Introduction to Combining Classifiers

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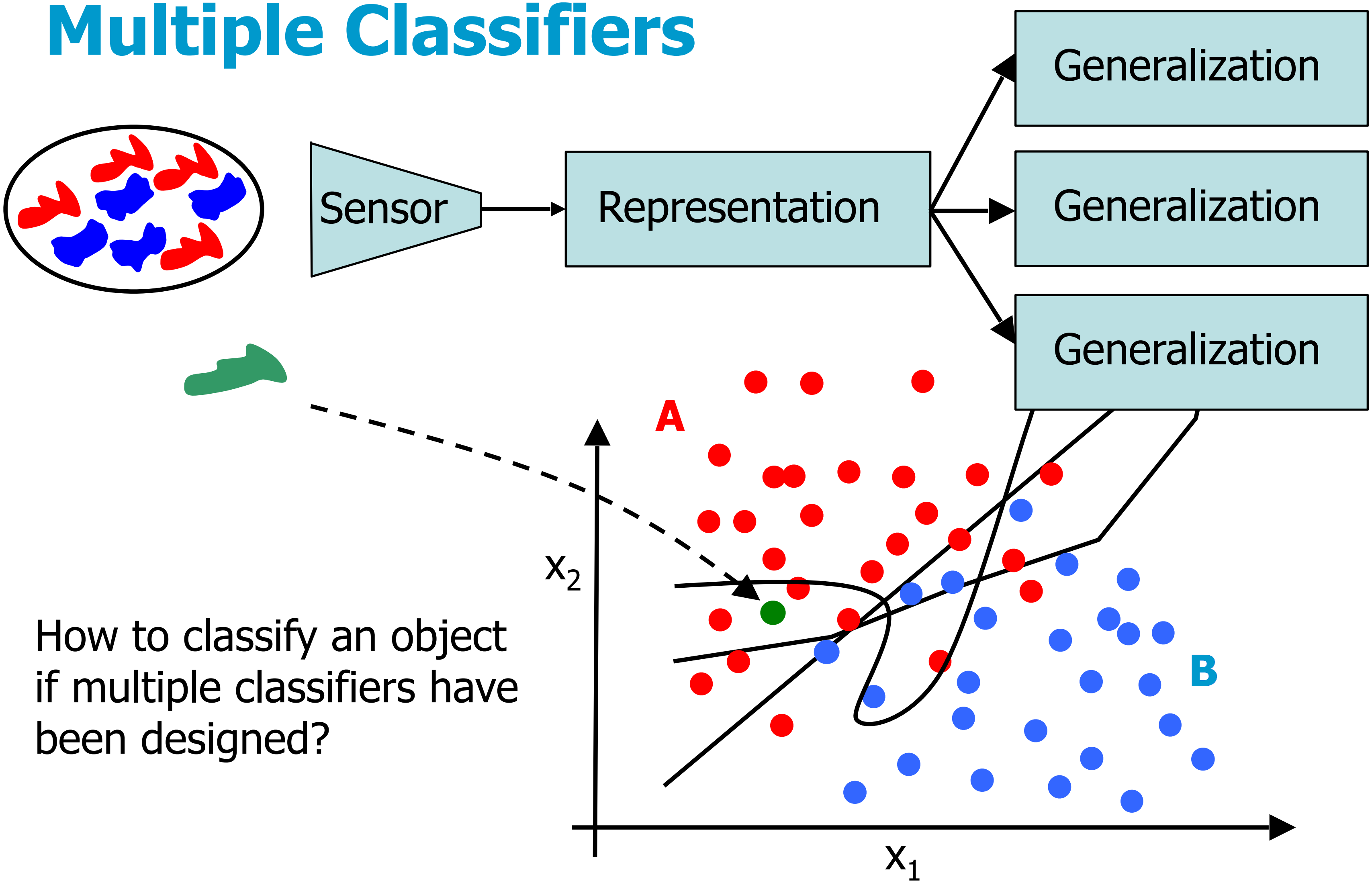
Multiple Classifiers



How to classify an object if multiple classifiers have been designed?

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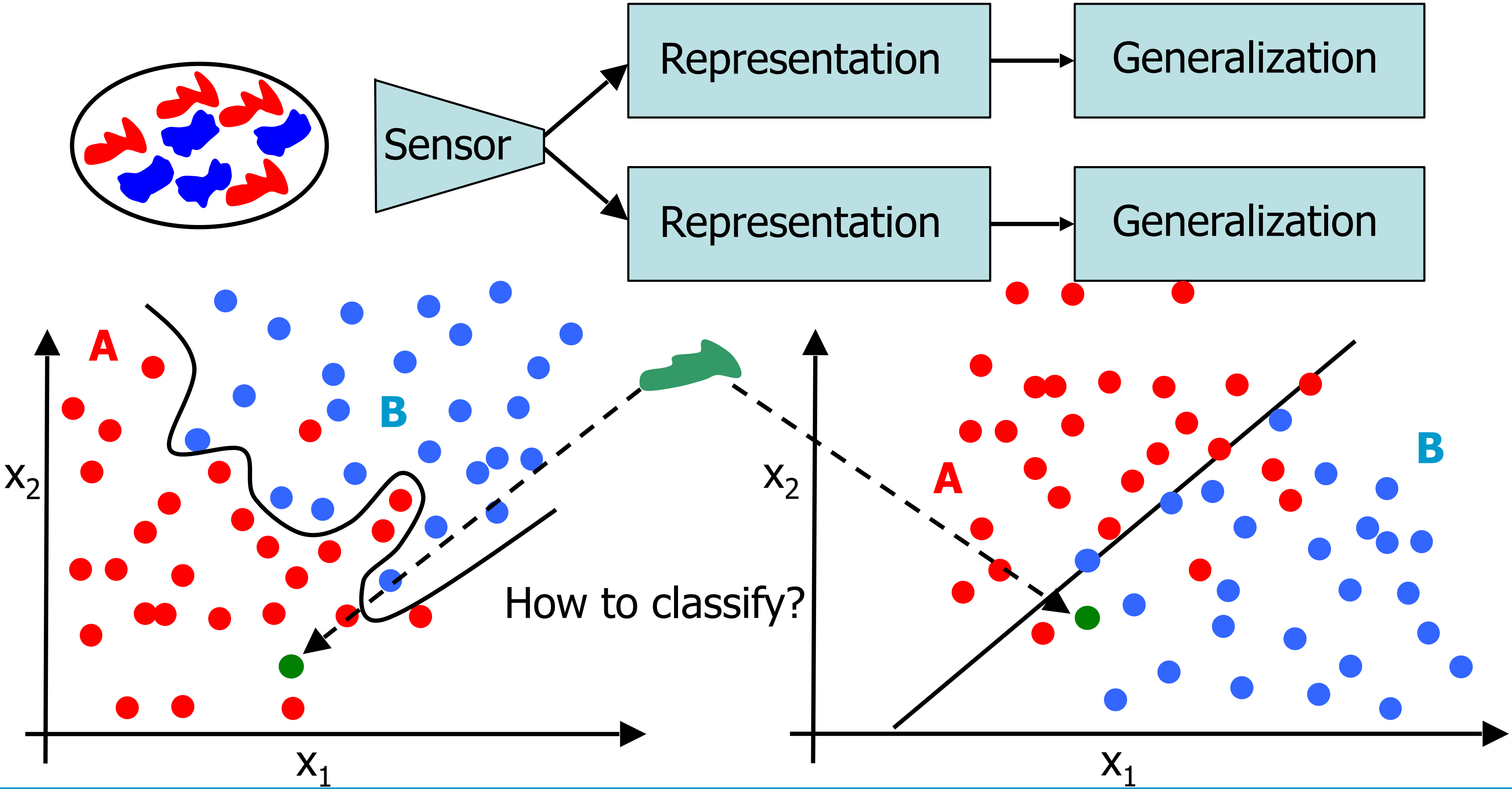
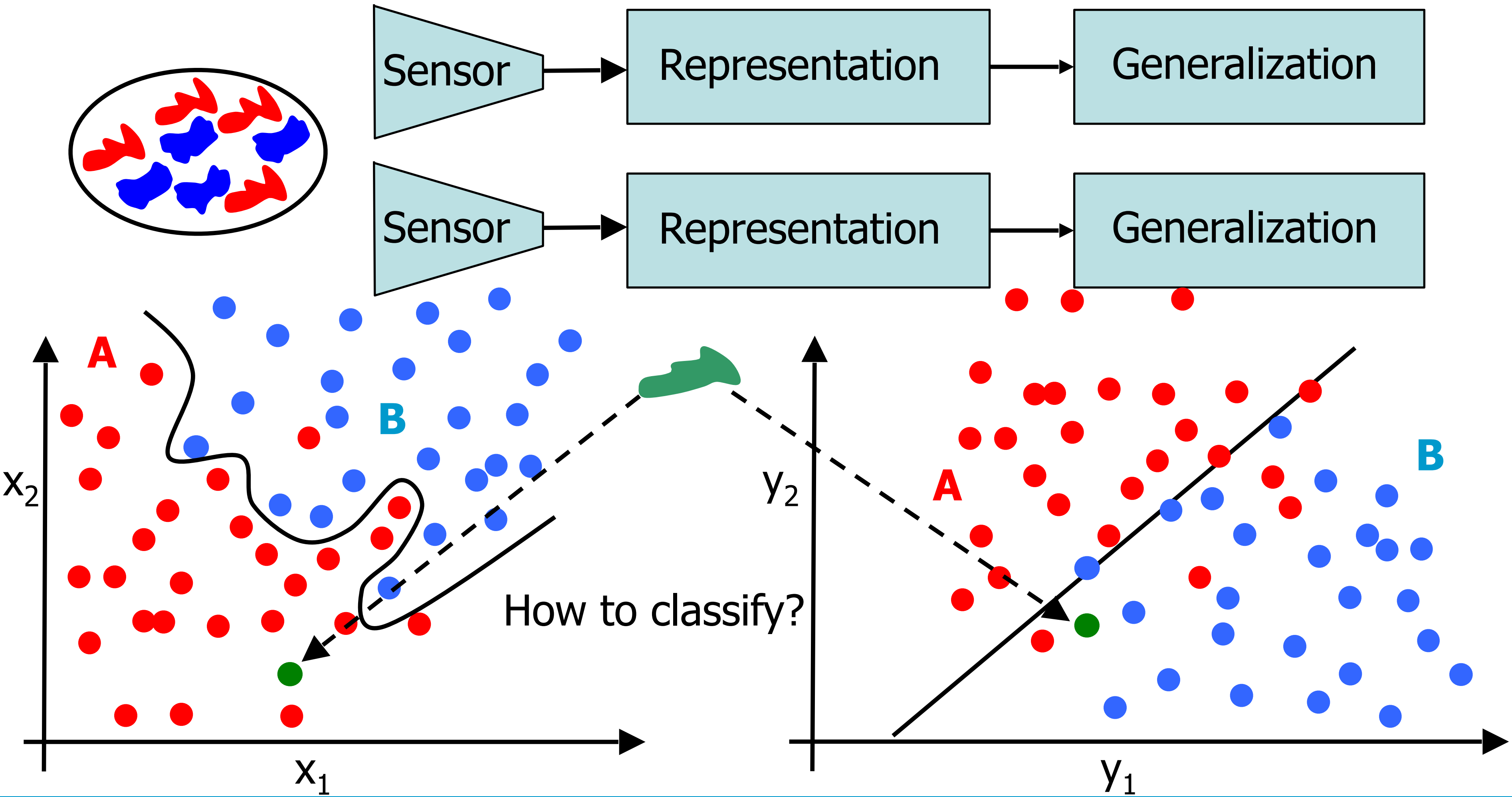
Multiple Representations



Multiple Sensors



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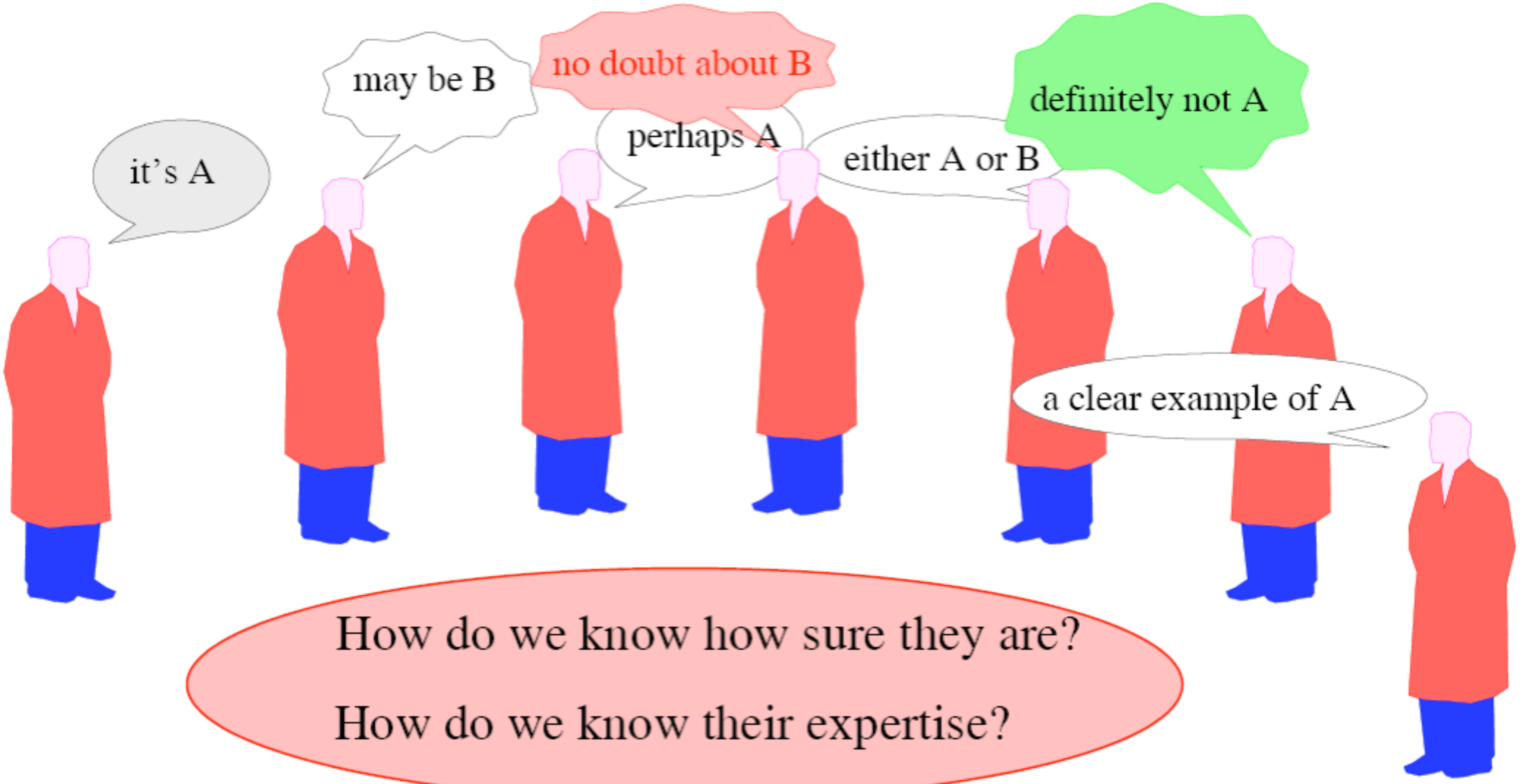
Multiple Experts



The Combiner and the Base Classifiers

The basic questions:

- How to reach a committee decision?

→ How to design a combining classifier?

- How to constitute a committee?

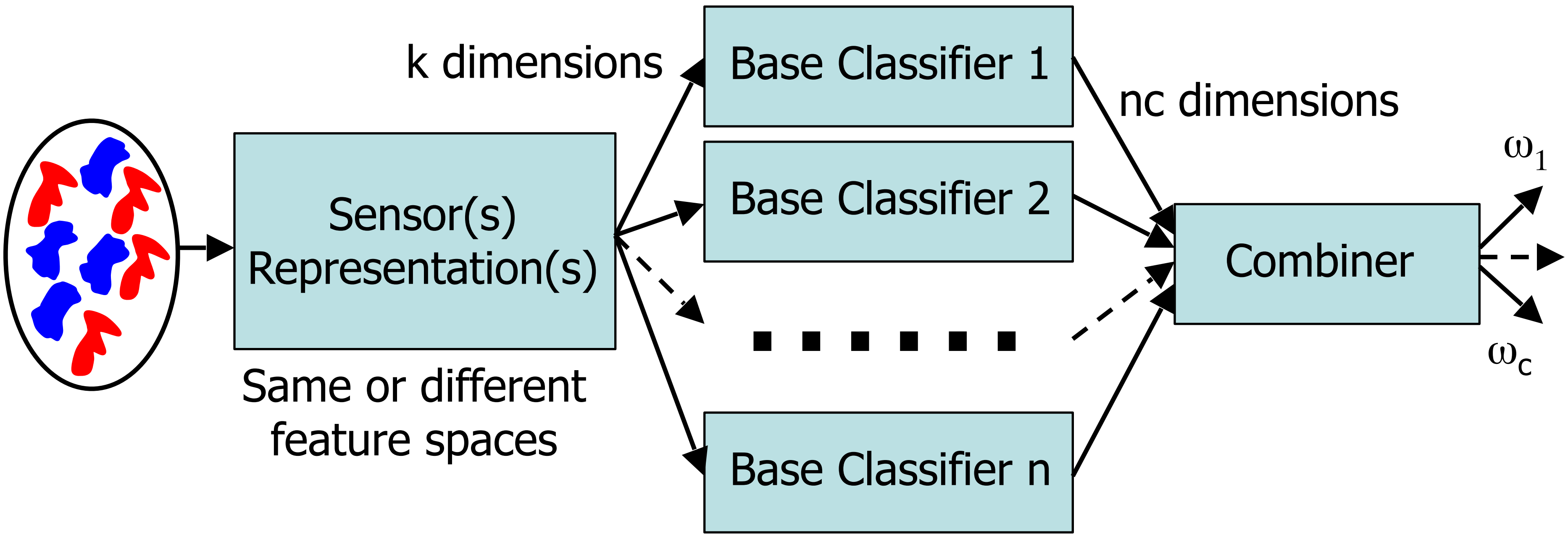
→ How to generate the base classifiers?

Combining Classifiers

Part I

The Combiner

Combining Classifier Architecture



Combining scheme

- Objects: $\{o_i\}$
- Features: $x = F(o)$

  User defined representation
- Base classifiers: $y = S(x \mid par\_base)$

  par_base : parameters optimized by training set
- Combining classifier $z = C(y \mid par\_comb)$

  par_comb : parameters optimized by training set
  (sometimes fixed, untrained combiners are used)

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Combiners

- Fixed rules based on crisp labels or confidences (estimated posterior probabilities).
- Special trained rules based on ‘classifier confidences’.
- General trained rules interpreting base-classifier outputs as features.

Fixed Combining Rules

$$C(y) = \omega_i \text{ if } \operatorname{argmax}_i(\text{comb\_rule}_{j|i}(y_{ij} = S_{ij}(x_j))) = i$$

An object is assigned to class ω_i if the combination of the outcomes y_{ij} for class ω_i over all classifiers $y_j = S_j(x)$ is maximum.

- Voting, over labels $y_{ij} \in \{0,1\}$
- Product, minimum $y_{ij} \in [0,1]$
- Sum, median $y_{ij} \in [0,1]$
- Maximum $y_{ij} \in [0,1]$

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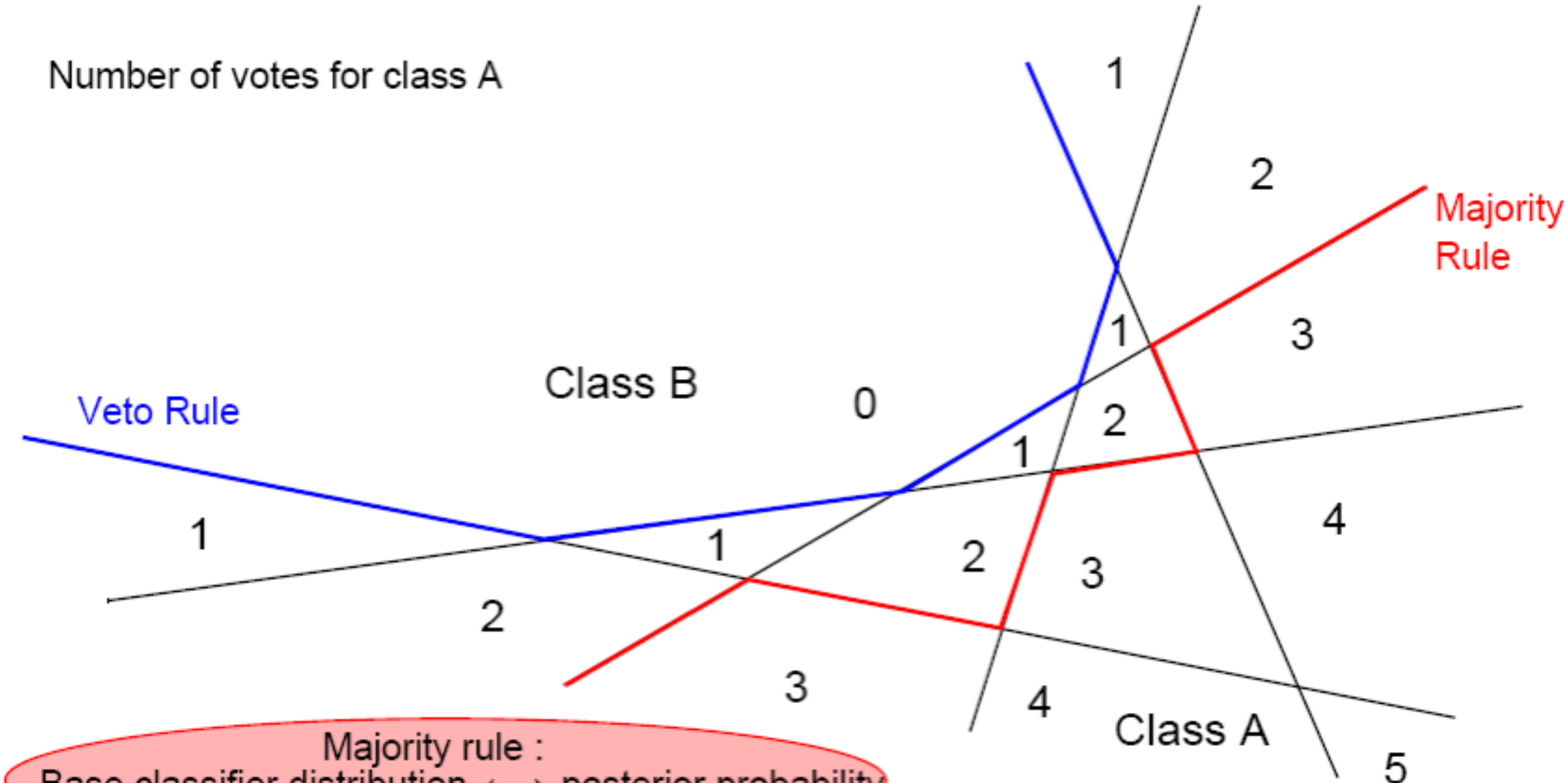
Voting; Majority Rule, Veto Rule



Majority rule :
Base classifier distribution $\longleftrightarrow$ posterior probability

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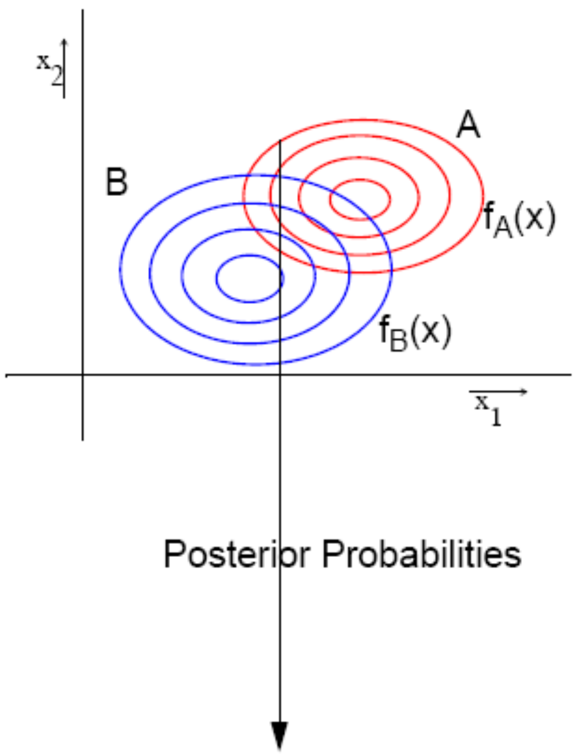
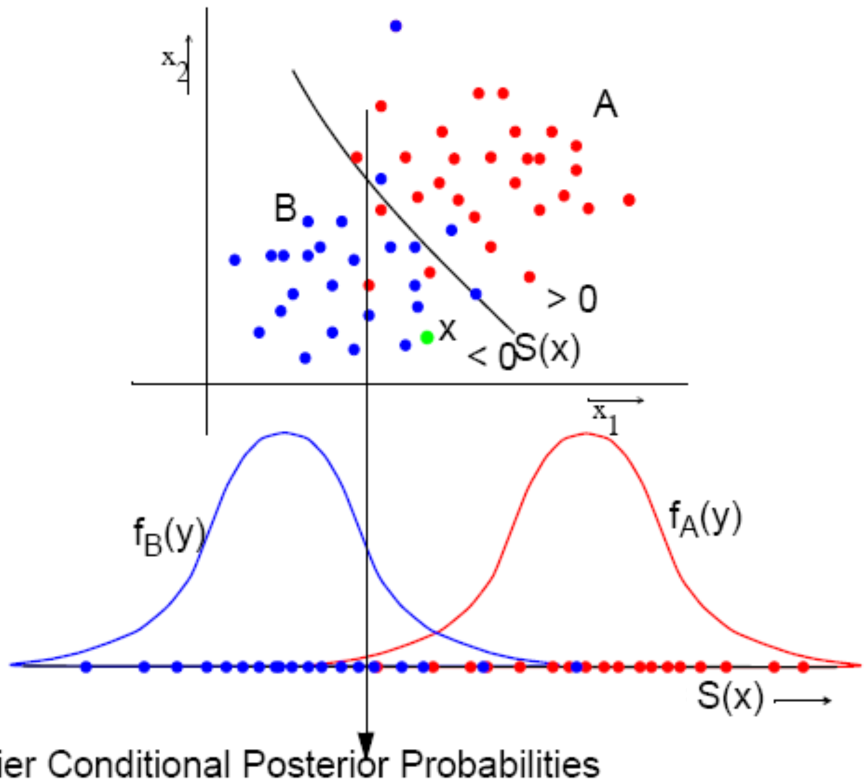
Confidences, Posterior Probabilities



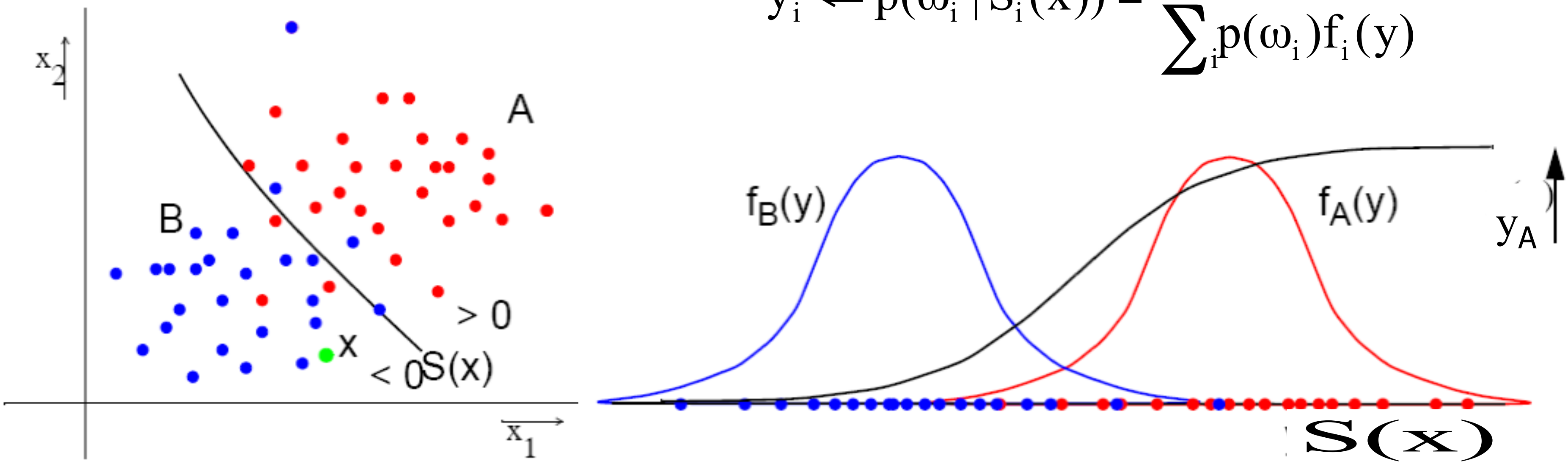


$$y_i = S_i(x) = p(\omega_i \mid x) = \frac{p(\omega_i) f_i(x)}{\sum_i p(\omega_i) f_i(x)}$$

$$y_i \Leftarrow p(\omega_i \mid S_i(x)) = \frac{p(\omega_i) f_i(y)}{\sum_i p(\omega_i) f_i(y)}$$

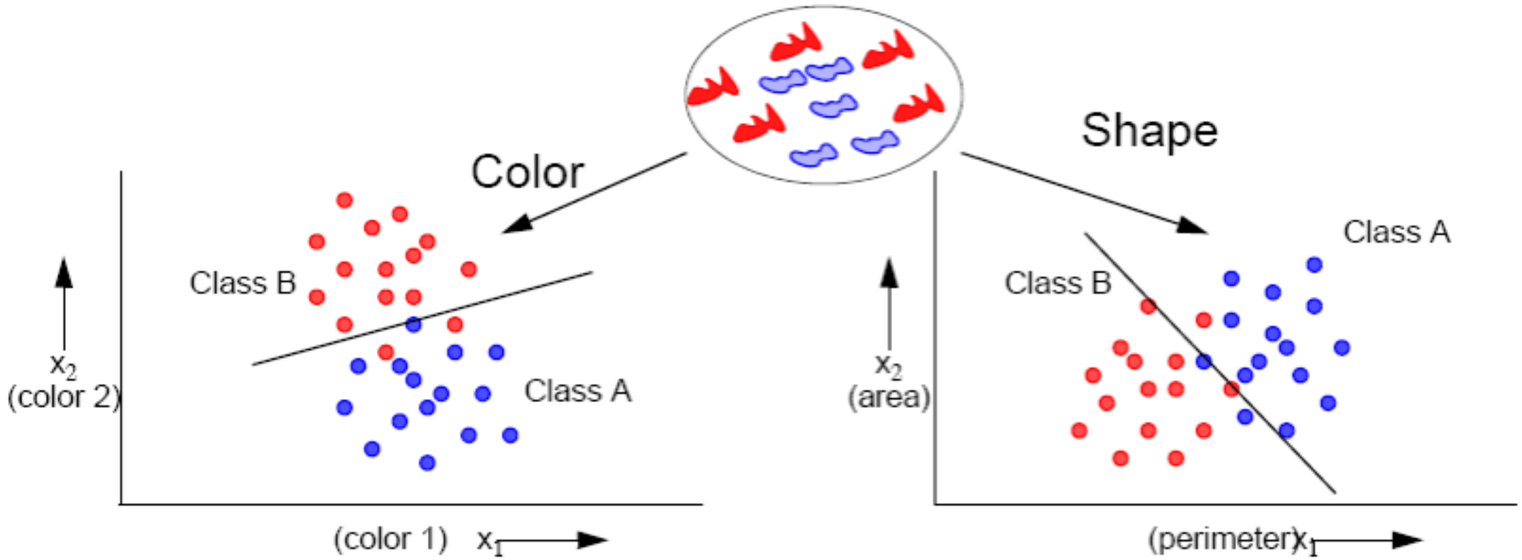
Optimal Scaling for Classifier Conditional Posterior Probabilities

$$y_i \Leftarrow p(\omega_i \mid S_i(x)) = \frac{p(\omega_i) f_i(y)}{\sum_i p(\omega_i) f_i(y)}$$



Fit a logistic function or sigmoid to the data such that $\prod_{x \in \text{Trainingset}} y(S(x))$ is maximum conditional to $y = 0.5$ for $S(x) = 0$.

Combining Different Representations



Base classifier j posterior probabilities for class A : $y_{A_j} = \mathrm{Prob}_j(A|x_j)$

Product Rule: $y_A = \prod \mathrm{Prob}_j(A|x_j)$, $y_B = \prod \mathrm{Prob}_j(B|x_j)$,

prodc

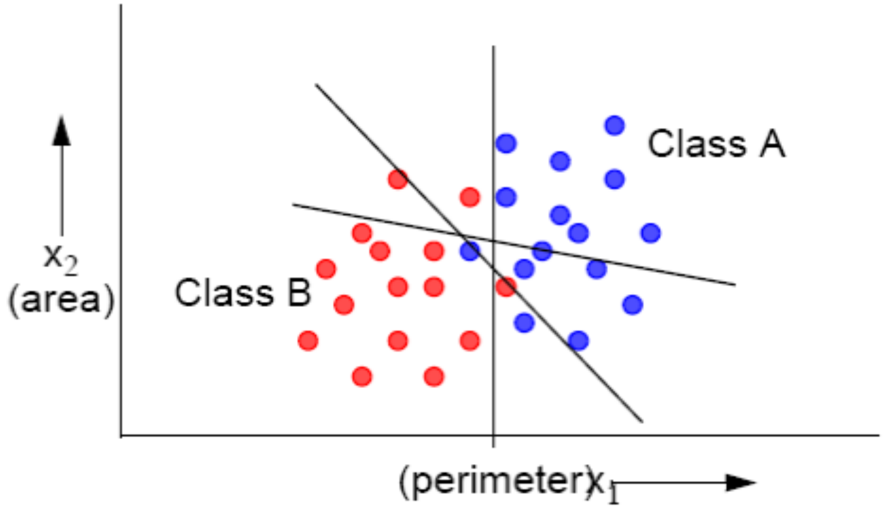
Useful for 'independent' feature spaces (logical 'AND', experts should agree)

Minimum Rule: $y_A = \mathrm{Min}\{\mathrm{Prob}_j(A|x_j)\}$, $y_B = \mathrm{Min}\{\mathrm{Prob}_j(B|x_j)\}$

Assign according to 'least objecting expert'

minc

Combining Different Classifier Estimates



Base classifier j posterior probabilities for class A : $y_{Aj} = \mathrm{Prob}_j(A|\mathbf{x})$

meanc

Sum (Mean) Rule: $y_A = \sum \mathrm{Prob}_j(A|\mathbf{x})$, $y_B = \sum \mathrm{Prob}_j(B|\mathbf{x})$,

Useful for improved estimates of posterior probabilities

Also: Median and Majority Voting

medianc

Improvement by averaging out mistakes of experts

The Product and the Minimum Rule

Base classifier j posterior probabilities for class A : $y_{A_j} = \mathrm{Prob}_j(A|x_j)$

Product Rule: $y_A = \prod \mathrm{Prob}_j(A|x_j)$, $y_B = \prod \mathrm{Prob}_j(B|x_j)$,

Useful for 'independent' feature spaces, see *Kittler, IEEE-PAMI-20(3),1998*

Minimum Rule: $y_A = \mathrm{Min}\{\mathrm{Prob}_j(A|x_j)\}$, $y_B = \mathrm{Min}\{\mathrm{Prob}_j(B|x_j)\}$

Assign according to 'least objecting classifier'

objects	Classifier 1		Classifier 2		Product		Minimum	
	Class A	Class B	Class A	Class B	Class A	Class B	Class A	Class B
1	0.4	0.6	0.2	0.8	0.08	0.48	0.2	0.6
2	0.1	0.9	0.7	0.3	0.07	0.27	0.1	0.3
3	0.3	0.7	0.4	0.6	0.12	0.42	0.3	0.6
4	0.5	0.5	0.2	0.8	0.10	0.40	0.2	0.5
5	0.0	1	0.9	0.1	0.00	0.10	0.0	0.1
6	0.8	0.2	0.2	0.8	0.16	0.16	0.2	0.2

Fixed Combining Rules Overview

Product, Minimum

- Independent feature spaces
- Different areas of expertise
- Error free posterior probability estimates

prodc minc

Ever optimal?

Sum (Mean), Median, Majority Vote

- Equal posterior-estimation distributions in same feature space
- Differently trained classifiers, but drawn from the same distribution
- Bad if some classifiers (experts) are very good or very bad

meanc majorc

Maximum

- Trust the most confident classifier / expert
- Bad if some classifiers (experts) are badly trained

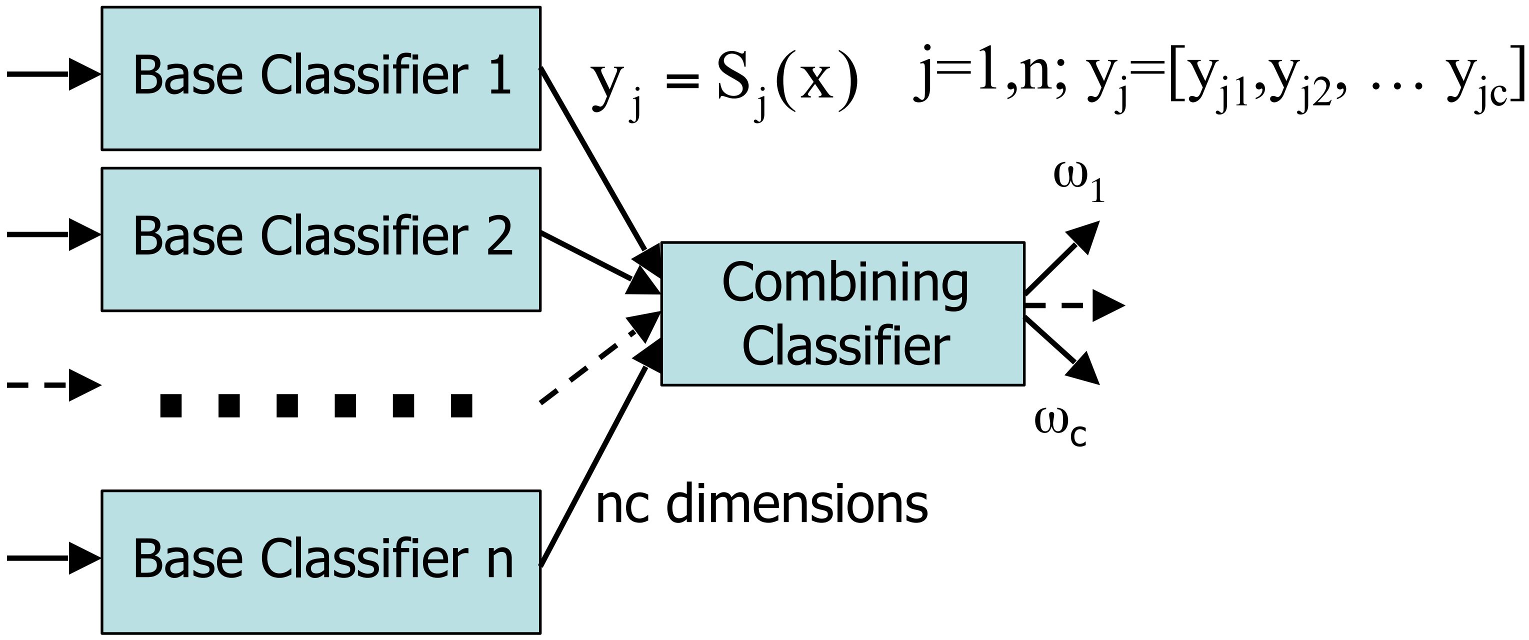
maxc

Fixed Combining Rules are Sub-optimal

- Base classifiers are never really independent (product)
- Base classifiers are never really equally imperfectly trained (sum, median, majority)
- Sensitivity to over-confident base classifiers (product, min, max)

- Fixed combining rules are never optimal
- Larger training sets do not really improve this (except max?)

Trained Combiners



General rules neglect the classification-confidence characteristic of the base classifier outputs, as they are treated as general feature values.

Trained Combiners (2)

Special Trained Combiners

- DT: Decision Templates (~ Nearest Mean)
- (BKS: Behavioral Knowledge Space)
- (DCS: Dynamic Classifier Selection)
- (ECOC: Error Correcting Output Coding)
- NN: Neural Networks

General Classifiers

- Nearest Mean
- Fisher
- Decision Trees
- ……

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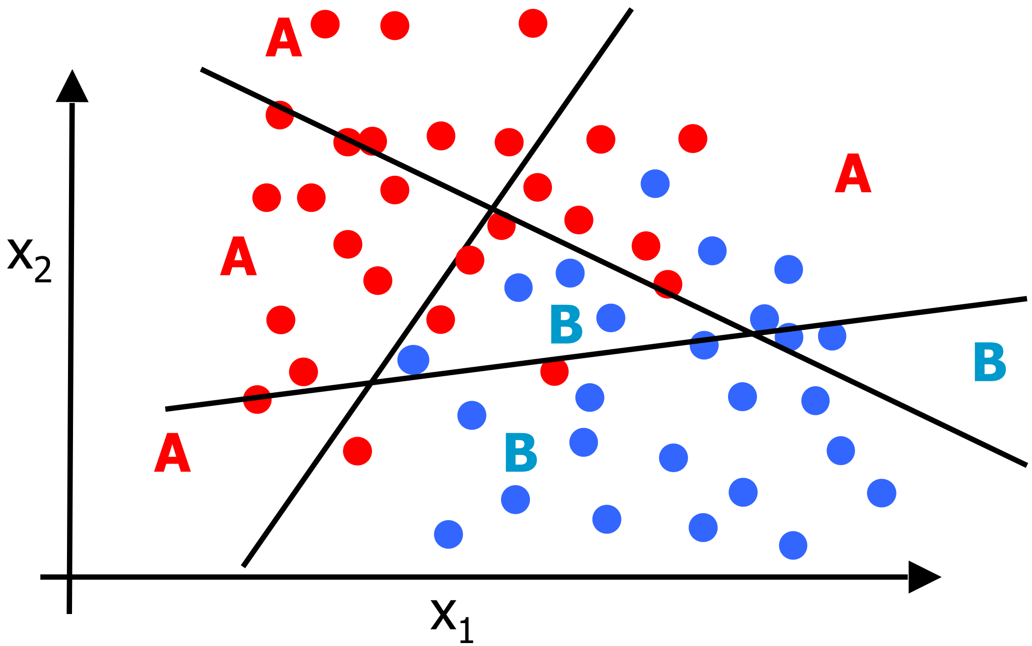
Decision Templates

- Determine, using a training set, the average outcomes of the base classifiers per class (decision templates, i.e. class means in the base-classifier outcome space).

- Assign new objects to the class of the nearest decision template in the base-classifier outcome space.

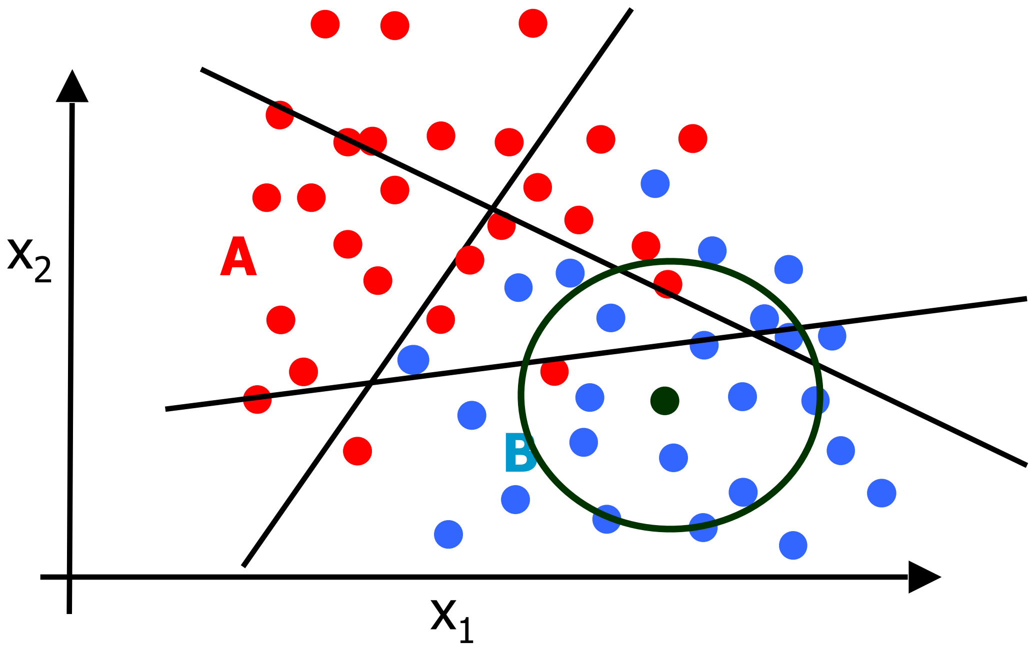
(Issue: is it good to have posterior probabilities for the base-classifier outputs, or yield inverse sigmoids a better scaling?)

Behavioral Knowledge Space



Determine on the basis of a training set for every cell in the original feature space the preferred class and assign new objects accordingly.

Dynamic Classifier Selection



- Select the classifier that classifies most of the k nearest neighbors of a test object correctly.

- Use this classifier to classify the test object.

ECOC: Error Correcting Output Coding

- ECOC is a system to use a small set of binary (i.e. two-class) classifiers for a large set of c classes.
- n classifiers can distinguish at most $c=2^n$ classes.
- If $n > {}^2\log(c)$ the system of classifiers is more robust
- ECOC studies mainly discuss the coding scheme, not the way base classifiers are trained. Combining is done by using the crisp, {0,1}-labels.

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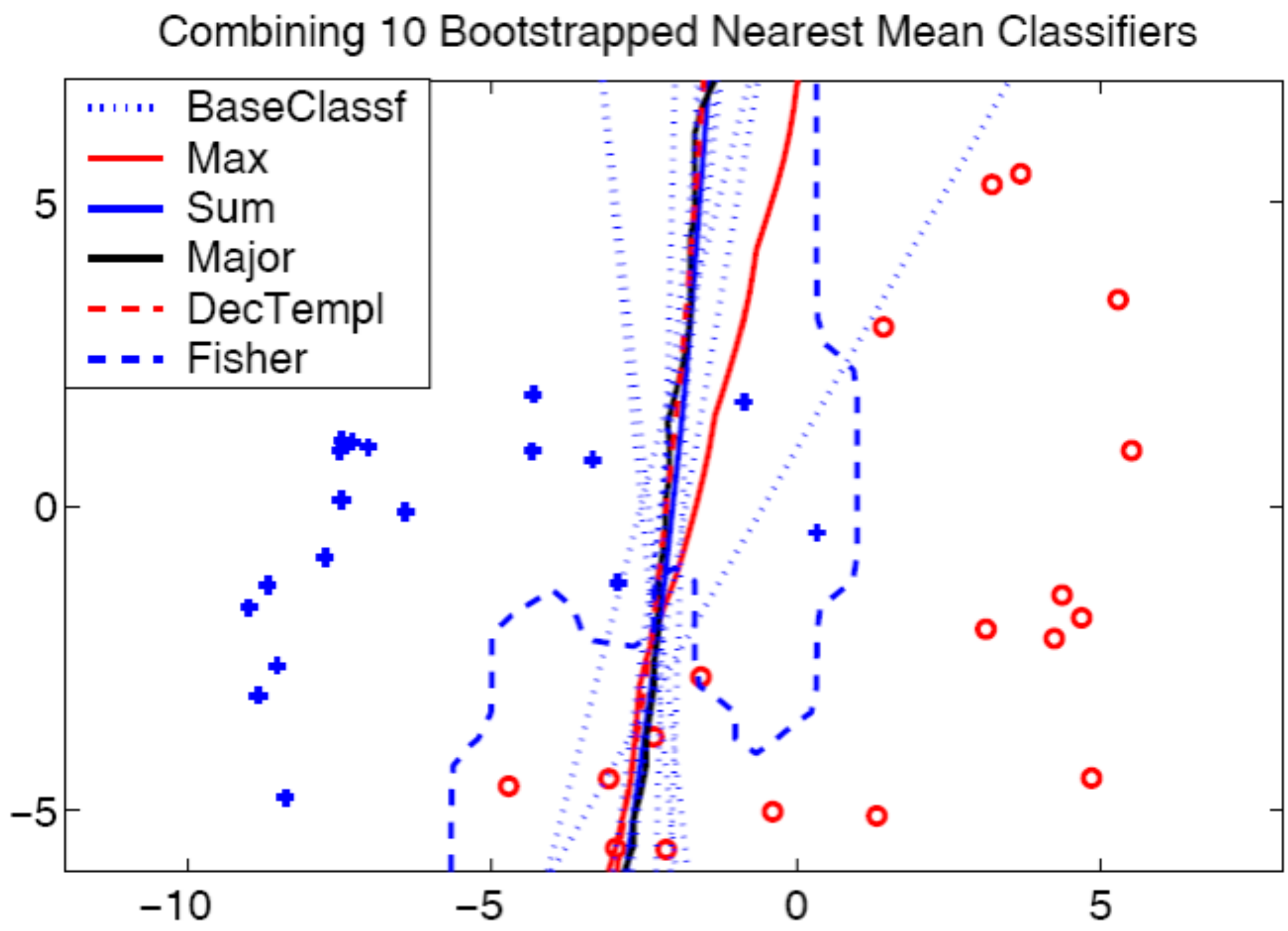
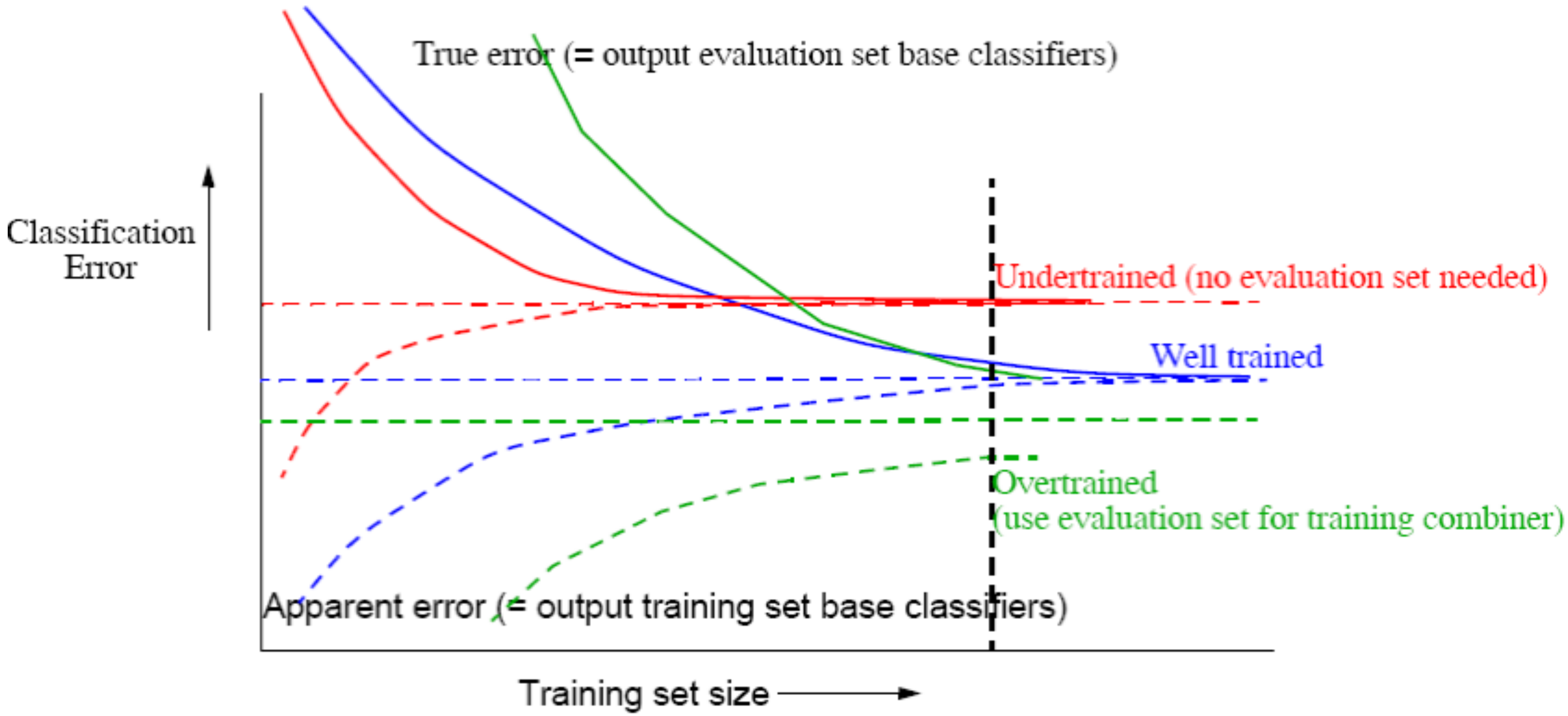
Example



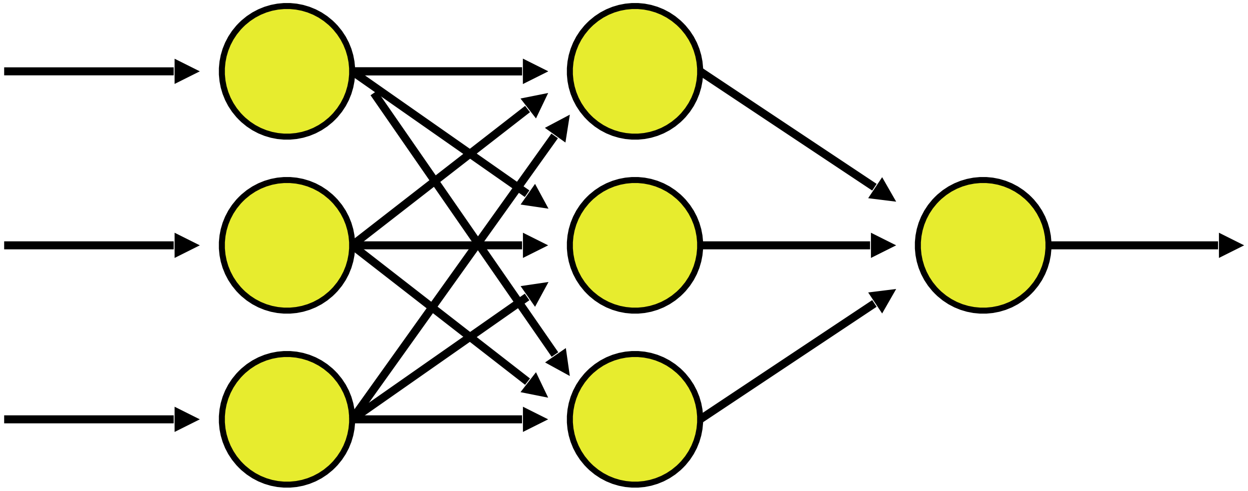
Combining 10 Bootstrapped Nearest Mean Classifiers
BaseClassf
Max
Sum
Major
DecTempl
Fisher
5
0
−5
−10
−5
0
5

Undertrained, Well Trained, Overtrained



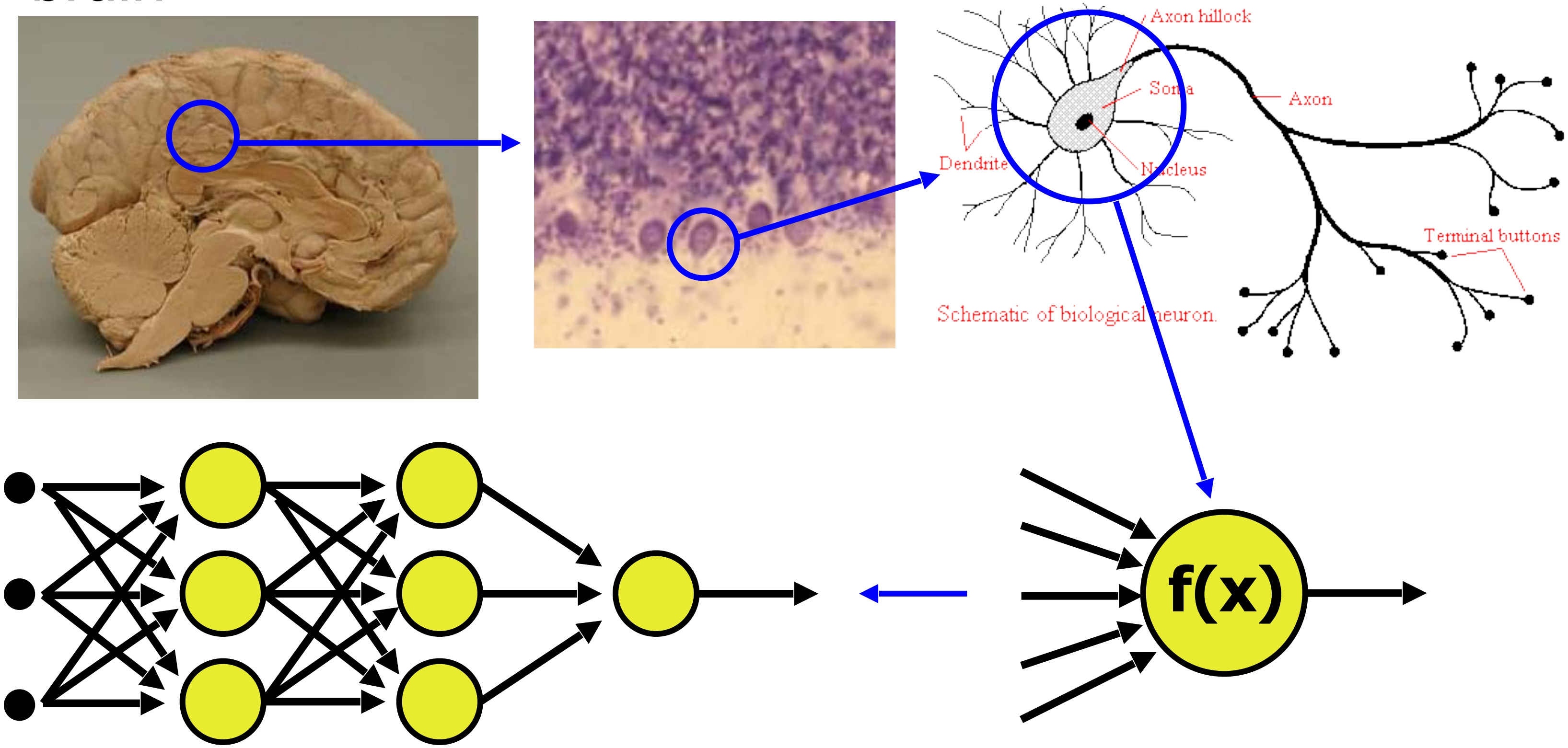
Artificial neural networks (1)

- Large, densely interconnected networks of simple processing units



Artificial neural networks (2)

- Some (not all!) networks originally inspired by the brain



Artificial neural networks (3)

- Research started in the 1950s
- Took off after 1986 – big hype for about 10-15 years
  - brought together psychologists, neurologists, philosophers, machine learners, statisticians...
  - helped thinking about, among others, pattern recognition
  - resulted in a lot of grant money

- Now: useful tool in many areas, with many pitfalls

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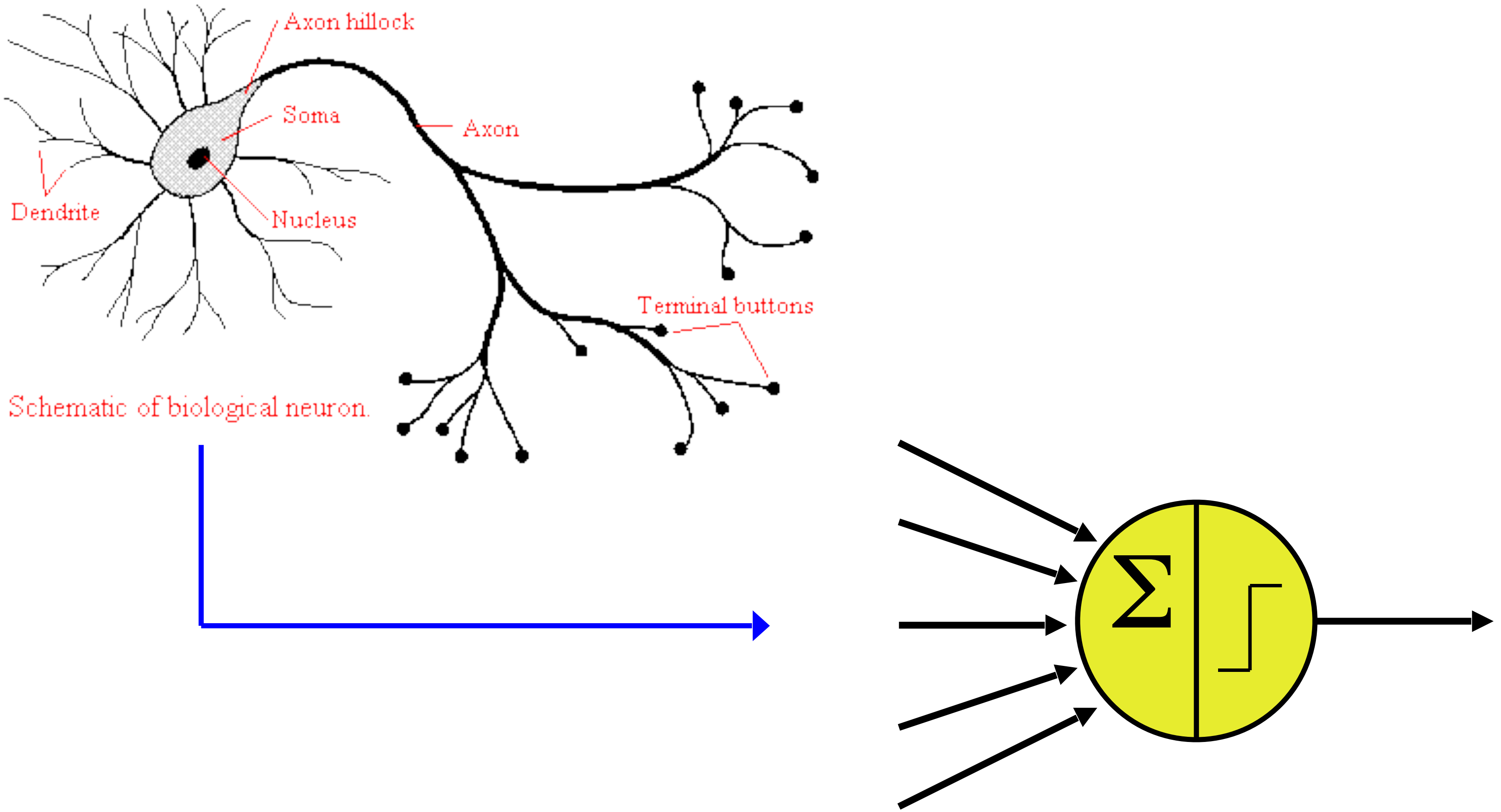
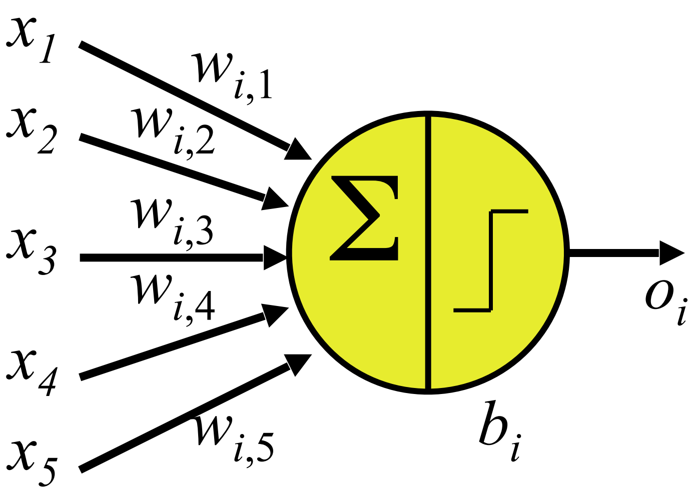
History

- 1943 : McCulloch and Pitts: model of neuron
- **1958** : Rosenblatt: perceptron
- 1960s : Rosenblatt, Nilsson work on perceptrons
- 1968 : Minsky and Papert point out limitations: perceptrons are linear
- 1982 : Hopfield network (associative memory), Kohonen's self-organising map (clustering), Fukushima's Neocognitron (vision)
- **1986** : Rumelhart, Hinton and Williams: training of nonlinear networks
- 1980s, 1990s: various theoretical developments
- 2010s : More data, faster hardware (GPUs)

McCulloch-Pitts model



McCulloch-Pitts model (2)



weights inputs

output $$o_i = \phi\left(\sum_j w_{ij} x_j - b_i\right)$$

threshold or bias

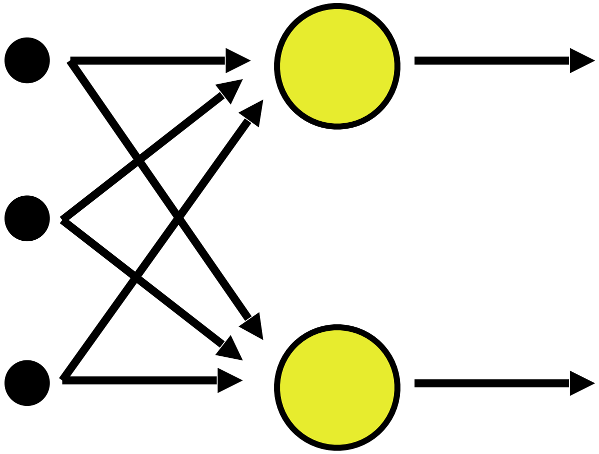
with $$\phi(a) = \begin{cases} 1 & a \geq 0 \\ 0 & a < 0 \end{cases}$$

or $$\phi(a) = \frac{1}{1 + \exp(-a)}$$

transfer function
or
activation function

Perceptron

- Networks of McCulloch-Pitts models can perform universal computation, given the right weights $\boldsymbol{w}$: it can do anything a binary computer can do
- ...but how can we find the right weights $\boldsymbol{w}$?
- Rosenblatt (1956): possible for single layer networks, perceptrons



Perceptron (2)

- Perceptron is a trainable two-class linear discriminant
- Training algorithm can be proven to converge to correct solution for separable classes
- Possible to extend to multiple classes
- When classes are not linearly seperable:
  - indefinite training, weights will blow up
  - solution: decrease ρ during training

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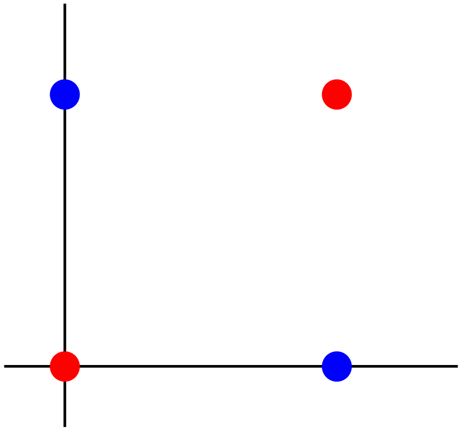
Perceptron (3)

- Minsky & Papert (1969): perceptrons are limited

x_1	x_2	ω
0	0	A
1	0	B
0	1	B
1	1	A



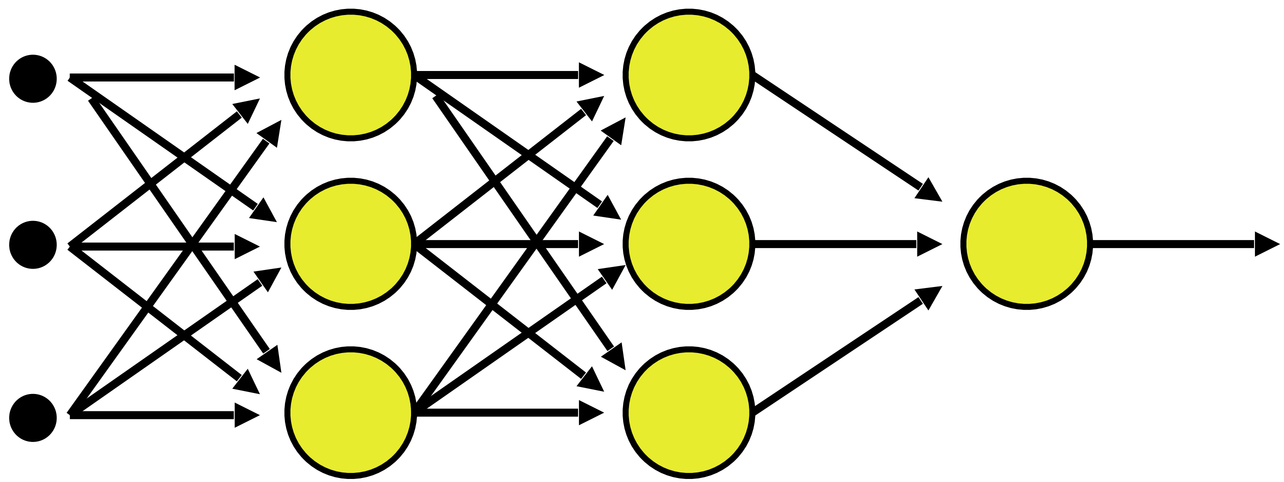
The XOR problem cannot be solved by a linear discriminant such as the perceptron

- When classes are nonlinearly separable:
  - nonlinear transfer functions
  - multilayer perceptron – but how to find weights...?
  - Rumelhart et al. (1986): use the chain rule

Multilayer perceptron

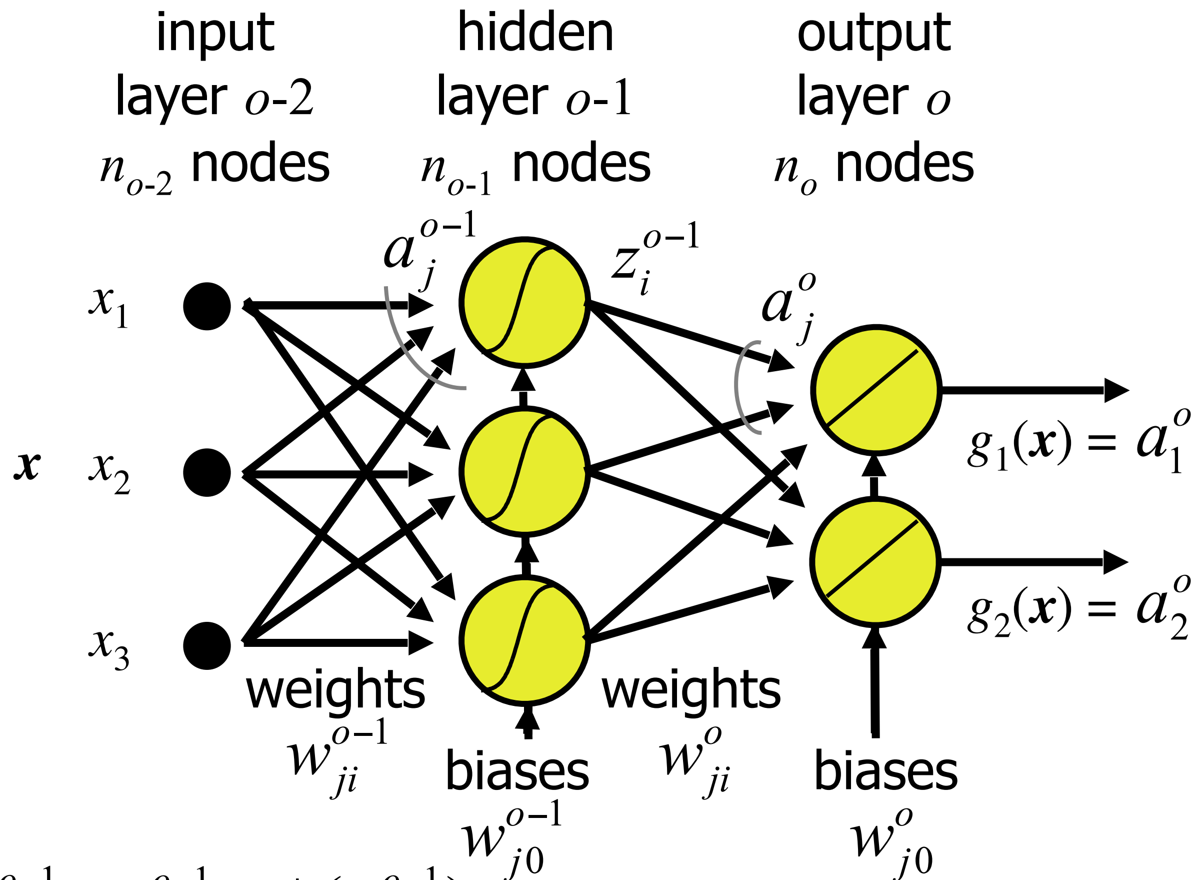
- Stacked perceptrons: feedforward networks
- Each unit has a nonlinear transfer function,

e.g. $\phi(a) = \dfrac{1}{1+\exp(-a)}$ sigmoid or logistic function



Backpropagation training

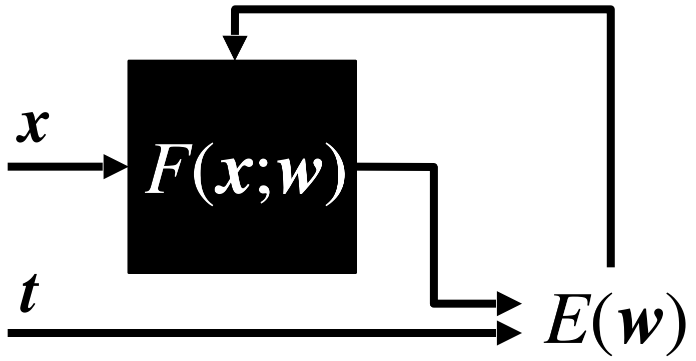
- To explain training: simple network
- One hidden layer, linear output units



- $a_j^o = \sum_{i=1}^{n_{o-1}} w_{ji}^o z_i^{o-1}, \quad z_j^{o-1} = \phi(a_j^{o-1})$

Other training algorithms

- Backpropagation training is simple gradient descent, but implemented in a useful way: all updates can be calculated locally (in parallel)



- Other view: simply optimise MSE E w.r.t. weight vector w
  using any optimisation routine, e.g.
  - second order (Newton, pseudo-Newton)
  - conjugate gradient descent
  - Broyden-Fletcher-Goldfarb-Shanno (BFGS)
  - Levenberg-Marquardt (LM, in PRTools)

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Multilayer perceptrons (2)

- Choices:
  - targets (0/1, 0.1/0.9, 0.2/0.8) t
  - **number of hidden layers**
  - **number of units per hidden layer** n_i
  - transfer functions $\phi\ (a)$
  - initialisation $w^{(0)}$
  - training algorithm
  - parameters (learning rate ρ etc.)
  - convergence decision E_{thr} or test set selection
  - ...
- All of these influence results!

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Multilayer perceptrons (3)

- Number of weights = number of parameters = $\sum_{l=1}^{o-1}(n_l+1)n_{l+1}$
  e.g. for p = 10, C = 2, 2 20-unit hidden layers:
  $(10+1)\cdot 20+(20+1)\cdot 20+(20+1)\cdot 2$ = 682 parameters

- Danger of overtraining!

- Prevention:
  - use small networks
  - regularise: minimise $E(\boldsymbol{w})+\lambda\|\boldsymbol{w}\|$
  - small w's: low complexity, training slowly increases w's;
    so when stopping in time: automatic regularisation!

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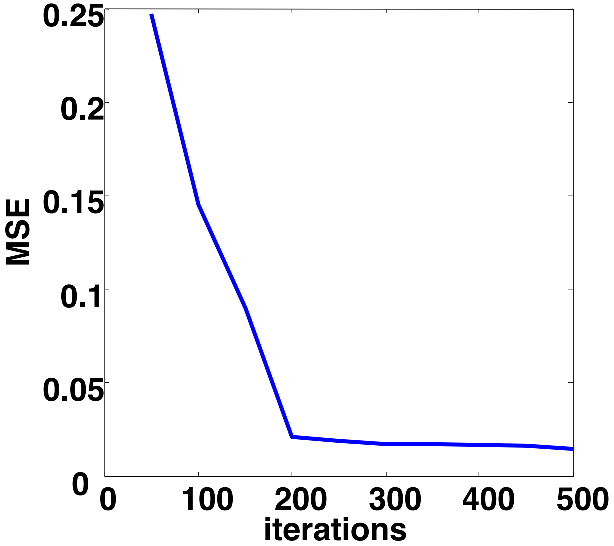
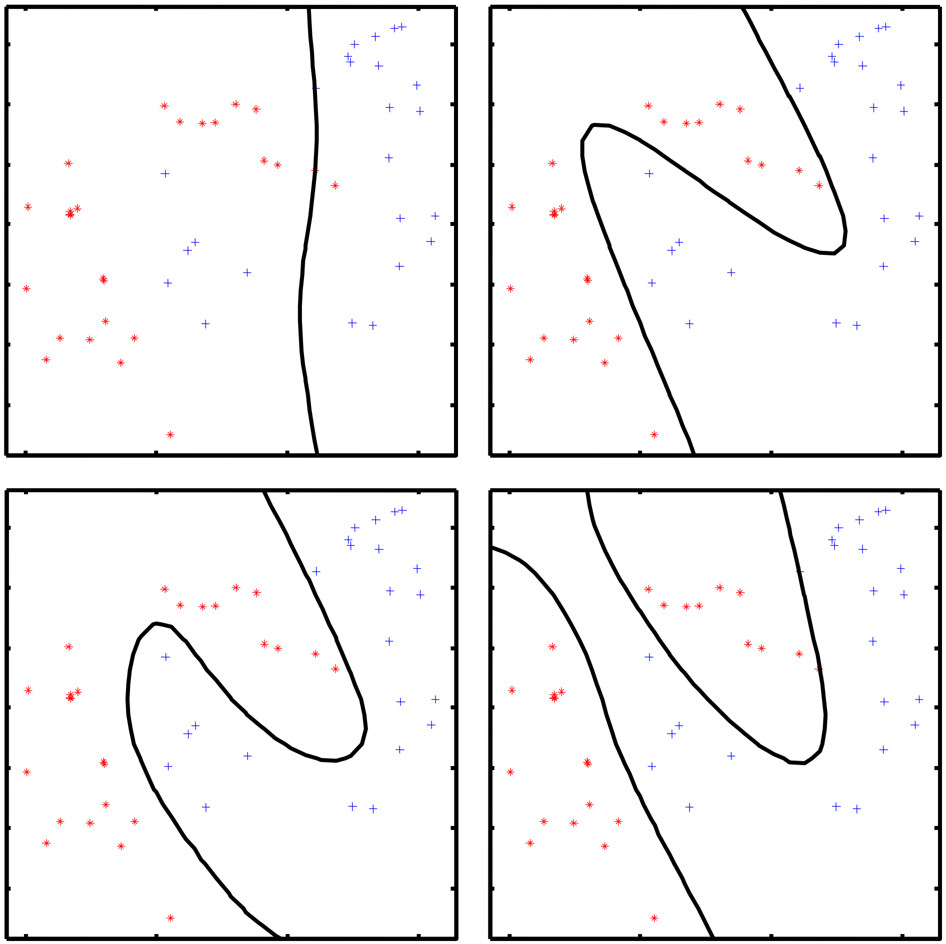
Multilayer perceptrons (4)

- Examples:

1 hidden layer
of 3 units,
2 initialisations





2 hidden layers
of 5 units each,
2 initialisations

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Combining Classifiers

Part II
Generation of Base Classifiers

Generation of base classifiers

- Random Subspace Approach
- Bagging
- Boosting

Random Subspace Approach

- Select a dimensionality k’ << k that fits well with the training size
- Select at random n subsets of k’ features
- Train n classifiers
- Combine

- When better than feature selection?
- When better than feature extraction?

Bagging (Bootstrap and Aggregate)

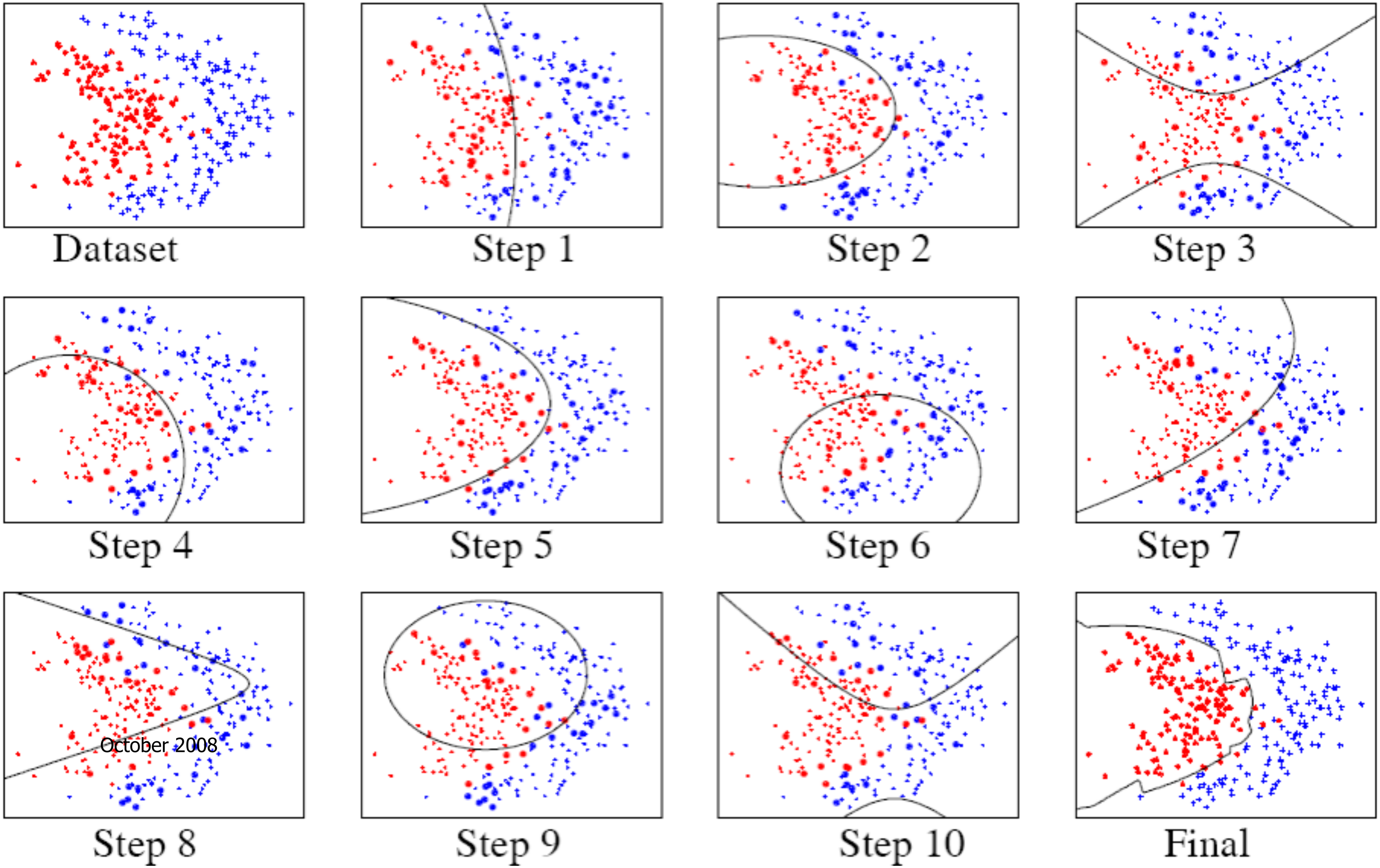
- Select a training set size m' < m
- Select at random n subsets of m' training objects (original: bootstrap)
- Train a classifier (original: decision tree)
- Combine (original: vote)

- Bagging decision trees combined with random subspace approach gives: Random Forest classifier

Boosting

- Initialize all objects with an equal weight
- Select a training set size m′ < m according to the object weights
- Train a weak classifier
- Increase the weights of the erroneously classified objects
- Repeat as long as needed
- Combine

Boosting: Emphasize Difficult Objects



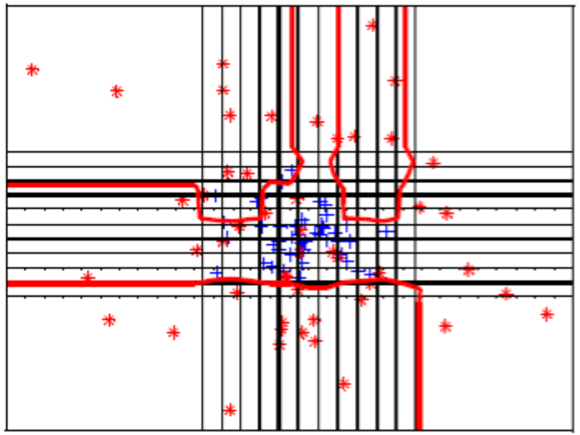
Adaboost Algorithm

1. **Sample** the training set according to a set of object weights (initially equal)
2. Use it for **training a** simple (weak) **classifier** w_i
3. **Classify** the entire data set, using the weights, **error** ε_i
   Store classifier weight $\alpha_i = 0.5 \log((1-\varepsilon_i)/\varepsilon_i)$
4. **Multiply weights** of erroneously classified objects with $\exp(\alpha_i)$
   Multiply weights of correctly classified objects with $\exp(-\alpha_i)$
5. **Goto 1** as long as needed
6. **Final classifier**: weighted voting, weights α_i

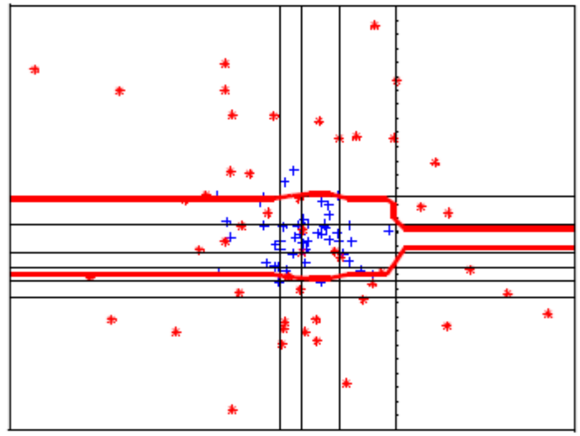
Assumes decision stump as weak classifier, and minimises exponential

loss (See course CS4230 Machine Learning 2)

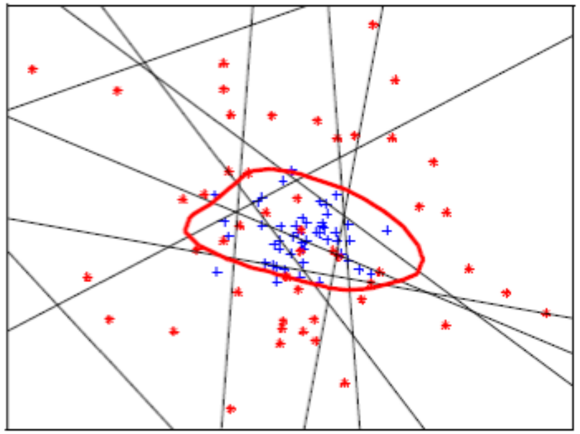
Adaboost - 2D Example



100 dec. stumps, wvote



10 dec. stumps, Fisher



10 Fisher, Fisher

```
w=adaboostc(a,stumpc,100)
```

```
w=adaboostc(a,fisherc,10,fisherc)
```

```
w=adaboostc(a,stumpc,10,fisherc)
```

Discussion on Base Classifiers

- Are to be combined
- Simple, not overtrained, especially not for trained combiners
- Many: fast training, fast execution
- Soft outputs might be helpful
- Traditional: decision trees, decision stumps, linear, quadratic
- Weak classifiers: simple, should do something,
- not sufficient for the problem,
- large bias, large variance

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Discussion on Combining

- Base classifiers are trained on systematically different training sets.
- They may be different in importance → weighting is appropriate.

$$S(x) = \text{sign}\left(\sum_i \alpha_i w_i(x)\right)$$

- Weights should follow from the performance → training
- Weights are not optimized for the ensemble of classifiers (avoid overtraining)
- Weights operate on the crisp outputs of wi(x): weighted voting
- Alternative:
  Fisher: soft outputs, optimize weights over ensemble of base classifiers
  Large set of base classifiers may overtrain

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