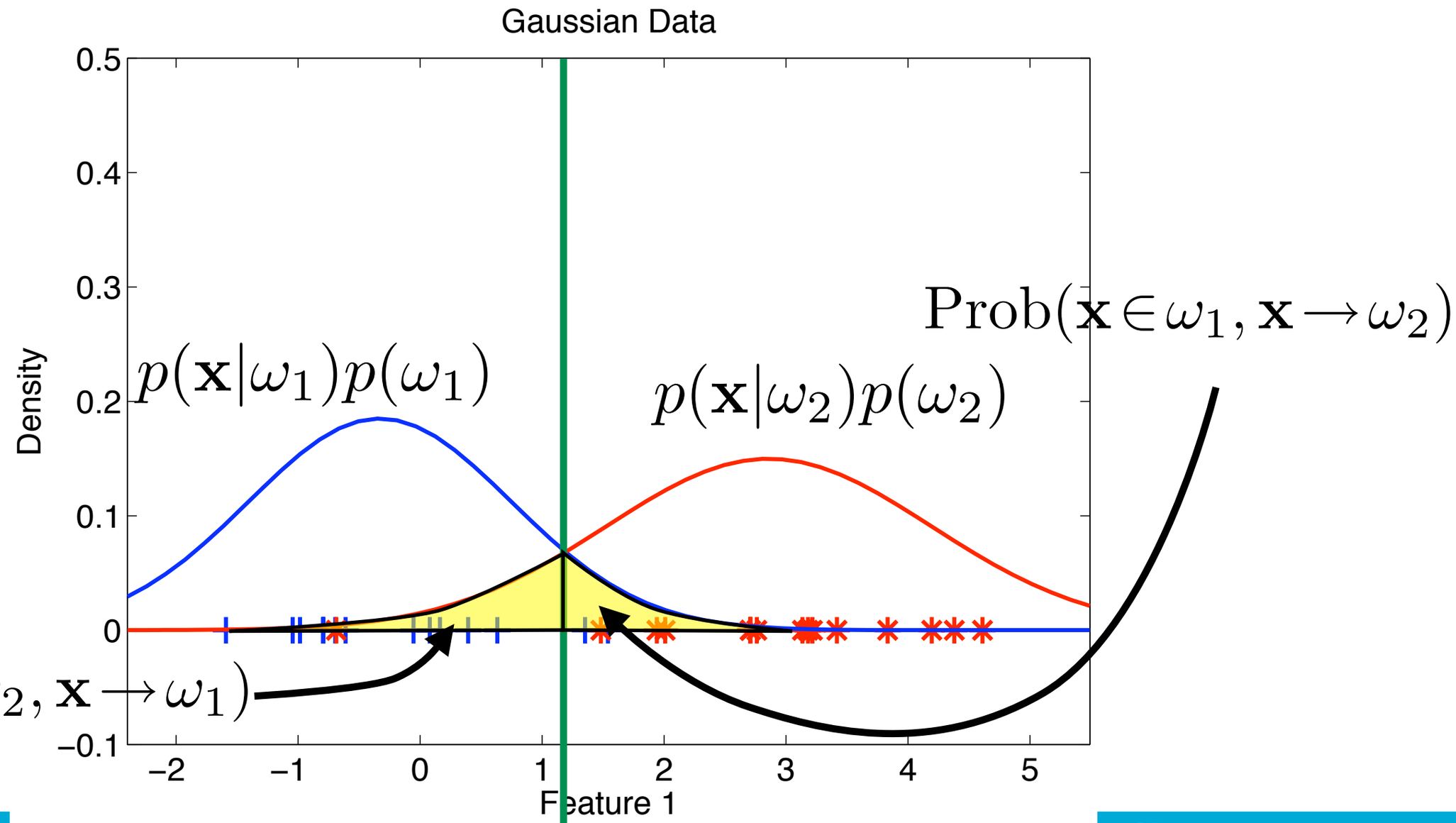
Bayes error ε^*

Bayes error is the **minimum** error: typically >0 !!



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Bayes' Error

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

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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' to 'ill'

misclassification:
classify 'ill' to 'healthy'

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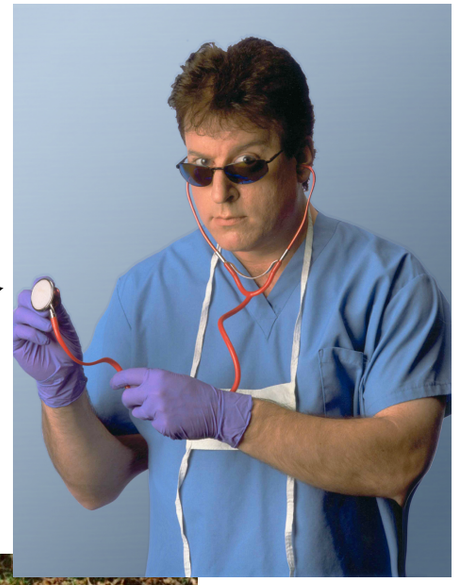
Misclassification cost

- Introduce a loss that measures the cost of assigning an object that came from class ω_j to class ω_i :

$$\lambda_{ji}$$

$$\lambda_{\text{healthy,ill}} = 10$$

$$\lambda_{\text{ill,healthy}} = 100$$



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Misclassification cost of some dataset

- Assume I have a labeled dataset $\mathcal{D} = \{(\mathbf{x}_i, \omega_i)\}_{i=1}^{N}$
- Further assume that these objects are classified by a classifier, and the estimated class labels are $\hat{\omega}_i$

- Then the total empirical risk on this dataset is

$$R = \frac{1}{N} \sum_{i=1}^{N} \lambda_{\omega_i, \hat{\omega}_i}$$

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Conditional risk, total risk

- The conditional risk of assigning object **x** to class ω_i :

$$l^i(\mathbf{x}) = \sum_{j=1}^{C} \lambda_{ji} p(\omega_j|\mathbf{x})$$

- The average risk over a region:

$$r^i = \int_{\Omega_i} l^i(\mathbf{x}) p(\mathbf{x}) d\mathbf{x}$$

- Overall risk:

$$= \int_{\Omega_i} \sum_{j=1}^{C} \lambda_{ji} p(\omega_j|\mathbf{x}) p(\mathbf{x}) d\mathbf{x}$$

$$r = \sum_{i=1}^{C} r^i = \sum_{i=1}^{C} \int_{\Omega_i} \sum_{j=1}^{C} \lambda_{ji} p(\omega_j|\mathbf{x}) p(\mathbf{x}) d\mathbf{x}$$

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Minimum total risk

- We minimize the risk when we define the regions Ω_i are chosen such that each of the integrals are as small as possible:

$$r = \sum_{i=1}^{C} r^i = \sum_{i=1}^{C} \int_{\Omega_i} \sum_{j=1}^{C} \lambda_{ji} p(\omega_j|\mathbf{x}) p(\mathbf{x}) d\mathbf{x}$$

- So make **x** part of Ω_i if:

$$\sum_{j=1}^{C} \lambda_{ji} p(\omega_j|\mathbf{x}) \leq \sum_{j=1}^{C} \lambda_{jk} p(\omega_j|\mathbf{x}) \quad k = 1, .., C$$

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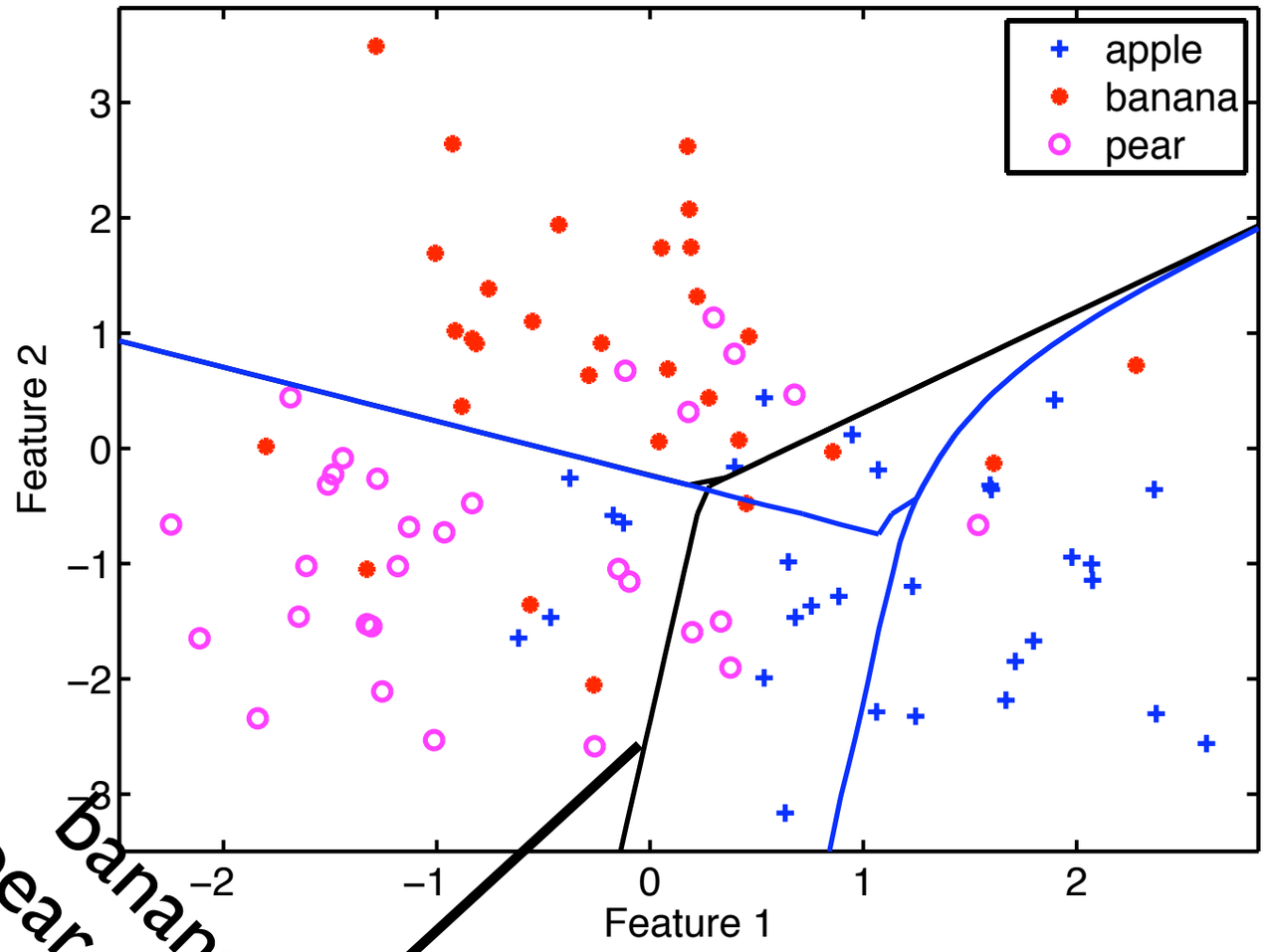
Example cost



classified

True	apple	pear	banana
apple	0	1	1
pear	1	0	1
banana	1	1	0

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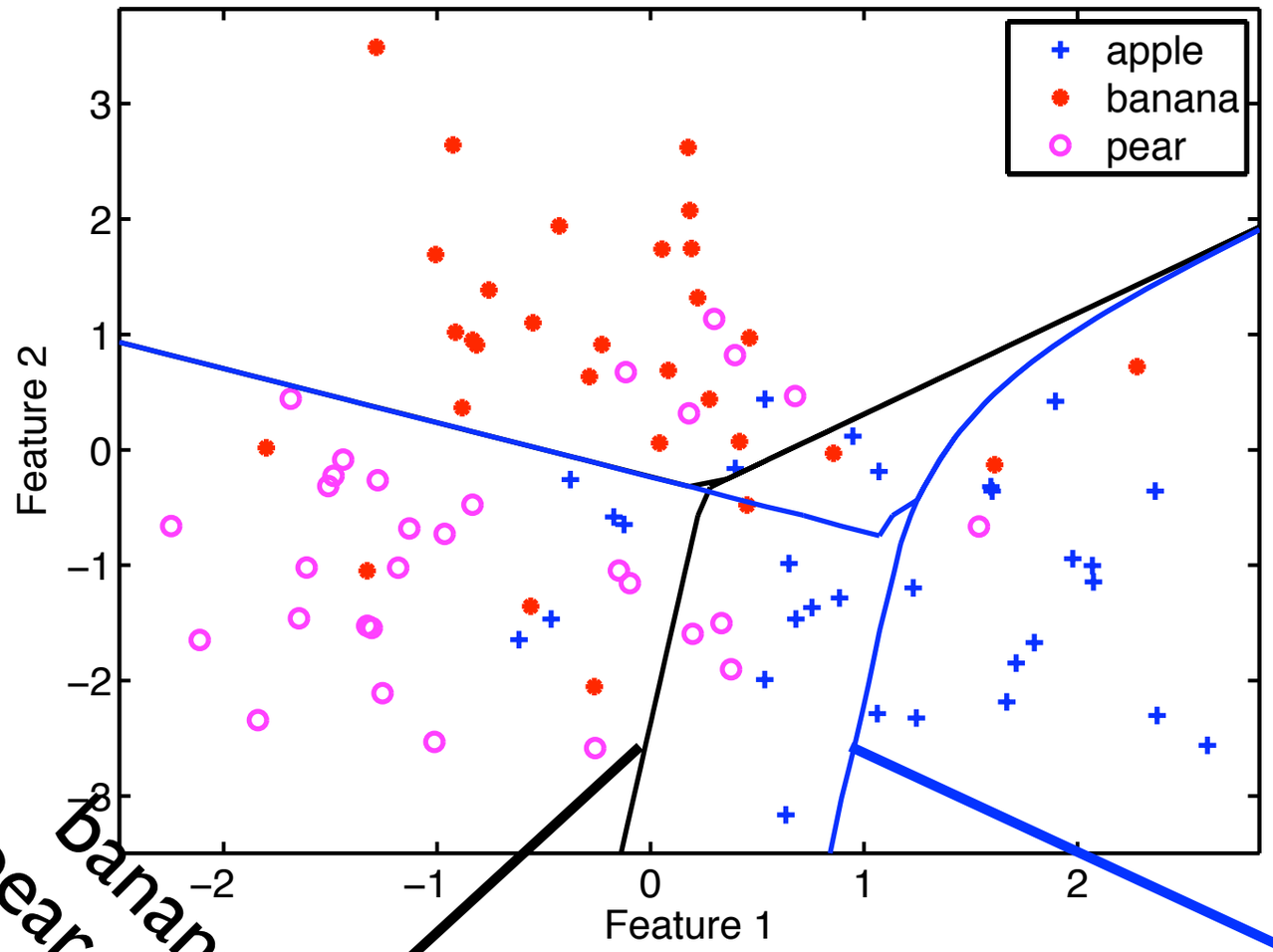
Example cost



$$\lambda_{2,1} = 9$$

Predicted: apple, pear, banana

True:

	apple	pear	banana
apple	0	1	1
pear	1	0	1
banana	1	1	0

Predicted: apple, pear, banana

	apple	pear	banana
apple	0	1	1
pear	9	0	1
banana	1	1	0

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What did we do?

- Objects, features, measurements,
- ... datasets and feature space
- Traditional pattern recognition: classification
- Class posterior probabilities and Bayes' rule
- Bayes' classifier and Bayes' error
- Misclassification costs

- Next week: how do we get these class-conditional probabilities?

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