Department of Mathematics and Computer Science
University of Southern Denmark, Odense

November 9, 2018
Marco Chiarandini

DM534 - Introduction to Computer Science

Training Session, Week 46, Autumn 2018

Solution
Included.

Exercise 1. k-Nearest Neighbors: Prediction

Suppose you are trying to predict a continuous response y to an input x and that you are given the set of training data $D = [(x_1, y_1), \ldots, (x_{11}, y_{11})]$ reported and plotted in Figure 1.

$$D = \begin{bmatrix} (8, & 8.31) \\ (14, & 5.56) \\ (0, & 12.1) \\ (6, & 7.94) \\ (3, & 10.09) \\ (2, & 9.89) \\ (4, & 9.52) \\ (7, & 7.77) \\ (8, & 7.51) \\ (11, & 8.0) \\ (8, & 10.59) \end{bmatrix}$$

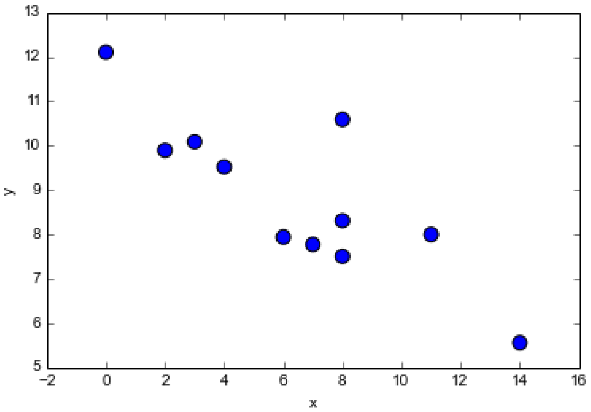


Figure 1: The data for Exercise 1.

Using 5-nearest neighbors, what would be the prediction on an new input $x = 8$?

Solution
First, we need to determine the set $N_5(x)$ of points from D with the 5 shortest distances from x. Hence, we calculate the distance from x to each point in D. For example, the distance between x and $\vec{x}_1$ is:

$$d(\vec{x}, \vec{x}_1) = \sqrt{(8-8)^2} = 0$$

Then, once we have calculated all Euclidean distances for x we rank them in increasing order and take the 5 data points whose corresponding distances are the shortest. Here, we can carry out this process more easily by inspection of the given plot and conclude that:

$$N_5(x) = \begin{bmatrix} (8, & 8.31) \\ (6, & 7.94) \\ (7, & 7.77) \\ (8, & 7.51) \\ (8, & 10.59) \end{bmatrix}$$

Then the prediction $\hat{y}$ can be calculated as:

$$\hat{y}(x) = \frac{1}{k} \sum_{i | x_i \in N_k(x)} y_i = \frac{1}{5}(8.31 + 7.94 + 7.77 + 7.51 + 10.59) = 8.424$$

What form of learning is this exercise about?

- Supervised learning, regression
- Supervised learning, classification
- Unsupervised learning
- Reinforcement learning

Solution

Supervised learning, regression

Exercise 2. k-Nearest Neighbors: Prediction

Suppose you are trying to predict the class $y \in \{0,1\}$ of an input (x_1, x_2) and that you are given the set of training data $D = [((x_{1,1}, x_{1,2}), y_1), \dots, ((x_{11,1}, x_{11,2}), y_{11})]$ reported and plotted in Figure 2.

$$D = \begin{bmatrix} ((10, & 2), & 1) \\ ((15, & 2), & 1) \\ ((6, & 11), & 1) \\ ((2, & 3), & 0) \\ ((5, & 15), & 1) \\ ((5, & 14), & 1) \\ ((10, & 1), & 0) \\ ((1, & 6), & 0) \\ ((17, & 19), & 1) \\ ((15, & 13), & 0) \\ ((19, & 9), & 0) \end{bmatrix}$$

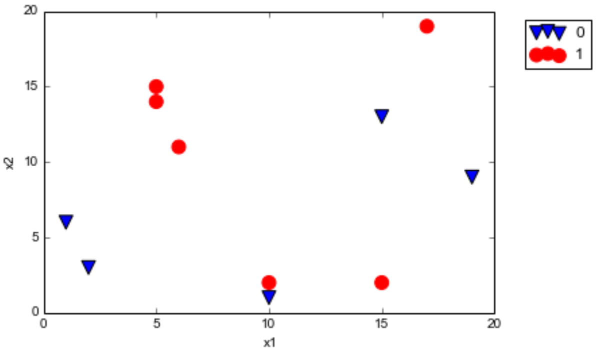


Figure 2: The data for Exercise 2.

Using the 5-nearest neighbors method, what would the prediction be on the new input $\vec{x} = (5, 10)$?

Solution

First, we need to determine the set $N_5(\vec{x})$ of points from D with the 5 shortest distances from $\vec{x}$. We choose to use the Euclidean distance. Hence, we calculate the Euclidean distance from $\vec{x}$ to each point in D. For example the distance between $\vec{x}$ and $\vec{x}_1$ is:

$$d(\vec{x}, \vec{x}_1) = \sqrt{(5-10)^2 + (10-2)^2} \approx 9.44$$

Then, once we have calculated all Euclidean distances for x we rank them in increasing order and take the 5 data points whose corresponding distances are the shortest. Here, we can carry out this process more easily by inspection of the given plot and conclude that:

$$N_5(\vec{x}) = \begin{bmatrix} ((6, & 11), & 1) \\ ((2, & 3), & 0) \\ ((5, & 15), & 1) \\ ((5, & 14), & 1) \\ ((1, & 6), & 0) \end{bmatrix}$$

Then, the prediction $\hat{y}$ is given by majority vote. Since 3 points in $N_5(x)$ have $y = 1$ and 2 points have $y = 0$ then 1 wins and $\hat{y} = 1$.

What form of learning is this exercise about?

- Supervised learning, regression
- Supervised learning, classification
- Unsupervised learning
- Reinforcement learning

Solution

Supervised learning, classification

Exercise 3. Linear Regression: Prediction

As in Exercise 1. you are trying to predict a response y to an input x and you are given the same set of training data $D = [(x_1, y_1), \dots, (x_{11}, y_{11})]$, also reported and plotted in Figure 3. However, now you want to use a linear regression model to make your prediction. After training, your model looks as follows:

$$g(x) = -0.37x + 11.22$$

The corresponding function is depicted in red in Figure 3. What is your prediction $\hat{y}$ for the new input $x = 8$?

$$D = \begin{bmatrix} (8, & 8.31) \\ (14, & 5.56) \\ (0, & 12.1) \\ (6, & 7.94) \\ (3, & 10.09) \\ (2, & 9.89) \\ (4, & 9.52) \\ (7, & 7.77) \\ (8, & 7.51) \\ (11, & 8.0) \\ (8, & 10.59) \end{bmatrix}$$

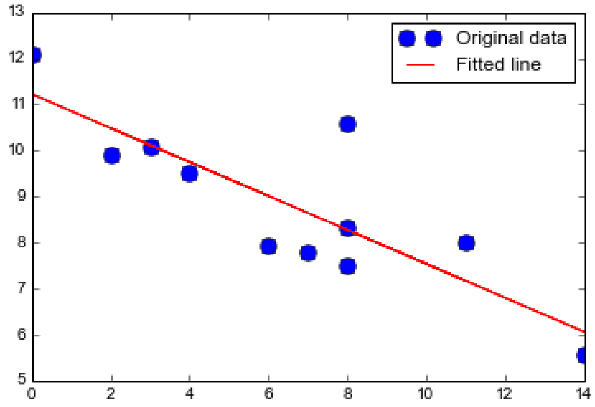


Figure 3: The data for Exercise 3.

Solution

$$\hat{y} = g(8) = -0.37 \times 8 + 11.22 = 8.26$$

Exercise 4. Linear Regression: Training

Calculate the linear regression line for the set of points:

$$D = \begin{bmatrix} (2, 2) \\ (3, 4) \\ (4, 5) \\ (5, 9) \end{bmatrix}$$

Calculate also the *loss* of using g to predict the data from D.
Plot the points and the regression line on the Cartesian coordinate system.
[You can carry out the calculations by hand or you can use any program of your choice. Similarly, you can draw the plot by hand or get aid from a computer program.]

Solution

We use the equations for the closed form solution from the slides:

$$\bar{x} = \frac{1}{m} \sum_{i=1}^{m} x_i \qquad \bar{y} = \frac{1}{m} \sum_{i=1}^{m} y_i$$

which yield:

$$\bar{x} = \frac{2+3+4+5}{4} = 3.5 \qquad \bar{y} = \frac{2+4+5+9}{4} = 5.0$$

and

$$a = \frac{\sum_{i=1}^{m} (x_i - \bar{x})(y_i - \bar{y})}{\sum_{i=1}^{m} (x_i - \bar{x})^2} \qquad b = \bar{y} - a\bar{x}$$

which yield:

$$\hat{b} = -2.7 \qquad \hat{a} = 2.2$$

We carry out these calculations in Python using the module Numpy.

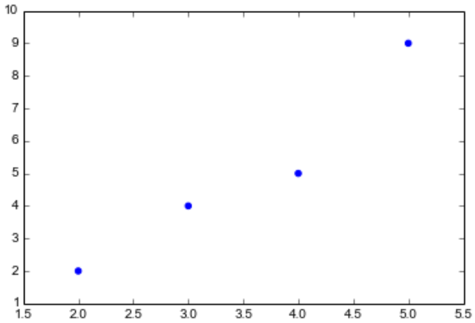
```
In [2]: import numpy as np

        m = 4
        input = np.array([
            [2, 2],
            [3, 4],
            [4, 5],
            [5, 9]
        ])
```

Then we can slice the matrix to extract only the x or y coordinates:

```
In [3]: xx = input[:,0]
        yy = input[:,1]
        xx

Out[3]: array([2, 3, 4, 5])
```

To plot we import the module pyplot from the 2D plotting library matplotlib

```
In [4]: import matplotlib.pyplot as plt

        plt.figure(1)
        plt.scatter(xx, yy, color='b', marker='o')
```



We are then ready to calculate the parameters of the linear regression using the formulas in the slides. We must be careful that the division in Python 2.7 by default returns the integral part. To allow float numbers we import another module:

```
In [5]: from __future__ import division

        x_bar = sum(xx)/m
        y_bar = sum(yy)/m

        print(x_bar)
        print(y_bar)

3.5
5.0
```

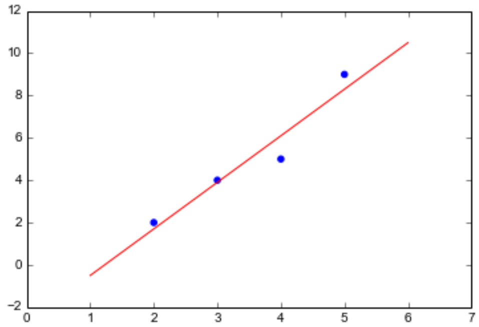
The calculations can be performed in vectorized form, that is, working with arrays. `sum()` sums over the elements of an array and `**` makes the element-wise square of the elements of an array. Hence:

```
In [6]: a_hat = sum((xx-x_bar)*(yy-y_bar))/sum((xx-x_bar)**2)
        b_hat = y_bar - a_hat * x_bar

        print(a_hat)
        print(b_hat)
```

```
2.2
-2.7
```

Finally, we can plot the line. In `pytplot` the easiest way to plot a line is by giving two points and plotting the segment between them. We generate the x coordinates and then calculate the corresponding y value:

```
In [7]: x12 = np.linspace(1, 6, 2)
        y12 = np.array(b_hat + a_hat * x12)

        plt.figure(1)
        plt.scatter(xx, yy, color='b', marker='o')
        plt.plot(x12, y12.T, color='r')
        plt.show()
```



To calculate the sum of squared errors for the training data we need to first calculate the predictions $\hat{y}$ of the linear model on each point of the training set. This can be done as follows:

```
In [8]: def g(var):
            return (b_hat + a_hat * var)
        vec_g = np.vectorize(g)
        y_hat = g(xx)
        L_hat = sum((yy-y_hat)**2)
        print L_hat
```

```
1.8
```

Exercise 5. Logical Functions and Perceptrons

Perceptrons can be used to compute the elementary logical functions that we usually think of as underlying computation. Examples of these functions are AND, OR and NOT.

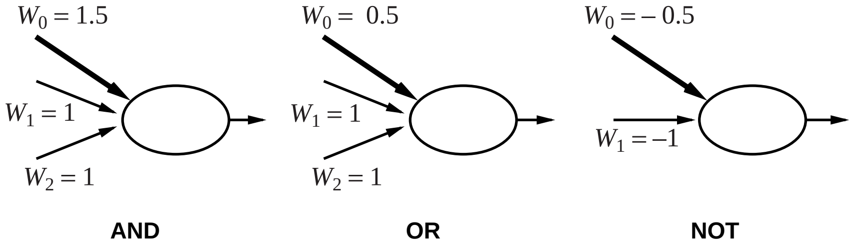


Figure 4: Logical functions and perceptrons. Exercise Exercise 5..

In class, we carried out the verification that the left most perceptron in Figure 4 is a correct representation of the AND operator.

- Verify that the perceptrons given for the OR and NOT cases in Figure 4 are also correct representations of the corresponding logical functions.

- Design a perceptron that implements the logical function NAND.

  Solution

  For example weighting the two inputs by -2 and the output by 3.

Later in this Assignment Sheet we will see that there are also Boolean functions that cannot be represented by a single perceptron alone.

Exercise 6. Multilayer Perceptrons

Determine the truth table of the Boolean function represented by the perceptron in Figure 5:

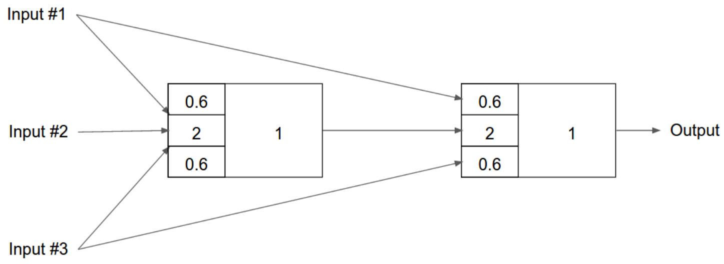


Figure 5: . The multilayer perceptron of Exercise 6.

Solution

x_1	x_2	x_3	y
0	0	0	0
0	0	1	0
0	1	0	1
1	0	0	0
0	1	1	1
1	1	0	1
1	0	1	1
1	1	1	1

Exercise 7. Feed-Forward Neural Networks: Single Layer Perceptron

Determine the parameters of a single perceptron (that is, a neuron with step function) that implements the majority function: for n binary inputs the function outputs a 1 only if more than half of its inputs are 1.

Solution

Set all input weights to 1 and the threshold (bias) to $n/2$.

Exercise 8. Single Layer Neural Networks: Prediction

In Exercise 2. we predicted the class $y \in \{0, 1\}$ of an input (x_1, x_2) with the 5-nearest neighbors method using the data from set D. We used those data to train a single layer neural network for the same task. The result is depicted in Figure 6. (We use the convention $x_0 = -1$ in the linear combination of the inputs.)

- Calculate the prediction of the neural network for the new input $\vec{x} = (5, 10)$. Assume a step function as activation function in the unit (i.e., a perceptron).

  Solution

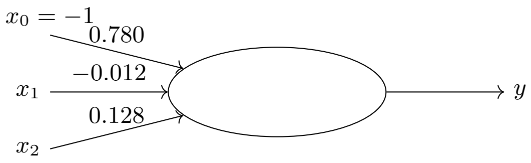


Figure 6: A single layer neural network for the task of Exercise 8.

The step function implemented by the neuron returns $\vec{\theta} \cdot \vec{x} > 0$. In our case:

$$\vec{\theta} \cdot \vec{x} = -0.780 - 0.012 \cdot x_1 + 0.128 \cdot x_2 = 0.44$$

Since the value is > 0 then $\hat{y} = 1$.

- Calculate the prediction of the neural network for the new input $\vec{x} = (5, 10)$. Assume a sigmoid function as activation function in the unit (which is therefore a sigmoid neuron).

Solution

$$g(\vec{x}) = \frac{1}{1 + \exp\left(-0.780 + 0.012 \cdot x_1 - 0.128 \cdot x_2\right)} = 0.608$$

and since $g(\vec{x}) > 0.5$ then $\hat{y} = 1$.

- Compare the results at the previous two points against the result in Exercise 2. Are they all consistent? Is this expected to be always the case? Which one is right?

Solution

The three methods return the same result in this case but they could return different results, in particular the k-nearest neighbors can be different from the single neuron cases. It is impossible to say who is right, because we do not know the actual response to x.

- In binary classification, the loss can be defined as the number of mispredicted cases. Calculate the loss for the network under the two different activation functions. Which one performs better according to the loss?

Solution

We need to repeat the operations at the previous point for all points in D. We can use Python, or any other program (eg, R), for that. The results are reported in the table, where we used $\hat{y}_p$ and $\hat{y}_s$ to indicate the predictions of the perceptron and sigmoid neuron, respectively:

x_1	x_2	y	$\vec{\theta} \cdot \vec{x}$	$\hat{y}_p$	$g(\vec{\theta} \cdot \vec{x})$	$\hat{y}_s$
10.	2.	1.	-0.64	0	0.34	0
15.	2.	1.	-0.7	0	0.33	0
6.	11.	1.	0.56	1	0.64	1
2.	3.	0.	-0.42	0	0.4	0
5.	15.	1.	1.08	1	0.75	1
5.	14.	1.	0.95	1	0.72	1
10.	1.	0.	-0.77	0	0.32	0
1.	6.	0.	-0.02	0	0.49	0
17.	19.	1.	1.45	1	0.81	1
15.	13.	0.	0.7	1	0.67	1
19.	9.	0.	0.14	1	0.54	1

We observe that both two types of neurons perform in the same way: they predict 4 cases wrong and 7 right. The training error defined as the number of wrong predictions is 4.

- Derive and draw in the plot of Exercise 2. the decision boundaries between 0s and 1s that is implied by the perceptron and the sigmoid neuron. [See Section 2.1.3 of the Lecture Notes.] Are the points linearly separable?

Solution

As explained in the answer to Exercise 10. we can derive the decision boundaries as follows. The decision boundary for the perceptron is $\vec{\theta} \cdot \vec{x} = 0$:

$$-0.012 * x_1 + 0.128 * x_2 - 0.780 = 0$$

which is a line indeed.

The decision boundary for the sigmoid neuron is $g(\vec{\theta} \cdot \vec{x}) = 0.5$. That is:

$$\frac{1}{1 + \exp\left(0.780 + 0.012x_1 - 0.128x_2\right)} = 0.5$$

Simplifying:

$$\begin{aligned} 1 &= 0.5(1 + \exp(0.780 + 0.012x_1 - 0.128x_2)) \\ 0.5 &= 0.5\exp(0.780 + 0.012x_1 - 0.128x_2) \\ \log_e 1 &= (0.780 + 0.012x_1 - 0.128x_2) \\ \log_e 1 &= (0.780 + 0.012x_1 - 0.128x_2) \\ 0.012x_1 - 0.128x_2 + 0.780 &= 0 \end{aligned}$$

which is also a line. The two neurons lead to the same separator function, which is depicted in Figure 7!

Note, however, that in the traing phase, that is, when the values of the weights have to be decided, using one or the other activation function can lead to different values for $\vec{\theta}$. This is because the output of the sigmoid function is a real value while the one of the step function is either 0 or 1. Hence, the loss function to optimize is different and may have minima in different points of the space of parameters $\vec{\theta}$.

In Figure 7 we can recognise the 4 points that are misclassified (the four red dots below the line). We can also see that the separator found is perhaps not the best one. It seems that a separator with only two points mispredicted should be possible. How can better parameters be found?

Finally, we can observe that the data points are not linealry separable and that hence a training error equal to zero on this training set is not possible with the single layer neurons analysed.

Below I report part of the Python code behind these calculations. It assumes that the module numpy is imported and that the data set D is put in the array C.

Training error:

```
In [13]: import math

         def stepfunc(x):
             return -0.780 -0.012*x[0] + 0.128*x[1]

         def logistic(x):
             return 1/(1+math.exp(0.780 +0.012*x[0] - 0.128*x[1]  ))

         print( stepfunc([5,10]) ) # > 0
         print( logistic([5,10]) ) # > 0.5

0.43999999999999995
0.6082590307465143
```

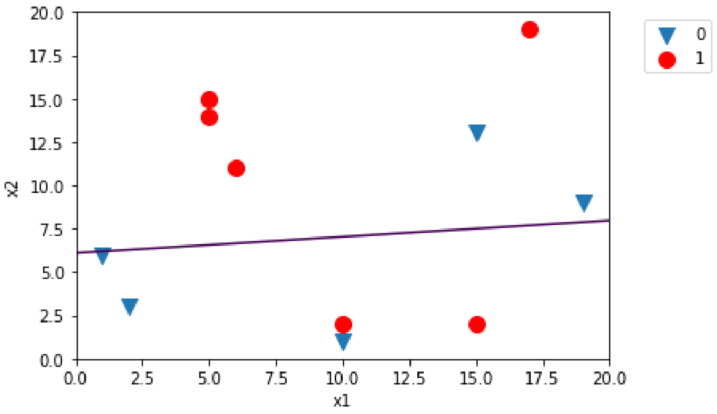


Figure 7: The linear separator for the Exercise Exercise 8.

```
In [14]: l = np.apply_along_axis(logistic,1,C[:,0:2])
         s = np.apply_along_axis(stepfunc,1,C[:,0:2])
         lb = np.where(l>0.5,1,0)
         sb = np.where(s>0,1,0)
         print("loss step function: ", sum(sb != C[:,2]))
         print("loss logistic: ", sum(lb != C[:,2]))

         # %%
```

```
loss step function:  4
loss logistic:  4
```

Separator:

```
In [15]: C0 = C[C[:,2]==0]
         C1 = C[C[:,2]==1]
         l1=plt.scatter(C1[:,0], C1[:,1], s=100, marker='o',color="red")
         l0=plt.scatter(C0[:,0], C0[:,1], s=100, marker="v")
         #plt.axis.xlabel=('x')
         #plt.axis.Axis.ylabel=('x')
         plt.xlabel('x1')
         plt.ylabel('x2')
         plt.legend((l0,l1),('0','1'),bbox_to_anchor=(1.05,1),loc=2)
         x1 = np.linspace(0, 20)
         x2 = np.linspace(0, 20)[:, None]
         plt.contour(x1, x2.ravel(), 0.780 +0.012*x1 - 0.128*x2,[0])
         plt.show()

         # %%
```

Exercise 9. Single Layer Perceptrons

Can you represent the two layer perceptron of Figure 8 as a single perceptron that implements the same function? If yes, then draw the perceptron.

Solution

It corresponds to a single perceptron with two inputs of weight .35 each. Indeed, the output of the first neuron is multiplied by 0 in the second, hence it has no influence whatever its output is. This can also be shown by the equivalent outputs of the two networks on all 4 possible combinations of inputs.

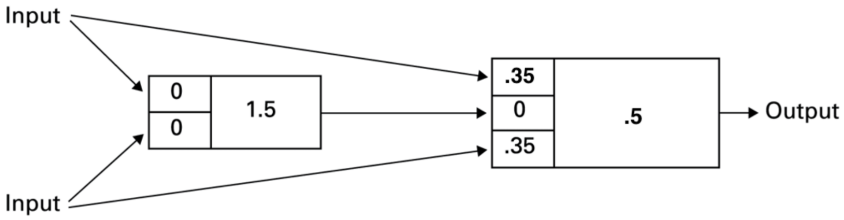


Figure 8: A two layer neural network

Exercise 10. Expressivness of Single Layer Perceptrons

Is there a Boolean (logical) function in two inputs that cannot be implemented by a single perceptron? Does the answer change for a single sigmoid neuron?

Solution

Yes, there is a Boolean (logical) function in two inputs that cannot be implemented by a single perceptron. We saw, for example, in the lecture notes that the algebraic expression of a perceptron is:

$$\text{output} := \begin{cases} 0 & \text{if } \sum_j w_j x_j \leq \text{threshold} \\ 1 & \text{if } \sum_j w_j x_j > \text{threshold} \end{cases}$$

Then the decision boundary is

$$\sum_{j=1}^{p} w_j x_j = \text{threshold}$$

In the case of two inputs, x_1 and x_2, this becomes: $w_1 x_2 + w_2 x_2 = \text{threshold}$, which corresponds to the equation of a line in the Cartesian plane:

$$x_2 = -\frac{w_1}{w_2} x_1 + \frac{1}{w_2} \text{threshold}$$

(you might have seen this with y in place of x_2 and x in place of x_1.) Figure 9 taken from the slides gives an example of a non separable case:

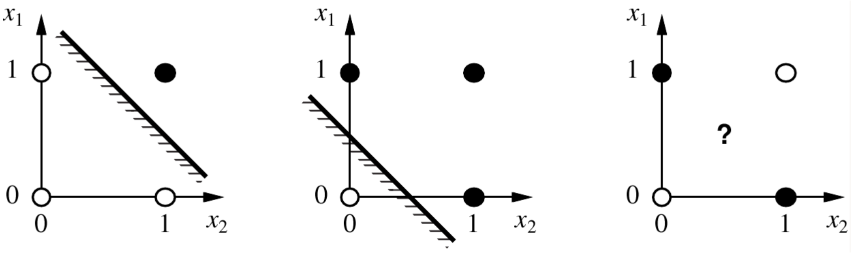


Figure 9: The figure is part of the solution only.

A sigmoid neuron would have the same problem. Indeed, if we use the value 0.5 as the discriminant on the output of a sigmoid neuron to answer 0 or 1 then the decision boundary corresponds to:

$$\frac{1}{1 + \exp(-\sum_{j=1}^{p} w_j x_j - w_0 x_0)} = 0.5$$

(We continue assuming $x_0 = -1$ and the term $b = w_0 x_0 = -w_0$ is called the *bias*. It controls a translation of the sigmoid while the other terms determine the shape of the curve.). Solving in $\vec{x}$ we obtain an equation of the form:

$$\sum_j w_j x_j - b = \text{constant}$$

which therefore is also a line.

Exercise 11. Logical Functions and Neural Networks

The NAND gate is universal for computation, that is, we can build any computation up out of NAND gates. We saw in Exercise 5. that a single perceptron can model a NAND gate. From here, it follows that using networks of perceptrons we can compute any logical function.
For example, we can use NAND gates to build a circuit which adds two bits, x_1 and x_2. This requires computing the bitwise sum, x_1 XOR x_2, as well as a carry bit which is set to 1 when both x_1 and x_2 are 1, i.e., the carry bit is just the bitwise product x_1x_2. The circuit is depicted in Figure 10.

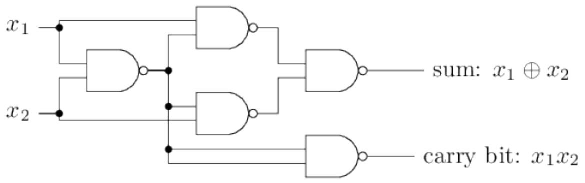
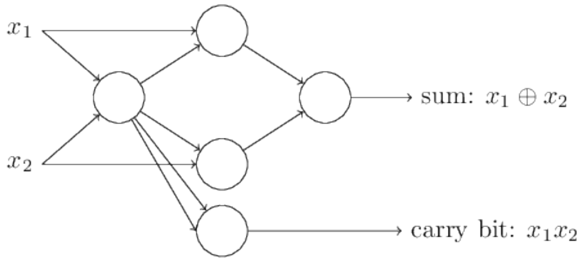


Figure 10: The adder circuit of Exercise 11.. All gates are NAND gates.

Draw a neural network of NAND perceptrons that would simulate the adder circuit from the figure. [You do not need to decide the weights. You have already discovered which weights for a single perceptron would implement a NAND function in Exercise 5.]

What is the advantage of neural networks over logical circuits when representing Boolean functions?

Solution



The exercise provides an example of how any logical function can be implemented by composition of perceptrons in a (multi-layered) network. The computational universality of perceptrons is reassuring because it tells us that perceptron networks can be as powerful as any other computing device. NN are however not merely a new type of NAND gate.
It turns out that we can devise learning algorithms which can automatically tune the weights and biases of a network of artificial neurons. This tuning happens in response to external stimuli, without direct intervention by a programmer. These learning algorithms enable us to use artificial neurons in a way which is radically different to conventional logic gates. Instead of explicitly laying out a circuit of NAND and other gates, our neural networks can simply learn to solve problems, sometimes problems where it would be extremely difficult to directly design a conventional circuit.

Exercise 12. Computer Performance Prediction

You want to predict the running time of a computer program on any computer architecture. To achieve this task you collect the running time of the program on all machines you have access to. At the end you have a spreadsheet with the following columns of data:

(1) MYCT: machine cycle time in nanoseconds (integer)

(2) MMIN: minimum main memory in kilobytes (integer)

(3) MMAX: maximum main memory in kilobytes (integer)

(4) CACH: cache memory in kilobytes (integer)

(5) CHMIN: minimum memory channels in units (integer)

(6) CHMAX: maximum memory channels in units (integer)

(7) Running time in seconds (integer)

Indicate which of the following machine learning approaches is correct:

a. It is a supervised learning, regression task. Therefore, we can apply 5-nearest neighbors using the data in columns (1)-(6) as features and those in column (7) as response.

b. It is a supervised learning, regression task. Therefore, we can apply a linear model that takes columns (1)-(6) as independent variables and attribute (7) as response variable.

c. It is a supervised learning, classification task. Therefore, we can train a multilayer neural network that has an input layer made by one input node for each of the columns (1)-(6); an output layer made by one single sigmoid node that outputs the predicted running time in seconds; an hidden layer of say 10 nodes made by sigmoid nodes.

d. It is a supervised learning, regression task. Therefore, we can train a multilayer neural network that has an input layer made by one input node for each of the columns (1)-(6); an output layer made by one single node implementing a linear activation function that outputs the predicted running time in seconds; an hidden layer of say 10 nodes made by sigmoid nodes.

e. It is an unsupervised learning task. We cluster the machines according to the data from columns (1)-(7). Then for a new machine we predict the time as the one of the cluster whose data are closer to the one of the new machine.

f. It is a reinforcement learning task. We program the computer to sequentially try machines and guess the correct time. We reward the guesses after each guess by a score that is higher when the guess is close to the true value.

Solution

a. b. d. are correct.
c. is not correct because the output would always be in $[0,1]$ while the running time of a program is not restricted to that interval. Thus, this is an example of neural network applied for regression rather than classification, as we saw so far.
e. is not correct because we would not have the run time for the new machine. Therefore we would not be able to identify the most similar cluster because we would miss one variable to calculate the distance. A similar approach that would work in this case is k-nearest neighbors.
f. is not correct because as it is described it falls back to be a supervised learning task. In reinforcement learning we do not have a supervision at every decision (guess) that is made but only at the end after a sequence of guesses.