Supervised Learning (Part 2)

GE 461, Spring 2022

Slide credits:
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Adding Nonlinearity to Linear Discriminants

(*revisited*)

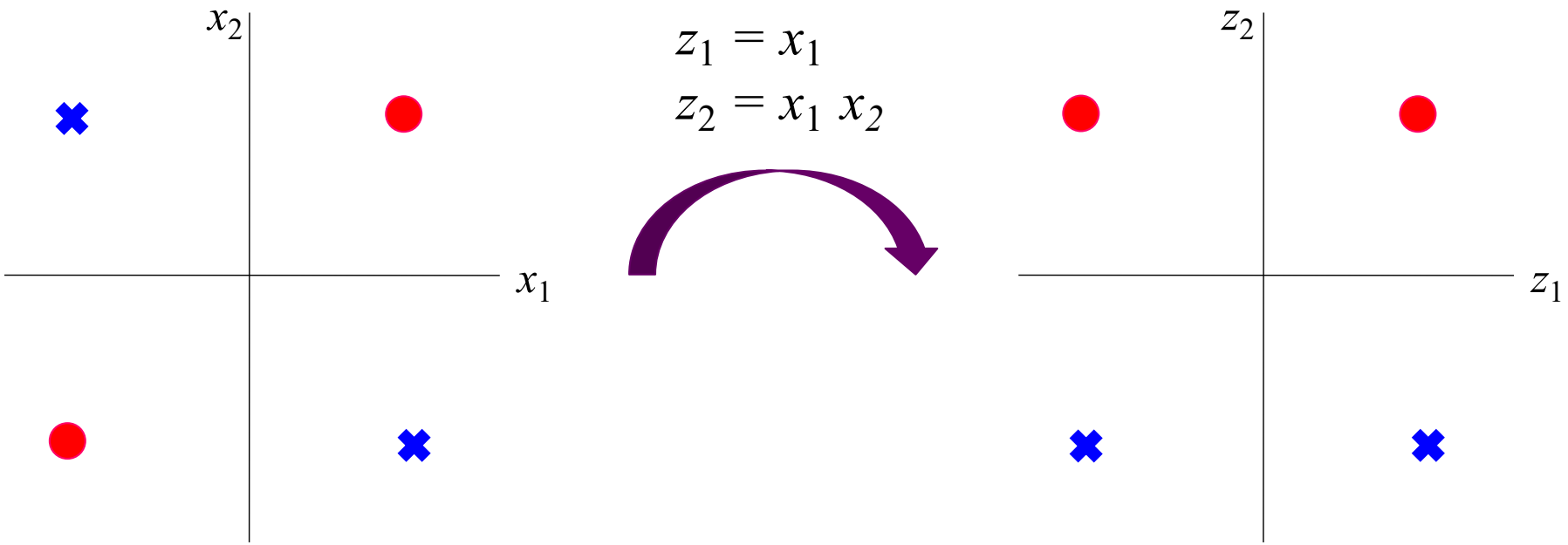
- Linear discriminants yield hyperplane decision boundaries

- If they are not sufficient to construct a "good" model

  1. Transform the space into a new one using nonlinear mappings and construct linear discriminants on the transformed space → **Support vector machines**

  2. Learn nonlinearity at the same time as you learn the linear discriminants → **Neural networks**

XOR Problem



Support vector machines use the idea of nonlinear mapping to find a linearly separable space

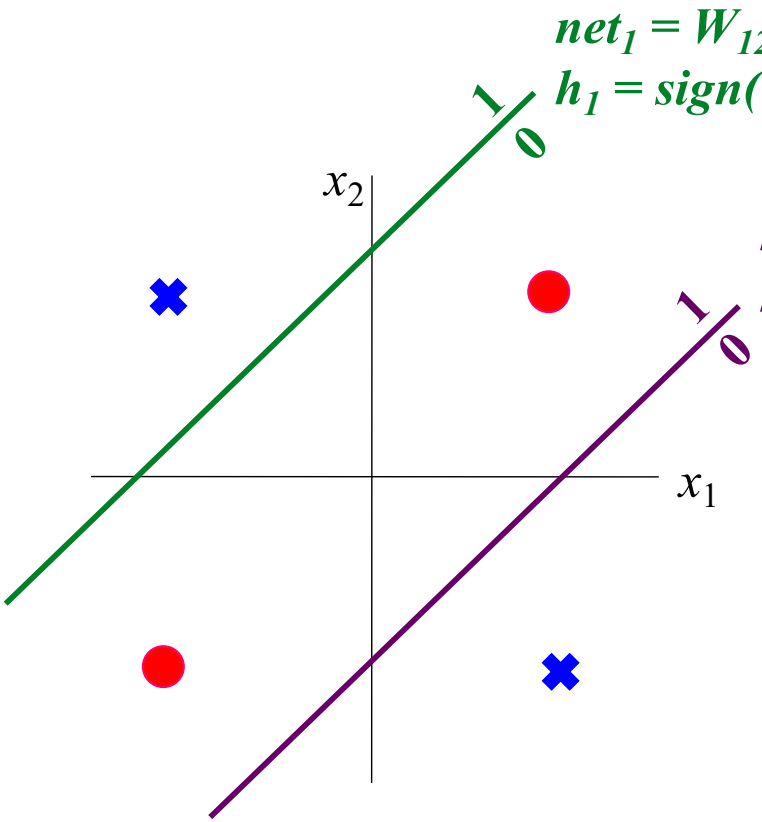
XOR Problem

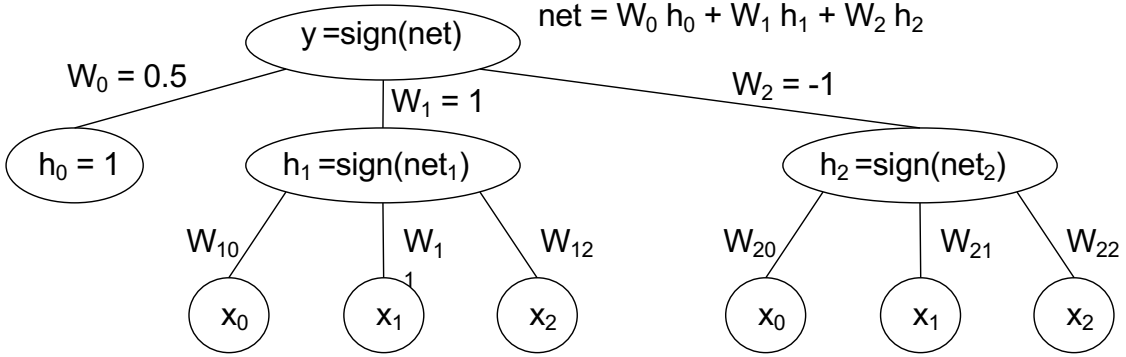
$net_1 = W_{12}\ x_2 + W_{11}\ x_1 + W_{10}$

$h_1 = sign(\ net_1\ )$

$net_2 = W_{22}\ x_2 + W_{21}\ x_1 + W_{20}$

$h_2 = sign(\ net_2\ )$





Neural networks learn the nonlinearity at the same time as they learn the linear discriminants (learn all the weights at the same time)

Support Vector Machines

(Slide credit: Selim Aksoy, CS Bilkent)

Generalized Linear Discriminant Functions

- The linear discriminant function $g(\mathbf{x})$ can be written as

$$g(\mathbf{x}) = w_0 + \sum_{i=1}^{d} \mathbf{w}_i \mathbf{x}_i$$

where $\mathbf{w} = (\mathbf{w}_1, \ldots, \mathbf{w}_d)^T$.

- We can obtain the *quadratic discriminant function* by adding second-order terms as

$$g(\mathbf{x}) = w_0 + \sum_{i=1}^{d} \mathbf{w}_i \mathbf{x}_i + \sum_{i=1}^{d} \sum_{j=1}^{d} \mathbf{w}_{ij} \mathbf{x}_i \mathbf{x}_j$$

which result in more complicated decision boundaries (hyperquadrics).

Generalized Linear Discriminant Functions

- Adding higher-order terms gives the *generalized linear discriminant function*

$$g(\mathbf{x}) = \sum_{i=1}^{d'} \mathbf{a}_i \mathbf{y}_i(\mathbf{x}) = \mathbf{a}^T \mathbf{y}$$

  where $\mathbf{a}$ is a d'-dimensional weight vector and d' functions $\mathbf{y}_i(\mathbf{x})$ are arbitrary functions of $\mathbf{x}$.

- The physical interpretation is that the functions $\mathbf{y}_i(\mathbf{x})$ map point $\mathbf{x}$ in d-dimensional space to point $\mathbf{y}$ in d'-dimensional space.

Generalized Linear Discriminant Functions

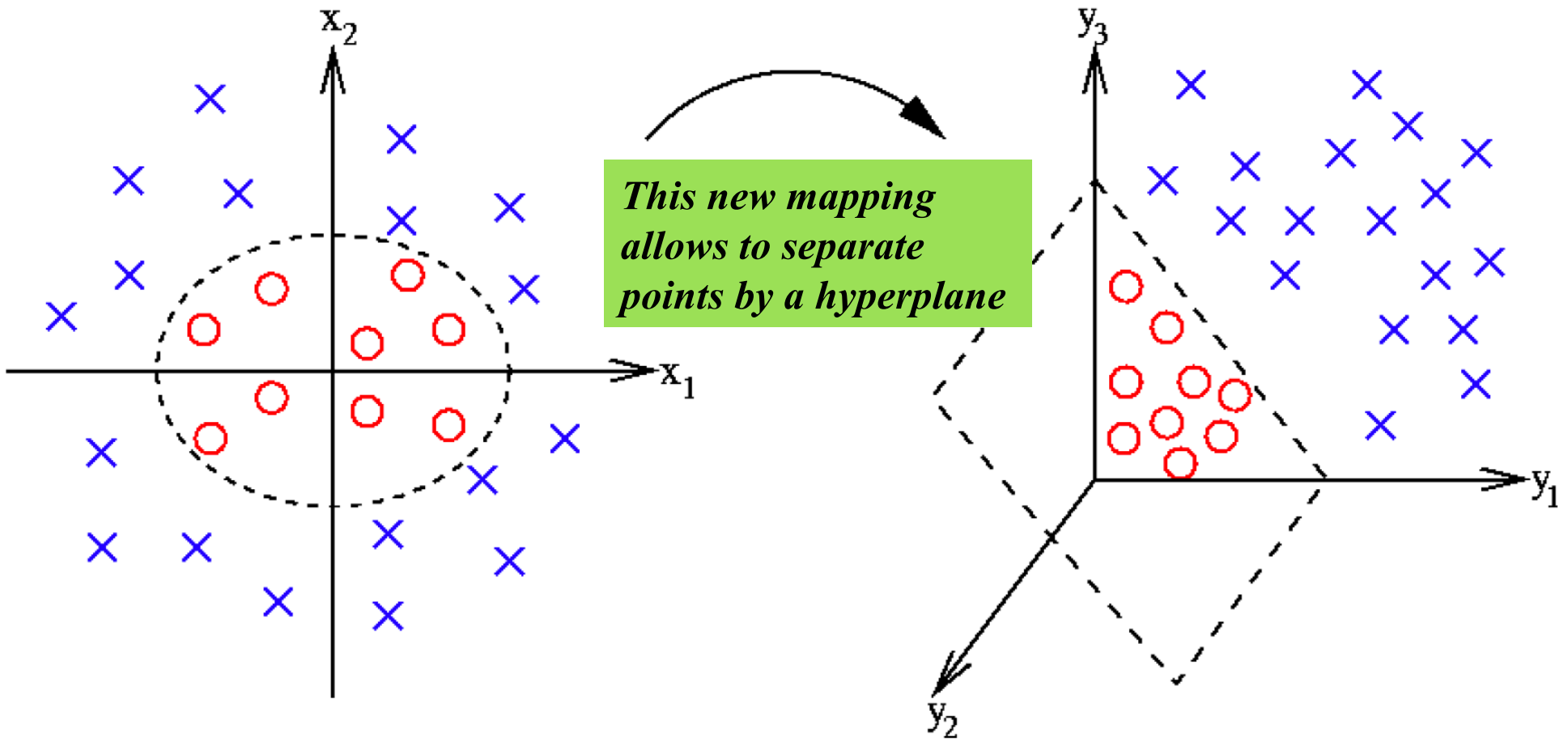


Figure 3: Mapping from $\mathbb{R}^2$ to $\mathbb{R}^3$ where points $(x_1, x_2)^T$ in the original space become $(y_1, y_2, y_3)^T = (x_1^2, \sqrt{2}x_1x_2, x_2^2)^T$ in the new space. The planar decision boundary in the new space corresponds to a non-linear decision boundary in the original space.

Generalized Linear Discriminant Functions

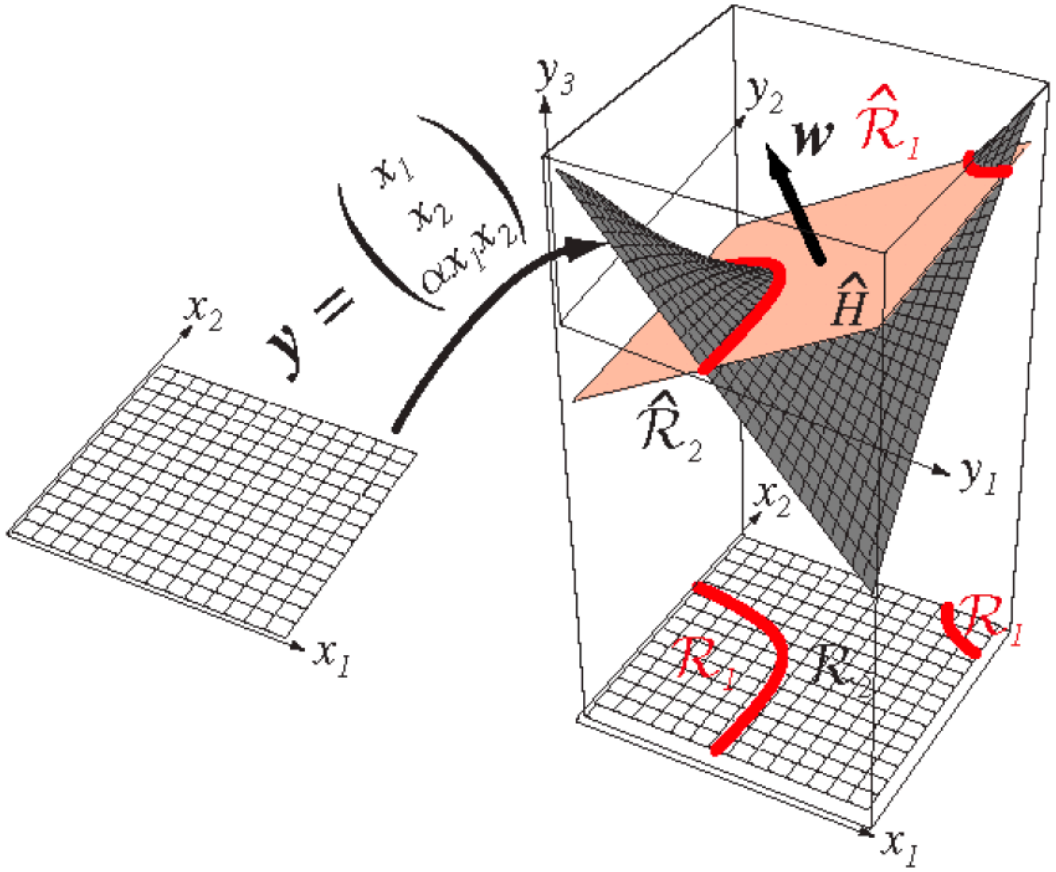


Figure 4: Mapping from $\mathbb{R}^2$ to $\mathbb{R}^3$ where points $(x_1, x_2)^T$ in the original space become $(y_1, y_2, y_3)^T = (x_1, x_2, \alpha x_1 x_2)^T$ in the new space. The decision regions $\hat{\mathcal{R}}_1$ and $\hat{\mathcal{R}}_2$ are separated by a plane in the new space where the corresponding regions $\mathcal{R}_1$ and $\mathcal{R}_2$ in the original space are separated by non-linear boundaries ($\mathcal{R}_1$ is also not connected).

Support Vector Machines

- In the general case, the problem of finding linear discriminant functions can be formulated as a problem of optimizing a criterion function.
- Among all hyperplanes separating the data, there exists a unique one yielding the maximum margin of separation between the classes.

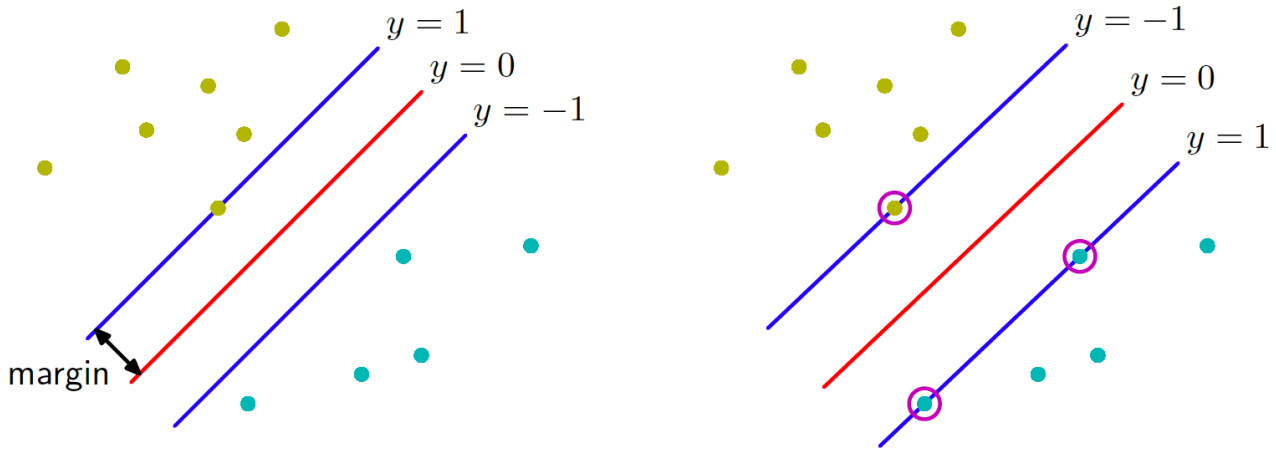


Figure 5: The margin is defined as the perpendicular distance between the decision boundary and the closest of the data points (left). Maximizing the margin leads to a particular choice of decision boundary (right). The location of this boundary is determined by a subset of the data points, known as the support vectors, which are indicated by the circles.

Support Vector Machines

- Given a set of training patterns and class labels as $(\mathbf{x_1}, y_1), \ldots, (\mathbf{x_n}, y_n) \in \mathbb{R}^d \times \{\pm 1\}$, the goal is to find a classifier function $f : \mathbb{R}^d \to \{\pm 1\}$ such that $f(\mathbf{x}) = y$ will correctly classify new patterns.
- *Support vector machines* are based on the class of hyperplanes

$$(\mathbf{w} \cdot \mathbf{x}) + b = 0, \quad \mathbf{w} \in \mathbb{R}^d, b \in \mathbb{R}$$

corresponding to decision functions

$$f(\mathbf{x}) = \text{sign}((\mathbf{w} \cdot \mathbf{x}) + b).$$

Support Vector Machines

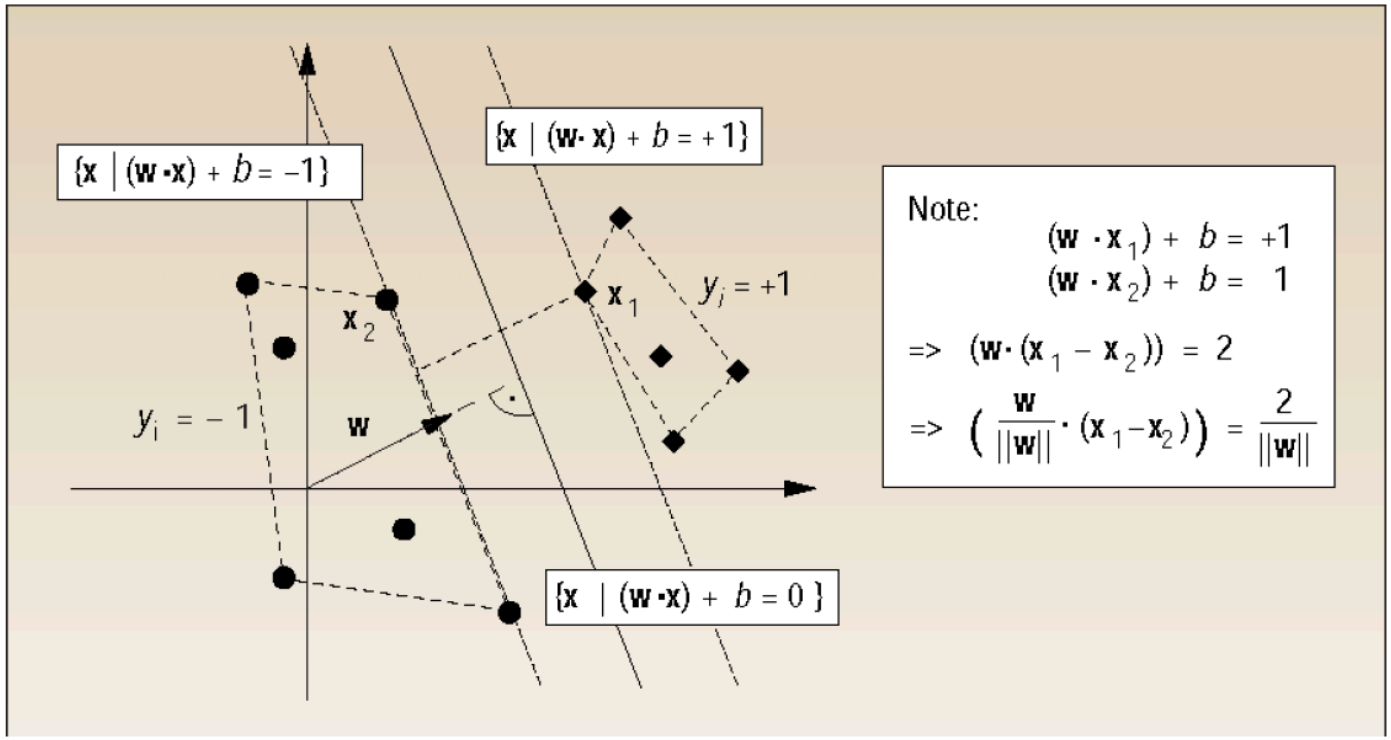


Figure 6: A binary classification problem of separating balls from diamonds. The optimal hyperplane is orthogonal to the shortest line connecting the convex hulls of the two classes (dotted), and intersects it half way between the two classes. There is a weight vector $\mathbf{w}$ and a threshold b such that the points closest to the hyperplane satisfy $|(\mathbf{w} \cdot \mathbf{x_i}) + b| = 1$ corresponding to $y_i((\mathbf{w} \cdot \mathbf{x_i}) + b) \geq 1$. The margin, measured perpendicularly to the hyperplane, equals $2/\|\mathbf{w}\|$.

Support Vector Machines

- To construct the optimal hyperplane, we can define the following optimization problem:

$$\text{minimize } \frac{1}{2}\|\mathbf{w}\|^2$$

$$\text{subject to } y_i((\mathbf{w}\cdot\mathbf{x_i})+b)\geq 1, \quad i=1,\ldots,n.$$

- This constrained optimization problem is solved using Lagrange multipliers $\alpha_i \geq 0$ and the Lagrangian

$$L(\mathbf{w},b,\boldsymbol{\alpha}) = \frac{1}{2}\|\mathbf{w}\|^2 - \sum_{i=1}^{n}\alpha_i(y_i((\mathbf{w}\cdot\mathbf{x_i})+b)-1)$$

where L has to be minimized w.r.t. the prime variables $\mathbf{w}$ and b, and maximized w.r.t. the dual variables α_i.

It gives a solution where the vector w is a linear combination of support vectors

- The maximum margin can be written as dot products between the support vectors and all samples
- When the input space is transformed using a mapping function Φ, the dot product between a support vector and a sample is $\Phi(x)\,.\,\Phi(x_i)$
- You do not need to know the mapping function itself but the dot product in the transformed space
- This is known as the **KERNEL TRICK** in support vector machines

polynomial kernel	$K(x,x_i) = (x\cdot x_i+1)^p$
radial basis function kernel	$K(x,x_i) = exp\,(-\gamma\,\|x-x_i\|^2)$
sigmoidal kernel	$K(x,x_i) = tanh(\eta\,x\cdot x_i+\nu)$

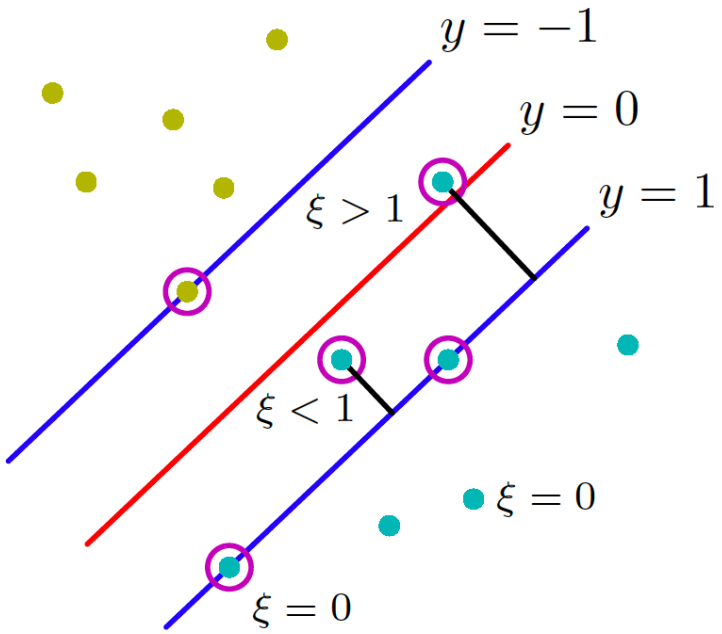
Support Vector Machines

For non-separable data, we relax the constraints

- The new optimization problem becomes:

$$\text{minimize} \quad \frac{1}{2}\|\mathbf{w}\|^2 + C\sum_{i=1}^{n}\xi_i$$

$$\begin{aligned}\text{subject to } (\mathbf{w}\cdot\mathbf{x_i}) + b &\geq +1 - \xi_i \quad \text{for } y_i = +1,\\ (\mathbf{w}\cdot\mathbf{x_i}) + b &\leq -1 + \xi_i \quad \text{for } y_i = -1,\\ \xi_i &\geq 0 \qquad\qquad\quad i = 1,\ldots,n\end{aligned}$$



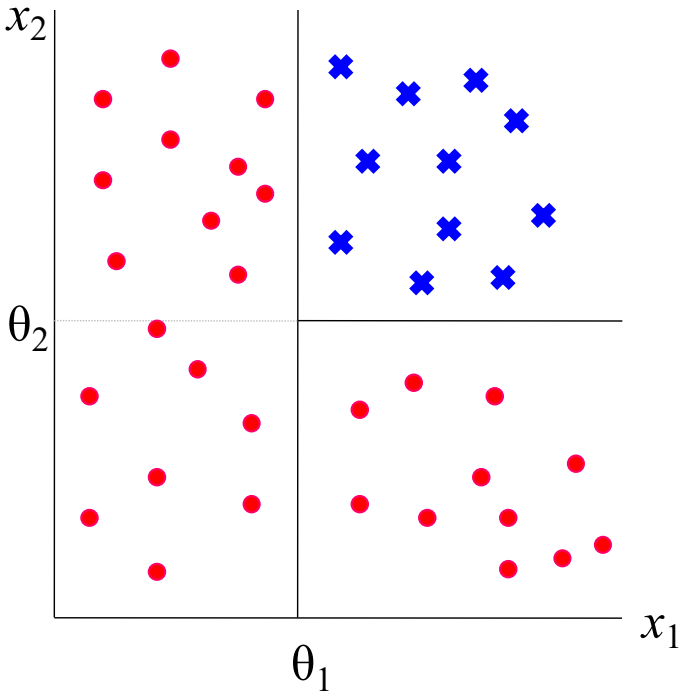
where ξ_i, $i = 1,\ldots,n$, are called the slack variables and C is a regularization parameter.

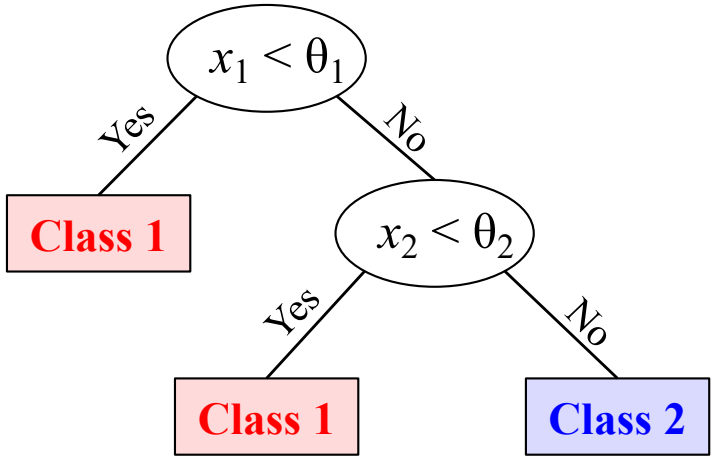
- The term $C\sum_{i=1}^{n}\xi_i$ can be thought of as measuring some amount of misclassification where lowering the value of C corresponds to a smaller penalty for misclassification (see references).

Decision Trees

Decision Trees

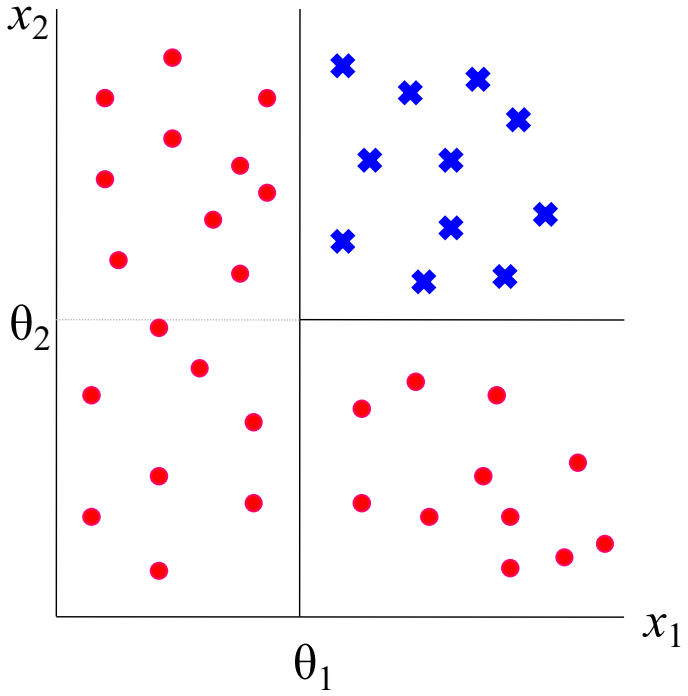
- A decision tree provides a classification or regression model built in the form of a tree structure
- It corresponds to partitioning the input space into localized regions, each of which can make different decision
- Decision tree learning aims to find these partitions

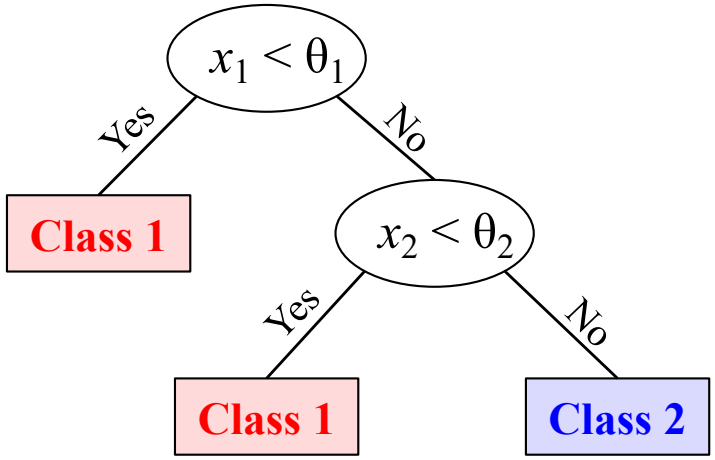




Decision Trees

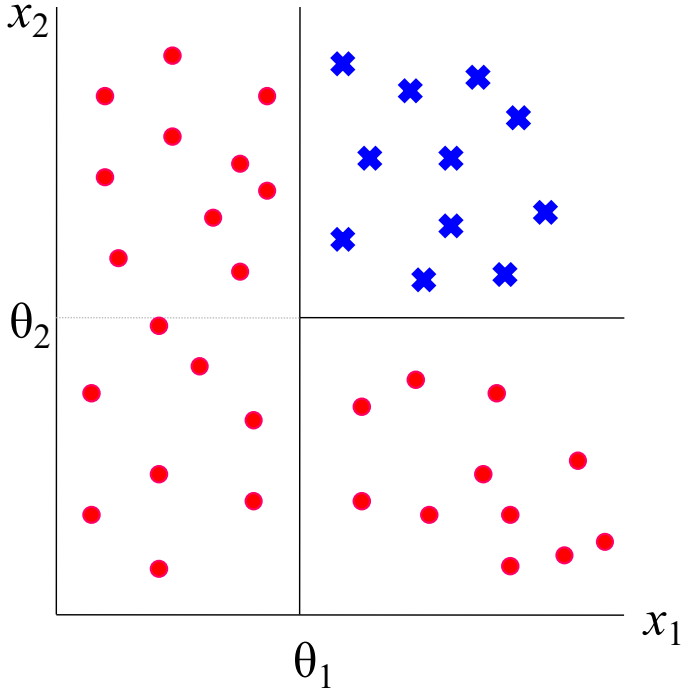
- It is composed of internal decision nodes and leaves
  - An internal node corresponds to a test function whose discrete outcomes label the branches
  - A leaf defines a localized region (and a class for classification and a numerical value for regression)

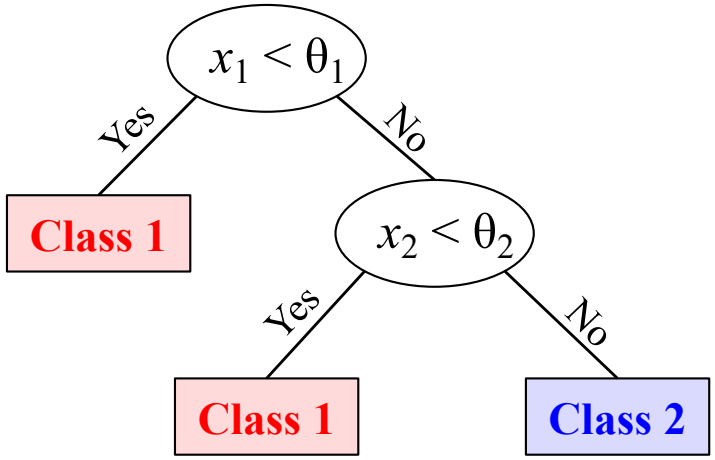




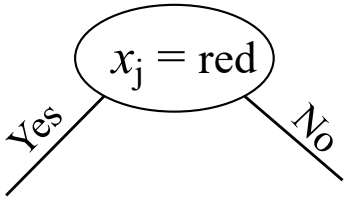
Decision Trees

- In training, the goal is to construct a tree yielding the minimum error
  - At each step, the "best" split is selected among all possible ones
  - Tree construction iteratively continues until all leaves are pure
  - This is the basis of CART, ID3, and C4.5 algorithms
- For an unseen instance, start at the root, take branches according to the test outcomes until a leaf is reached
  - The value in the leaf is the output

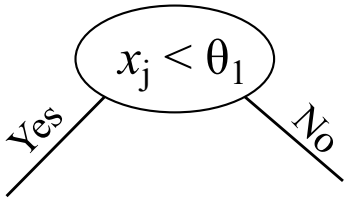




Decision Trees

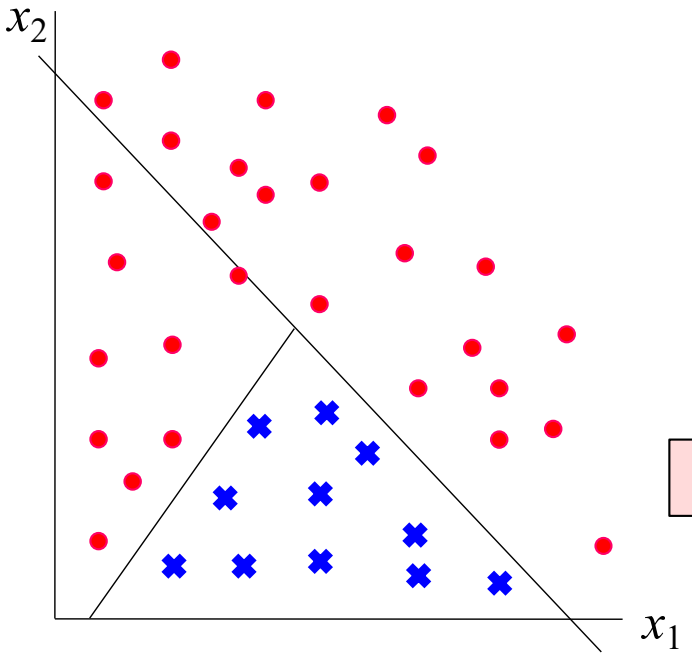


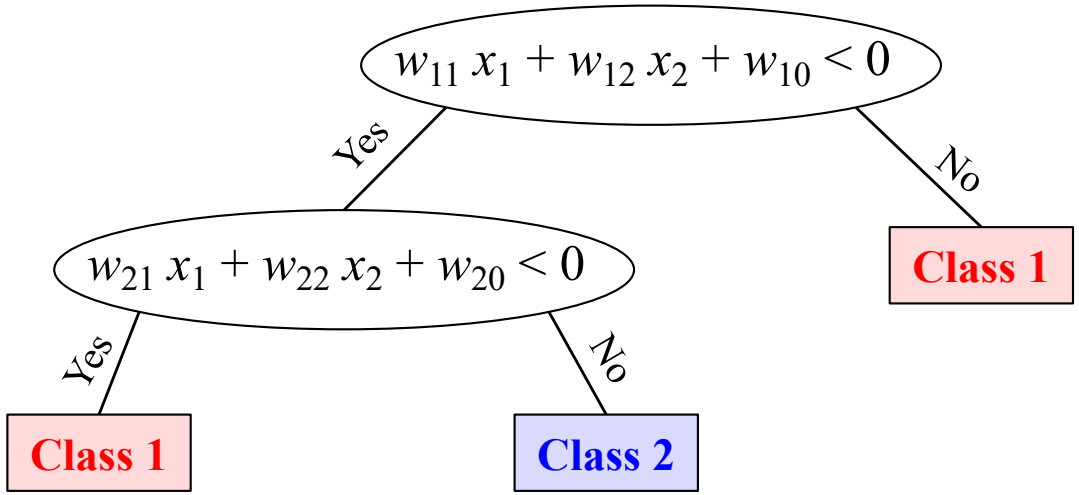
Discrete features



Continuous features

- Univariate trees
  - Test functions use one feature at a time
  - Define splits orthogonal to the coordinate axes
- Multivariate trees
  - Test functions use more than one feature at a time





Classification Trees

- For tree construction, iteratively select the "best" split until all leaves are pure
- What is the "best" split?
  - The goodness of a split is quantified by an impurity measure
  - Entropy is one of the most commonly used measures

$$\underbrace{I(m)}_{\textbf{Entropy at node m}} = -\sum_{i=1}^{\overbrace{C}^{\text{number of classes}}} \underbrace{P_m(C_i)}_{\text{Probability of having i-th class at node m}} \log P_m(C_i)$$

$$\underbrace{I(S)}_{\textbf{Entropy of a binary split S}} = P_{left}\, I(left) + P_{right}\, I(right)$$

Classification Trees

Construct a tree for the training instances below

	x_1	x_2	class
S_1	red	0.5	**1**
S_2	red	0.2	**2**
S_3	green	0.5	**2**
S_4	blue	0.1	**1**
S_5	red	-0.5	**2**
S_6	green	0.1	**1**
S_7	green	0.4	**2**
S_8	blue	0.0	**2**

- At every step
  1. List all possible splits
  2. Calculate the entropy for every split
  3. Select the one with the minimum entropy

Classification Trees

Construct a tree for the training instances below

	x_1	x_2	class
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S_3	green	0.5	**2**
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S_5	red	-0.5	**2**
S_6	green	0.1	**1**
S_7	green	0.4	**2**
S_8	blue	0.0	**2**

- For classification
  - Each different value of a **discrete feature** will define a split
  - Halfway between **continuous feature** values of the samples belonging to different classes will be split points
  - Possible splits:

    x_1 = red x_1 = green x_1 = blue

    $x_2 \leq 0.05$ $x_2 \leq 0.15$ $x_2 \leq 0.45$

Classification Trees

Construct a tree for the training instances below

	x_1	x_2	class
S_1	red	0.5	**1**
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S_3	green	0.5	**2**
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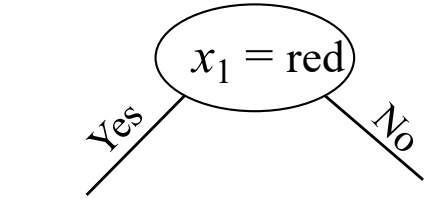
S_5	red	-0.5	**2**
S_6	green	0.1	**1**
S_7	green	0.4	**2**
S_8	blue	0.0	**2**

- Calculate the entropy for all possible splits

$$I(x_1 = red) = P_{Yes}\, I(Yes) + P_{No}\, I(No)$$

$$= \frac{3}{8}\left(-\frac{1}{3}\log\frac{1}{3} - \frac{2}{3}\log\frac{2}{3}\right) + \frac{5}{8}\left(-\frac{2}{5}\log\frac{2}{5} - \frac{3}{5}\log\frac{3}{5}\right)$$

$$= 0.9512$$



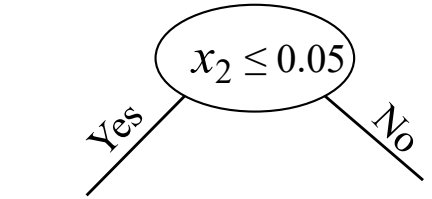
S_1 – Class 1
S_2 – Class 2
S_5 – Class 2

S_3 – Class 2
S_4 – Class 1
S_6 – Class 1
S_7 – Class 2
S_8 – Class 2

$$I(x_2 \le 0.05) = P_{Yes}\, I(Yes) + P_{No}\, I(No)$$

$$= \frac{2}{8}\left(-0\log 0 - 1\log 1\right) + \frac{6}{8}\left(-\frac{3}{6}\log\frac{3}{6} - \frac{3}{6}\log\frac{3}{6}\right)$$

$$= 0.7500$$



S_5 – Class 2
S_8 – Class 2

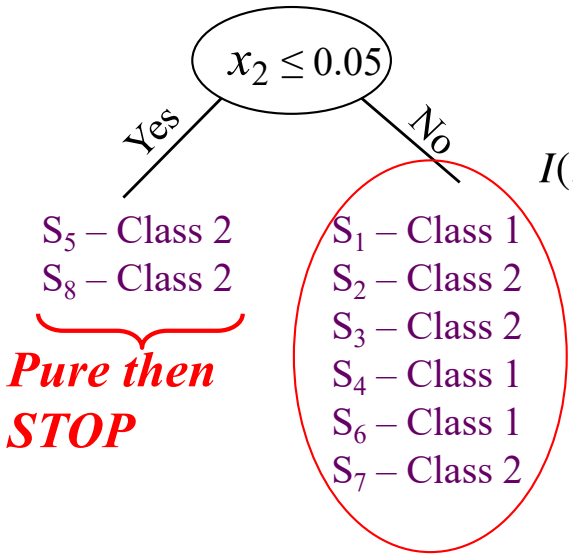
S_1 – Class 1
S_2 – Class 2
S_3 – Class 2
S_4 – Class 1
S_6 – Class 1
S_7 – Class 2

Classification Trees

Construct a tree for the training instances below

	x_1	x_2	class
S_1	red	0.5	**1**
S_2	red	0.2	**2**
S_3	green	0.5	**2**
S_4	blue	0.1	**1**
S_5	red	-0.5	**2**
S_6	green	0.1	**1**
S_7	green	0.4	**2**
S_8	blue	0.0	**2**

- Select the split with the minimum entropy and continue



$$I(x_1 = red) = P_{Yes}\, I(Yes) + P_{No}\, I(No)$$

$$= \frac{2}{6}\left(-\frac{1}{2}\log\frac{1}{2} - \frac{1}{2}\log\frac{1}{2}\right) + \frac{4}{6}\left(-\frac{2}{4}\log\frac{2}{4} - \frac{2}{4}\log\frac{2}{4}\right)$$

...

Continue for this branch

List all possible splits for this branch, calculate the entropy for each, and select the one with the min entropy

Alternative Splitting Criteria

Entropy at node m

$$I(m) = -\sum_{i=1}^{C} \underbrace{P_m(C_i)}_{\text{Probability of having i-th class at node m}} \log P_m(C_i)$$

Gini impurity at node m

$$I(m) = \sum_{i \neq j} P_m(C_i) \;\; P_m(C_j) = \frac{1}{2}\left[1 - \sum_i \left(P_m(C_i)\right)^2\right]$$

Misclassification impurity at node m

$$I(m) = 1 - \max_i \; P_m(C_i)$$

When to Stop Splitting

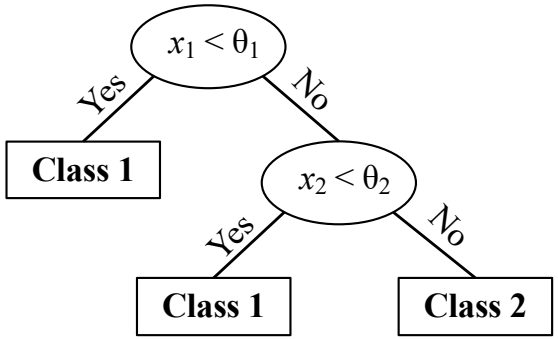
- Until all leaves are pure → **Overfitting**
- To prevent overfitting
  - Set a small threshold value in the reduction in impurity
  - Use cross validation techniques (e.g., continue splitting if the cross validation error is decreasing)
  - Use an explicit measure of the complexity to encode the training samples and the tree, stop growing when the encoding size is minimized (*minimum description length principle*)
  - Use statistical tests (e.g., use chi-squared statistic to understand if a split differs significantly from a random one)
- Then, it might be useful to keep the classes existing in a leaf together with their class probabilities

Pruning

- Prepruning: Stop growing the tree earlier before it overfits the training samples
- Postpruning: Grow the tree until it overfits the training samples (all leaves are pure) then prune the grown tree
  - *Reduced error pruning:* Remove nodes (or subtrees) only if the pruned tree performs no worse than the unpruned one over the validation set
  - *Rule post pruning:* Convert a tree into a set of rules and simplify (prune) each rule by removing any preconditions that result in no-worse-than validation performance

if $\underbrace{(x_1 \geq \theta_1)}_{\mathbf{A}}$ and $\underbrace{(x_2 \geq \theta_2)}_{\mathbf{B}}$ then Class 2

Try removing A or B and see what happens on the validation set

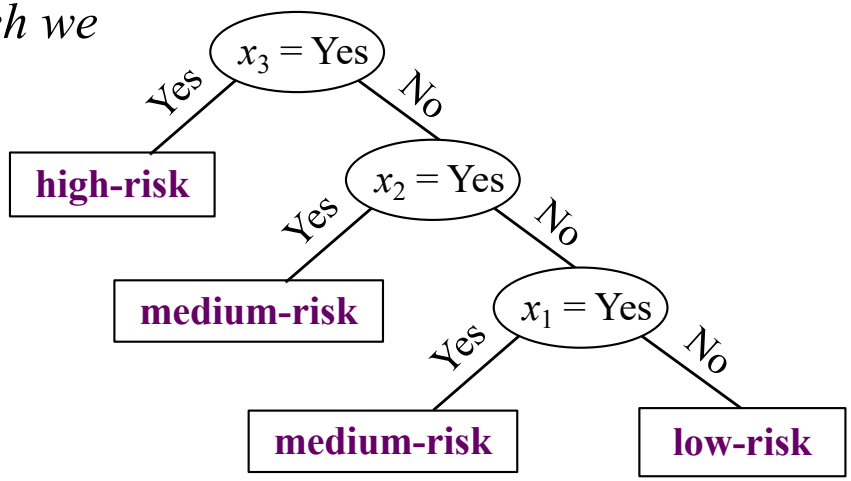


Rule Extraction

- One advantage of using a decision tree classifier is its ability to extract human interpretable rules

Consider the following problem setting in which we estimate the risk of getting avian flu

x_1: living close to migration routes (Yes / No)
x_2: feeding poultry (Yes / No)
x_3: contact with sick poultry (Yes / No)
x_4: gender (Male / Female)

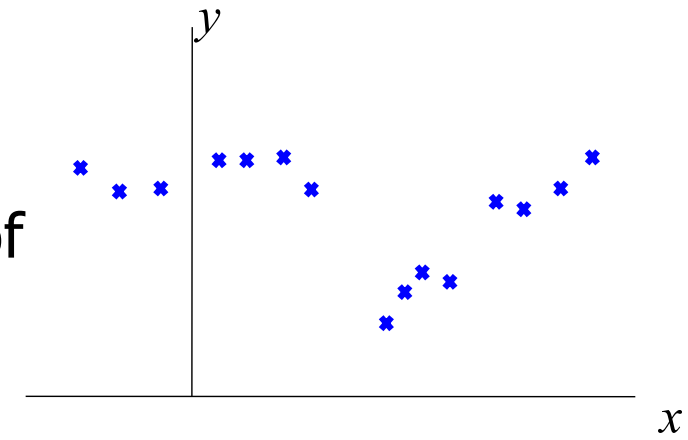


Rule 1: if (contact = yes) then high-risk
Rule 2: if (contact = no) and (feeding = yes) then medium-risk
Rule 3: if (contact = no) and (feeding = no) and (close-living = yes) then medium-risk
Rule 4: if (contact = no) and (feeding = no) and (close-living = no) then low-risk

Rule support is the percentage of the training samples covered by the rule

Regression Trees

- Continuous outputs at leaves (instead of class labels)
- Error measure is used for the goodness of a split (instead of an impurity measure)
- Iteratively grow the tree until the error measure falls below a certain threshold



$$\underbrace{E(m)}_{\textbf{Mean square error at node m}} = \frac{1}{|D_m|} \sum_{x_i \in D_m} (y_i - f_m)^2$$

training samples at node m

estimated output at node m

$$\underbrace{E(S)}_{\textbf{Mean square error of a binary split S}} = P_{left}\, E(left) + P_{right}\, E(right)$$

To estimate f_m

The mean (median) over the outputs of the training samples at node m could be used (piecewise constant approx.)

A linear function is fit over the outputs of the training samples at node m and its output value could be used (piecewise linear approx.)