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Review: The General Learning Problem

- ▶ We want to learn functions from inputs to outputs, where each input has n features:

Inputs $\langle x_1, x_2, \dots, x_n \rangle$, with each feature x_i from domain X_i .
Outputs y from domain Y .

Function to learn: $f : X_1 \times X_2 \times \dots \times X_n \rightarrow Y$

- ▶ The type of learning problem we are solving really depends upon the type of the output domain, Y
 1. If $Y \subseteq \mathcal{R}$ (i.e., is real-valued), this is **regression**
 2. If Y is a finite discrete set, this is **classification**

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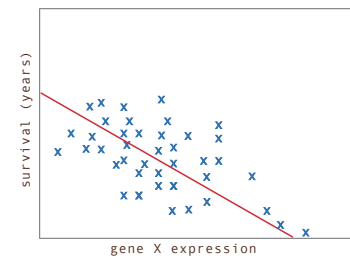
Decisions to Make

- ▶ When collecting our training example pairs, $(x, f(x))$, we still have some decisions to make
- ▶ **Example:** Medical Informatics
 - ▶ We have some genetic information about patients
 - ▶ Some get sick with a disease and some don't
 - ▶ Patients live for a number of years (sick or not)
- ▶ **Question:** what do we want to learn from this data?
- ▶ Depending upon what we decide, we may use:
 - ▶ Different models of the data
 - ▶ Different machine learning approaches
 - ▶ Different measurements of successful learning

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One Approach: Regression

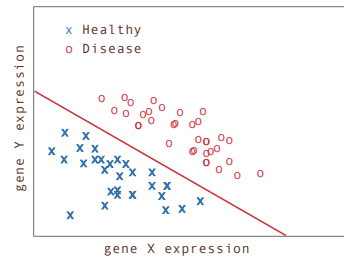
- ▶ We decide that we want to try to learn to predict how long patients will live
- ▶ We base this upon information about the degree to which they express a specific gene
- ▶ A **regression problem**: the function we learn is the "best (linear) fit" to the data we have



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Another Approach: Classification

- ▶ We decide instead that we simply want to decide whether a patient will get the disease or not
- ▶ We base this upon information about expression of two genes
- ▶ A **classification problem**: function separates data into two different groups (binary classes)

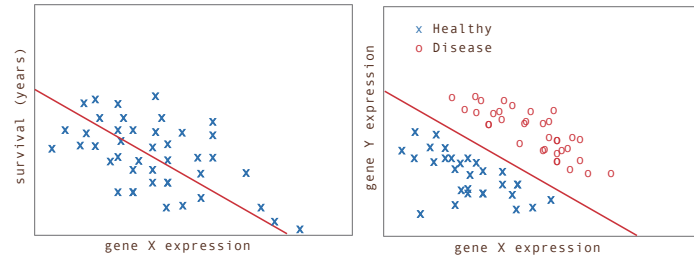


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Which is the Correct Approach?



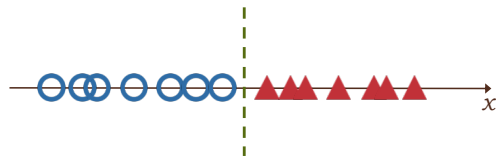
- ▶ The approach we use depends upon what we want to achieve, and what works best based upon the data we have
- ▶ Much machine learning involves investigating different approaches

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From Regression to Classification



- ▶ Suppose we have two classes of data, defined by a single attribute x
- ▶ We seek a **decision boundary** that splits the data in two
- ▶ When such a boundary can be defined using a linear function, it is called a **linear separator**

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Threshold Functions

1. We have data-points with n features:
 $\mathbf{x} = (x_1, x_2, \dots, x_n)$
2. We have a linear function defined by $n+1$ weights:
 $\mathbf{w} = (w_0, w_1, w_2, \dots, w_n)$
3. We can write this linear function as:
 $\mathbf{w} \cdot \mathbf{x}$
4. We can then find the **linear boundary**, where:
 $\mathbf{w} \cdot \mathbf{x} = 0$
5. And use it to define our **threshold** between classes:

$$h_{\mathbf{w}} = \begin{cases} 1 & \mathbf{w} \cdot \mathbf{x} \geq 0 \\ 0 & \mathbf{w} \cdot \mathbf{x} < 0 \end{cases}$$

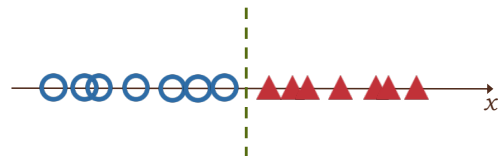
Outputs 1 and 0 here are **arbitrary labels** for one of two possible classes

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From Regression to Classification



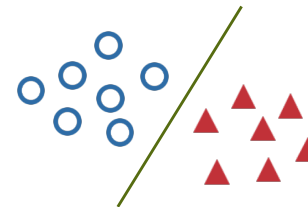
- ▶ Data is **linearly separable** if it can be divided into classes using a linear boundary:

$$\mathbf{w} \cdot \mathbf{x} = 0$$

- ▶ Such a boundary, in 1-dimensional space, is a **threshold value**

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From Regression to Classification



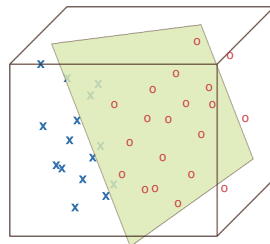
- ▶ Data is **linearly separable** if it can be divided into classes using a linear boundary:

$$\mathbf{w} \cdot \mathbf{x} = 0$$

- ▶ Such a boundary, in 2-dimensional space, is a **line**

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From Regression to Classification



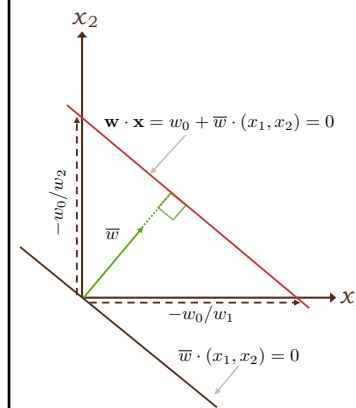
- ▶ Data is **linearly separable** if it can be divided into classes using a linear boundary:

$$\mathbf{w} \cdot \mathbf{x} = 0$$

- ▶ Such a boundary, in 3-dimensional space, is a **plane**
- ▶ In higher dimensions, it is a **hyper-plane**

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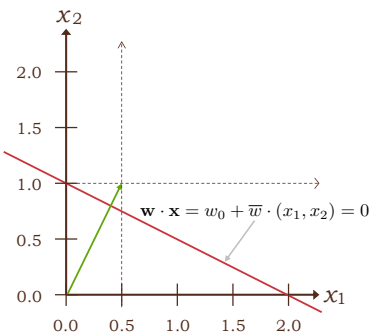
The Geometry of Linear Boundaries



- ▶ Suppose we have 2-dimensional inputs $\mathbf{x} = (x_1, x_2)$
- ▶ The “real” weights $\bar{\mathbf{w}} = (w_1, w_2)$ define a **vector**
- ▶ The boundary where our linear function is zero, $\mathbf{w} \cdot \mathbf{x} = w_0 + \bar{\mathbf{w}} \cdot (x_1, x_2) = 0$ is an orthogonal line, parallel to $\bar{\mathbf{w}} \cdot (x_1, x_2) = 0$
- ▶ Its offset from origin is determined by w_0 (which is called the **bias weight**)

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The Geometry of Linear Boundaries

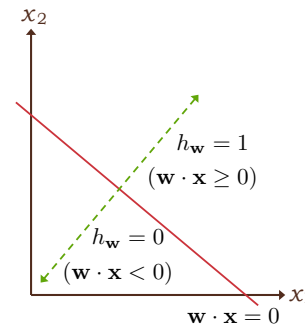


- ▶ For example, with “real” weights:
 $\bar{w} = (w_1, w_2) = (0.5, 1.0)$
 we get the vector shown as a green arrow
- ▶ Then, for a bias weight $w_0 = -1.0$
 the boundary where our linear function is zero,
 $\mathbf{w} \cdot \mathbf{x} = w_0 + \bar{w} \cdot (x_1, x_2) = 0$
 is the line shown in red, crossing origin at $(2,0)$ & $(0,1)$

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The Geometry of Linear Boundaries



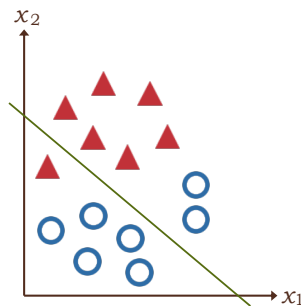
- ▶ Once we have our linear boundary, data points are classified according to our threshold function

$$h_{\mathbf{w}} = \begin{cases} 1 & \mathbf{w} \cdot \mathbf{x} \geq 0 \\ 0 & \mathbf{w} \cdot \mathbf{x} < 0 \end{cases}$$

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Zero-One Loss



- ▶ For a training set made up of input/output pairs, $\{(\mathbf{x}_1, y_1), (\mathbf{x}_2, y_2), \dots, (\mathbf{x}_k, y_k)\}$
 we could define the **zero/one loss**

$$L(h_{\mathbf{w}}(\mathbf{x}_i), y_i) = \begin{cases} 0 & \text{if } h_{\mathbf{w}}(\mathbf{x}_i) = y_i \\ 1 & \text{if } h_{\mathbf{w}}(\mathbf{x}_i) \neq y_i \end{cases}$$
- ▶ Summed for the entire set, this is simply the **count** of examples that we get wrong

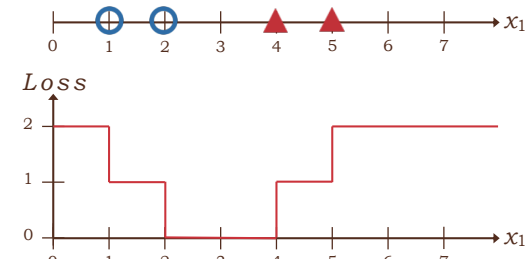
- ▶ In this example, if data-points marked should be in class 0 (below the line) and those marked should be in class 1 (above the line) the loss would be equal to 3

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Minimizing Zero/One Loss

- ▶ Sadly, it is not easy to compute weights that minimize zero/one loss
 - ▶ It is a piece-wise constant function of weights
 - ▶ It is not continuous, however, and gradient descent won't work
- ▶ E.g., for the following one-dimensional data, we get loss shown below:



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Perceptron Loss

- Instead, we define the **perceptron loss** on a training item:

$$\mathbf{x}_i = (x_{i,1}, x_{i,2}, \dots, x_{i,n})$$

$$L_\pi(h_{\mathbf{w}}(\mathbf{x}_i), y_i) = \sum_{j=0}^n (y_i - h_{\mathbf{w}}(\mathbf{x}_i)) \times x_{i,j}$$

- For example, suppose we have a 2-dimensional element in our training set for which the correct output is 0, but our threshold function says 1:

$$\mathbf{x}_i = (0.5, 0.4) \quad y_i = 1 \quad h_{\mathbf{w}}(\mathbf{x}_i) = 0$$

$$L_\pi(h_{\mathbf{w}}(\mathbf{x}_i), y_i) = (1 - 0)(1 + 0.5 + 0.4) = 1.9$$

The difference between what output **should** be, and what our weights make it

Sum of input attributes (1 is the "dummy" attribute that is multiplied by bias weight w_0)

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Perceptron Learning

- To minimize perceptron loss we can start from initial weights—perhaps chosen uniformly from interval $[-1, 1]$ —and then:

- Choose an input \mathbf{x}_i from our data set that is wrongly classified.
- Update vector of weights, $\mathbf{w} = (w_0, w_1, w_2, \dots, w_n)$, as follows:

$$w_j \leftarrow w_j + \alpha(y_i - h_{\mathbf{w}}(\mathbf{x}_i)) \times x_{i,j}$$

- Repeat until no classification errors remain.

- The update equation means that:

- If correct output should be *below* the boundary ($y_i = 0$) but our threshold has placed it *above* ($h_{\mathbf{w}}(\mathbf{x}_i) = 1$) then we *subtract* each feature ($x_{i,j}$) from the corresponding weight (w_i)
- If correct output should be *above* the boundary ($y_i = 1$) but our threshold has placed it *below* ($h_{\mathbf{w}}(\mathbf{x}_i) = 0$) then we *add* each feature ($x_{i,j}$) to the corresponding weight (w_i)

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Perceptron Updates

$$w_j \leftarrow w_j + \alpha(y - h_{\mathbf{w}}(\mathbf{x}_i)) \times x_{i,j}$$

- The perceptron update rule shifts the weight vector positively or negatively, trying to get all data on the right side of the linear decision boundary

- Again, supposing we have an error as before, with weights as given below:

$$\mathbf{x}_i = (0.5, 0.4) \quad \mathbf{w} = (0.2, -2.5, 0.6) \quad y_i = 1$$

$$\mathbf{w} \cdot \mathbf{x}_i = 0.2 + (-2.5 \times 0.5) + (0.6 \times 0.4) = -0.81 \quad h_{\mathbf{w}}(\mathbf{x}_i) = 0$$

- This means we add the value of each attribute to its matching weight (assuming again that "dummy" $x_{i,0} = 1$, and that parameter $\alpha = 1$):

$$w_0 \leftarrow (w_0 + x_{i,0}) = (0.2 + 1) = 1.2$$

$$w_1 \leftarrow (w_1 + x_{i,1}) = (-2.5 + 0.5) = -2.0$$

$$w_2 \leftarrow (w_2 + x_{i,2}) = (0.6 + 0.4) = 1.0$$

$$\mathbf{w} \cdot \mathbf{x}_i = 1.2 + (-2.0 \times 0.5) + (1.0 \times 0.4) = 0.6$$

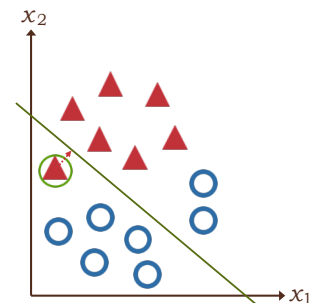
After adjusting weights, our function is now correct on this input

$$h_{\mathbf{w}}(\mathbf{x}_i) = 1$$

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Progress of Perceptron Learning



- For an example like this, we:

- Choose a mis-classified item (marked in green)
- Compute the weight updates, based on the "distance" away from the boundary (so weights shift more based upon errors in boundary placement that are more extreme)

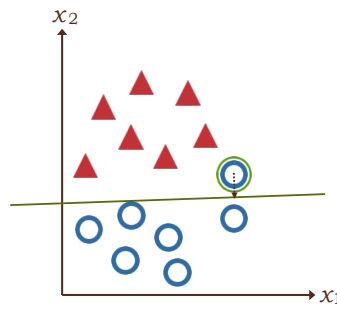
- Here, this **adds** to each weight, changing the decision boundary

- In this example, data-points marked \circ should be in class 0 (below the line) and those marked \triangle should be in class 1 (above the line)

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Progress of Perceptron Learning

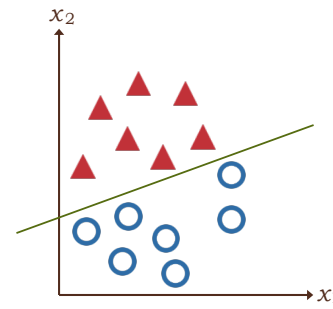


- ▶ Once we get a new boundary, we repeat the process
- 1. Choose a mis-classified item (marked in green)
- 2. Compute the weight updates, based on the “distance” away from the boundary (so weights shift more based upon errors in boundary placement that are more extreme)
- ▶ Here, this **subtracts** from each weight, changing the decision boundary in the other direction

▶ In this example, data-points marked ● should be in class 0 (below the line) and those marked ▲ should be in class 1 (above the line)

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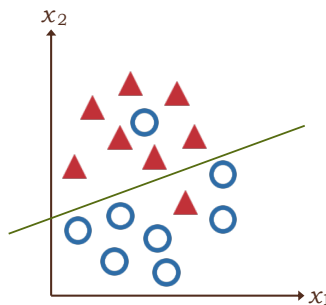
Linear Separability



- ▶ The process of adjusting weights stops when there is no classification error left
- ▶ A data-set is linearly separable if a linear separator exists for which there will be no error
- ▶ It is possible that there are **multiple** linear boundaries that achieve this
- ▶ It is also possible that there is **no such** boundary!

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Linearly Inseparable Data



- ▶ Some data **can't** be separated using a linear classifier
- ▶ Any line drawn will always leave some error
- ▶ The perceptron update method is guaranteed to eventually **converge** to an error-free boundary **if** such a boundary really exists
- ▶ If it **doesn't** exist, then the most basic version of the algorithm will never terminate

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Linearly Inseparable Data

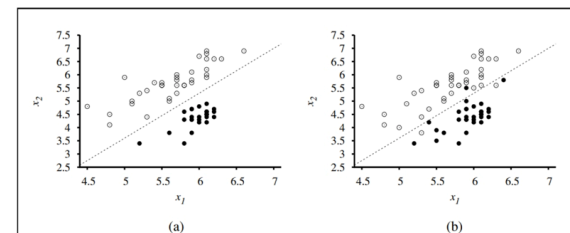


Figure 18.15 (a) Plot of two seismic data parameters, body wave magnitude x_1 and surface wave magnitude x_2 , for earthquakes (white circles) and nuclear explosions (black circles) occurring between 1982 and 1990 in Asia and the Middle East (Kebeasy *et al.*, 1998). Also shown is a decision boundary between the classes. (b) The same domain with more data points. The earthquakes and explosions are no longer linearly separable.

Image source: Russel & Norvig, *AI: A Modern Approach* (Prentice Hall, 2010)

- ▶ Unfortunately, data that can't be separated linearly is very common...

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Modifying Perceptron Learning

► To minimize error, we can modify the algorithm slightly:

1. Choose an input \mathbf{x}_i from our data set that is wrongly classified.
2. Update vector of weights, $\mathbf{w} = (w_0, w_1, w_2, \dots, w_n)$, as follows:

$$w_j \leftarrow w_j + \alpha(y_i - h_{\mathbf{w}}(\mathbf{x}_i)) \times x_{i,j}$$

~~3. Repeat until no classification errors remain.~~

3. Repeat until weights no longer change; modify learning parameter α over time to guarantee this.

► If we make α smaller and smaller over time, then as $\alpha \rightarrow 0$, the weights will quit changing, and the algorithm converges

► To get down to a **least-error** possible final separator, we do this slowly, e.g., setting $\alpha(t) = 1000/(1000 + t)$, where t is the current iteration of the update algorithm

Modifying Perceptron Learning

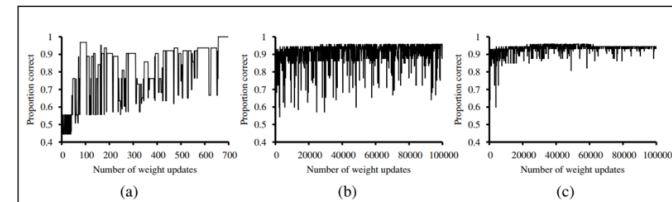


Figure 18.16 (a) Plot of total training-set accuracy vs. number of iterations through the training set for the perceptron learning rule, given the earthquake/explosion data in Figure 18.15(a). (b) The same plot for the noisy, non-separable data in Figure 18.15(b); note the change in scale of the x-axis. (c) The same plot as in (b), with a learning rate schedule $\alpha(t) = 1000/(1000 + t)$.

Image source: Russel & Norvig, *AI: A Modern Approach* (Prentice Hall, 2010)