Machine Learning – Classifiers and Boosting

Reading

Ch 18.6-18.12, 20.1-20.3.2

Outline

- Different types of learning problems
- Different types of learning algorithms
- Supervised learning
  - Decision trees
  - Naïve Bayes
  - Perceptrons, Multi-layer Neural Networks
  - Boosting
- Applications: learning to detect faces in images

You will be expected to know

- Classifiers:
  - Decision trees
  - K-nearest neighbors
  - Naïve Bayes
  - Perceptrons, Support vector Machines (SVMs), Neural Networks
- Decision Boundaries for various classifiers
  - What can they represent conveniently? What not?

Inductive learning

- Let $\underline{x}$ represent the input vector of attributes
  - x_j is the jth component of the vector x
  - x_j is the value of the jth attribute, j = 1,…d

- Let f($\underline{x}$) represent the value of the target variable for $\underline{x}$
  - The implicit mapping from x to f($\underline{x}$) is unknown to us
  - We just have training data pairs, D = {$\underline{x}$, f($\underline{x}$)} available

- We want to learn a mapping from $\underline{x}$ to f, i.e.,
  h($\underline{x}$; θ) is "close" to f(x) for all training data points $\underline{x}$

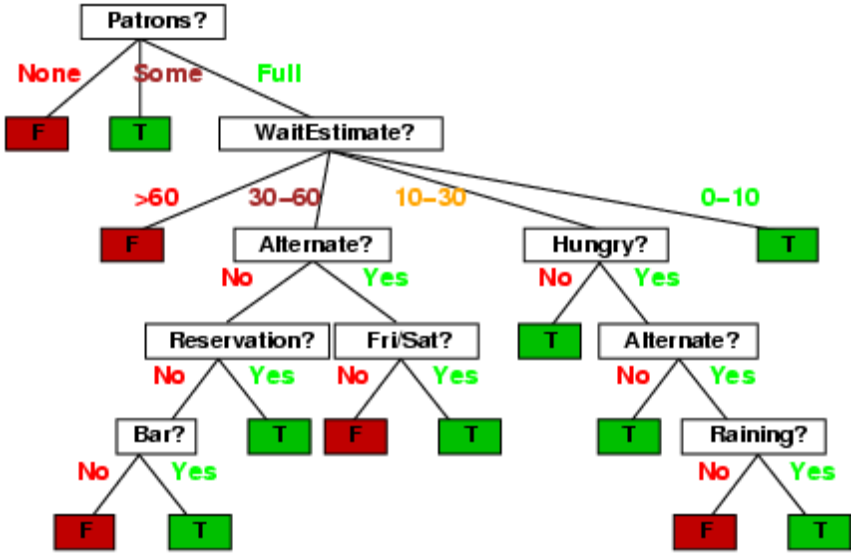
  θ are the parameters of our predictor h(..)

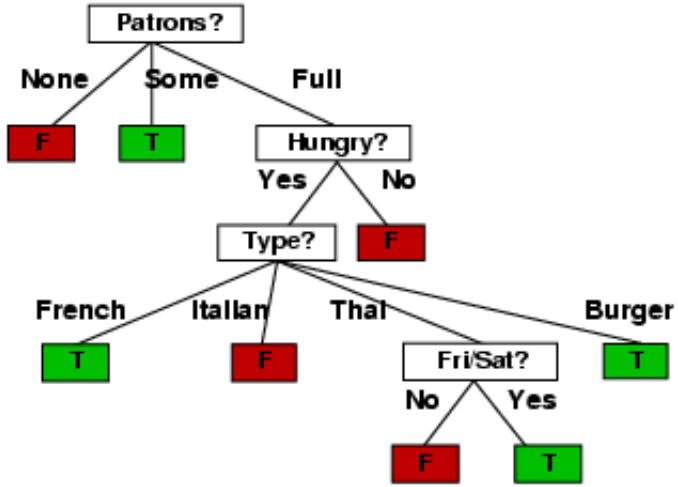
- Examples:
  - $h(\underline{x}; \theta) = \text{sign}(w_1x_1 + w_2x_2 + w_3)$
  - $h_k(\underline{x})$ = (x1 OR x2) AND (x3 OR NOT(x4))

Training Data for Supervised Learning

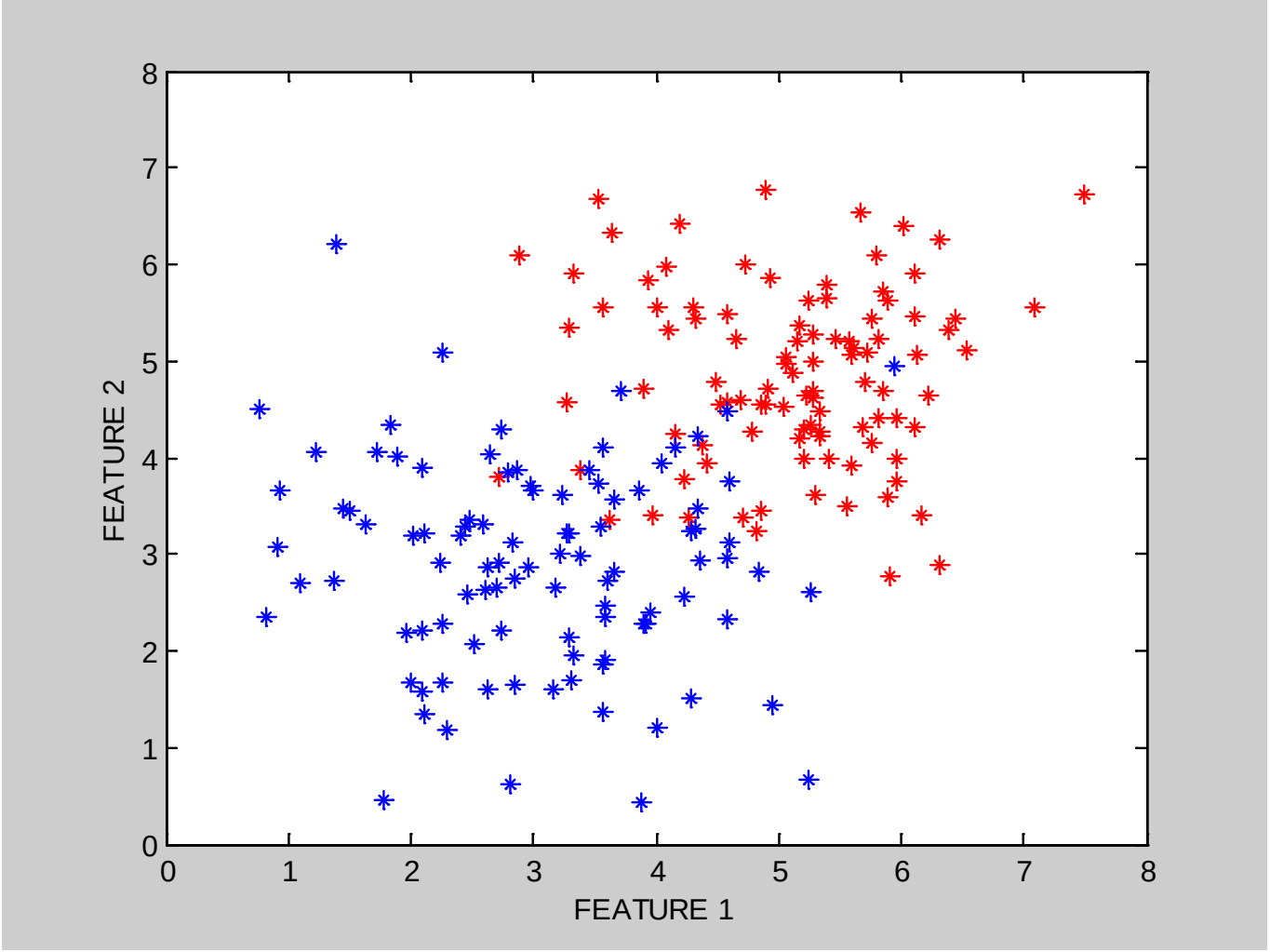
Example	Attributes										Target
	Alt	*Bar*	*Fri*	*Hun*	*Pat*	*Price*	*Rain*	*Res*	*Type*	*Est*	*Wait*
X_1	T	F	F	T	Some	$$$	F	T	French	0–10	T
X_2	T	F	F	T	Full	$	F	F	Thai	30–60	F
X_3	F	T	F	F	Some	$	F	F	Burger	0–10	T
X_4	T	F	T	T	Full	$	F	F	Thai	10–30	T
X_5	T	F	T	F	Full	$$$	F	T	French	>60	F
X_6	F	T	F	T	Some	$$	T	T	Italian	0–10	T
X_7	F	T	F	F	None	$	T	F	Burger	0–10	F
X_8	F	F	F	T	Some	$$	T	T	Thai	0–10	T
X_9	F	T	T	F	Full	$	T	F	Burger	>60	F
X_{10}	T	T	T	T	Full	$$$	F	T	Italian	10–30	F
X_{11}	F	F	F	F	None	$	F	F	Thai	0–10	F
X_{12}	T	T	T	T	Full	$	F	F	Burger	30–60	T

True Tree (left) versus Learned Tree (right)

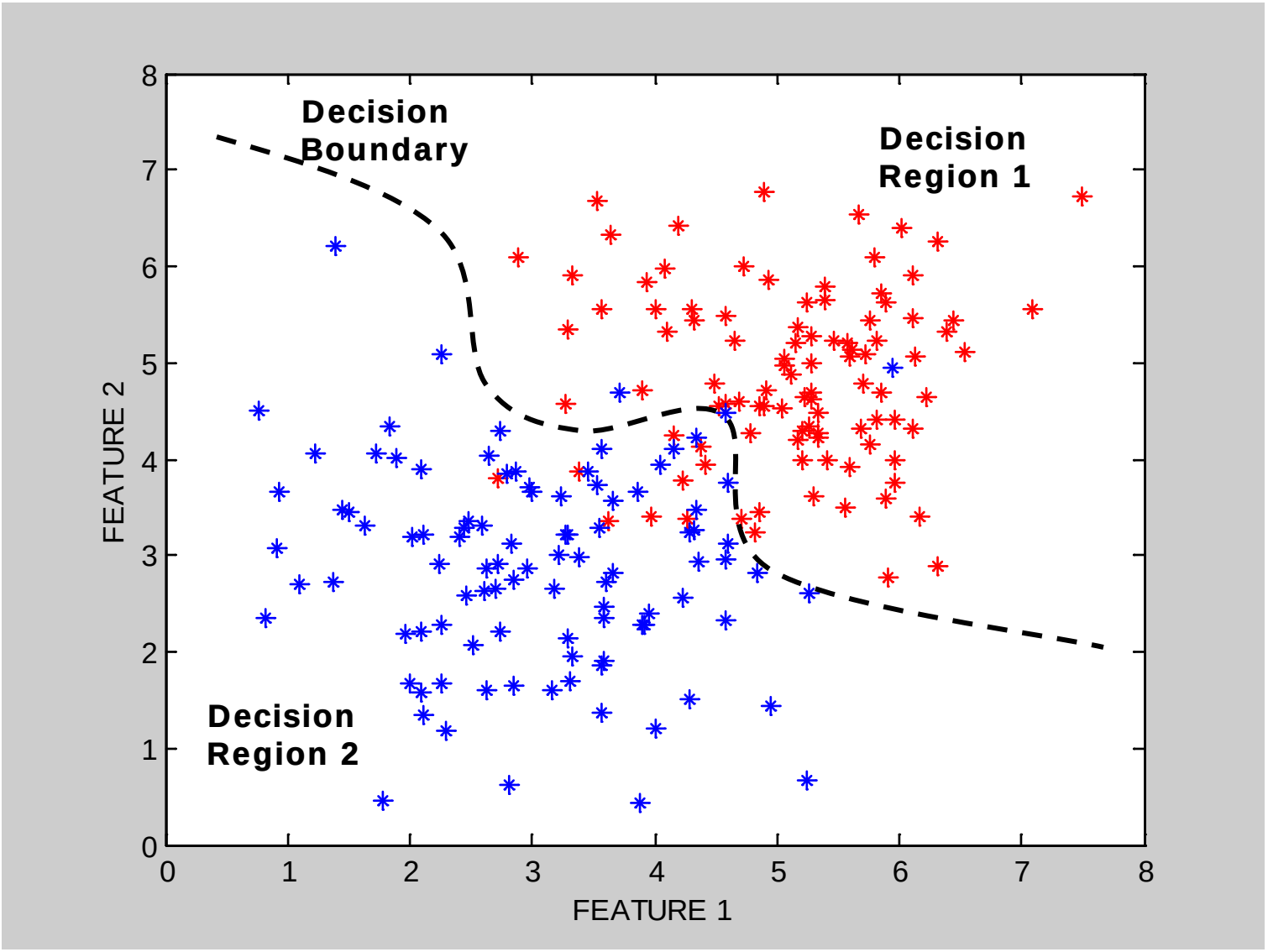




Classification Problem with Overlap



Decision Boundaries



Classification in Euclidean Space

- A classifier is a partition of the space $\underline{x}$ into disjoint decision regions
  - Each region has a label attached
  - Regions with the same label need not be contiguous
  - For a new test point, find what decision region it is in, and predict the corresponding label

- Decision boundaries = boundaries between decision regions
  - The “dual representation” of decision regions

- We can characterize a classifier by the equations for its decision boundaries

- Learning a classifier ⇔ searching for the decision boundaries that optimize our objective function

Example: Decision Trees

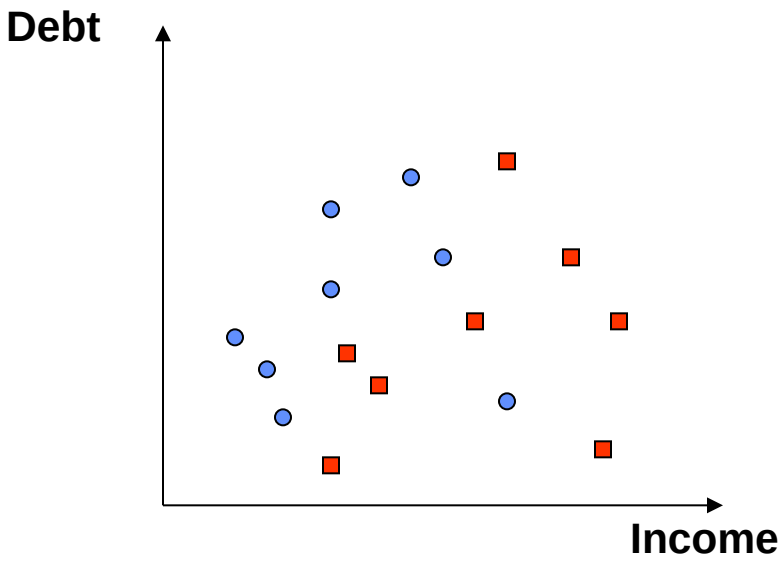
- When applied to real-valued attributes, decision trees produce "axis-parallel" linear decision boundaries

- Each internal node is a binary threshold of the form
  $x_j > t$?

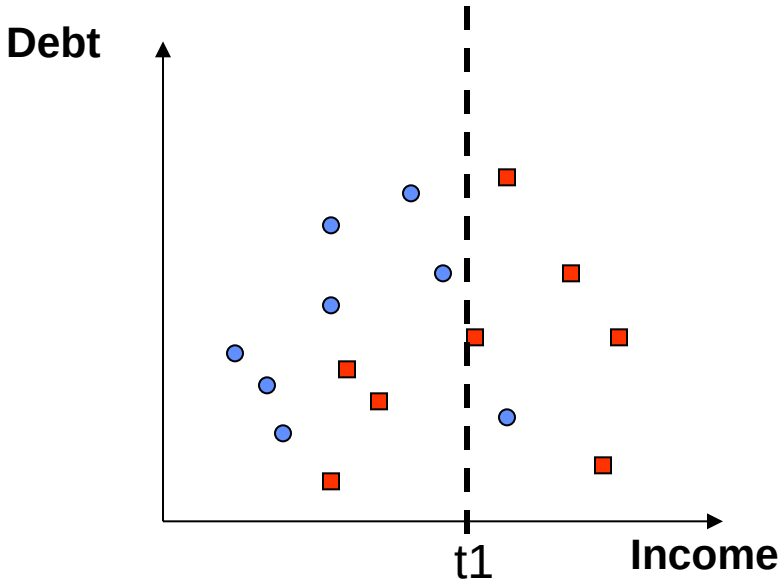
  converts each real-valued feature into a binary one

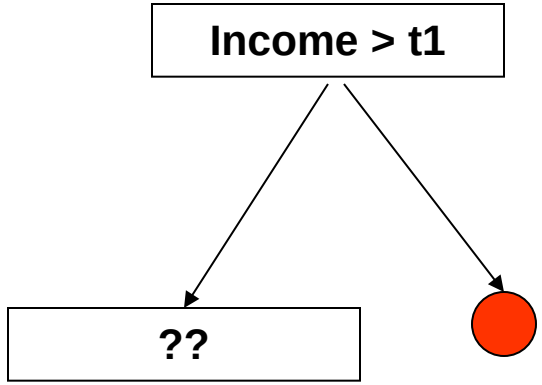
  requires evaluation of N-1 possible threshold locations for N data points, for each real-valued attribute, for each internal node

Decision Tree Example

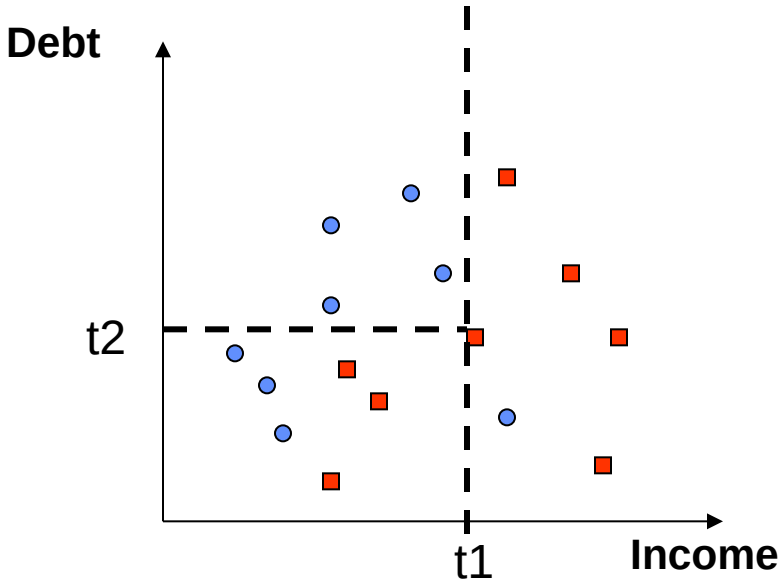


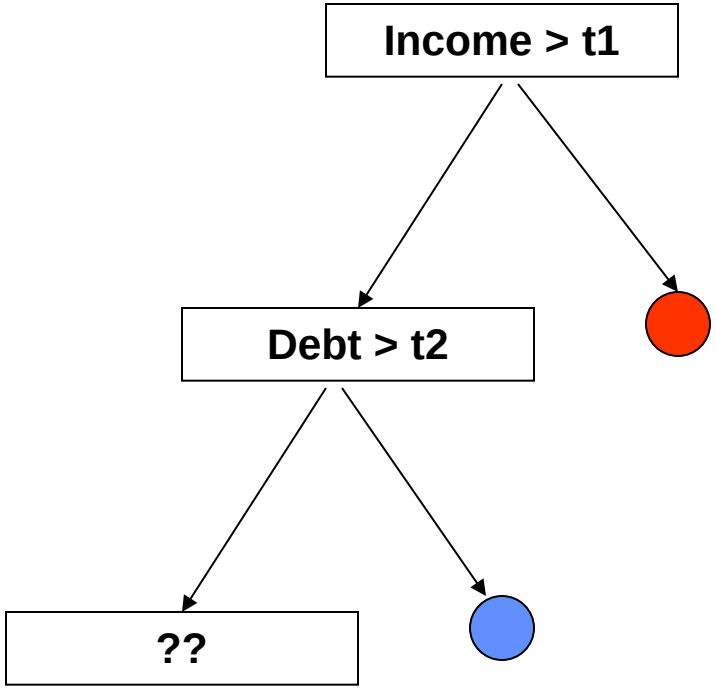
Decision Tree Example



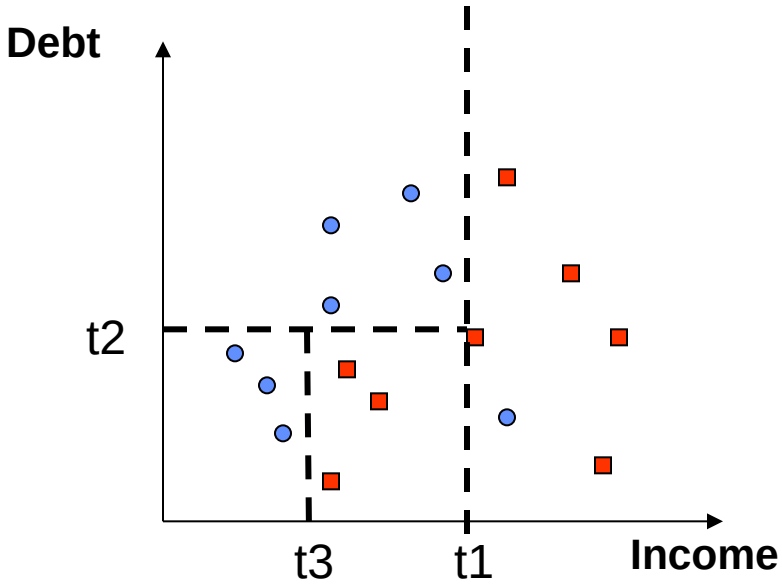


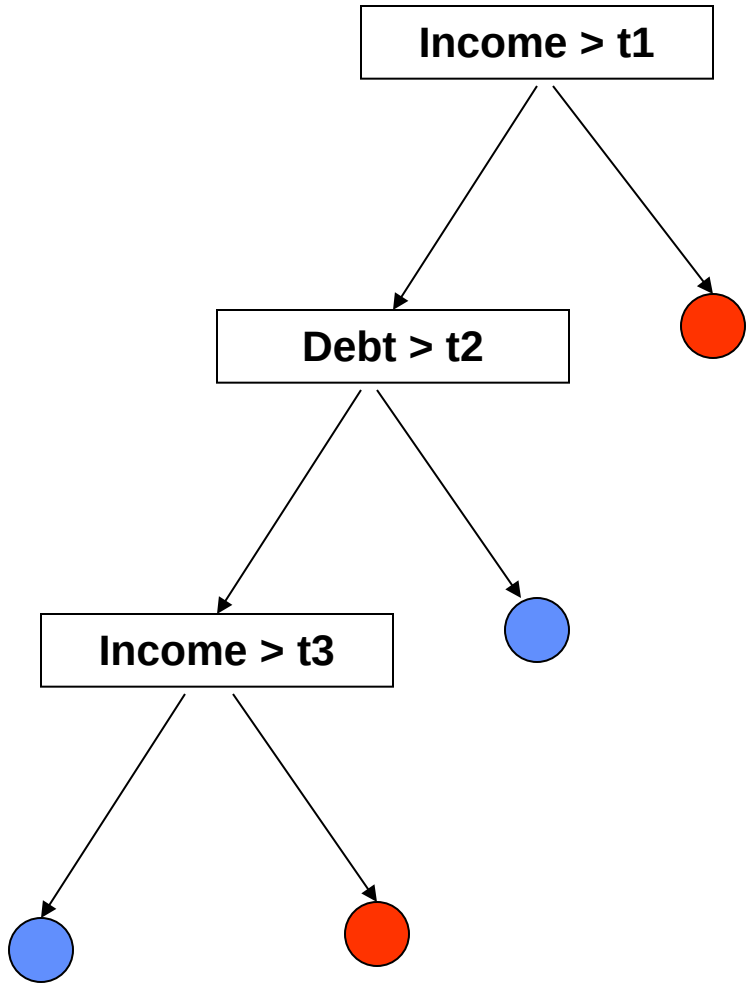
Decision Tree Example



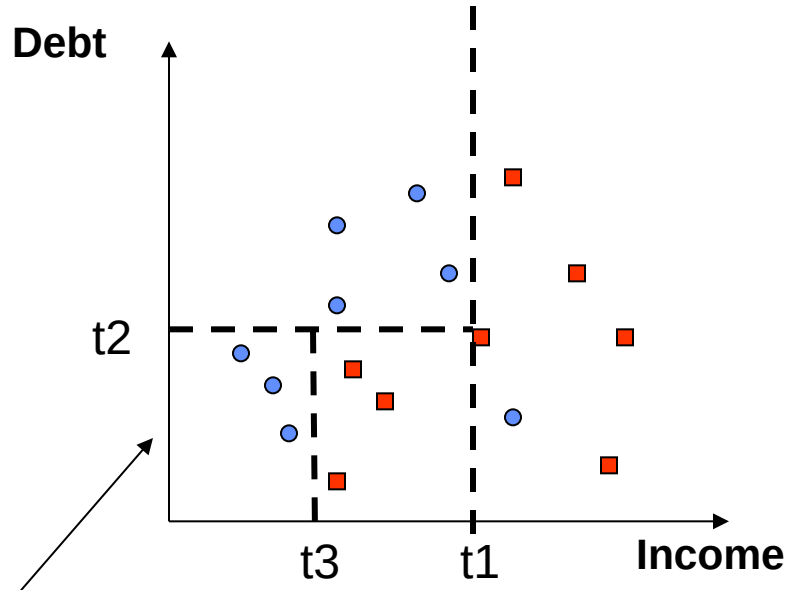


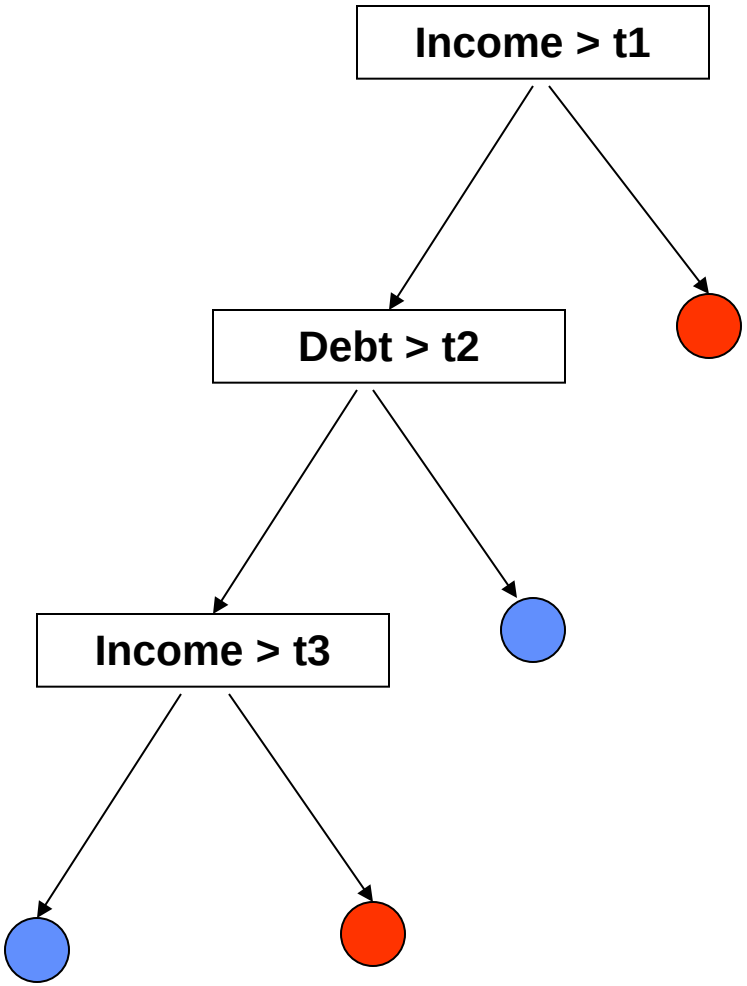
Decision Tree Example





Decision Tree Example



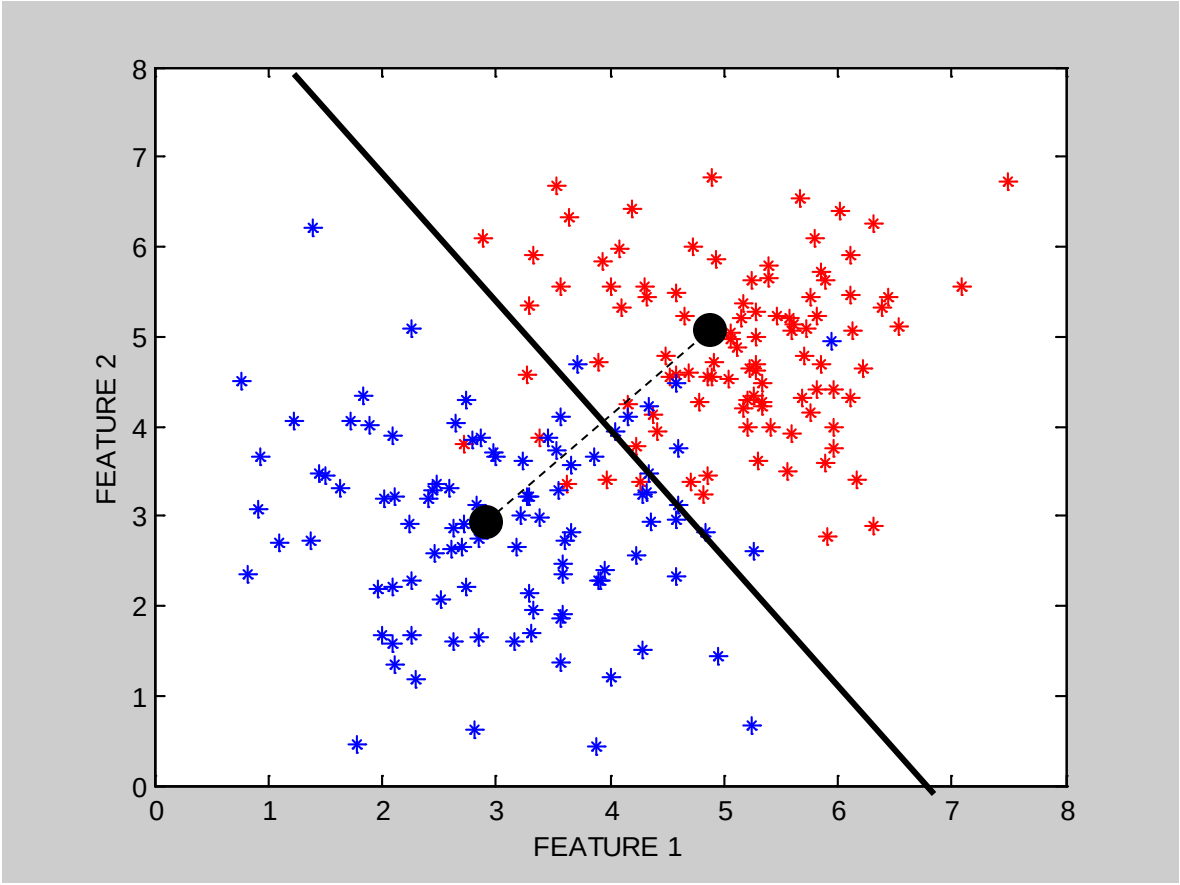


Note: tree boundaries are linear and axis-parallel

A Simple Classifier: Minimum Distance Classifier

- Training
  - Separate training vectors by class
  - Compute the mean for each class, $\underline{\mu}_k$, $k = 1, \ldots m$
- Prediction
  - Compute the closest mean to a test vector $\underline{x}$' (using Euclidean distance)
  - Predict the corresponding class
- In the 2-class case, the decision boundary is defined by the locus of the hyperplane that is halfway between the 2 means and is orthogonal to the line connecting them
- This is a very simple-minded classifier – easy to think of cases where it will not work very well

Minimum Distance Classifier



Another Example: Nearest Neighbor Classifier

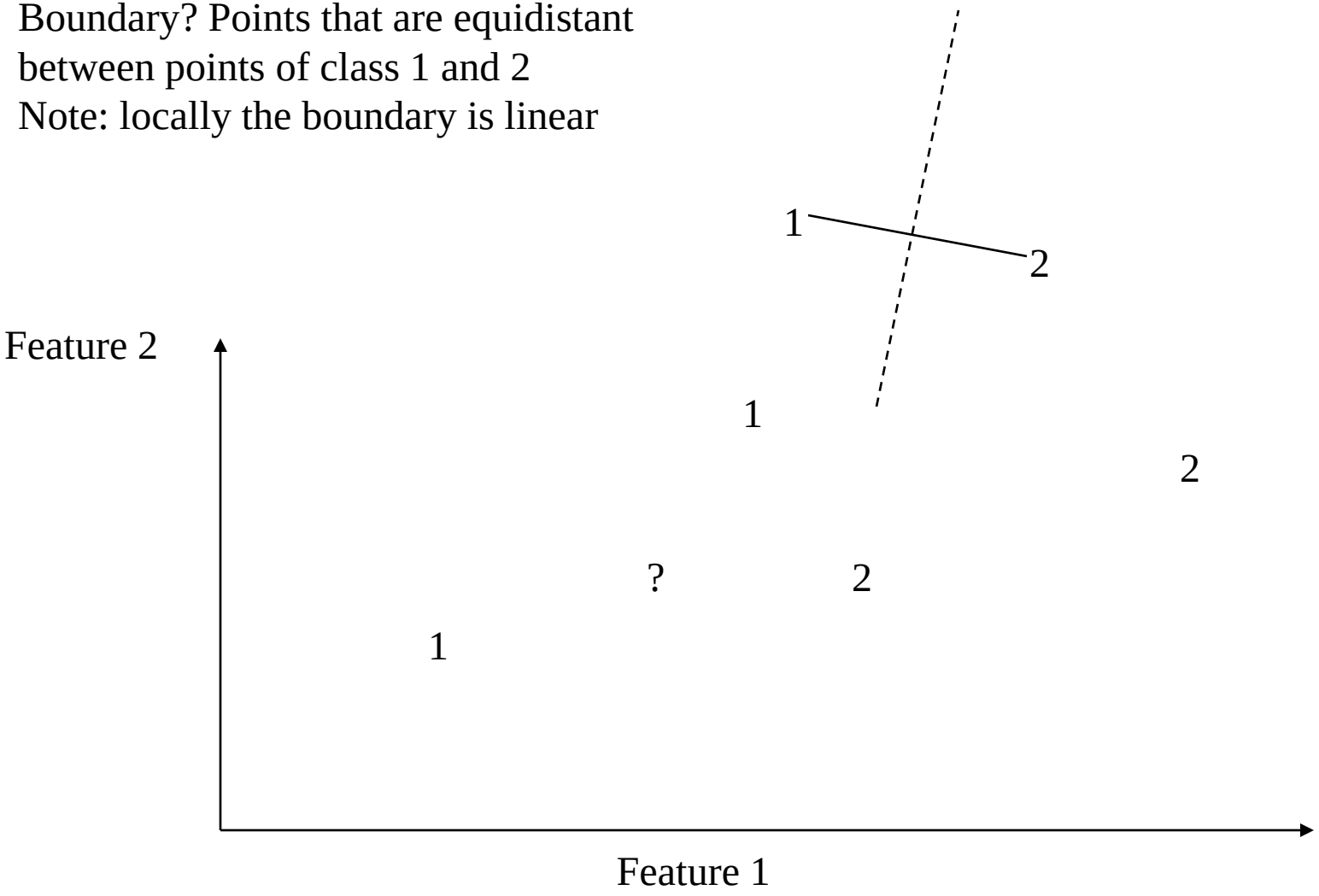
- The nearest-neighbor classifier
  - Given a test point $\underline{x}$', compute the distance between $\underline{x}$' and each input data point
  - Find the closest neighbor in the training data
  - Assign $\underline{x}$' the class label of this neighbor
  - (sort of generalizes minimum distance classifier to exemplars)

- If Euclidean distance is used as the distance measure (the most common choice), the nearest neighbor classifier results in piecewise linear decision boundaries

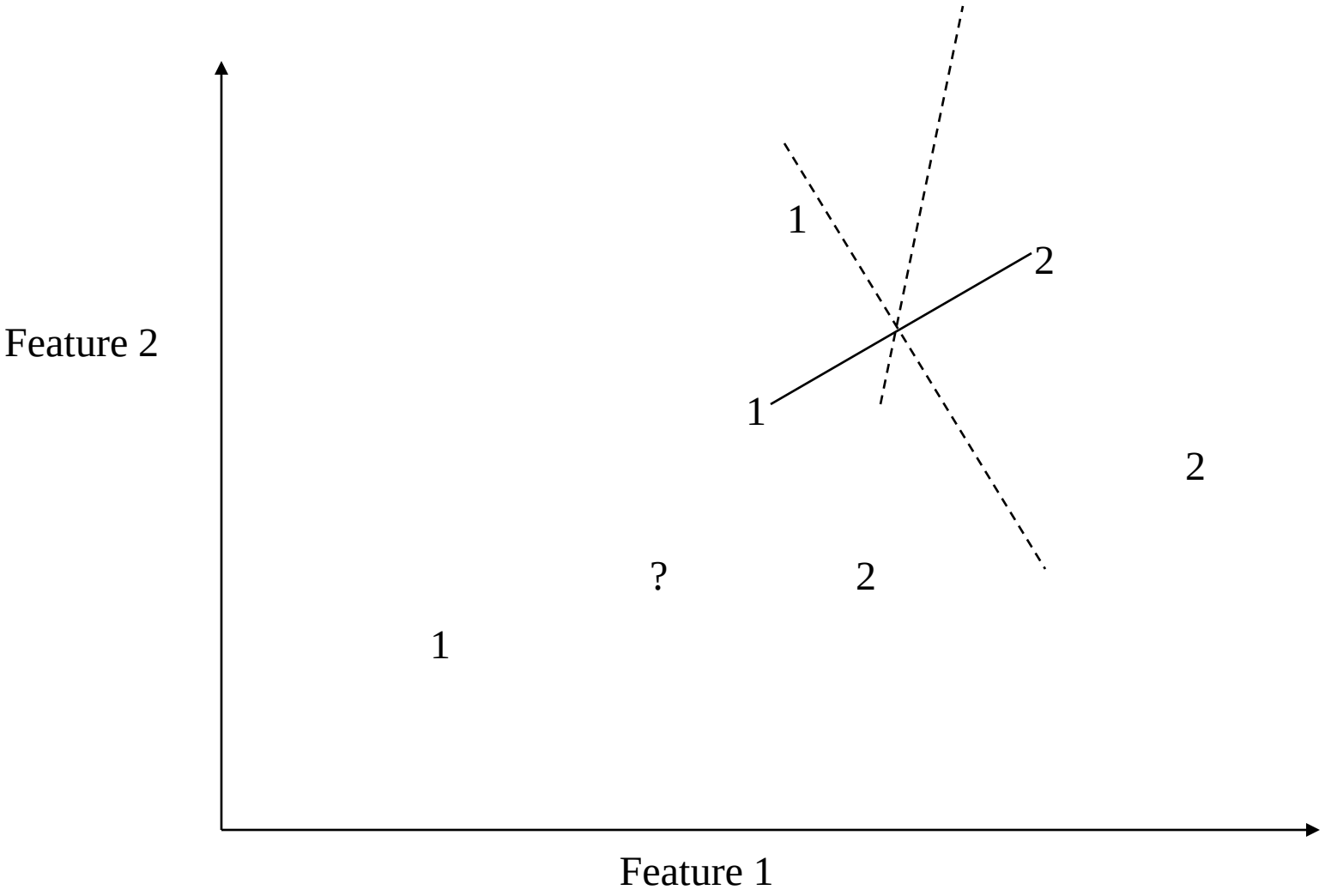
- Many extensions
  - e.g., kNN, vote based on k-nearest neighbors
  - k can be chosen by cross-validation

Local Decision Boundaries

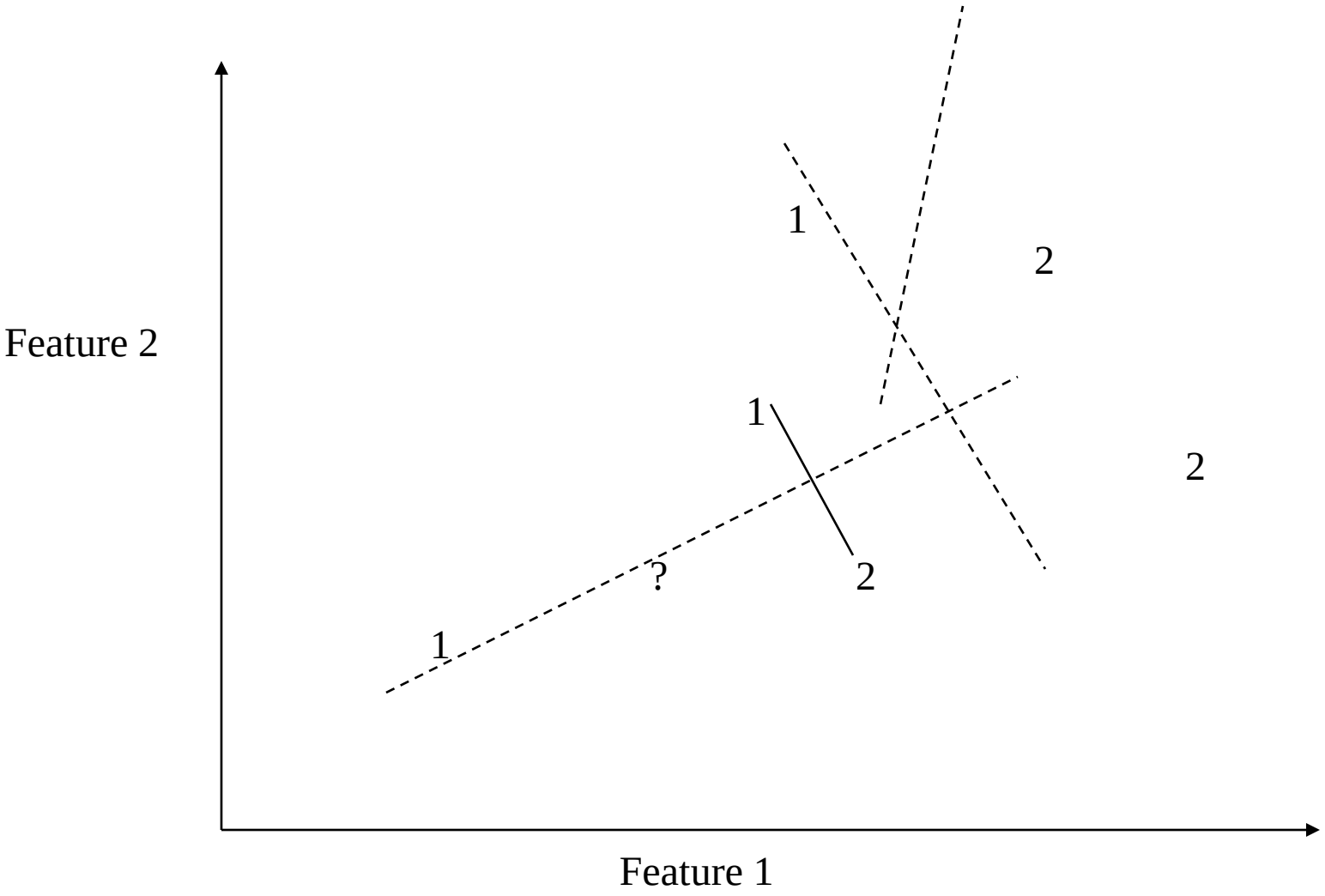
Boundary? Points that are equidistant between points of class 1 and 2
Note: locally the boundary is linear



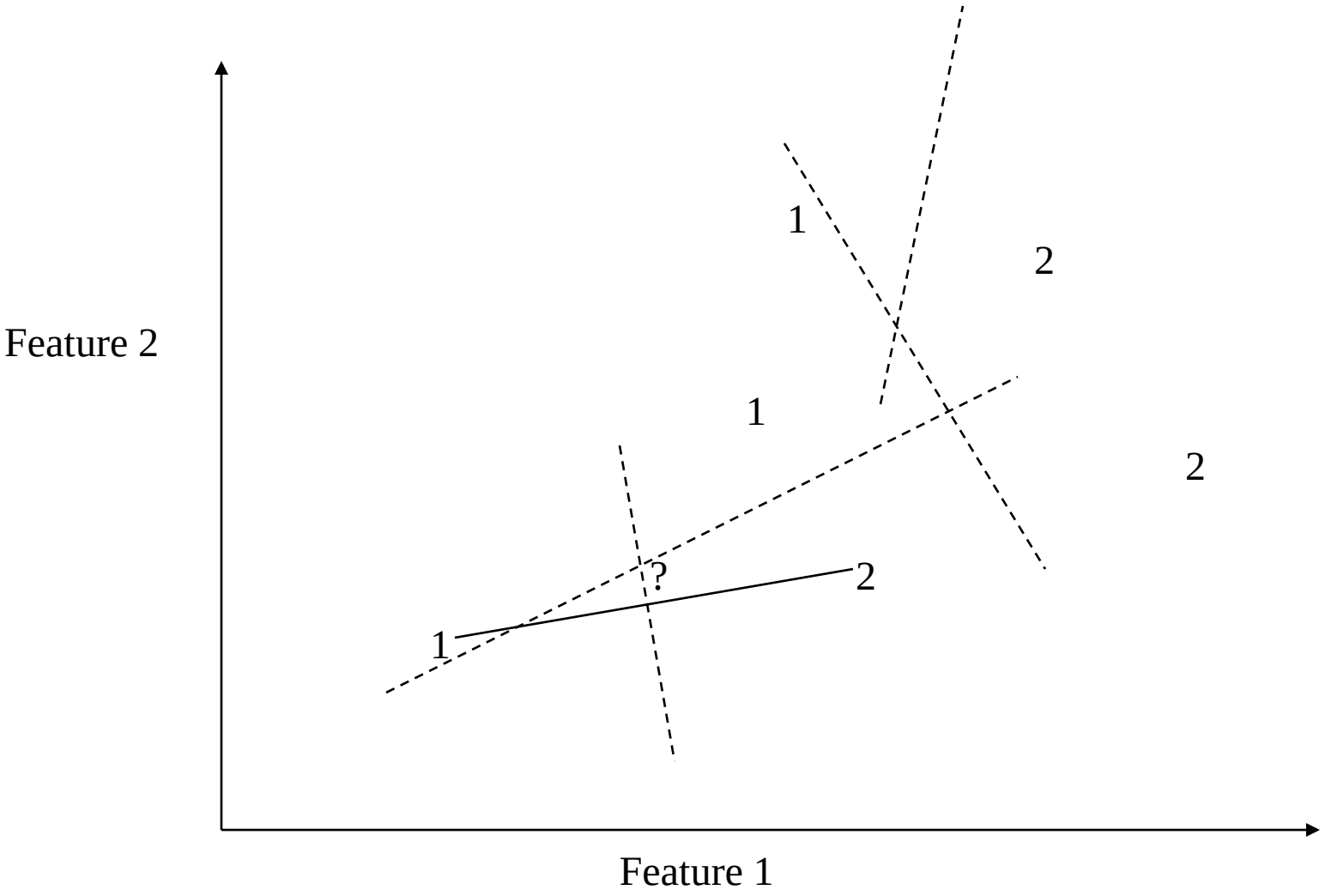
Finding the Decision Boundaries



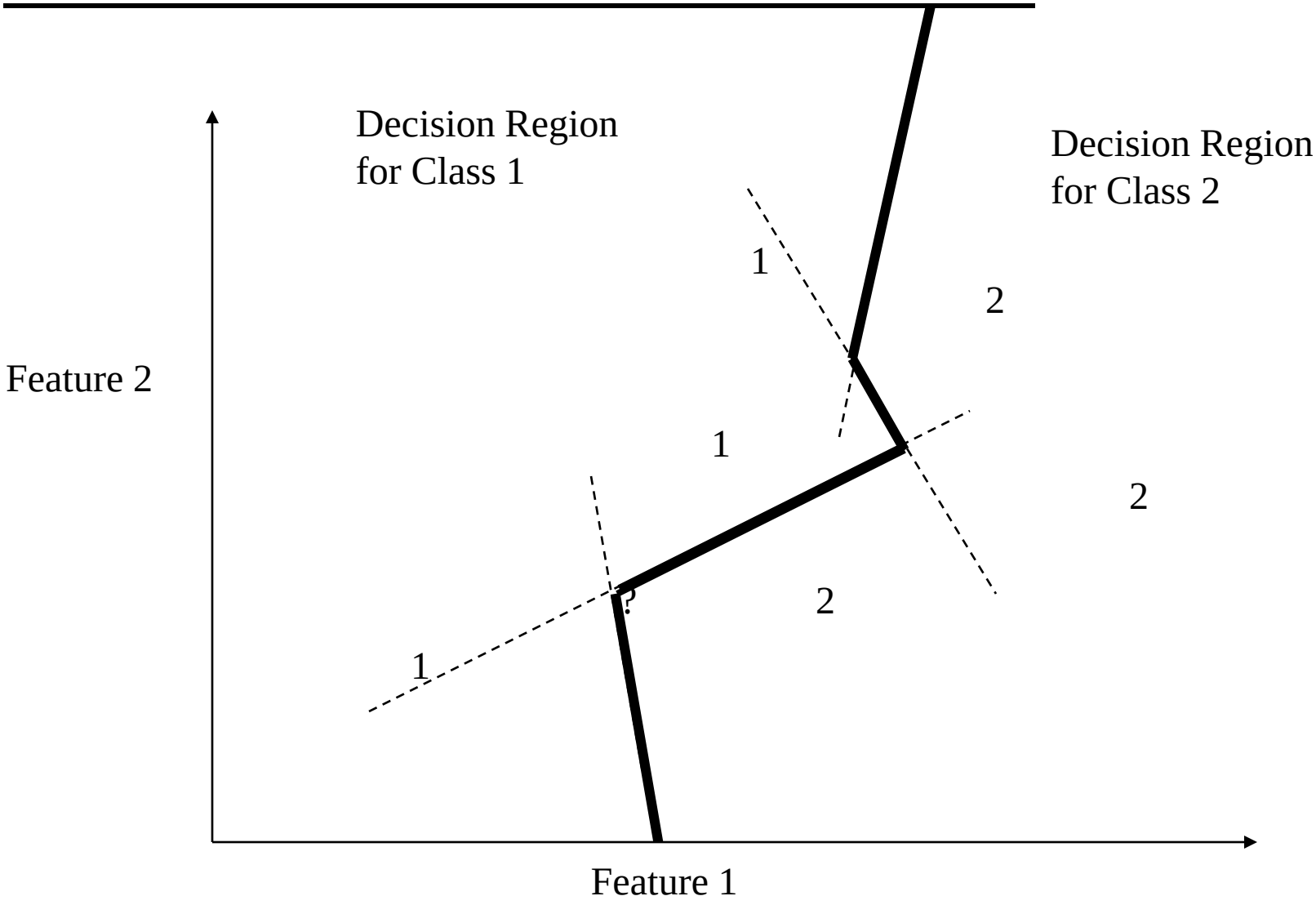
Finding the Decision Boundaries



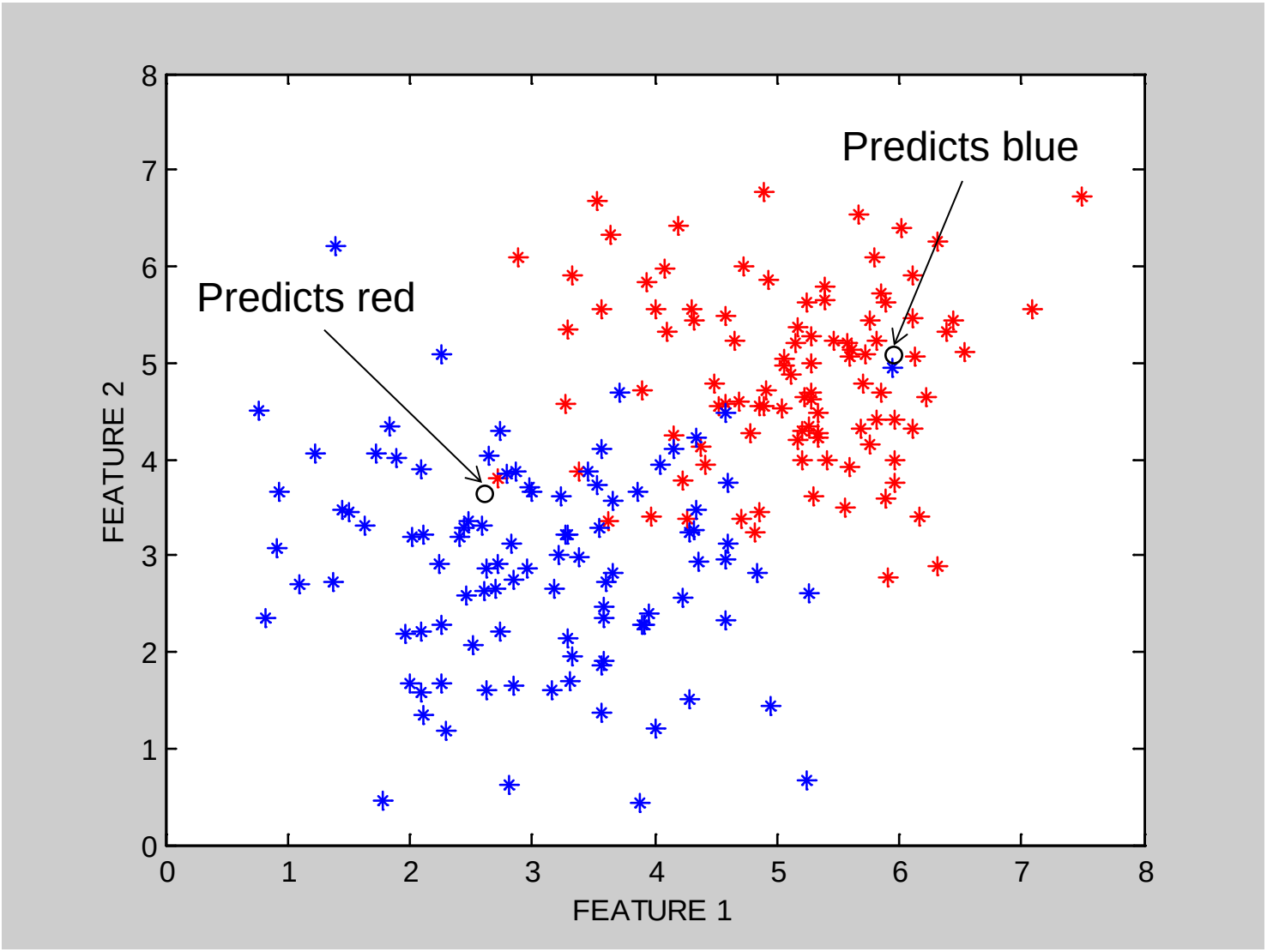
Finding the Decision Boundaries



Overall Boundary = Piecewise Linear



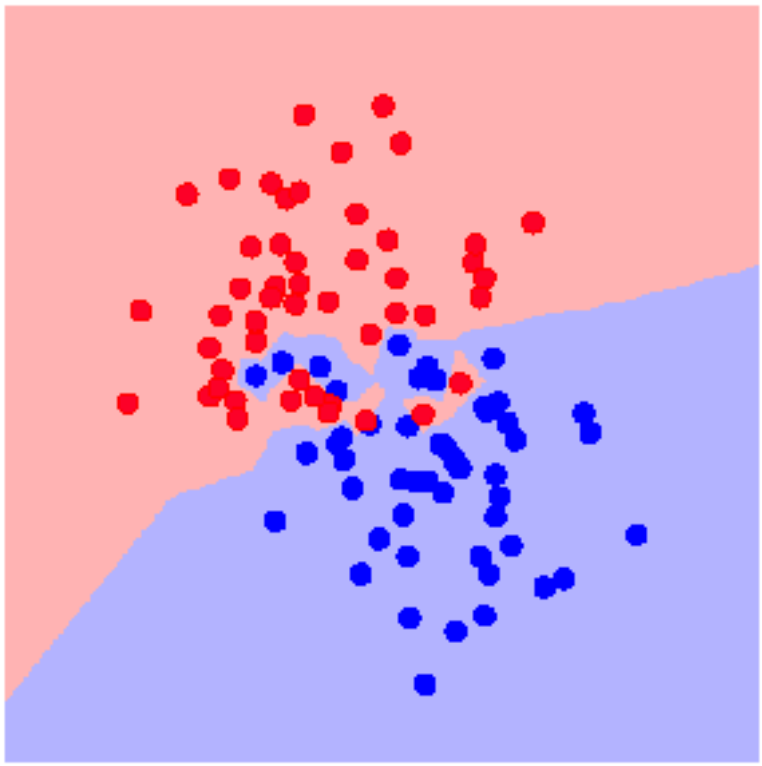
Nearest-Neighbor Boundaries on this data set?



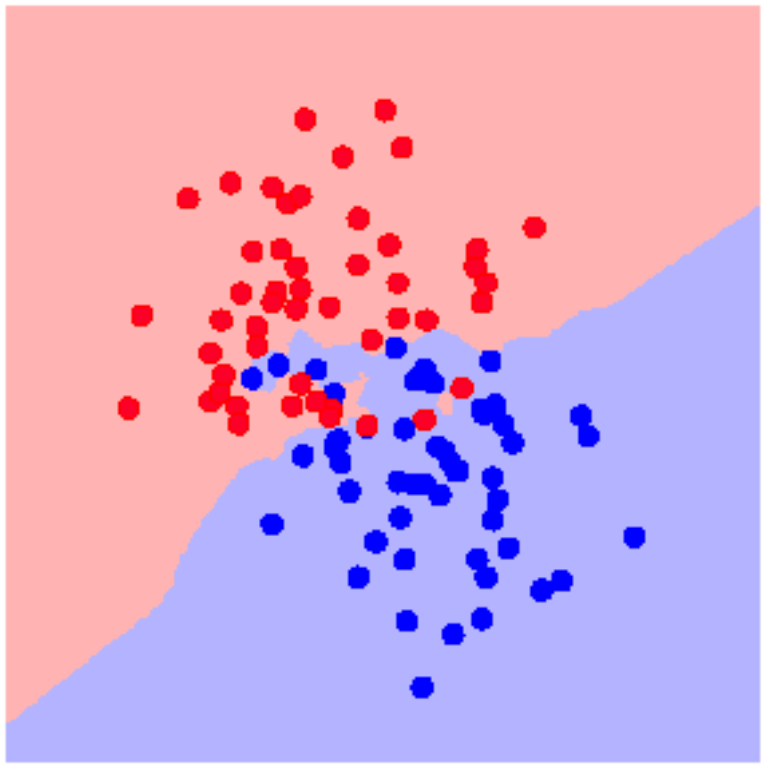
kNN Decision Boundary

- piecewise linear decision boundary
- Increasing k "simplifies" decision boundary
  - Majority voting means less emphasis on individual points

K = 1



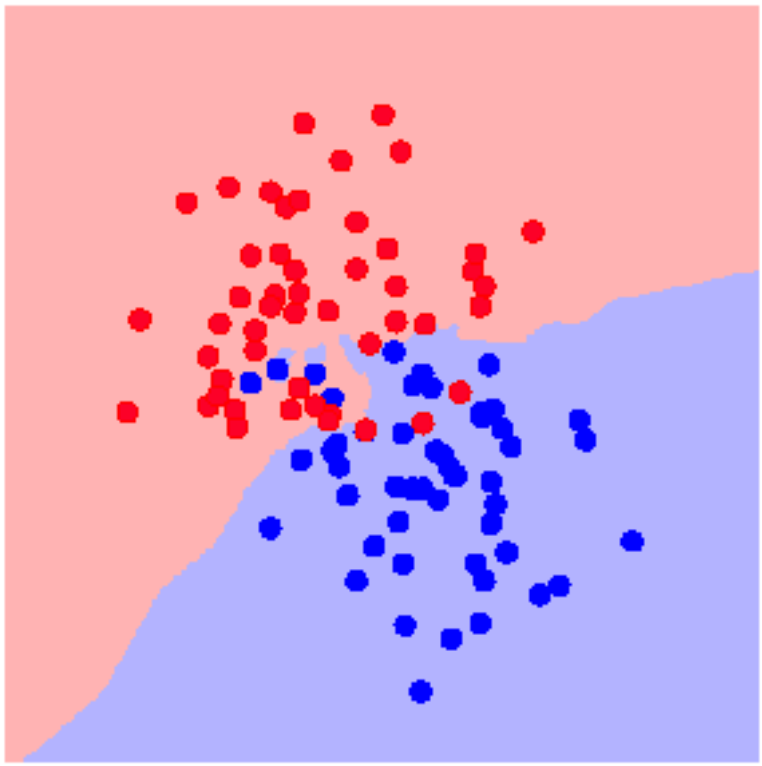
K = 3



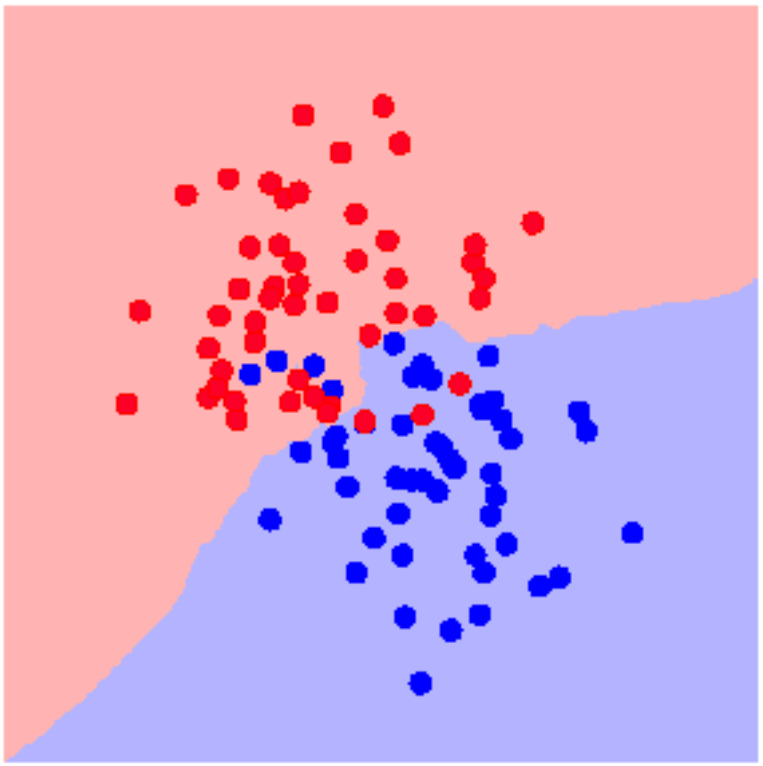
kNN Decision Boundary

- piecewise linear decision boundary
- Increasing k "simplifies" decision boundary
  - Majority voting means less emphasis on individual points

K = 5



K = 7

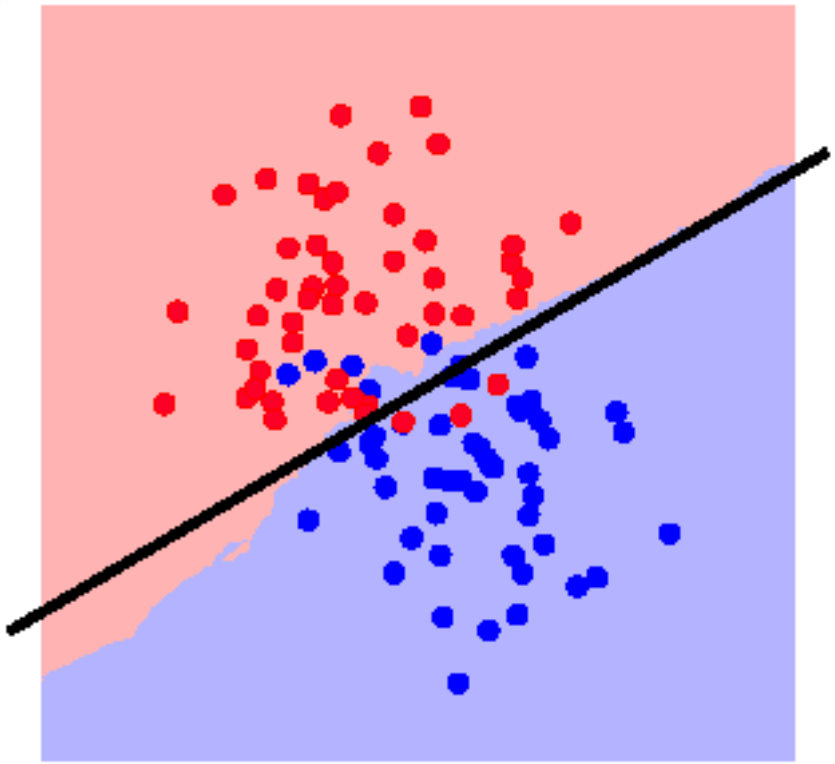


kNN Decision Boundary

- piecewise linear decision boundary
- Increasing k "simplifies" decision boundary
  - Majority voting means less emphasis on individual points

- True ("best") decision boundary
  - In this case is linear
  - Compared to kNN: not bad!

K = 25



The kNN Classifier

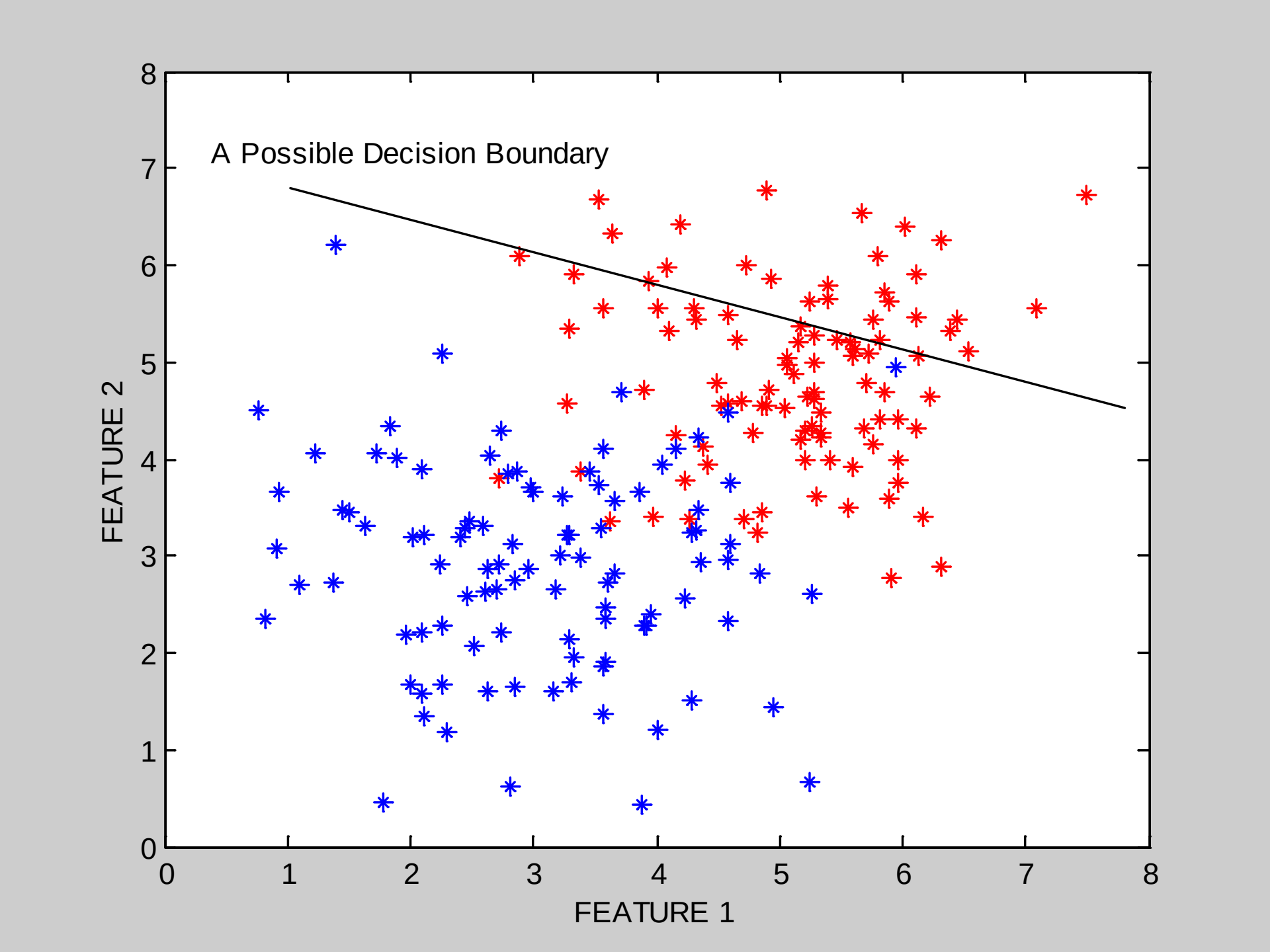
- The kNN classifier often works very well.
- Easy to implement.
- Easy choice if characteristics of your problem are unknown.
- Can be sensitive to the choice of distance metric.
  - Often normalize feature axis values, e.g., z-score or [0, 1]
  - Categorical feature axes are difficult, e.g., Color as Red/Blue/Green
- Can encounter problems with sparse training data.
- Can encounter problems in very high dimensional spaces.
  - Most points are corners.
  - Most points are at the edge of the space.
  - Most points are neighbors of most other points.

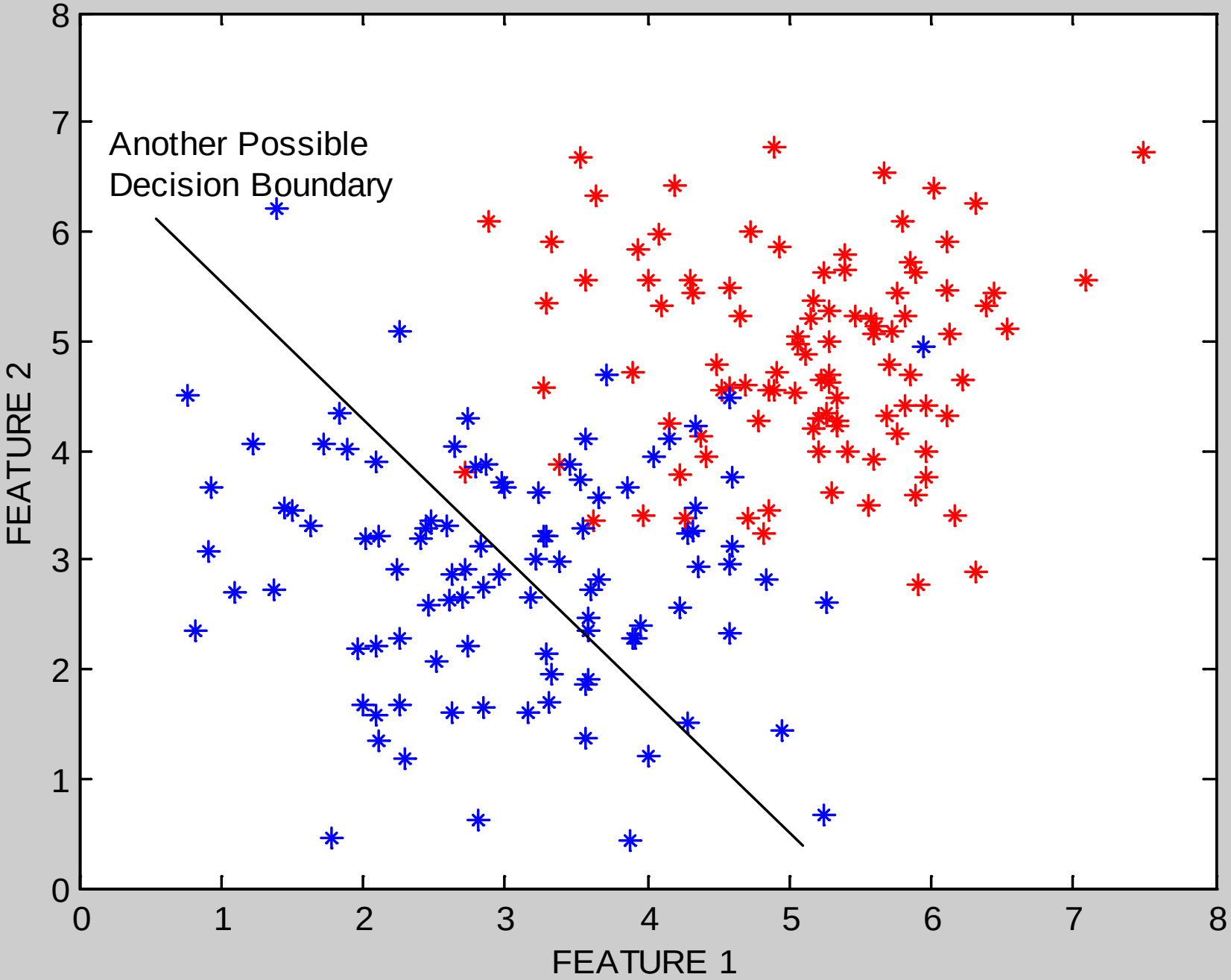
Linear Classifiers

- Linear classifier ⇔ single linear decision boundary (for 2-class case)
- We can always represent a linear decision boundary by a linear equation:

$$w_1 x_1 + w_2 x_2 + \ldots + w_d x_d = \sum w_j x_j = \underline{w}^t \underline{x} = 0$$

- In d dimensions, this defines a (d-1) dimensional hyperplane
  - d=3, we get a plane; d=2, we get a line
- For prediction we simply see if $\sum w_j x_j > 0$
- The w_i are the weights (parameters)
  - Learning consists of searching in the d-dimensional weight space for the set of weights (the linear boundary) that minimizes an error measure
  - A threshold can be introduced by a "dummy" feature that is always one; its weight corresponds to (the negative of) the threshold
- Note that a minimum distance classifier is a special (restricted) case of a linear classifier


A Possible Decision Boundary
FEATURE 2
FEATURE 1
0
1
2
3
4
5
6
7
8


Another Possible
Decision Boundary
FEATURE 2
FEATURE 1
0
1
2
3
4
5
6
7
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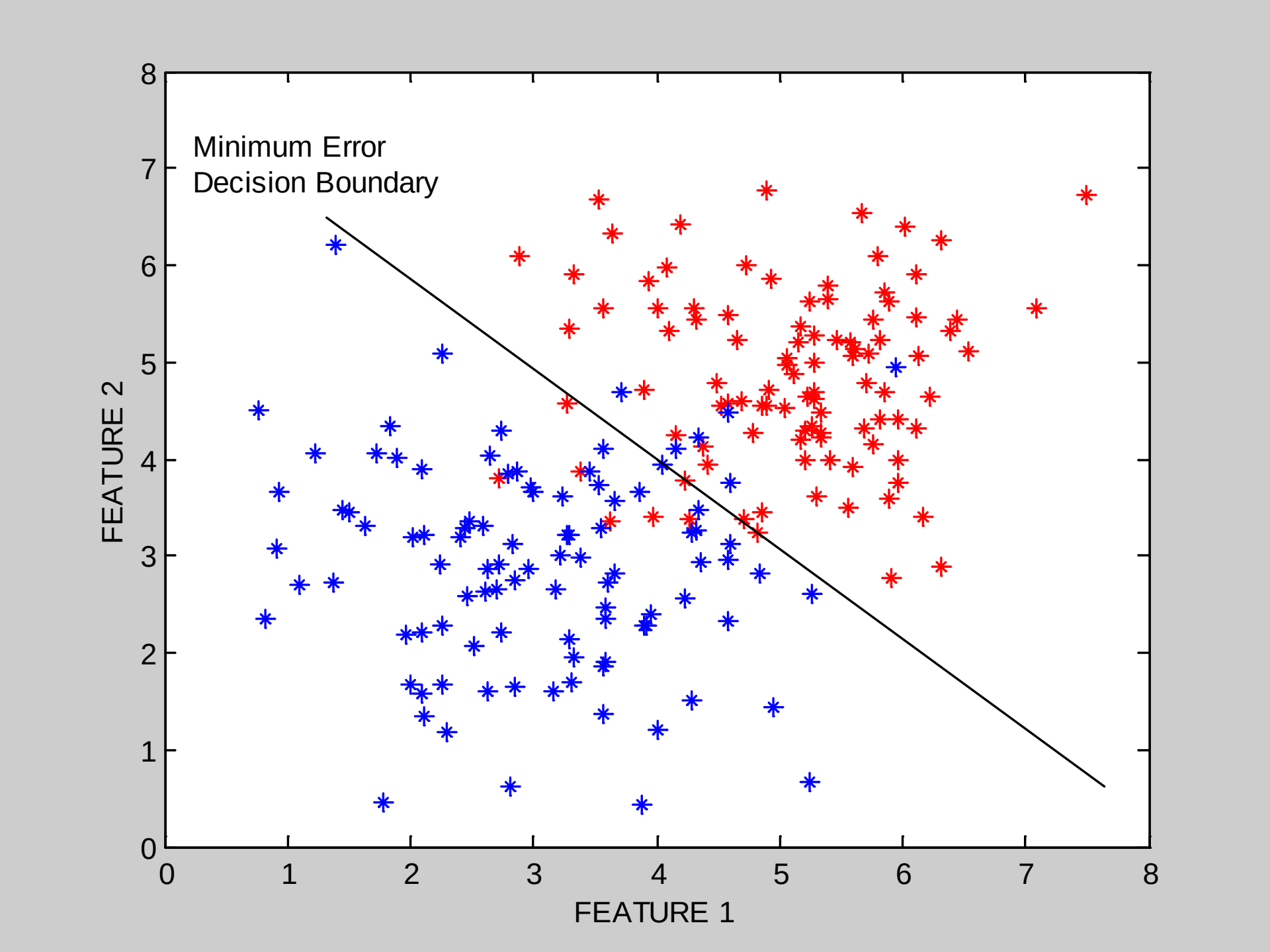

Minimum Error
Decision Boundary
FEATURE 2
FEATURE 1
0
1
2
3
4
5
6
7
8

The Perceptron Classifier (pages 729-731 in text)

- The perceptron classifier is just another name for a linear classifier for 2-class data, i.e.,

  $$\text{output}(\underline{x}) = \text{sign}\left(\sum w_j x_j \right)$$

- Loosely motivated by a simple model of how neurons fire

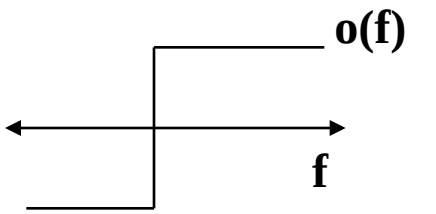
- For mathematical convenience, class labels are +1 for one class and -1 for the other

- Two major types of algorithms for training perceptrons
  - Objective function = classification accuracy ("error correcting")
  - Objective function = squared error (use gradient descent)

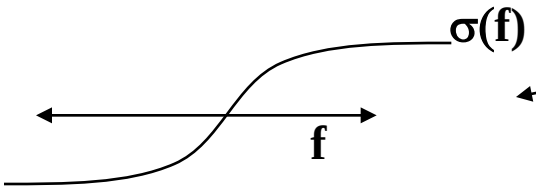
  - Gradient descent is generally faster and more efficient – but there is a problem! No gradient!

Two different types of perceptron output

x-axis below is f(x) = f = weighted sum of inputs
y-axis is the perceptron output



Thresholded output (step function), takes values +1 or -1



Sigmoid output, takes real values between -1 and +1

The sigmoid is in effect an approximation to the threshold function above, but has a gradient that we can use for learning

- Sigmoid function is defined as

$$\sigma[f] = [2 / (1 + \exp[- f])] - 1$$

- Derivative of sigmoid

$$\partial\sigma/\delta f [f] = .5 * (\sigma[f]+1) * (1-\sigma[f])$$

Squared Error for Perceptron with Sigmoidal Output

- Squared error = $E[\underline{w}] = \sum_i [\sigma(f[\underline{x}(i)]) - y(i)]^2$

where $\underline{x}(i)$ is the ith input vector in the training data, i=1,..N
$y(i)$ is the ith target value (-1 or 1)

$f[\underline{x}(i)] = \sum w_j x_j$ is the weighted sum of inputs
$\sigma(f[\underline{x}(i)])$ is the sigmoid of the weighted sum

- Note that everything is fixed (once we have the training data) except for the weights $\underline{w}$

- So we want to minimize $E[\underline{w}]$ as a function of $\underline{w}$

Gradient Descent Learning of Weights

Gradient Descent Rule:

$$\underline{\mathbf{w}}_{\text{new}} = \underline{\mathbf{w}}_{\text{old}} - \eta \, \Delta (E[\underline{\mathbf{w}}])$$

where

$\Delta (E[\underline{w}])$ is the gradient of the error function E wrt weights, and

η is the learning rate (small, positive)

Notes:

1. This moves us downhill in direction $\Delta (E[\underline{\mathbf{w}}])$ (steepest downhill)
2. How far we go is determined by the value of η

Gradient Descent Update Equation

- From basic calculus, for perceptron with sigmoid, and squared error objective function, gradient for a single input $\underline{x}(i)$ is

$$\Delta (E[\underline{w}]) = - (y(i) - \sigma[f(i)]) \partial\sigma[f(i)] x_j(i)$$

- Gradient descent weight update rule:

$$w_j = w_j + \eta (y(i) - \sigma[f(i)]) \partial\sigma[f(i)] x_j(i)$$

  - can rewrite as:

$$w_j = w_j + \eta * error * c * x_j(i)$$

Pseudo-code for Perceptron Training

Initialize each w_j (e.g.,randomly)

While (termination condition not satisfied)
    for i = 1: N % loop over data points (an iteration)
        for j= 1 : d % loop over weights
            deltawj = η (y(i) – σ[f(i)]) $\partial\sigma$[f(i)] x_j(i)
            w_j = w_j + deltawj
        end
    calculate termination condition
    end

- Inputs: N features, N targets (class labels), learning rate η
- Outputs: a set of learned weights

Comments on Perceptron Learning

- Iteration = one pass through all of the data
- Algorithm presented = incremental gradient descent
  - Weights are updated after visiting each input example
  - Alternatives
    - Batch: update weights after each iteration (typically slower)
    - Stochastic: randomly select examples and then do weight updates
- A similar iterative algorithm learns weights for thresholded output (step function) perceptrons
- Rate of convergence
  - E[$\underline{w}$] is convex as a function of $\underline{w}$, so no local minima
  - So convergence is guaranteed as long as learning rate is small enough
    - But if we make it too small, learning will be *very* slow
  - But if learning rate is too large, we move further, but can overshoot the solution and oscillate, and not converge at all

Support Vector Machines (SVM): "Modern perceptrons" (section 18.9, R&N)

- A modern linear separator classifier
  - Essentially, a perceptron with a few extra wrinkles

- Constructs a **"maximum margin separator"**
  - A linear decision boundary with the largest possible distance from the decision boundary to the example points it separates
  - "Margin" = Distance from decision boundary to closest example
  - The "maximum margin" helps SVMs to generalize well

- Can embed the data in a non-linear higher dimension space
  - Constructs a linear separating hyperplane in that space
    - **This can be a non-linear boundary in the original space**
  - Algorithmic advantages and simplicity of linear classifiers
  - Representational advantages of non-linear decision boundaries

- **Currently most popular "off-the shelf" supervised classifier.**

Multi-Layer Perceptrons (Artificial Neural Networks)

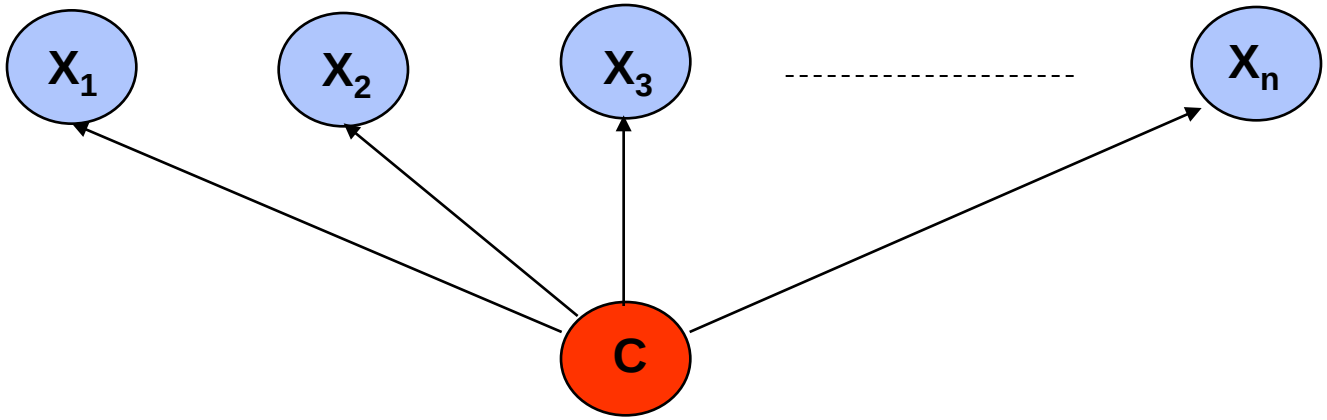
(sections 18.7.3-18.7.4 in textbook)

- What if we took K perceptrons and trained them in parallel and then took a weighted sum of their sigmoidal outputs?
  - This is a multi-layer neural network with a single "hidden" layer (the outputs of the first set of perceptrons)
  - If we train them jointly in parallel, then intuitively different perceptrons could learn different parts of the solution
    - They define different local decision boundaries in the input space
- What if we hooked them up into a general Directed Acyclic Graph?
  - Can create simple "neural circuits" (but no feedback; not fully general)
  - Often called neural networks with hidden units

- How would we train such a model?
  - Backpropagation algorithm = clever way to do gradient descent
  - Bad news: many local minima and many parameters
    - training is hard and slow
  - Good news: can learn general non-linear decision boundaries
  - Generated much excitement in AI in the late 1980's and 1990's
  - Techniques like boosting, support vector machines, are often preferred

Naïve Bayes Model

(section 20.2.2 R&N 3rd ed.)



Bayes Rule: $P(C \mid X_1,\ldots X_n)$ is proportional to $P(C) \ \Pi_i \ P(X_i \mid C)$
[note: denominator $P(X_1,\ldots X_n)$ is constant for all classes, may be ignored.]

Features Xi are conditionally independent given the class variable C

- choose the class value c_i with the highest $P(c_i \mid x_1,\ldots, x_n)$
- simple to implement, often works very well
- e.g., spam email classification: X's = counts of words in emails

Conditional probabilities $P(X_i \mid C)$ can easily be estimated from labeled date

- Problem: Need to avoid zeroes, e.g., from limited training data
- Solutions: Pseudo-counts, beta[a,b] distribution, etc.

Naïve Bayes Model (2)

$$P(C \mid X_1,\ldots X_n) = \alpha \prod P(X_i \mid C)\ P(C)$$

Probabilities P(C) and P(Xi | C) can easily be estimated from labeled data

P(C = cj) ≈ #(Examples with class label cj) / #(Examples)

P(Xi = xik | C = cj)
≈ #(Examples with Xi value xik and class label cj)
/ #(Examples with class label cj)

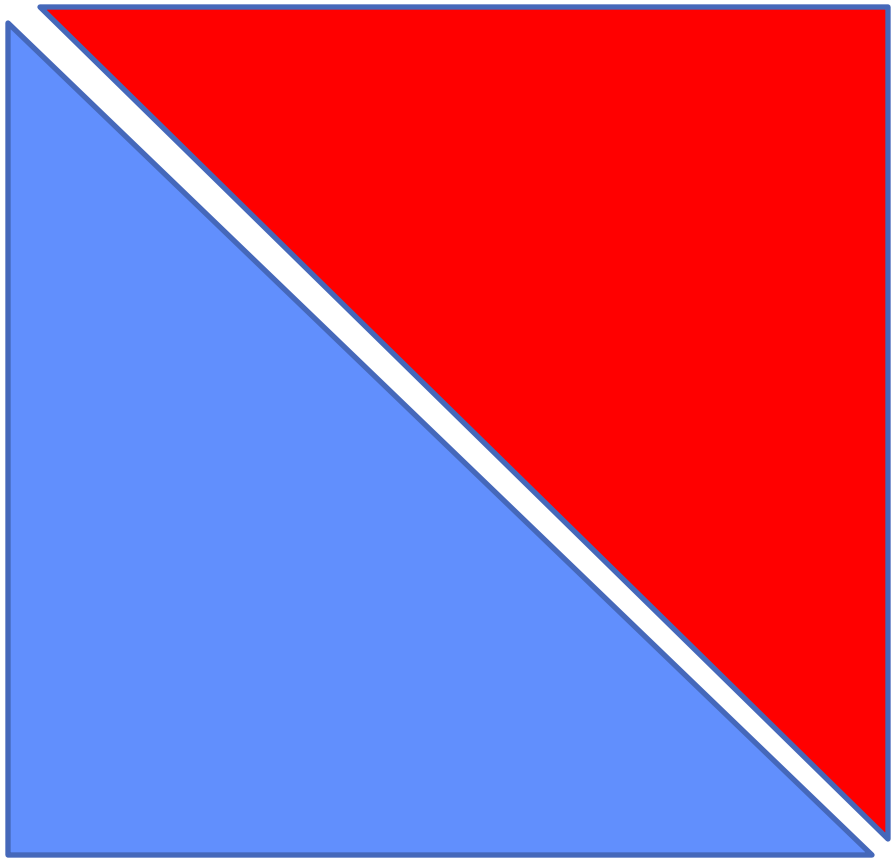
Usually easiest to work with logs

$$\log [\ P(C \mid X_1,\ldots X_n)\ ] = \log \alpha + \sum [\ \log P(X_i \mid C) + \log P(C)\ ]$$

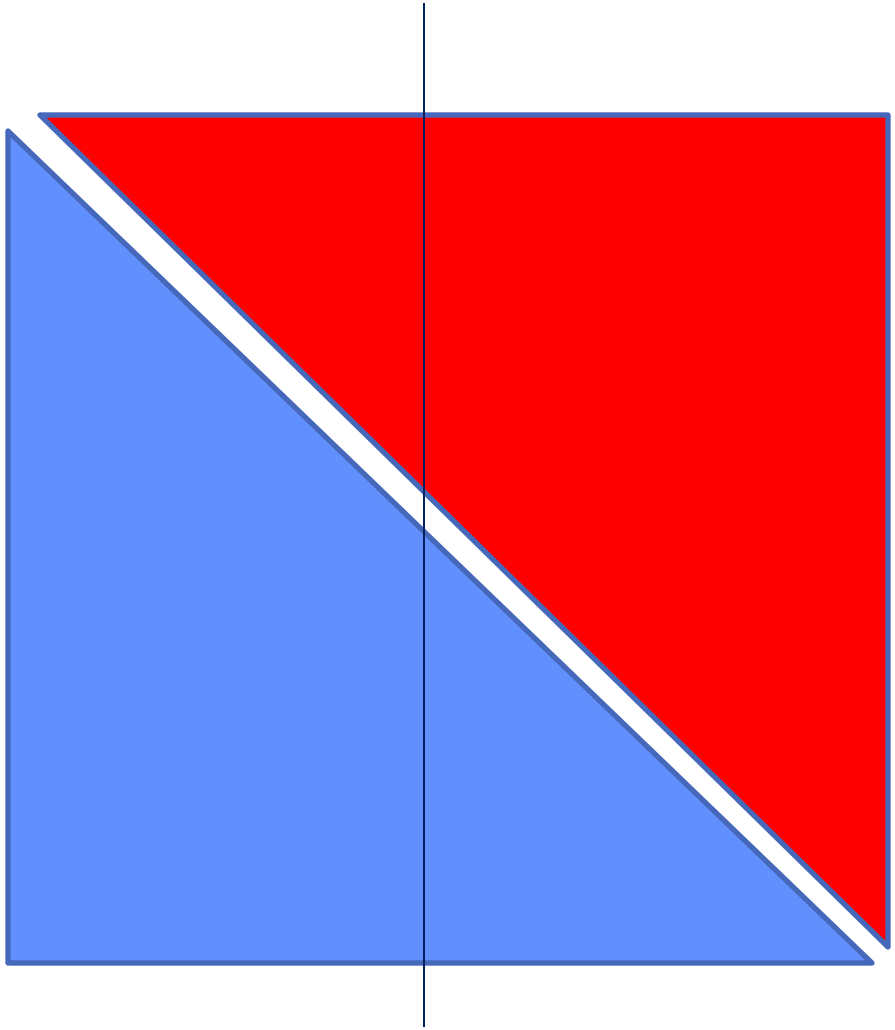
DANGER: Suppose ZERO examples with Xi value xik and class label cj ?
An unseen example with Xi value xik will NEVER predict class label cj !

Practical solutions: Pseudocounts, e.g., add 1 to every #() , etc.
Theoretical solutions: Bayesian inference, beta distribution, etc.

Classifier Bias — Decision Tree or Linear Perceptron?



Classifier Bias — Decision Tree or Linear Perceptron?



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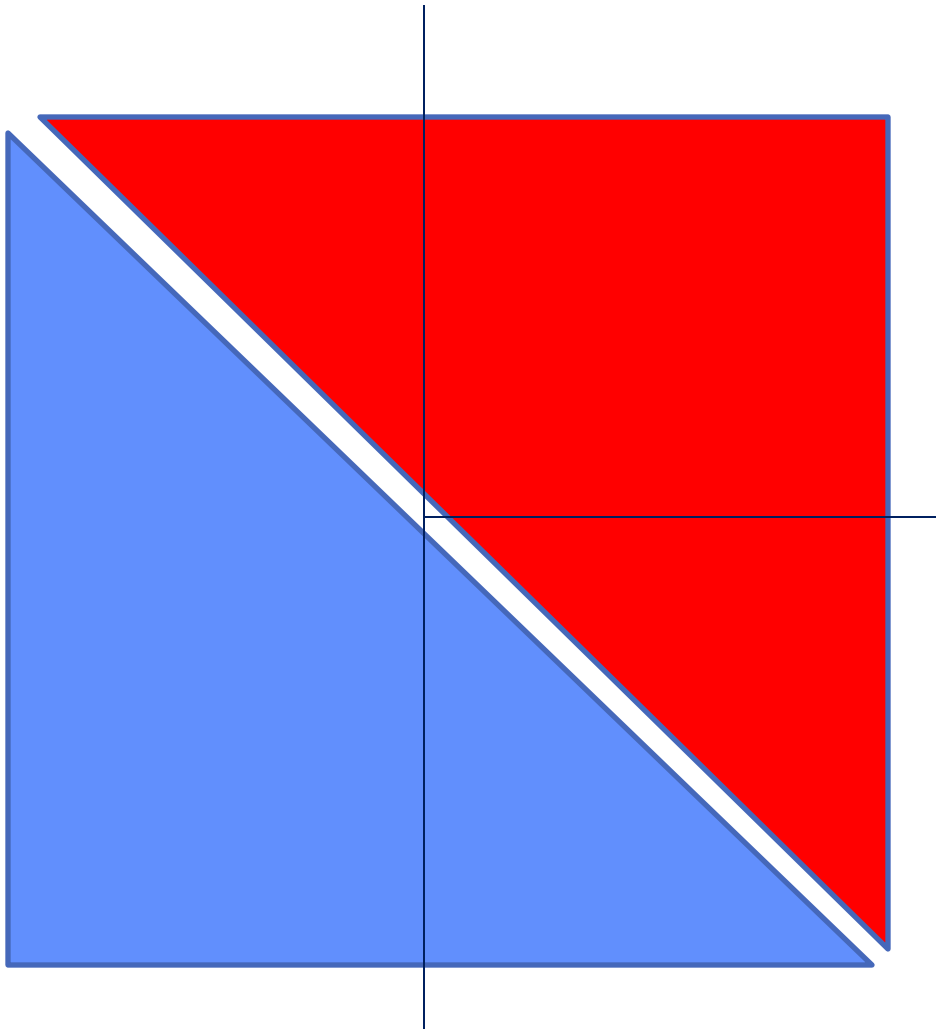

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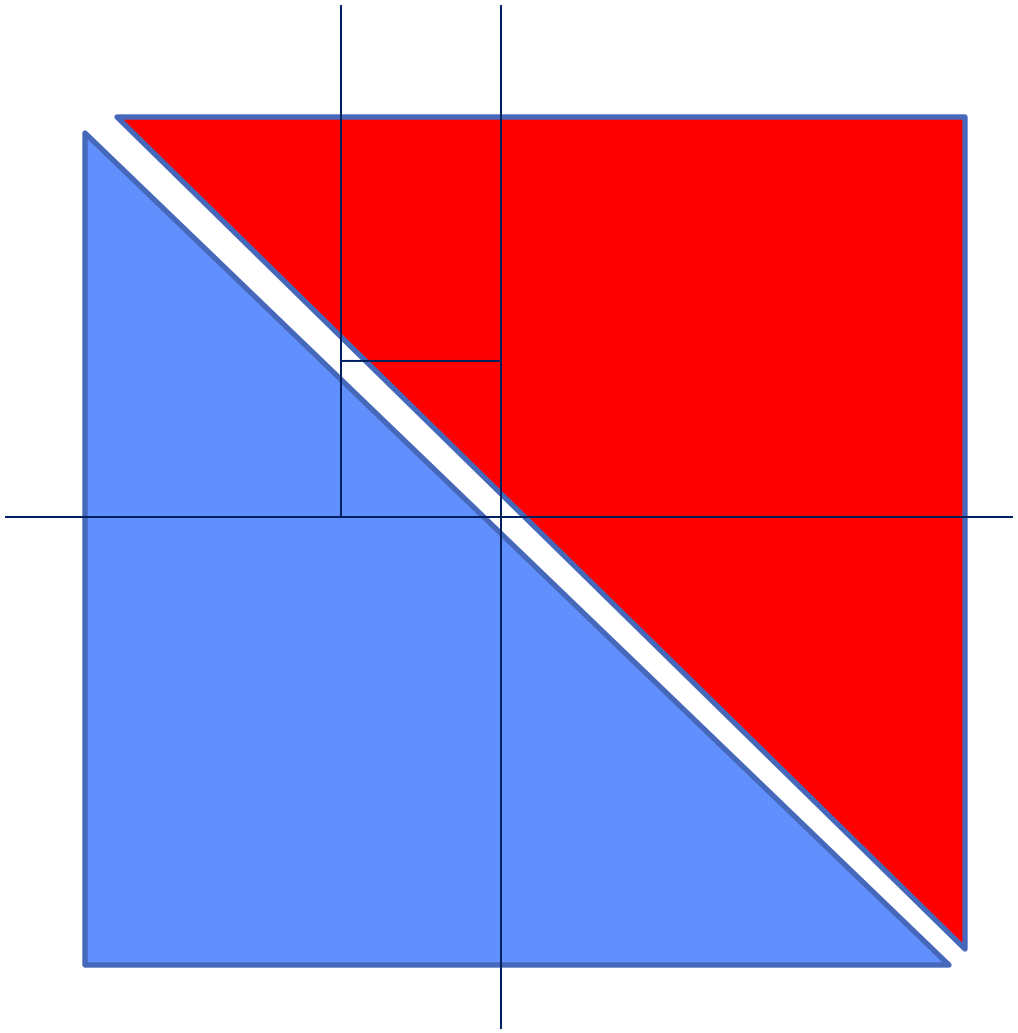

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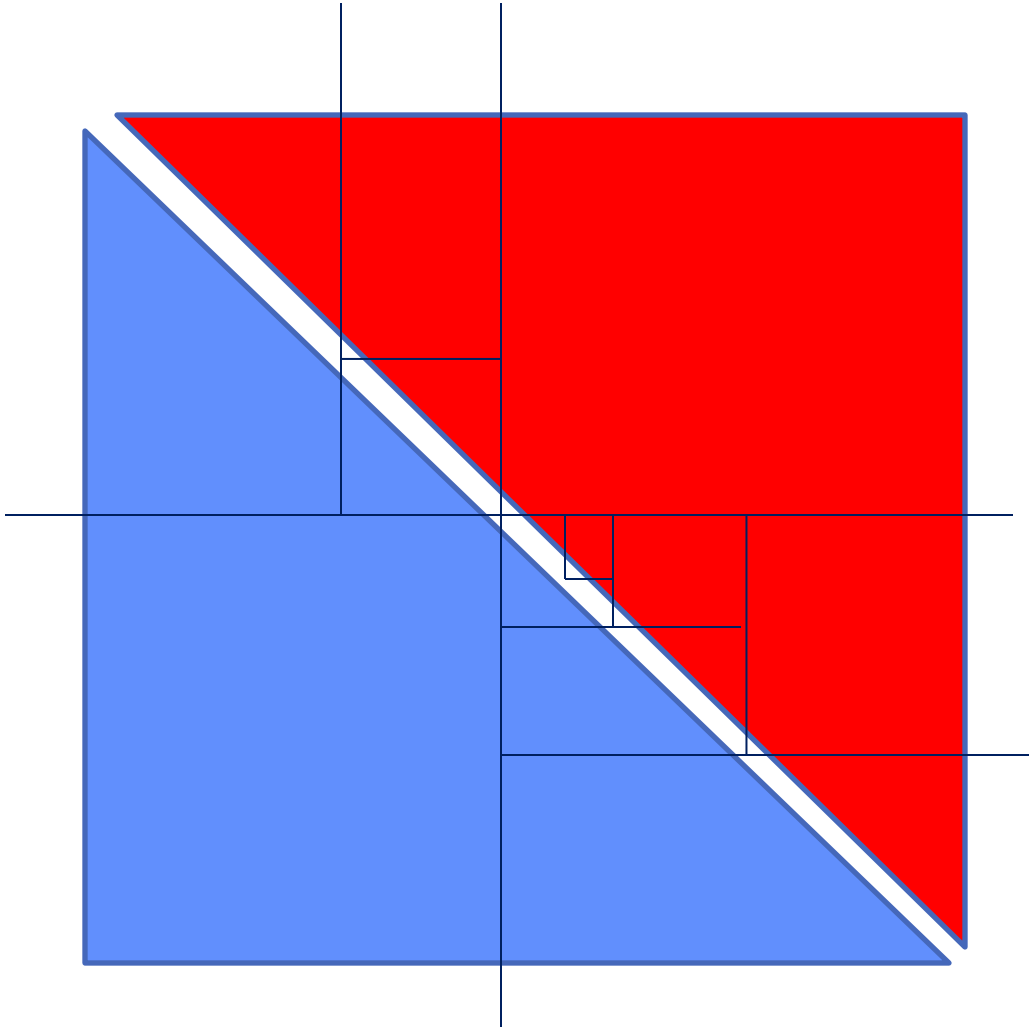

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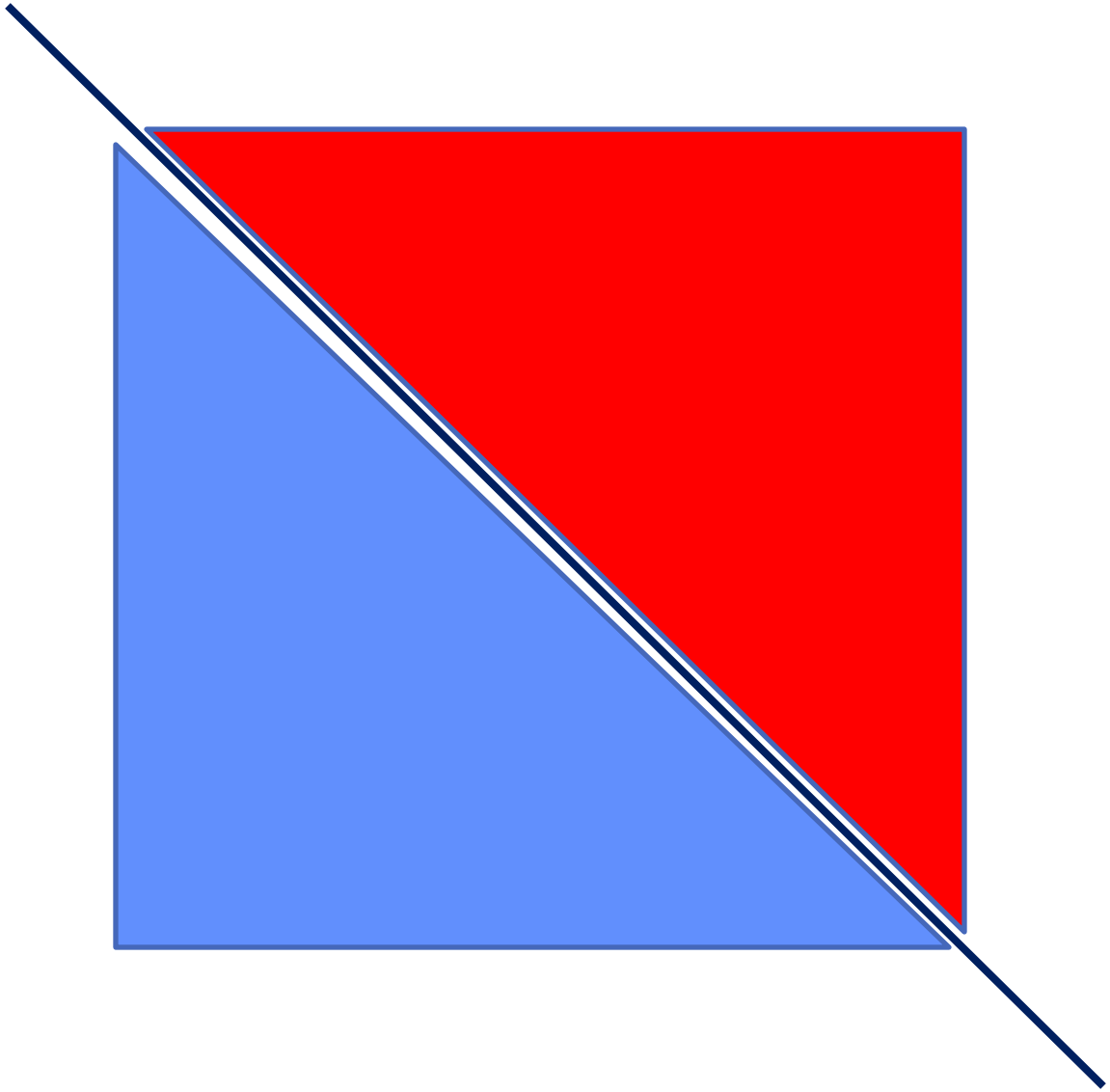

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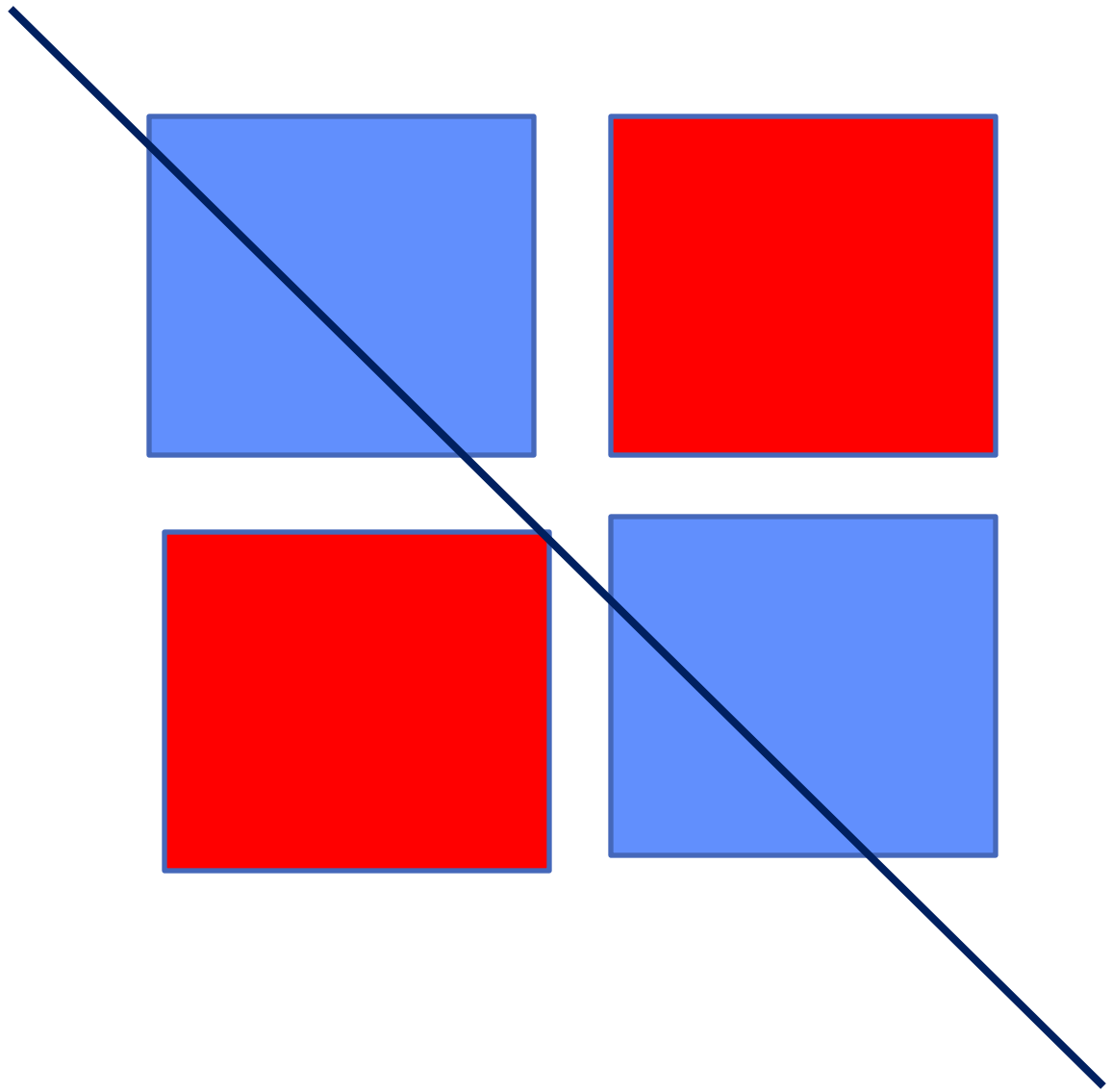

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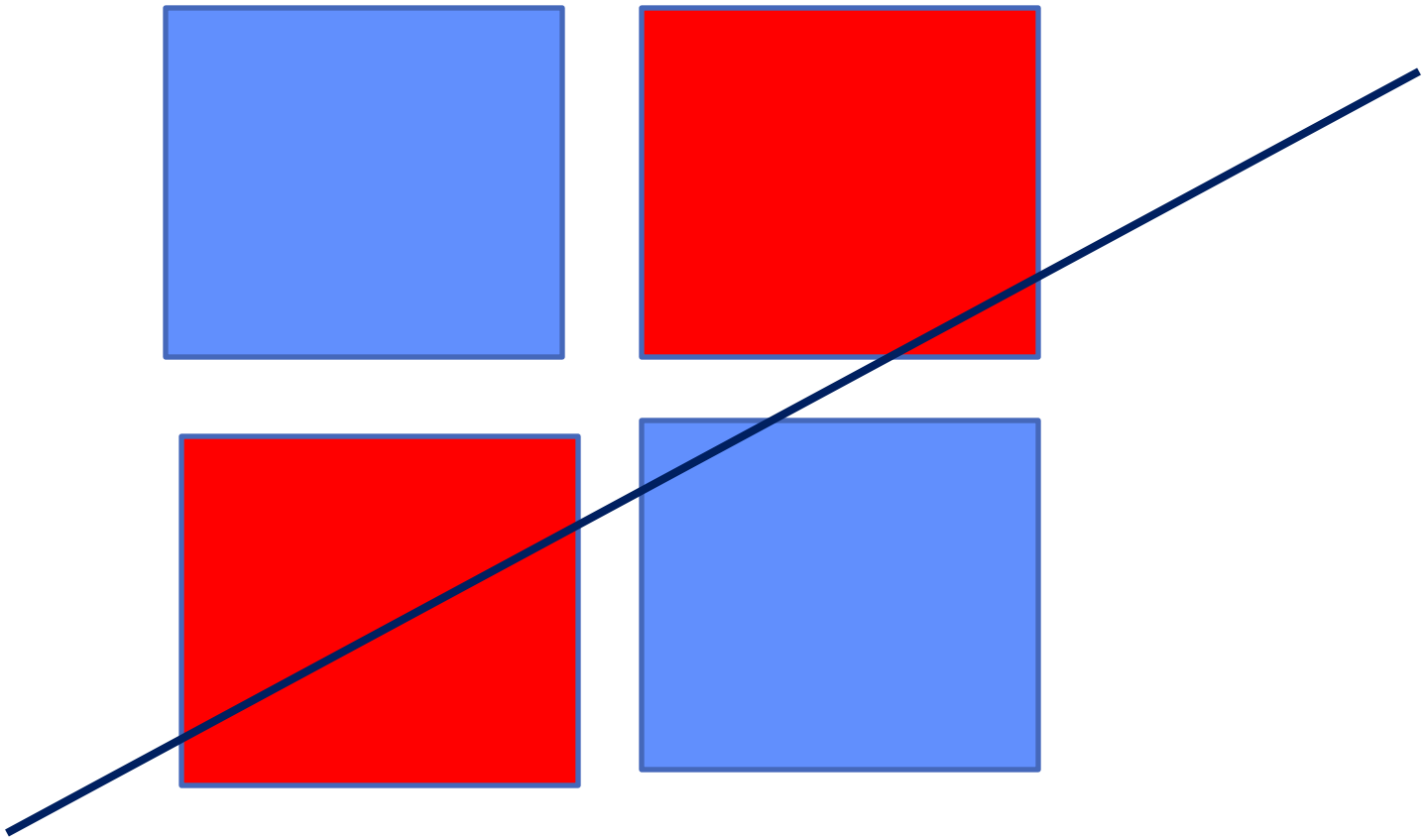

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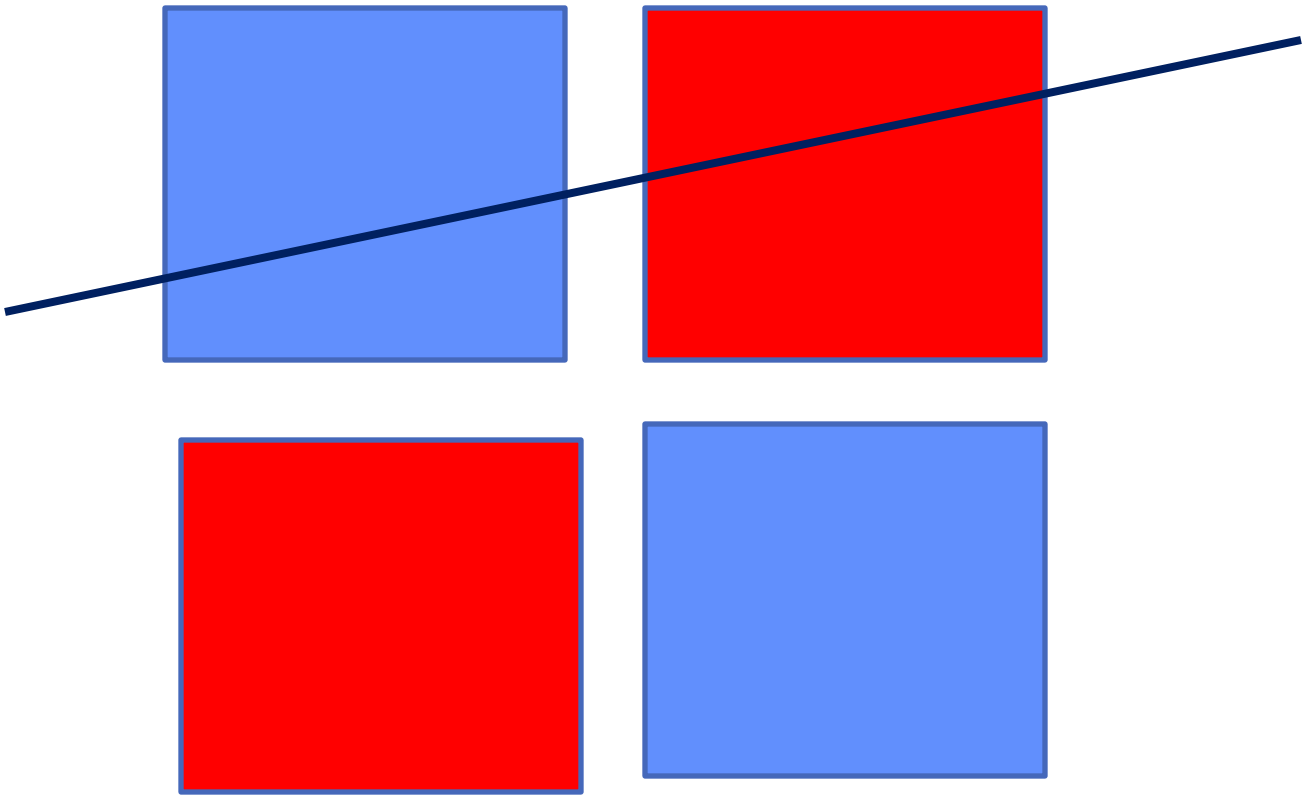

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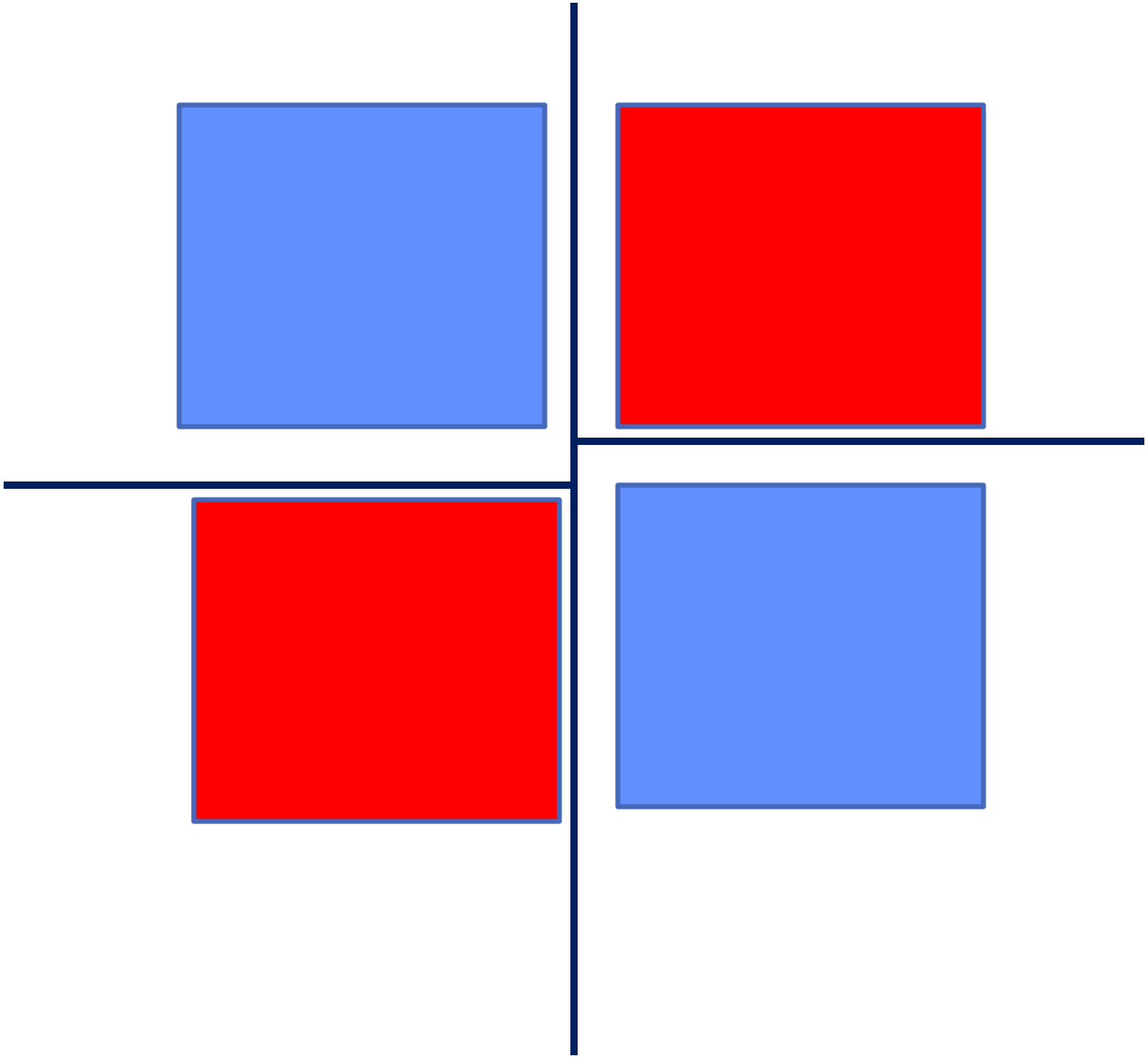

Summary

- Learning
  - Given a training data set, a class of models, and an error function, this is essentially a search or optimization problem
- Different approaches to learning
  - Divide-and-conquer: decision trees
  - Global decision boundary learning: perceptrons
  - Constructing classifiers incrementally: boosting
- Learning to recognize faces
  - Viola-Jones algorithm: state-of-the-art face detector, entirely learned from data, using boosting+decision-stumps