Machine Learning

Topic: Linear Discriminants

Bryan Pardo, EECS 349 Machine Learning, 2021

Thanks to Mark Cartwright for his contributions to these slides
Thanks to Alpaydin, Bishop, and Duda/Hart/Stork for images and ideas

Recall: Regression Learning Task

There is a set of possible examples $X = \{\mathbf{x_1}, \ldots \mathbf{x_n}\}$

Each example is a **vector** of k **real valued attributes**

$$\mathbf{x}_i = < x_{i1}, \ldots, x_{ik} >$$

A target function maps *X* onto some **real value** *Y*

$$f : X \to Y$$

The DATA is a set of tuples <example, response value>

$$\{< \mathbf{x}_1, y_1 >, \ldots < \mathbf{x_n}, y_n >\}$$

Find a hypothesis ***h*** such that...

$$\forall \mathbf{x}, h(\mathbf{x}) \approx f(\mathbf{x})$$

Discrimination Learning Task

There is a set of possible examples $X = \{\mathbf{x_1}, \ldots \mathbf{x_n}\}$

Each example is a **vector** of k **real valued attributes**

$$\mathbf{x}_i = < x_{i1}, \ldots, x_{ik} >$$

A target function maps *X* onto some **categorical variable** *Y*

$$f : X \rightarrow Y$$

The DATA is a set of tuples <example, response value>

$$\{< \mathbf{x}_1, y_1 >, \ldots < \mathbf{x_n}, y_n >\}$$

Find a hypothesis ***h*** such that...

$$\forall \mathbf{x}, h(\mathbf{x}) \approx f(\mathbf{x})$$

Reminder about notation

- $\mathbf{x}$ is a vector of attributes $<x_1,\ x_2,\ldots x_k>$
- $\mathbf{w}$ is a vector of weights $<w_1,\ w_2,\ldots w_k>$
- Given this…

$$g(x) = w_0 + w_1 x_1 + w_2 x_2 \ldots + w_k x_k$$

- We can notate it with linear algebra as

$$g(x) = w_0 + \mathbf{w}^{\mathrm{T}} \mathbf{x}$$

Recall: w_0

- $g(x) = w_0 + \mathbf{w}^\mathrm{T}\mathbf{x}$ is ALMOST what we want, but that pesky offset w_0 is not in the linear algebra part yet.

- If we define **w** to include w_0 and **x** to include an x_0 that is always 1, now…

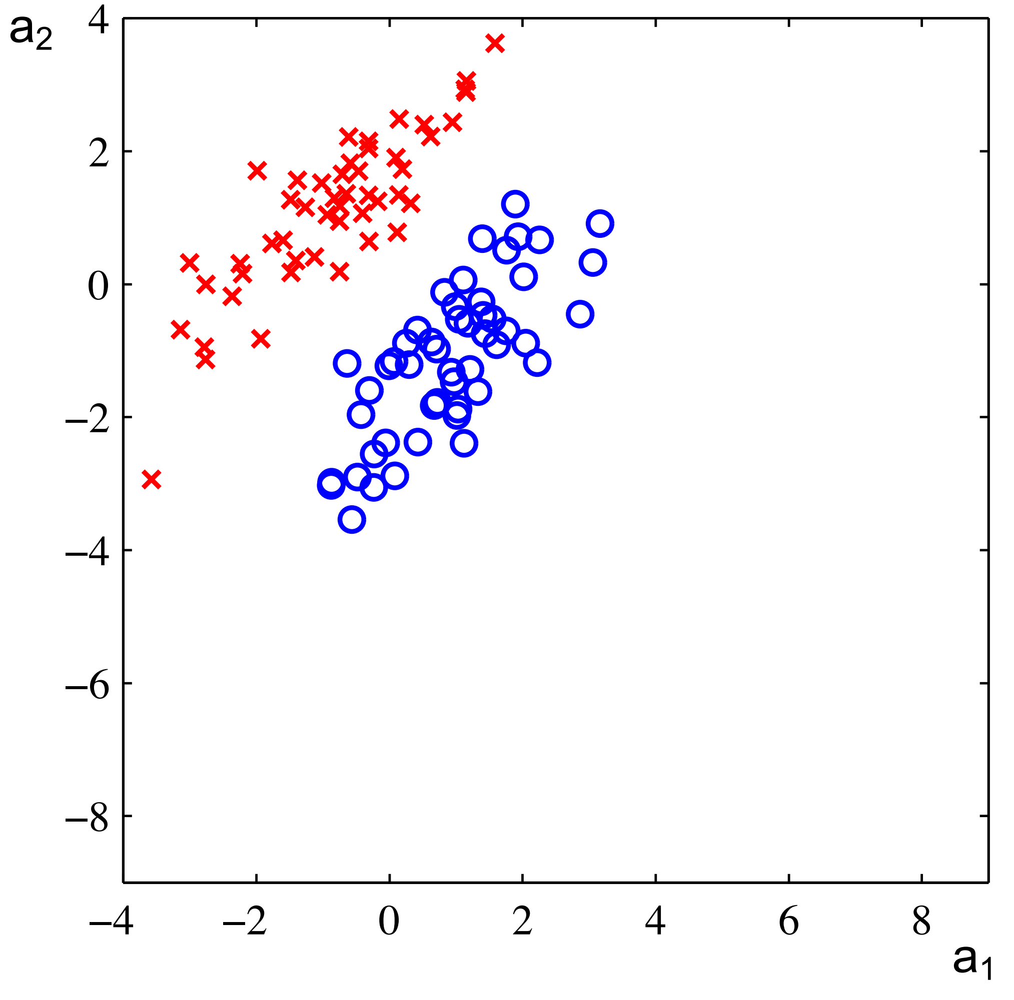
  x is a vector of attributes $<1, x_1, x_2, \ldots x_k>$

  w is a vector of weights $<w_0, w_1, w_2, \ldots w_k>$

- This lets us notate things as…

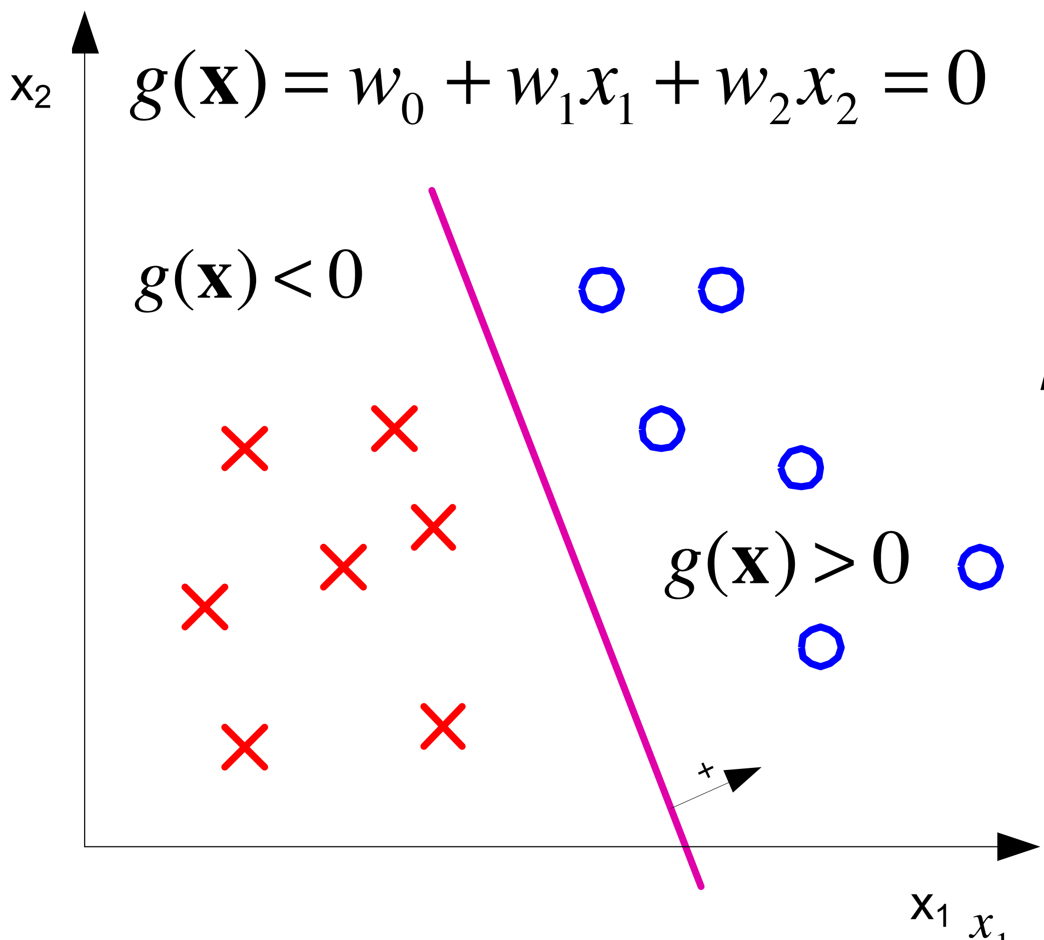
$$g(x) = \mathbf{w}^\mathrm{T}\mathbf{x}$$

Visually: Where to draw the line?



Two-Class Classification

$g(\mathbf{x}) = 0$ defines a decision boundary that splits the space in two

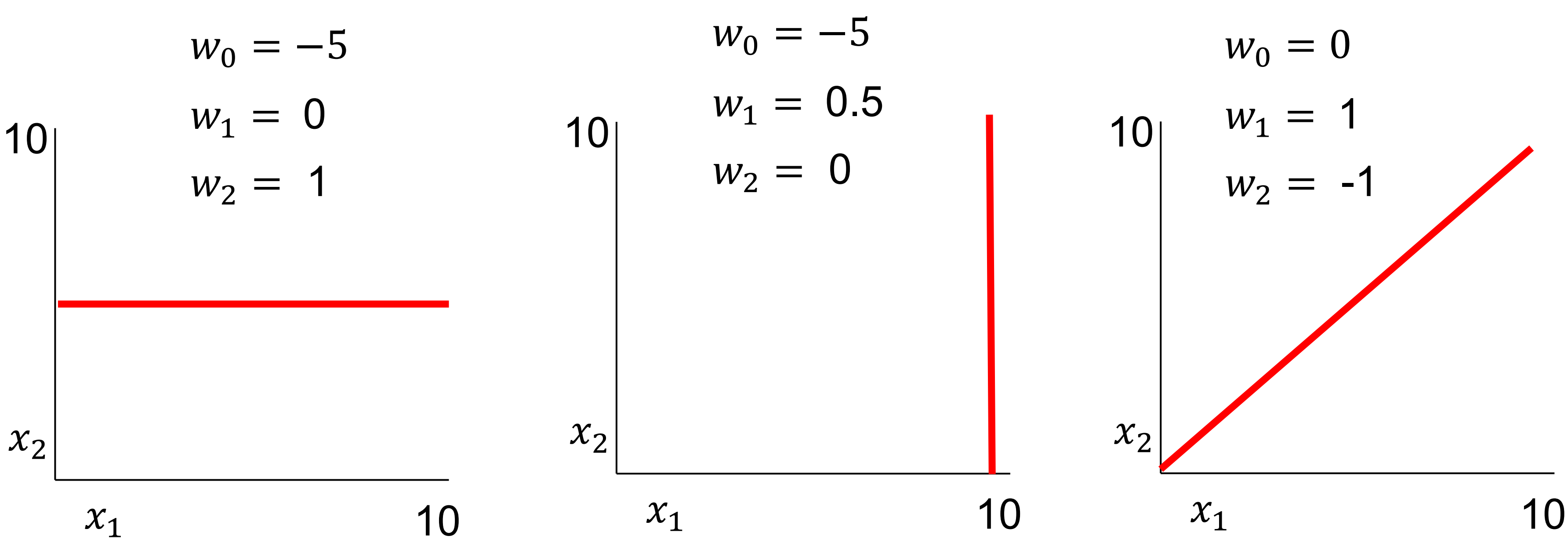


If a line exists that does this without error, the classes are *linearly separable*

$$h(\mathbf{x}) = \begin{cases} 1 & \text{if } g(\mathbf{x}) > 0 \\ -1 & \text{otherwise} \end{cases}$$

Example 2-D decision boundaries

$$0 = g(x) = w_0 + w_1 x_1 + w_2 x_2 = \mathbf{w}^T \mathbf{x}$$



What’s the difference?

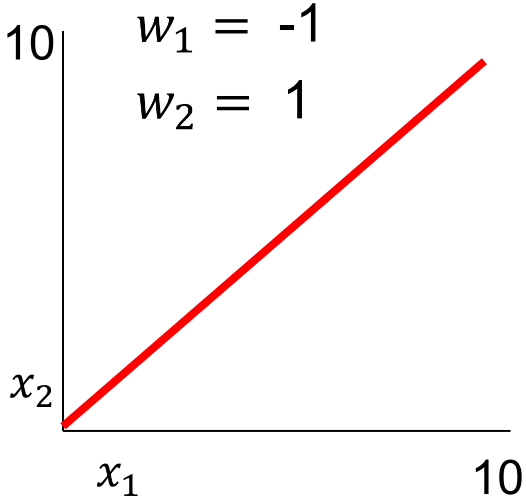
$$0 = g(x) = w_0 + w_1 x_1 + w_2 x_2 = \mathbf{w}^T \mathbf{x}$$

What’s the difference between these two?

$w_0 = 0$

$w_1 =$ -1

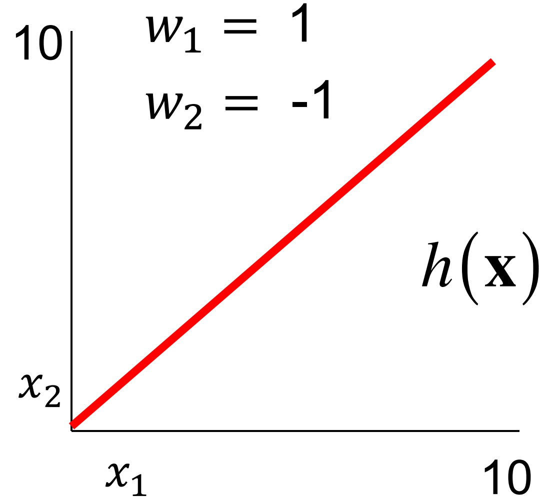
$w_2 =$ 1



$w_0 = 0$

$w_1 =$ 1

$w_2 =$ -1



$$h(\mathbf{x}) = \begin{cases} 1 & \text{if } g(\mathbf{x}) > 0 \\ -1 & \text{otherwise} \end{cases}$$

Loss/Objective function

- To train a model (e.g. learn the weights of a useful line) we define a measure of the ”goodness” of that model. (e.g. the number of misclassified points).

- We make that measure a function of the parameters of the model (and the data).

- This is called a loss function, or an objective function.

- We want to minimize the loss (or maximize the objective) by picking good model parameters.

Classification via regression

- Linear regression's loss function is the the squared distance from a data point to the line, summed over all data points.

- The line that minimizes this function can be calculated by applying a simple formula.

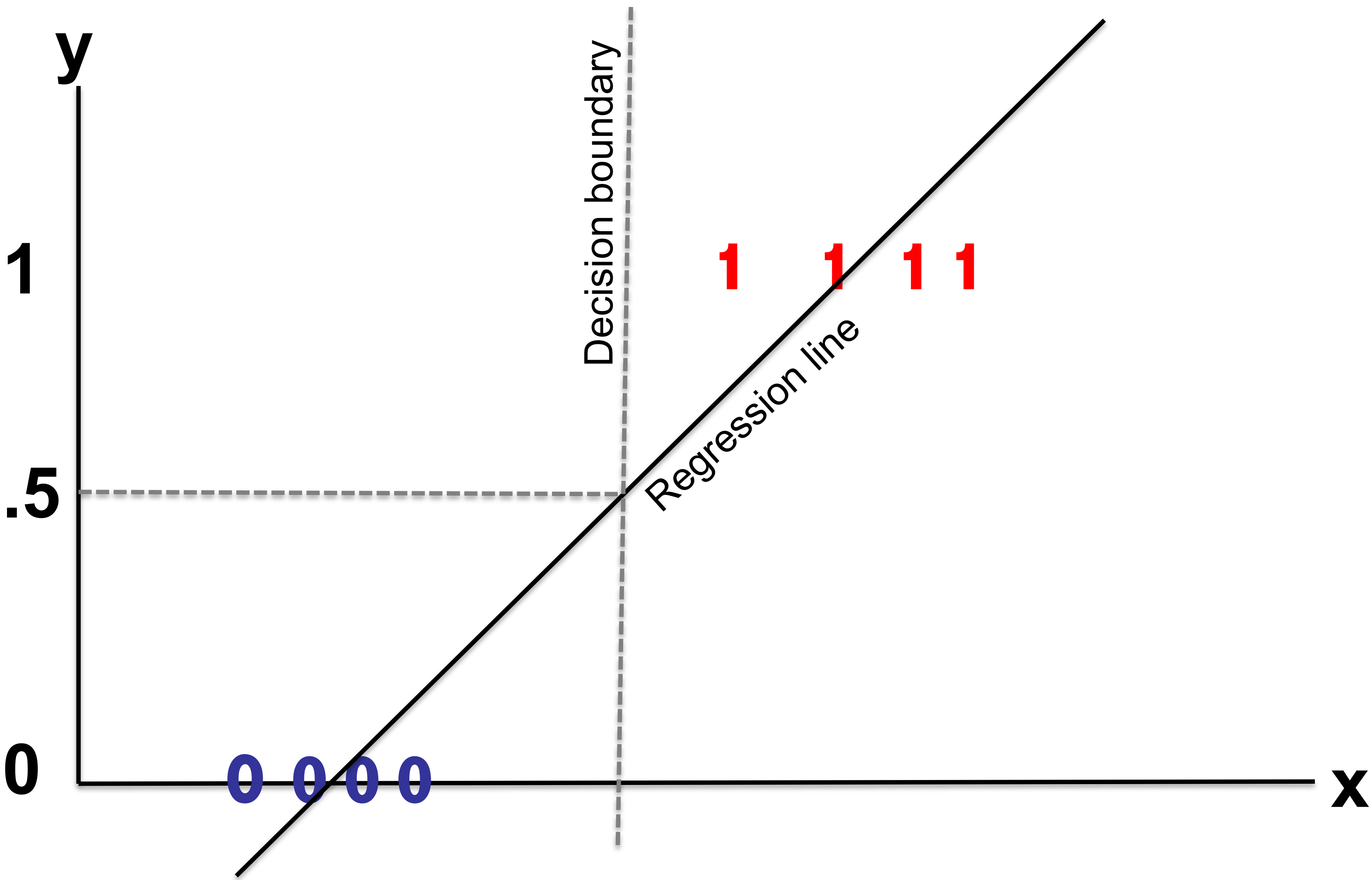
$$\mathbf{w} = (\mathbf{X}^T \mathbf{X})^{-1} \mathbf{X}^T \mathbf{y}$$

- Can we find a decision boundary in one step, by just repurposing the math we used for finding a regression line?

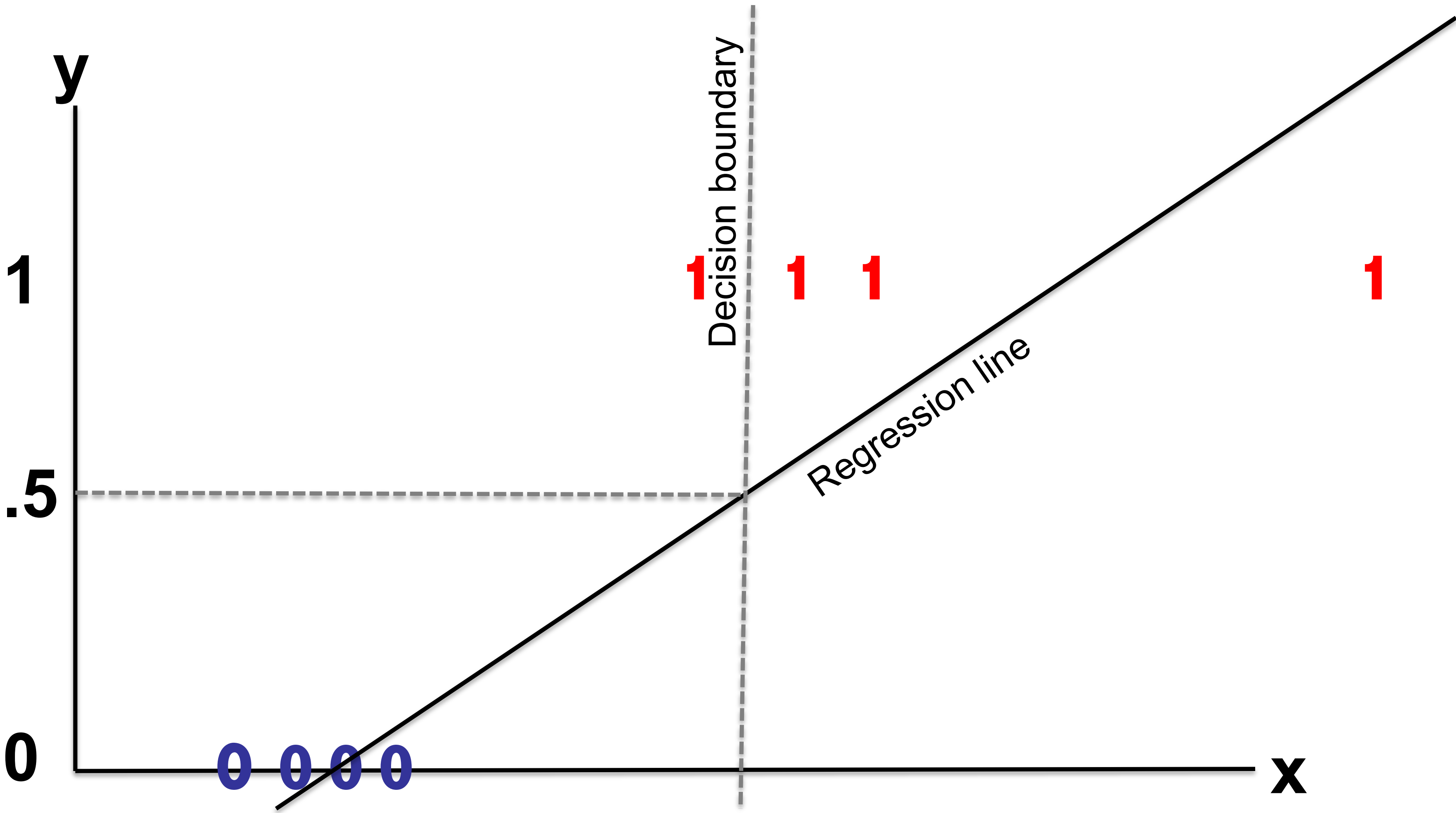
Classification via regression

- Label each class by a number
- Call that number the response variable
- Derive closed-form regression solution
- Round the regression prediction to the nearest label number

An example



What happens now?



Classification via regression take-away

- Closed form solution: simple formula for getting the regression line

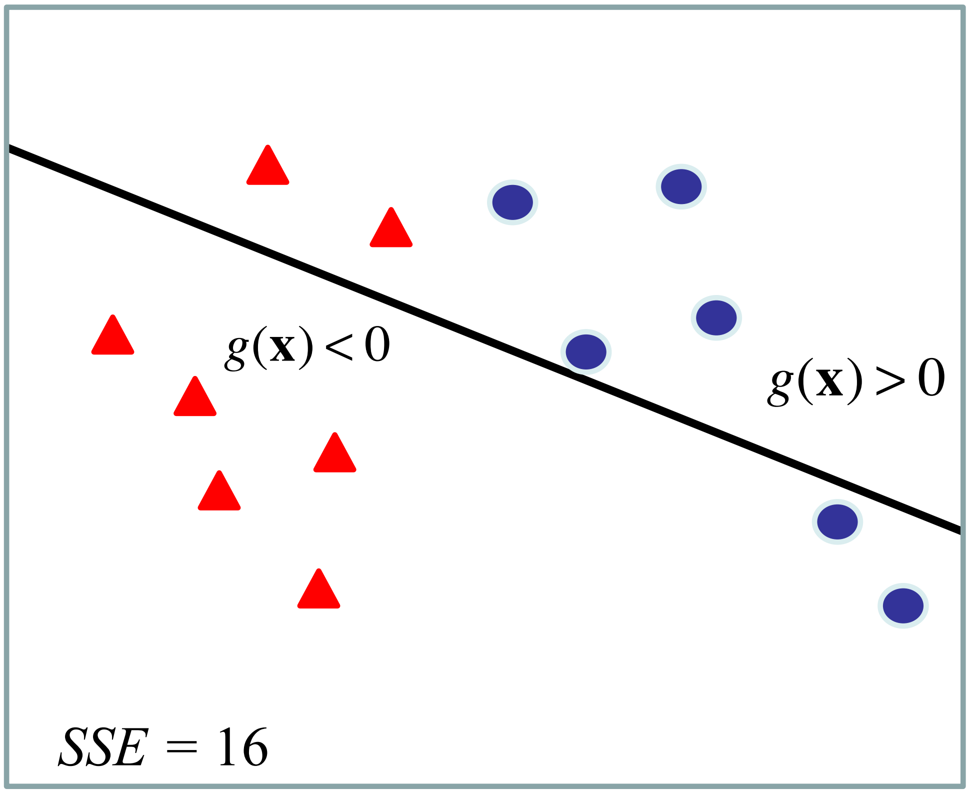
- Residual sum of squares is a bad fit for classification: very sensitive to outliers

- What’s the natural mapping from categories to the real numbers?

What can we do instead?

- Let's define an objective (aka "loss") function that directly measures the thing we want to get right
- Then let's try and find the line that minimizes the loss.
- How about basing our loss function on the number of misclassifications?

sum of squared errors (SSE)

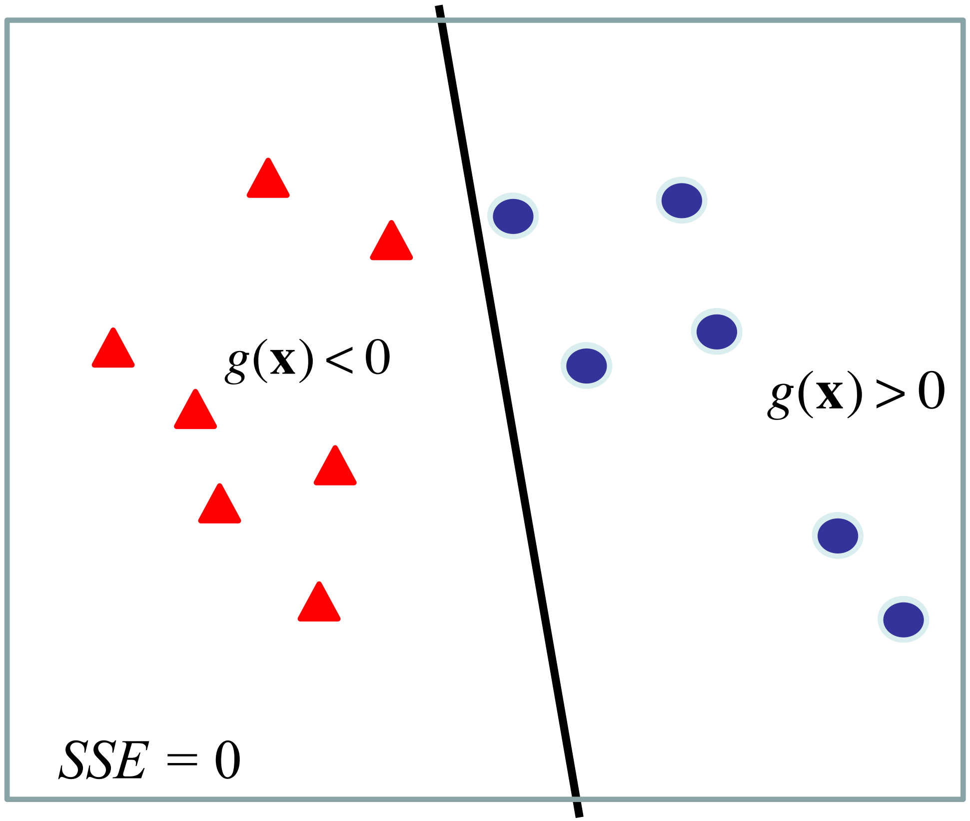


$$g(\mathbf{x}) = w_0 + w_1 x_1 + w_2 x_2 = 0$$
$$= \mathbf{w}^T \mathbf{x}$$

$$h(\mathbf{x}) = \begin{cases} 1 & \text{if } g(\mathbf{x}) > 0 \\ -1 & \text{otherwise} \end{cases}$$

$$SSE = \sum_i^n (y_i - h(\mathbf{x}_i))^2$$

sum of squared errors (SSE)



$$g(\mathbf{x}) = w_0 + w_1 x_1 + w_2 x_2 = 0$$
$$= \mathbf{w}^T \mathbf{x}$$

$$h(\mathbf{x}) = \begin{cases} 1 & \text{if } g(\mathbf{x}) > 0 \\ -1 & \text{otherwise} \end{cases}$$

$$SSE = \sum_{i}^{n} (y_i - h(\mathbf{x}_i))^2$$

No closed form solution!

- For many objective functions we can’t find a formula to to get the best model parameters, like we could with regression.
- The objective function from the previous slide is one of those ”no closed form solution” functions.
- This means we have to try various guesses for what the weights should be and try them out.
- Let’s look at the perceptron approach.

Let’s learn a decision boundary

- We’ll do 2-class classification
- We’ll learn a linear decision boundary

$$0 = g(x) = \mathbf{w}^{\mathrm{T}}\mathbf{x}$$

- Things on each side of 0 get their class labels according to the sign of what g(x) outputs.

$$h(\mathbf{x}) = \begin{cases} 1 & \text{if } g(\mathbf{x}) > 0 \\ -1 & \text{otherwise} \end{cases}$$

- We will use the Perceptron algorithm.

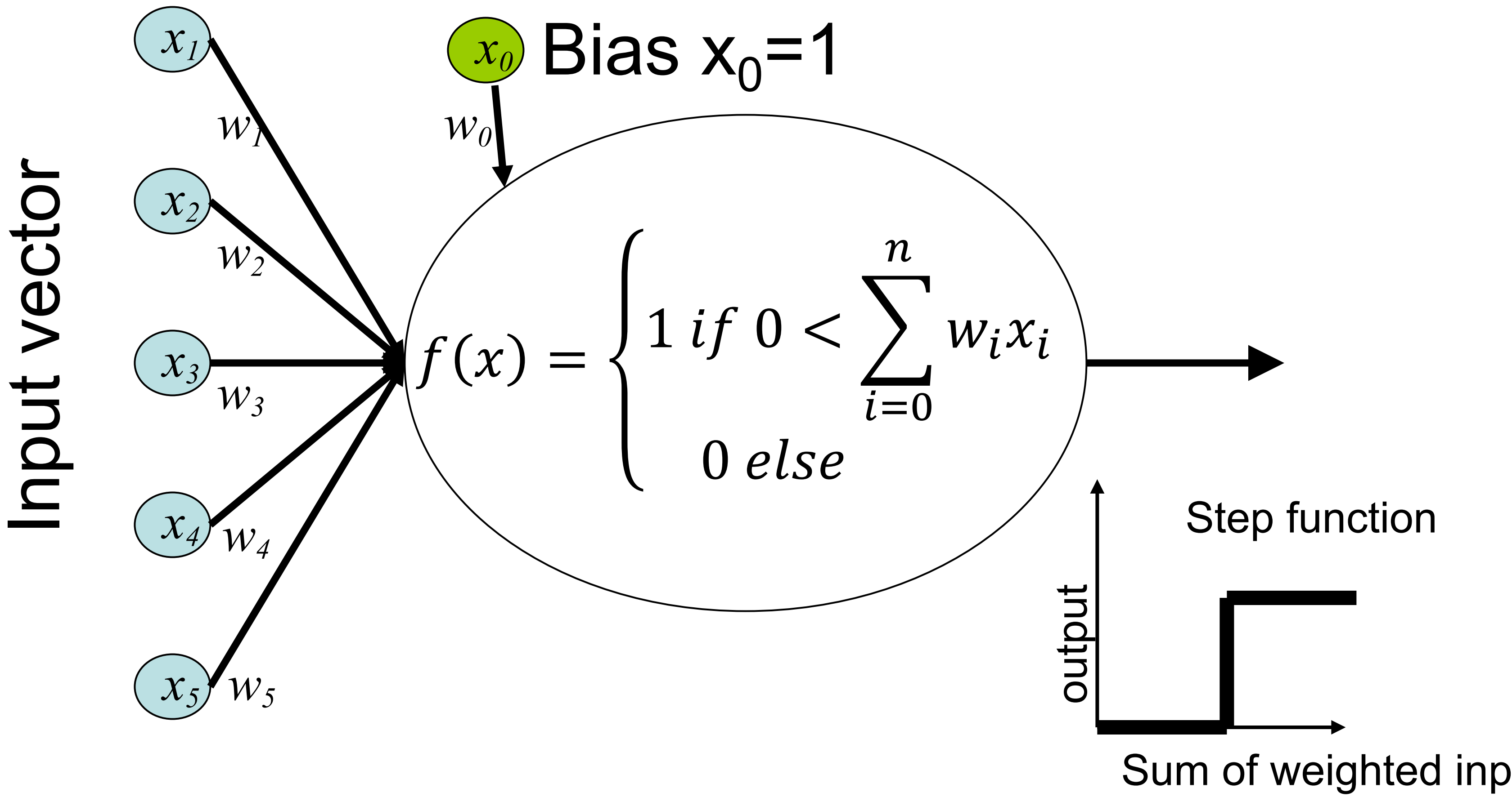
The Perceptron

- Rosenblatt, F. (1958). The perceptron: A probabilistic model for information storage and organization in the brain. Psychological Review, 65(6), 386-408

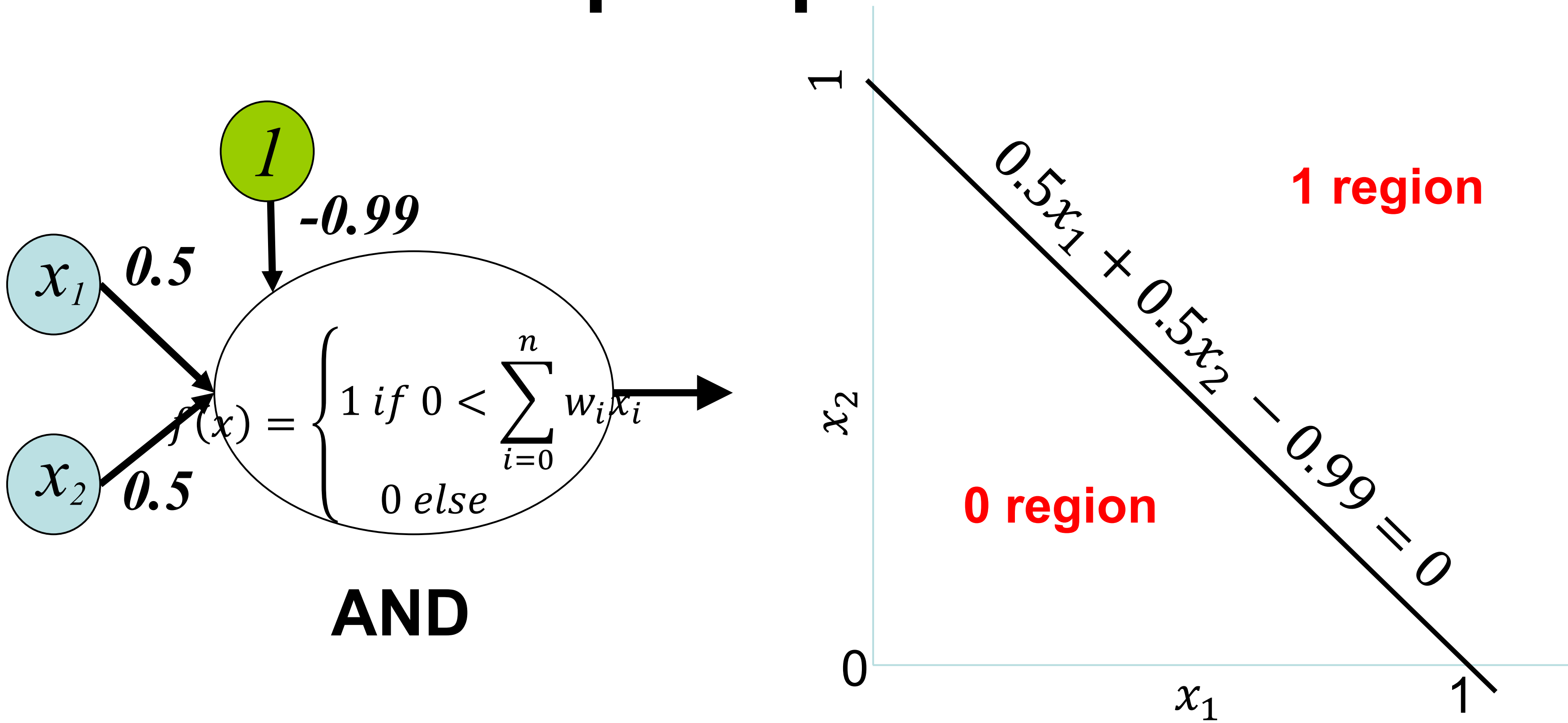
- The “first wave” in neural networks

- A linear classifier

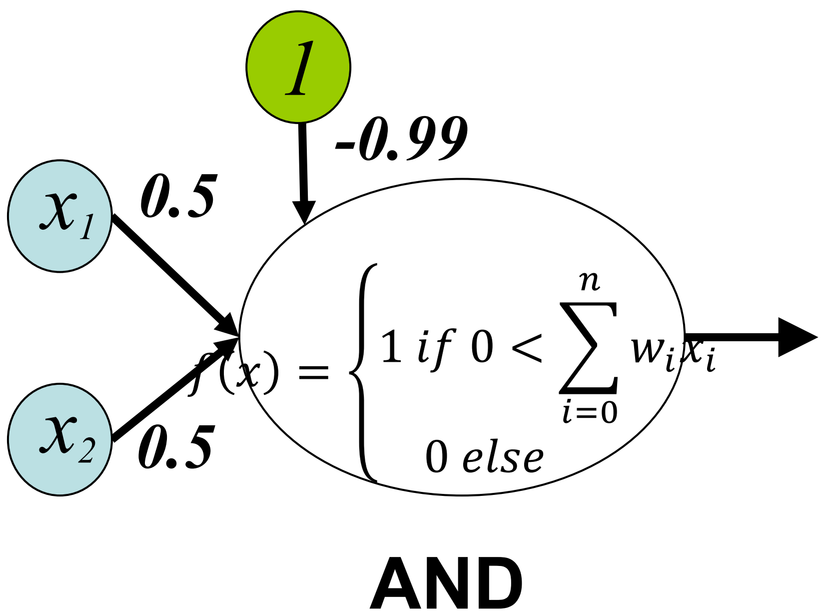
A single perceptron

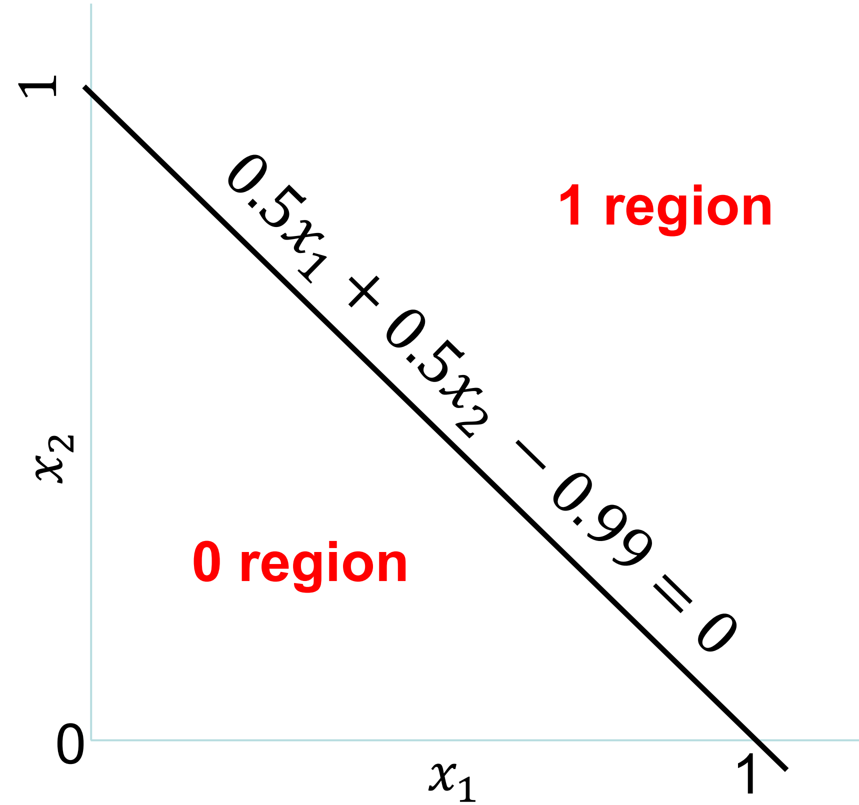


Weights define a hyperplane in the input space

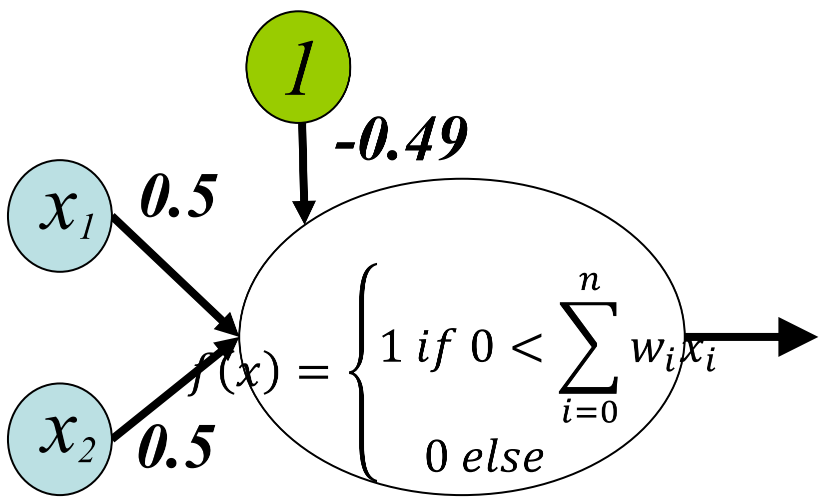


Classifies any (linearly separable) data

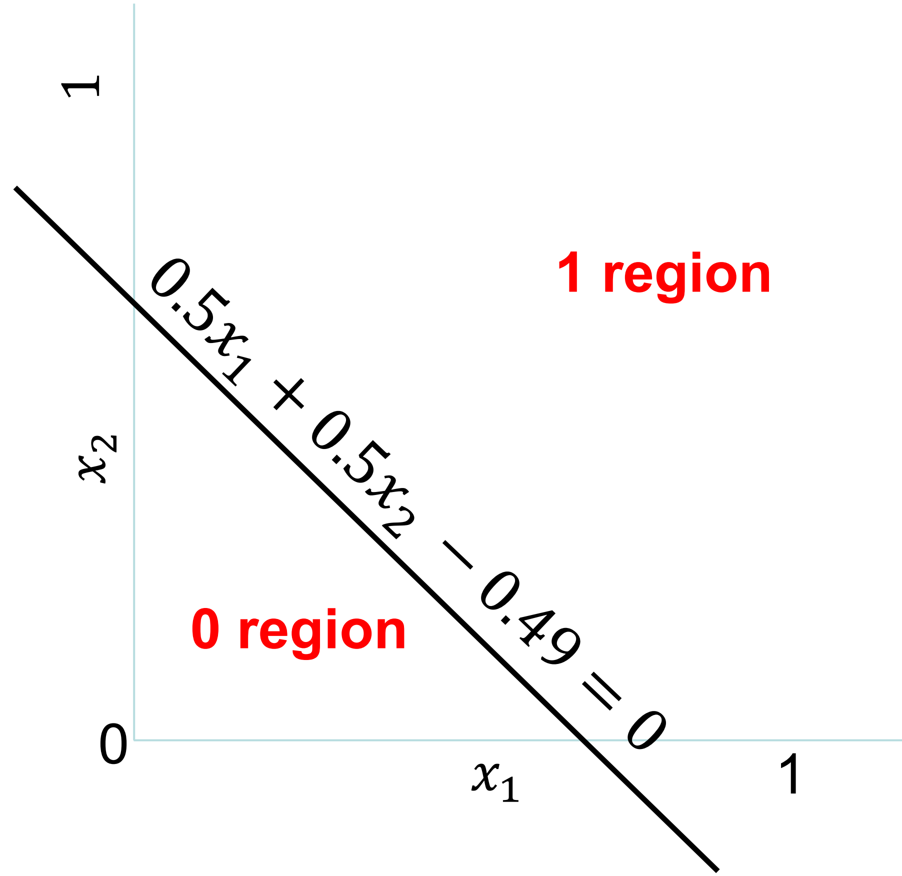




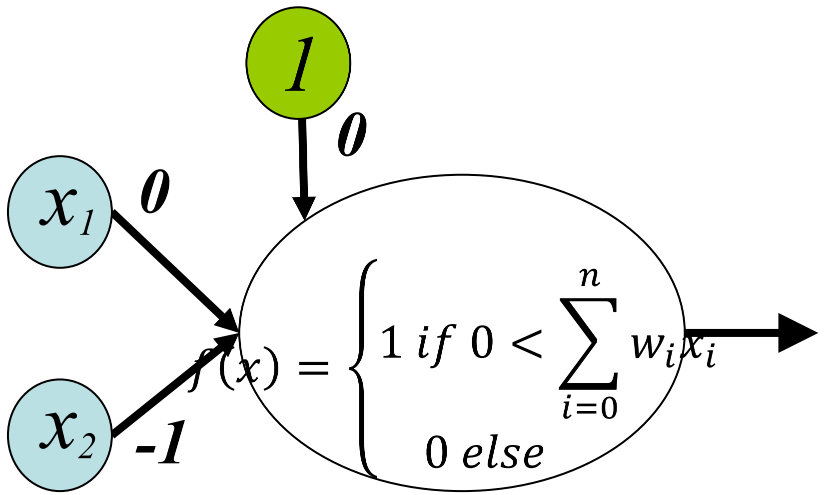
Different logical functions are possible



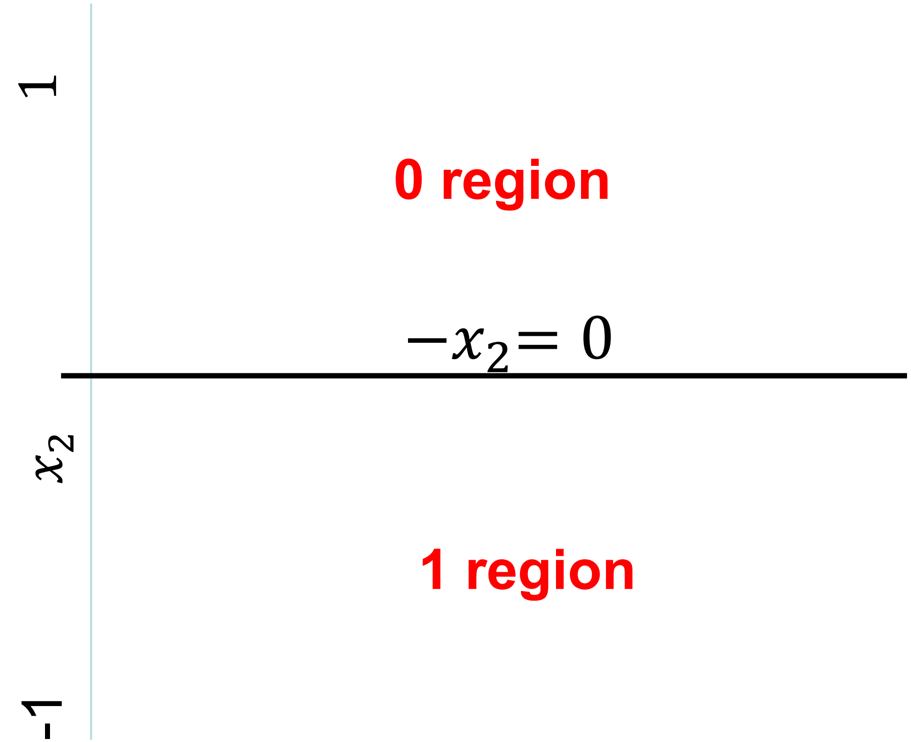
OR



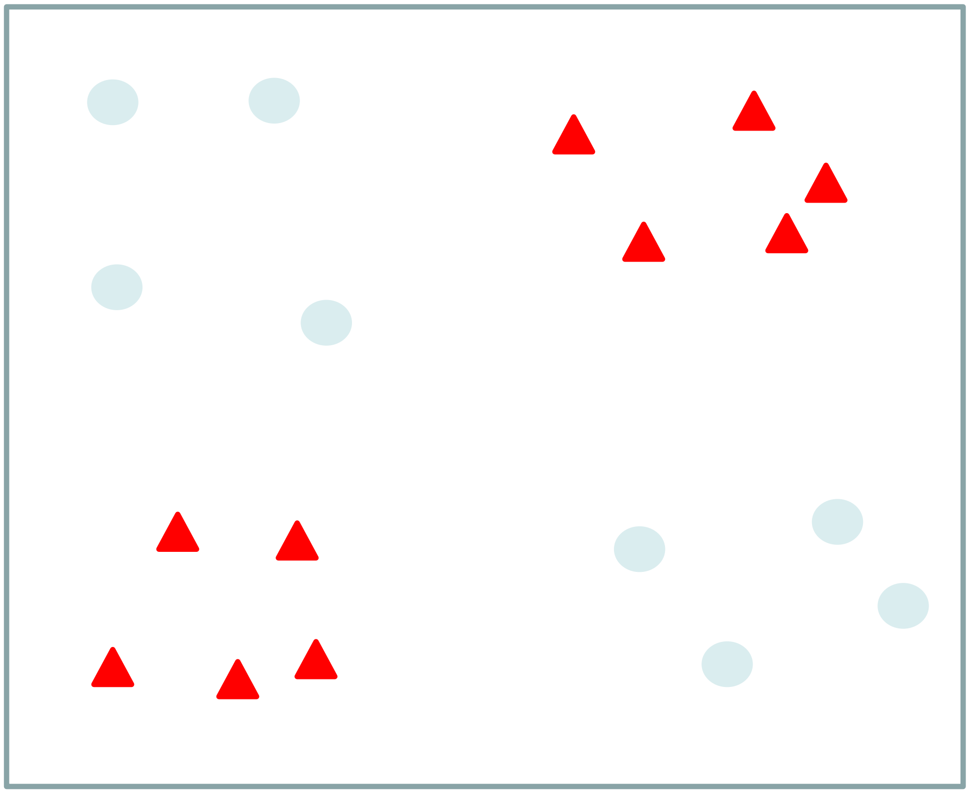
And, Or, Not are easy to define



NOT



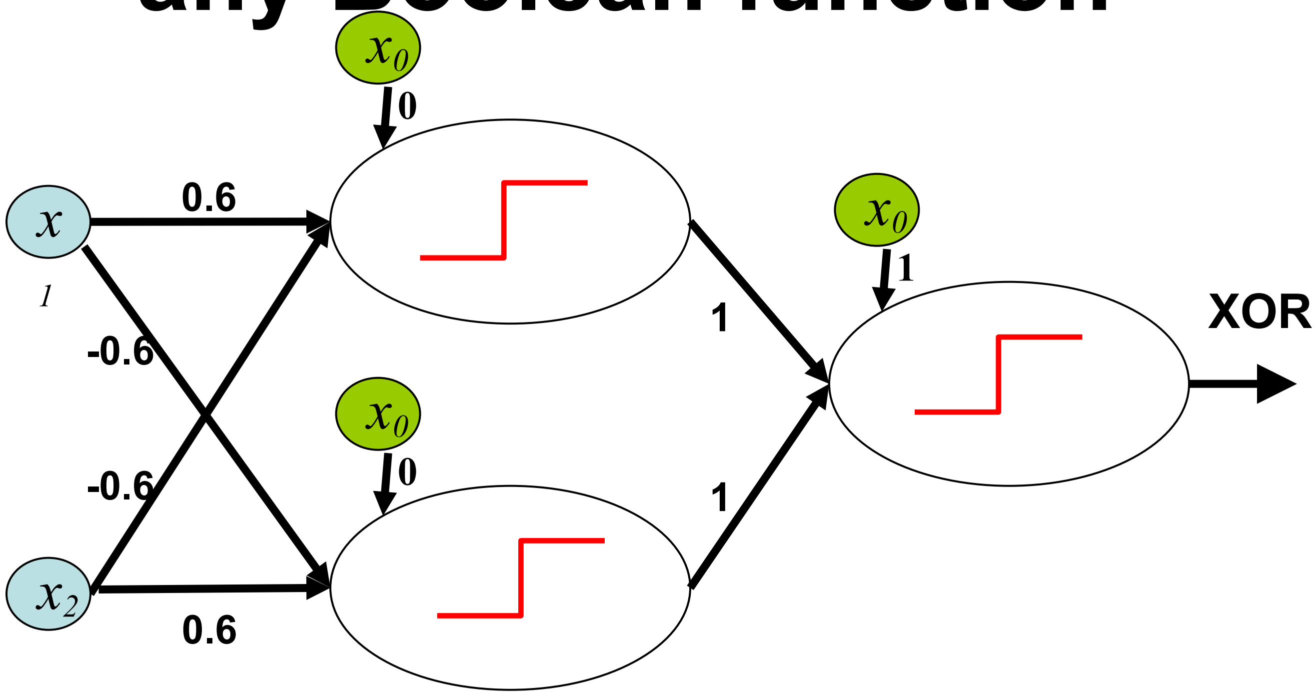
One perceptron: Only linear decisions



This is XOR.

It can’t learn XOR.

Combining perceptrons can make any Boolean function



…if you can set the weights & connections right

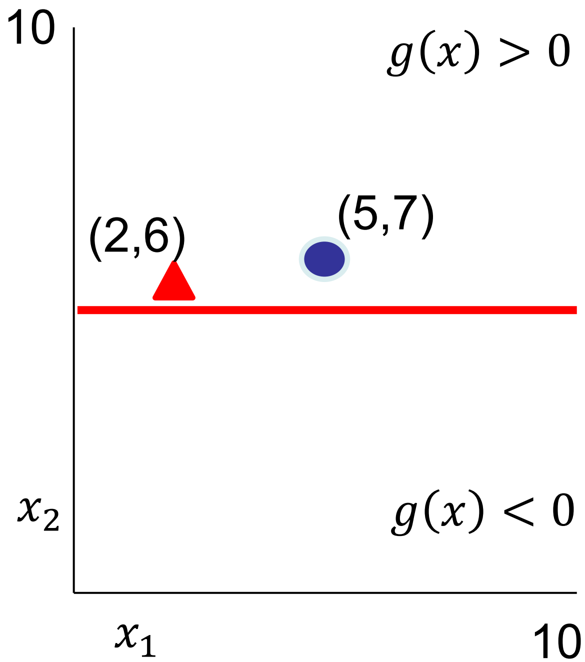
Defining our goal

D is our data, consisting of training examples $< \mathbf{x}, y >$. Remember y is the true label (drawn from {1,-1} and **x** is the thing being labeled.

Our goal : make $(\mathbf{w}^T\mathbf{x})y > 0$ for all $< \mathbf{x}, y > \in D$

Think about why this is the goal.

An example



Goal: classify ● as +1 and ▲ as -1 by putting a line between them.

Our objective function is…

$$(\mathbf{w}^T\mathbf{x})y > 0$$

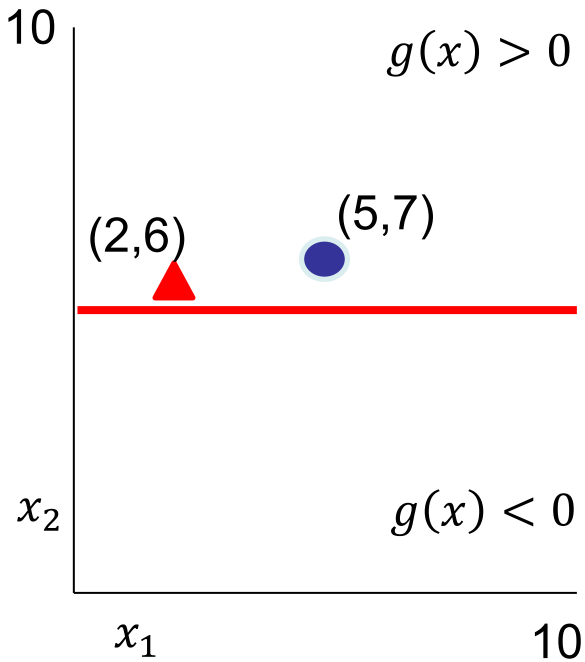
Start with a randomly placed line.

$$\mathbf{w} = [w_0, w_1, w_2] = [-5, 0, 1]$$

Measure the objective for each point.

Move the line if the objective isn't met.

An example



Goal: classify ● as +1 and ▲ as -1 by putting a line between them.

Our objective function is…

$$(\mathbf{w}^T\mathbf{x})y > 0$$

Start with a randomly placed line.

$$\mathbf{w} = [w_0, w_1, w_2] = [-5, 0, 1]$$

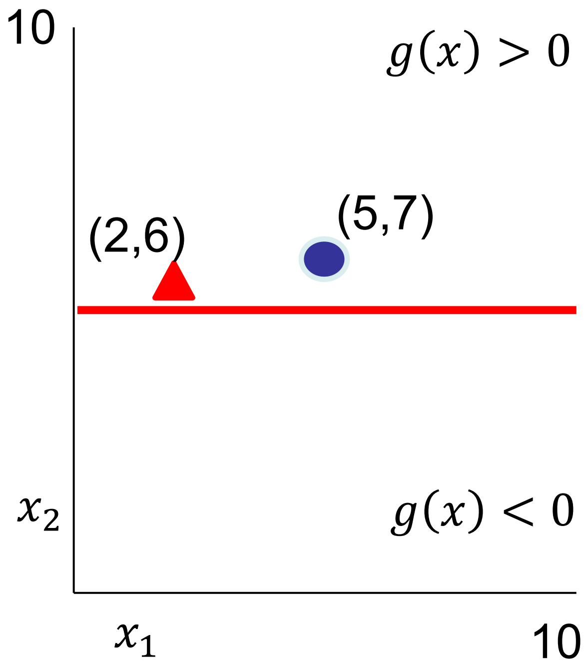
● $(\mathbf{w}^T\mathbf{x})y = [-5,0,1]^T[1,5,7](1)$

$= 2$

> 0

Objective met. Don't move the line.

An example



Goal: classify ● as +1 and ▲ as -1 by putting a line between them.

Our objective function is…

$$(\mathbf{w}^T\mathbf{x})y > 0$$

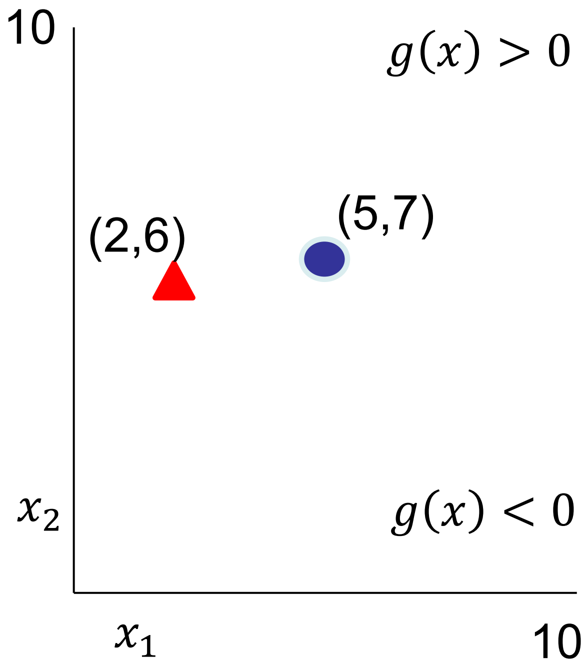
Start with a randomly placed line.

$$\mathbf{w} = [w_0, w_1, w_2] = [-5, 0, 1]$$

▲ $(\mathbf{w}^T\mathbf{x})y = [-5,0,1]^T[1,2,6](-1)$
$= (-5 + 6)(-1)$
$= -1$
< 0

Objective not met. Move the line.

An example



Goal: classify as +1 and as -1 by putting a line between them.

Our objective function is…

$$(\mathbf{w}^T\mathbf{x})y > 0$$

Start with a randomly placed line.

$$\mathbf{w} = [w_0, w_1, w_2] = [-5, 0, 1]$$

Let's update the line by doing $\mathbf{w} = \mathbf{w} + \mathbf{x}(y)$.

$$\mathbf{w} = \mathbf{w} + \mathbf{x}(y) = [-5,0,1] + [1,2,6](-1)$$
$$= [-6, -2, -5]$$

Now what ?

- What does the decision boundary look like when **w**$= [-6, -2, -5]$? Does it misclassify the blue dot now?

- What if we update it the same way, each time we find a misclassified point?

- Could this approach be used to find a good separation line for a lot of data?

Perceptron Algorithm

The decision boundary

$$0 = \ g(x) = \mathbf{w}^{\mathrm{T}}\mathbf{x}$$

The classification function

$$h(\mathbf{x}) = \begin{cases} 1 & \text{if } g(\mathbf{x}) > 0 \\ -1 & \text{otherwise} \end{cases}$$

$$m = |D| = size\ of\ data\ set$$

The weight update algorithm

$$\mathbf{w} = \ \ some\ random\ setting$$

Do

$$k = (k+1)\mathrm{mod}(m)$$

$$\text{if } h(\mathbf{x}_k)! = y_k$$

$$\mathbf{w} = \mathbf{w} + \mathbf{x}_k y$$

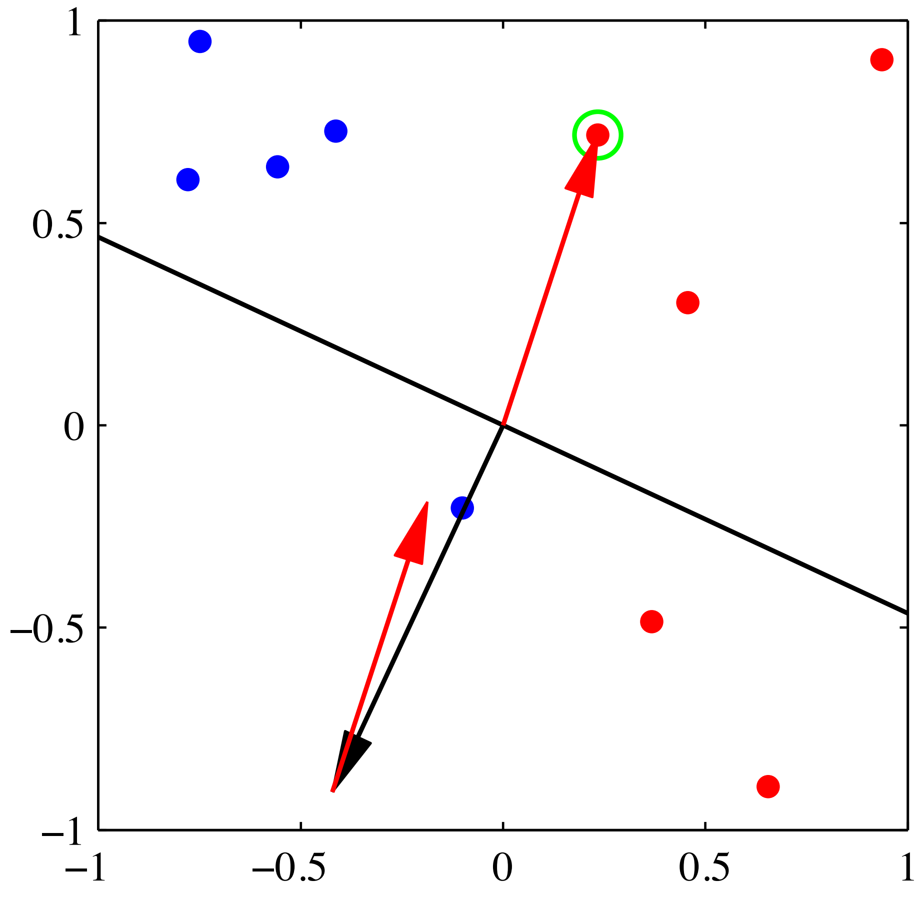
$\boxed{\text{Until } \forall k,\ \ h(\mathbf{x}_k) = y_k}$

Warning: Only guaranteed to terminate if classes are linearly separable!

This means you have to add another exit condition for when you've gone through the data too many times and suspect you'll never terminate.

Perceptron Algorithm

- Example:

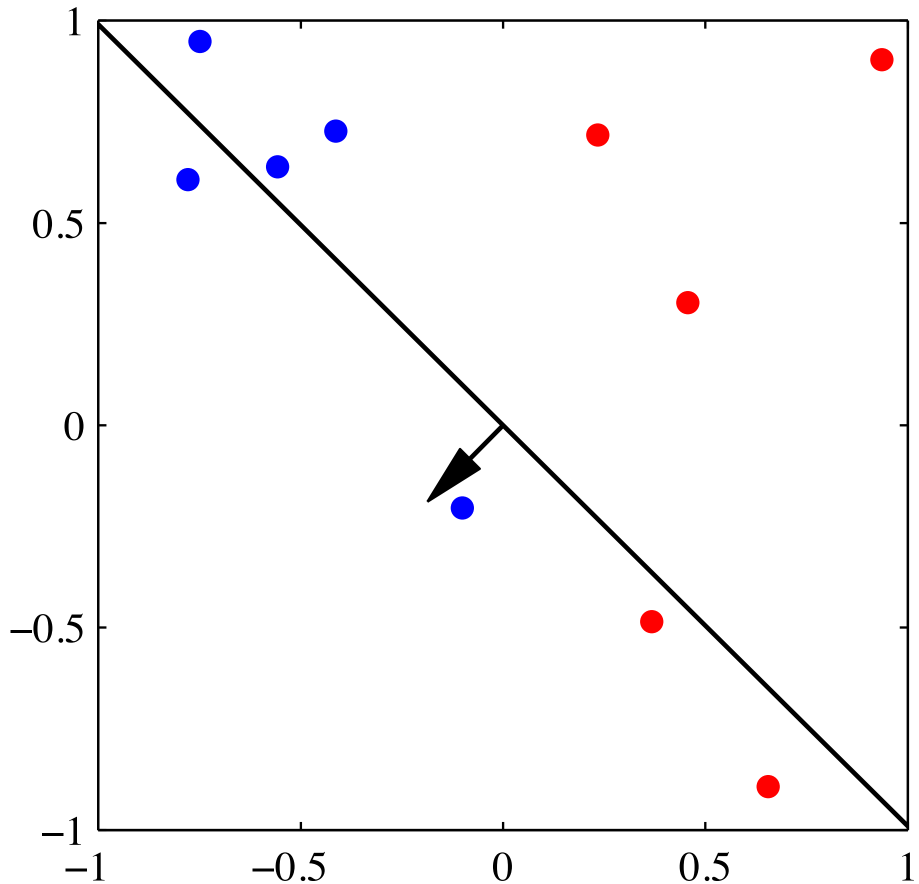


Red is the positive class

Blue is the negative class

Perceptron Algorithm

- Example (cont'd):

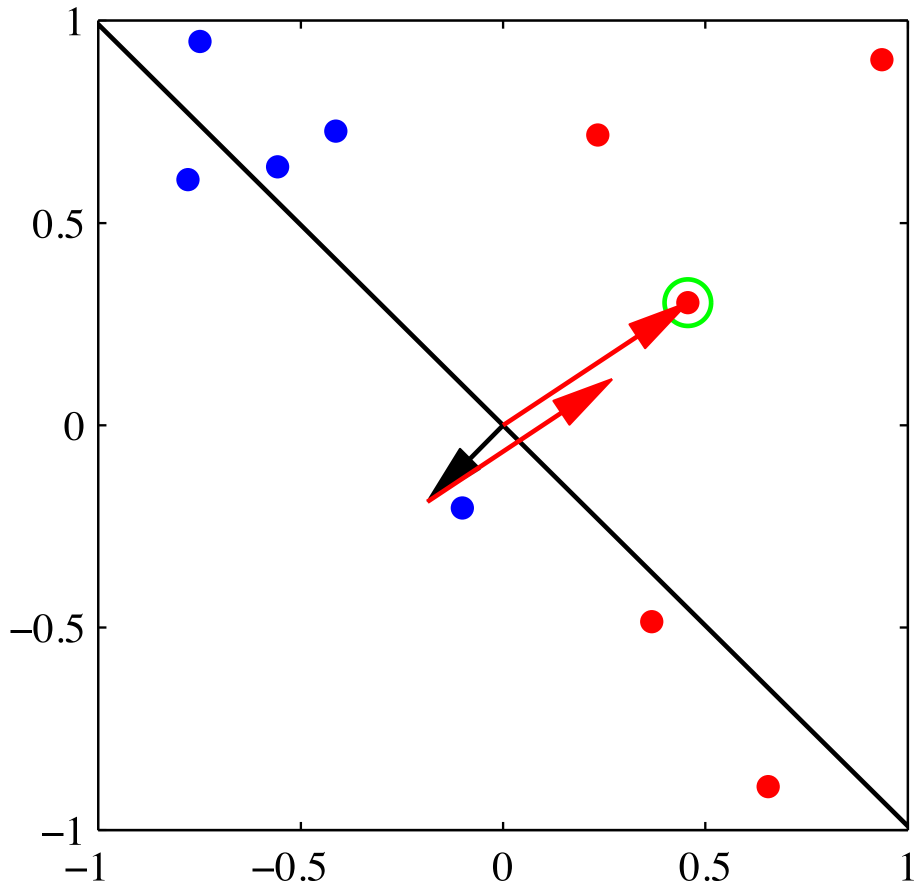


Red is the positive class

Blue is the negative class

Perceptron Algorithm

- Example (cont'd):

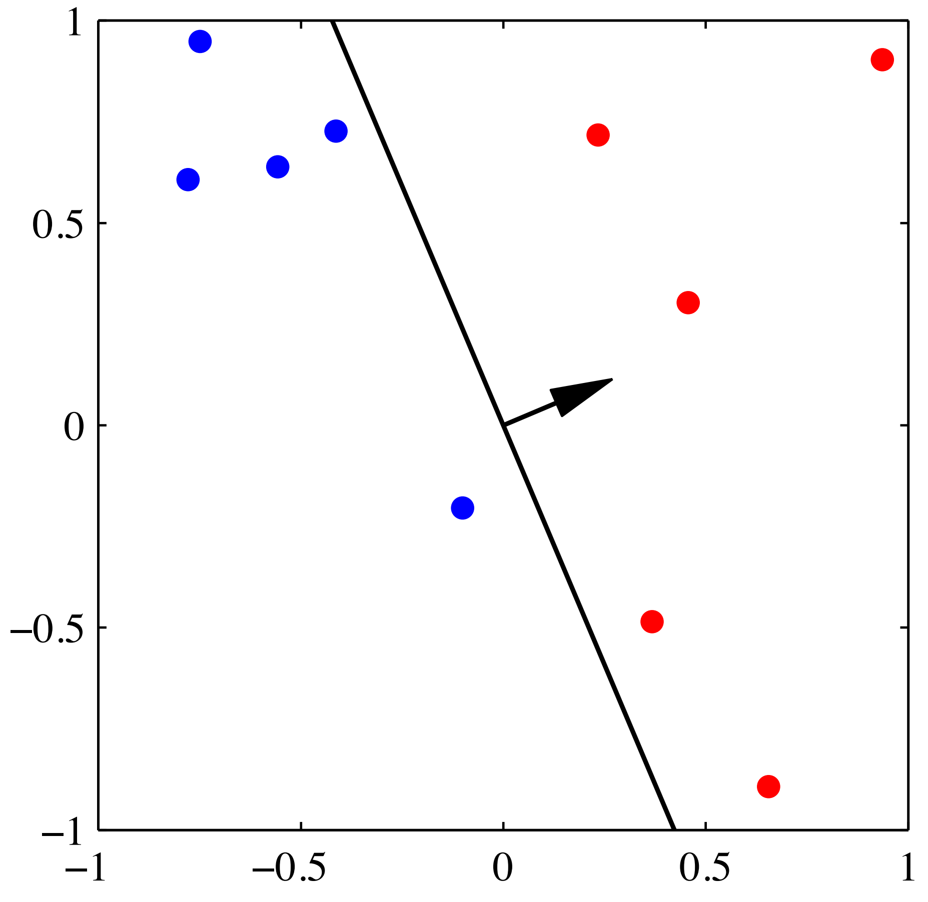


Red is the positive class

Blue is the negative class

Perceptron Algorithm

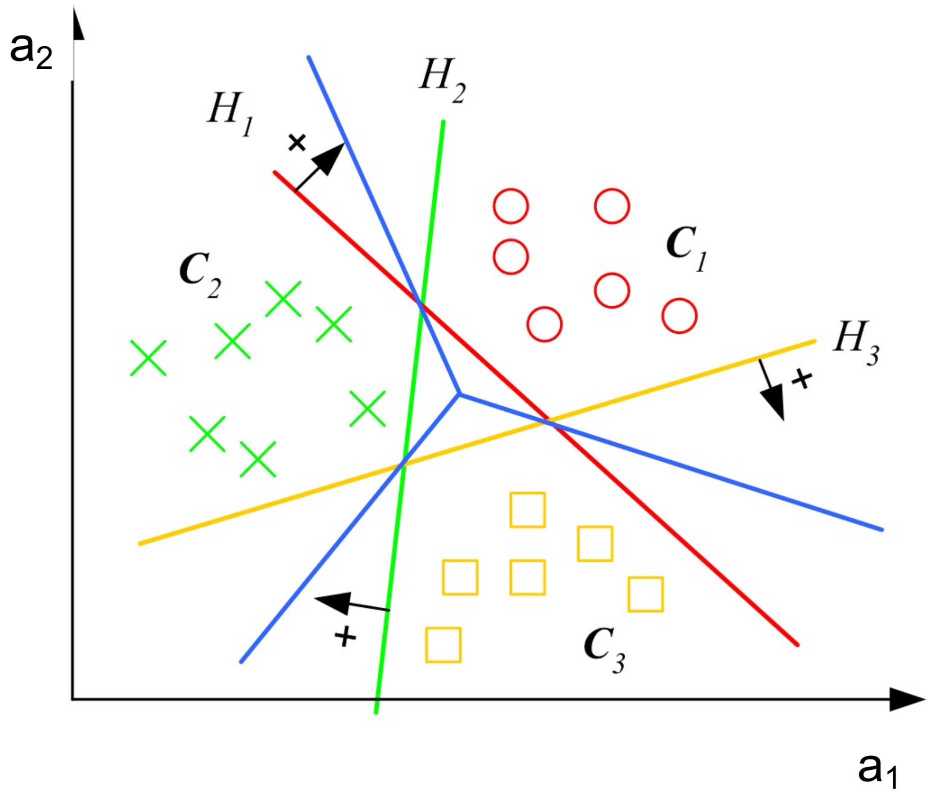
- Example (cont'd):



Red is the positive class

Blue is the negative class

Multi-class Classification



When there are N classes you can classify using N discriminant functions.

Choose the class c from the set of all classes C whose function $g_c(\mathbf{x})$ has the maximum output

Geometrically divides feature space into N **convex** decision regions

$$h(\mathbf{x}) = \underset{c \in C}{\operatorname{argmax}}\, g_c(\mathbf{x})$$

Multi-class Classification

A class label

$$c = h(\mathbf{x}) = \underset{c \in C}{\operatorname{argmax}}\, g_c(\mathbf{x})$$

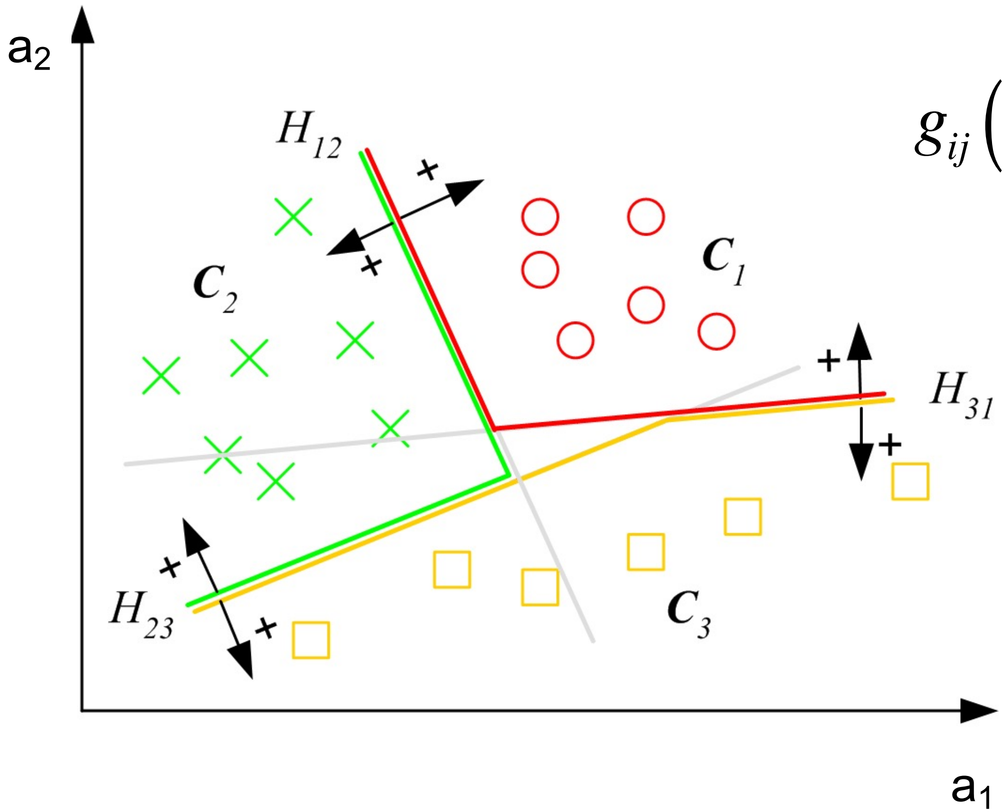
Set of all classes

Remember $g_c(\mathbf{x})$ is the inner product of the feature vector for the example $(\mathbf{x})$with the weights of the decision boundary hyperplane for class c. If $g_c(\mathbf{x})$ is getting more positive, that means $(\mathbf{x})$ is deeper inside its "yes" region.

Therefore, if you train a bunch of 2-way classifiers (one for each class) and pick the output of the classifier that says the example is deepest in its region, you have a multi-class classifier.

Pairwise Multi-class Classification

If they are not linearly separable (singly connected convex regions), may still be pair-wise separable, using N(N-1)/2 linear discriminants.



$$g_{ij}\left(\vec{x} \mid \vec{w}_{ij}, w_{ij0}\right) = w_{ij0} + \sum_{l=1}^{K} w_{ijl} x_l$$

choose C_i if

$$\forall j \neq i, g_{ij}\left(\mathbf{x}\right) > 0$$

Appendix

(stuff I didn't have time to discuss in class…and for which I haven't updated the notation.)

Linear Discriminants

- A linear combination of the attributes.

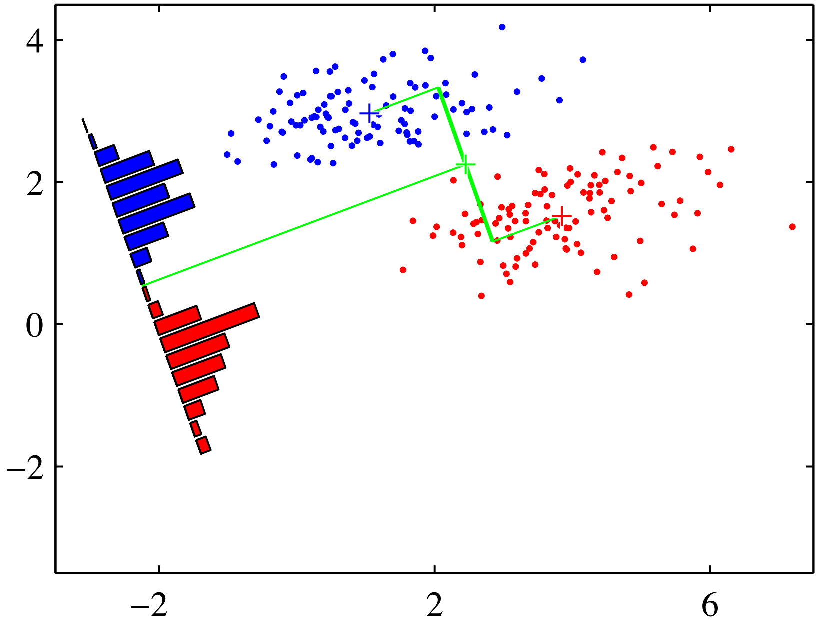
$$g\left(\vec{x} \mid \vec{w}, w_0\right) = w_0 + \vec{w}^T \vec{x} = w_0 + \sum_{i=1}^{k} w_i a_i$$

- Easily interpretable

- Are optimal when classes are Gaussian and share a covariance matrix

Fisher Linear Discriminant Criteria

- Can think of $\vec{w}^T \vec{x}$ as dimensionality reduction from K-dimensions to 1
- Objective:
  - Maximize the difference between class means
  - Minimize the variance within the classes



$$J(\vec{w}) = \frac{(m_2 - m_1)^2}{s_1^2 + s_2^2}$$

where s_i and m_i are the sample variance and mean for class i in the projected dimension. We want to maximize J.

Fisher Linear Discriminant Criteria

- Solution:

$$\vec{w} = \mathbf{S}_W^{-1}(\vec{m}_2 - \vec{m}_1)$$

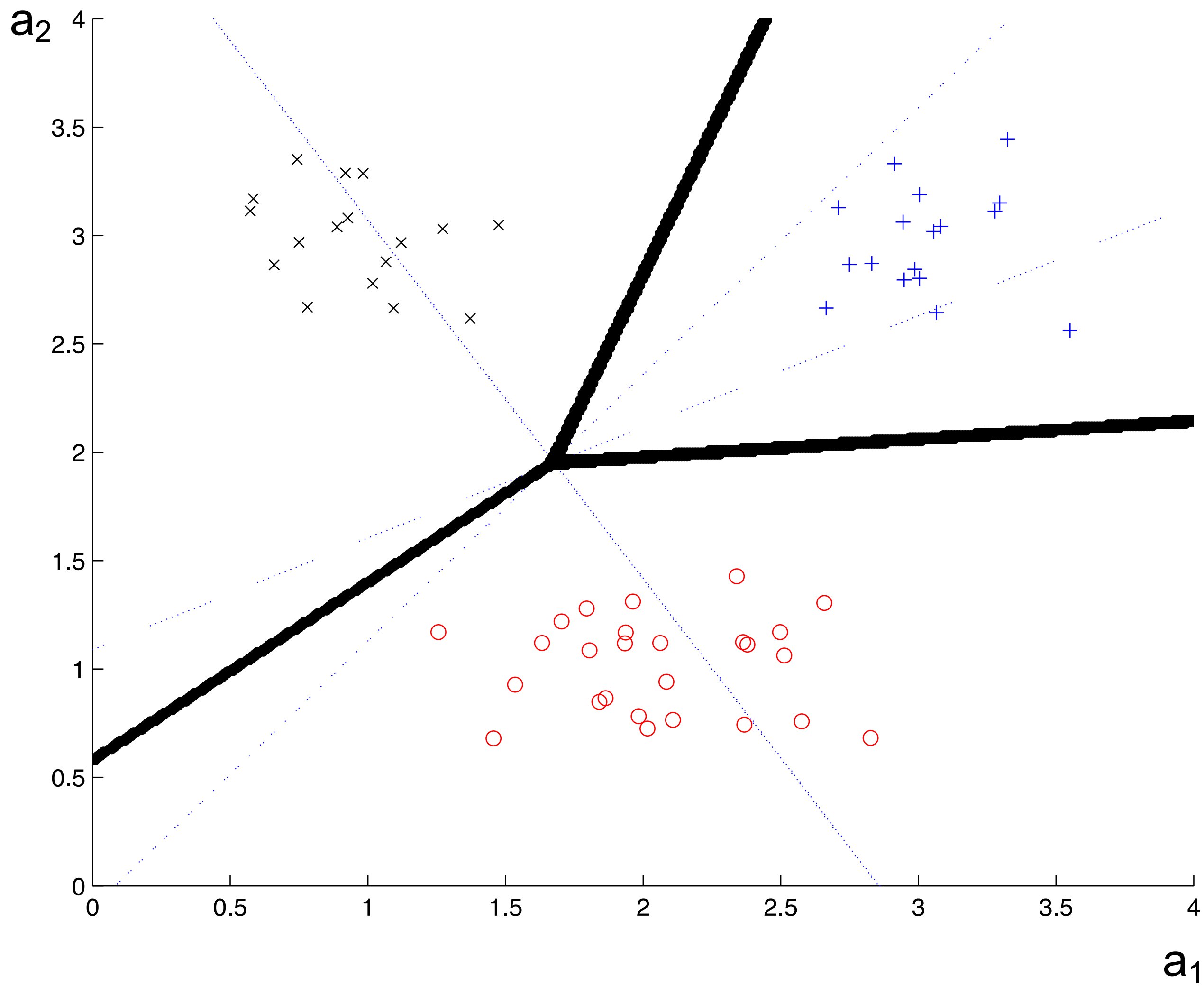
where

$$\mathbf{S}_W = \sum_{n \in C_1} (\vec{x}_n - \vec{m}_1)(\vec{x}_n - \vec{m}_1)^T + \sum_{n \in C_2} (\vec{x}_n - \vec{m}_2)(\vec{x}_n - \vec{m}_2)^T$$

- However, while this finds finds the direction ($\vec{w}$) of decision boundary. Must still solve for w_0 to find the threshold.

- Can be expanded to multiple classes

Logistic Regression (Discrimination)



Logistic Regression (Discrimination)

- Discriminant model but well-grounded in probability
- Flexible assumptions (exponential family class-conditional densities)
- Differentiable error function (“cross entropy”)
- Works very well when classes are linearly separable

Logistic Regression (Discrimination)

- Probabilistic discriminative model
- Models posterior probability $p(C_1|\overrightarrow{x})$
- To see this, let's start with the 2-class formulation:

$$\begin{aligned}
p(C_1|x) &= \frac{p(\overrightarrow{x}|C_1)p(C_1)}{p(\overrightarrow{x}|C_1)p(C_1) + p(\overrightarrow{x}|C_2)p(C_2)} \\
&= \frac{1}{1 + \exp\left(-\log\frac{p(\overrightarrow{x}|C_1)p(C_1)}{p(\overrightarrow{x}|C_2)p(C_2)}\right)} \\
&= \frac{1}{1 + \exp(-\alpha)} \\
&= \sigma(\alpha)
\end{aligned}$$

logistic sigmoid function

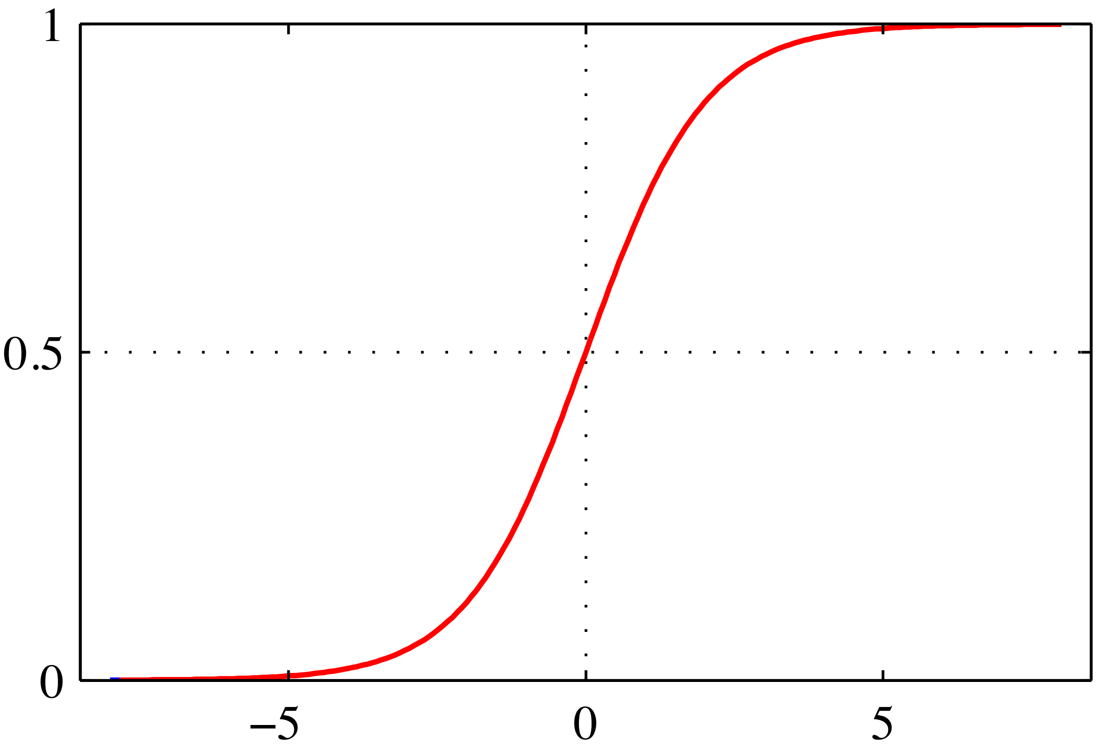
where

$$\alpha = \log\frac{p(\overrightarrow{x}|C_1)p(C_1)}{p(\overrightarrow{x}|C_2)p(C_2)}$$

Logistic Regression (Discrimination)

logistic sigmoid function

$$\sigma(\alpha) = \frac{1}{1 + \exp(-\alpha)}$$



"Squashing function" that maps $(-\infty, +\infty) \rightarrow (0, 1)$

Logistic Regression (Discrimination)

For exponential family of densities,

$$\alpha = \log \frac{p(\overrightarrow{x}|C_1)p(C_1)}{p(\overrightarrow{x}|C_2)p(C_2)}$$

is a linear function of x.

Therefore we can model the posterior probability as a logistic sigmoid acting on a linear function of the attribute vector, and simply solve for the weight vector **w** (e.g. treat it as a discriminant model):

$$y = p(C_1|\overrightarrow{x}) = \sigma(w_0 + \sum_{i=1}^{k} w_i a_i) \qquad p(C_2|\overrightarrow{x}) = 1 - p(C_1|\overrightarrow{x})$$

To classify: $h(\overrightarrow{x}_i) = \begin{cases} C_1 & y_i > 0.5 \\ C_2 & o.w. \end{cases}$