intro_mlp_xor

March 26, 2018

1 Introduction to Neural Networks

- Some material from peterroelants
- Goal: understand neural networks so they are no longer a black box

```
In [121]: # do all of the imports here
          import numpy  # Matrix and vector computation package
          import matplotlib.pyplot as plt  # Plotting library
          from sklearn import datasets
          import seaborn as sns
          %matplotlib inline
          sns.set(style='ticks', palette='Set2')
          import pandas as pd
          import numpy as np
          import math
          from __future__ import division
          numpy.random.seed(seed=1)
```

Suppose you are to write some kind of function. You know what inputs it's going to take (x) and what kinds of outputs that are expected (y):

1.1

$$y = f(x)$$

You find out, however, that your inputs are very complicated data points and your task is to write a function that can classify those data points into one of several classes. What do you do?

- Option 1: You can write $f(x)$, i.e., a rule-based algorithm, like we always have. Programmers do this all the time.
- Option 2: You can write a different kind of $f(x)$ that learns the function on its own using data.
- **x = data** (i.e., input features)
- **y = class label** (i.e., output)

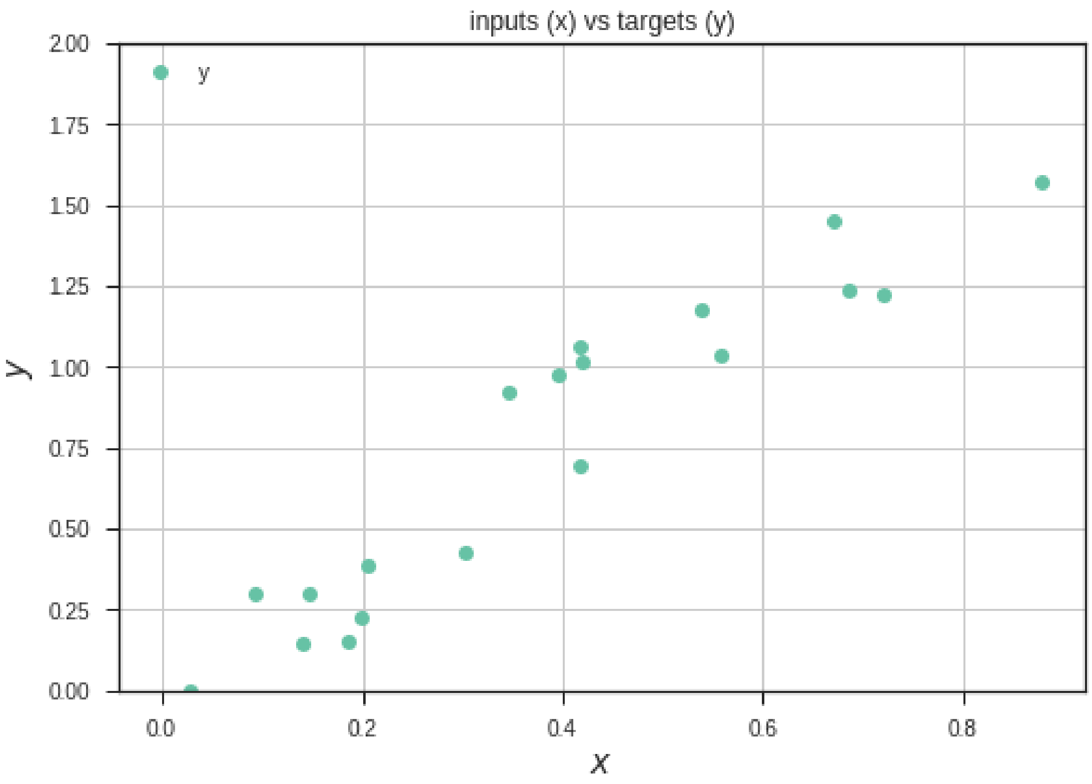
What do we mean when we say that a machine learns? Let's start with an intuitive example: linear regression.

first, we need some data (i.e., x and y)

```
In [122]: x = numpy.random.uniform(0, 1, 20)
          def f(x): return x * 2
          noise_variance = 0.2  # Variance of the gaussian noise
          noise = numpy.random.randn(x.shape[0]) * noise_variance
          t = f(x) + noise
```

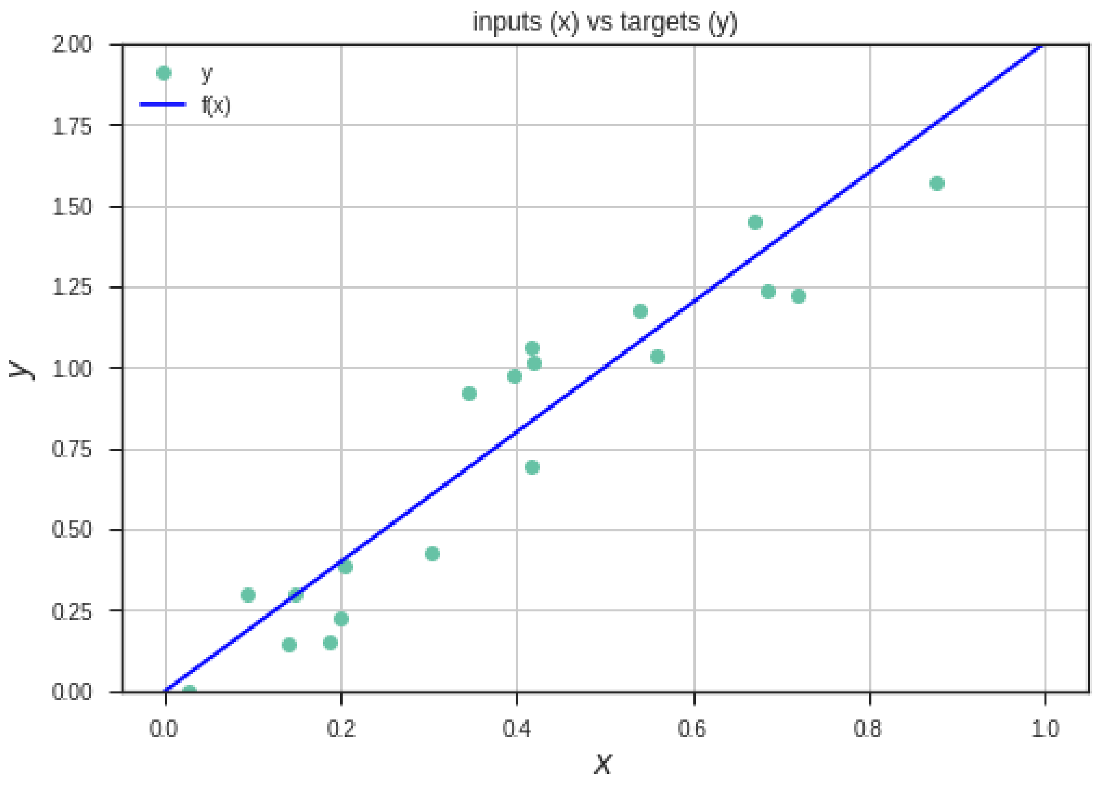
plot the data

```
In [123]: plt.plot(x, t, 'o', label='y')
          plt.xlabel('$x$', fontsize=15)
          plt.ylabel('$y$', fontsize=15)
          plt.ylim([0,2])
          plt.title('inputs (x) vs targets (y)')
          plt.grid()
          plt.legend(loc=2)
          plt.show()
```



now you want to use the data to make predictions That is, given a novel x that isn't already there, what would you predict y to be? We need to model that somehow.

```
In [124]: plt.plot(x, t, 'o', label='y')
          plt.plot([0, 1], [f(0), f(1)], 'b-', label='f(x)')
          plt.xlabel('$x$', fontsize=15)
          plt.ylabel('$y$', fontsize=15)
          plt.ylim([0,2])
          plt.title('inputs (x) vs targets (y)')
          plt.grid()
          plt.legend(loc=2)
          plt.show()
```



That's called a linear regression line. How did we come up with that? First, we need to define what a line is:

1.1.1

$$y = mx + b$$

That means we need to find out what m and b are, using the data x and the labels y.

Cost functions: To find the proper values of m and b using the data, we need to define a way to determine how well some arbitrary values of m and b represent / fit the data. This is what a cost function is for. In this case, we can calculate the vertical distance (aka the residual) between all of the data points and the line and sum up those distances. (This is well known for linear regression; the cost function is the least squares, or the sum of the squared residuals.)

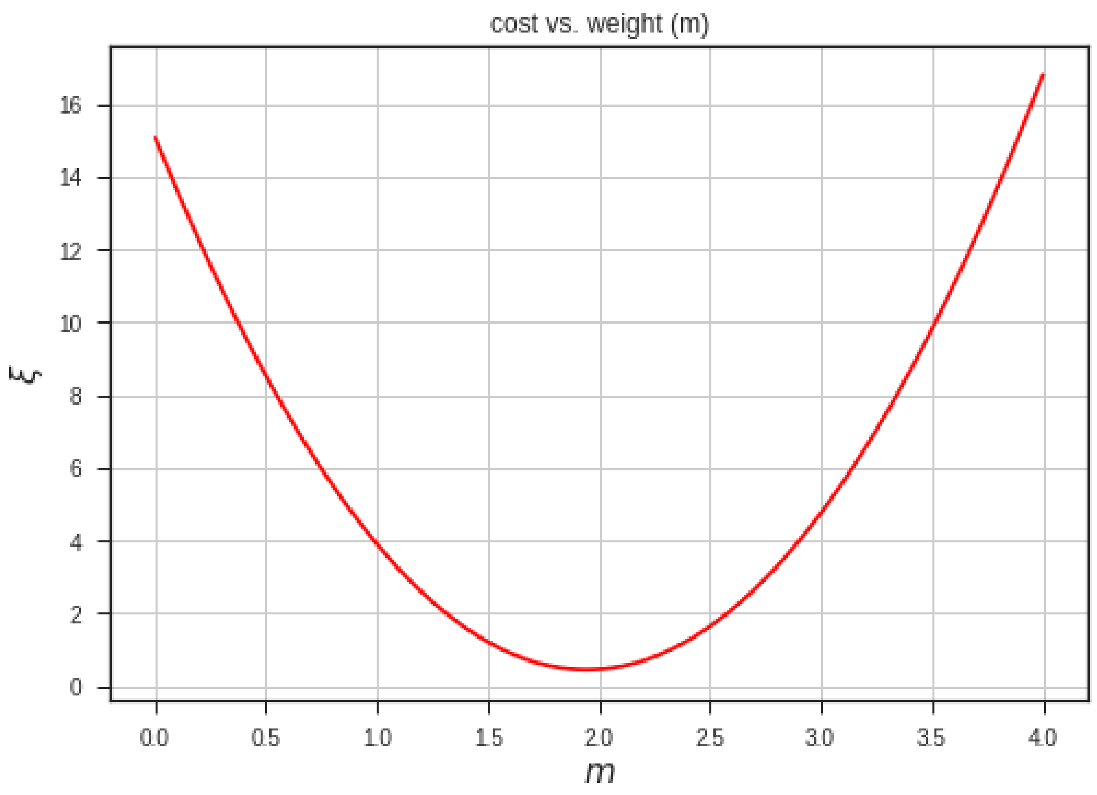
The goal is to find a line represented by the values m and b such that the sum of the vertical distances is minimized.

```
In [125]: def nn(x, w): return x * w

          # Define the cost function
          def cost(y, t): return ((t - y)**2).sum()
```

Randomly choose some values for m and b then check against the cost function.

The battle is only part way over: we have to apply our cost function to different values of m and b and find the best line for the data. The cost function tells us which way we should adjust m and b. If we range over all possible values for m and b, we can plot the cost.

```
In [126]: # Plot the cost vs the given weight w (m, in our explanation)

          # Define a vector of weights for which we want to plot the cost
          ws = numpy.linspace(0, 4, num=100)  # weight values
          cost_ws = numpy.vectorize(lambda w: cost(nn(x, w) , t))(ws)  # cost for each weight in

          # Plot
          plt.plot(ws, cost_ws, 'r-')
          plt.xlabel('$m$', fontsize=15)
          plt.ylabel('$\\xi$', fontsize=15)
          plt.title('cost vs. weight (m)')
          plt.grid()
          plt.show()
```



Range over all possible values of m and calculate the cost (ignore b for the moment). Notice above that if we plot the cost for a bunch of m values, we can find a value where the cost is at its lowest.

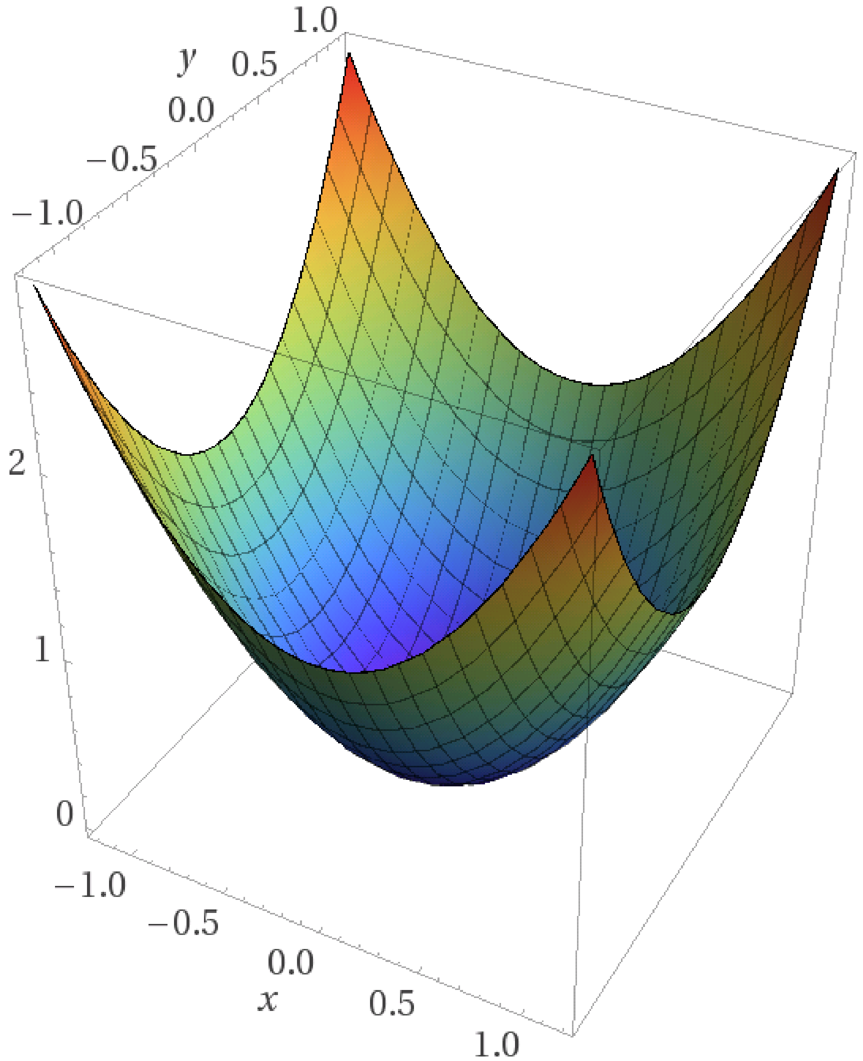
Here's another example of a plotted cost function in more dimensions (of course, using different data and a different cost function):

How do we get to the minimal point? That lowest point is the best "fit" line for the data. How do we find that line?

- Option 1: range over all possible values (very, very time consuming)
- Option 2: range until we reach a minimum (okay, but still time consuming, and how do we know which way to go with m, higher or lower?)
- Option 3: gradient descent

Gradient descent. The **gradient** is a functional way of representing the increase or decrease in the magnitude of something. Applied to our cost function, the gradient descent algorithm begins with some random initial point, computes the cost function, then computes a gradient step by determining the slope of where the initial point is, then goes in the desired direction; in our case, down towards a minimum.

```
In [127]: # define the gradient function. Remember that y = nn(x, w) = x * w
          def gradient(w, x, t):
              return 2 * x * (nn(x, w) - t)
```



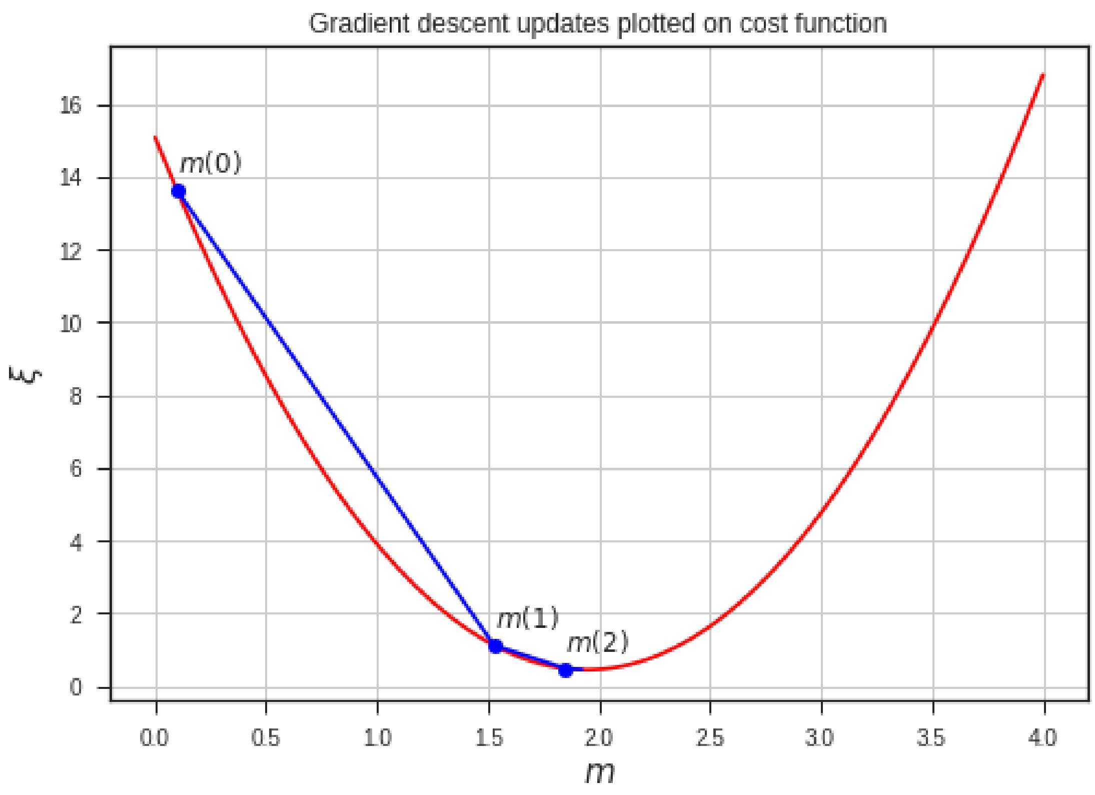
Computed by Wolfram|Alpha

nonconvex

```
# define the update function delta w
def delta_w(w_k, x, t, learning_rate):
    return learning_rate * gradient(w_k, x, t).sum()

# Set the initial weight parameter
w = 0.1
# Set the learning rate
learning_rate = 0.1

# Start performing the gradient descent updates, and print the weights and cost:
nb_of_iterations = 4  # number of gradient descent updates
w_cost = [(w, cost(nn(x, w), t))] # List to store the weight,costs values
for i in range(nb_of_iterations):
    dw = delta_w(w, x, t, learning_rate)  # Get the delta w update
    w = w - dw  # Update the current weight parameter
    w_cost.append((w, cost(nn(x, w), t)))  # Add weight,cost to list

# Print the final w, and cost
for i in range(0, len(w_cost)):
    print('m({}): {:.4f} \t cost: {:.4f}'.format(i, w_cost[i][0], w_cost[i][1]))
```

```
m(0): 0.1000         cost: 13.6197
m(1): 1.5277         cost: 1.1239
m(2): 1.8505         cost: 0.4853
m(3): 1.9234         cost: 0.4527
m(4): 1.9399         cost: 0.4510
```

```
In [128]: # Plot the first 2 gradient descent updates
          plt.plot(ws, cost_ws, 'r-')  # Plot the error curve
          # Plot the updates
          for i in range(0, len(w_cost)-2):
              w1, c1 = w_cost[i]
              w2, c2 = w_cost[i+1]
              plt.plot(w1, c1, 'bo')
              plt.plot([w1, w2],[c1, c2], 'b-')
              plt.text(w1, c1+0.5, '$m({})$'.format(i))
          # Show figure
          plt.xlabel('$m$', fontsize=15)
          plt.ylabel('$\\xi$', fontsize=15)
          plt.title('Gradient descent updates plotted on cost function')
          plt.grid()
          plt.show()
```



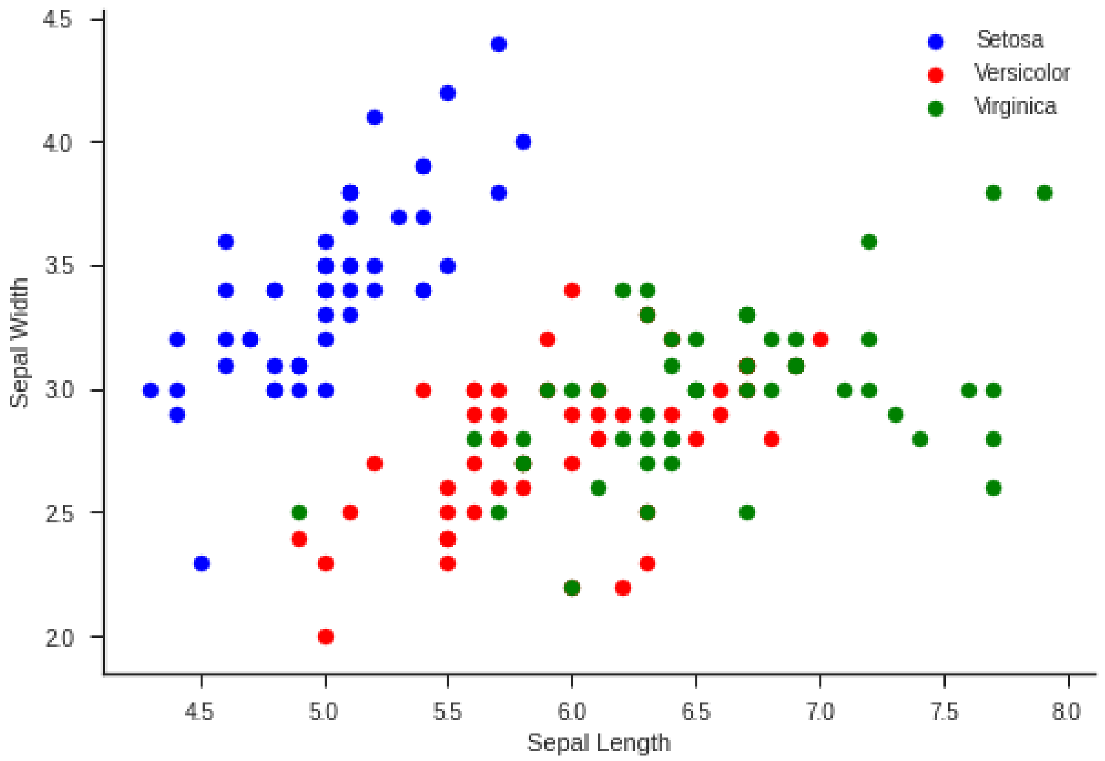
This is the intuition for a lot of classification approaches in machine learning: define a cost function then use data and a gradient to determine a best fit of the model (in the linear regression case, the weight m and the bias term b constitute the model). Machine "learning" often amounts to minimizing a cost function like this.

A linear regression line doesn't really help us do classification, however. For classification, we usually have two different sets of data. We can plot the data like we did before, but instead of drawing a regression line to fit the data, we want to draw a decision boundary between different classes in the data.

1.1.2 Example: Iris Dataset

```
In [40]: data = datasets.load_iris()
         X = data.data[:150, :3]
         y = data.target[:150]
         X_full = data.data[:150, :]
```

```
In [41]: setosa = plt.scatter(X[:50,0], X[:50,1], c='b')
         versicolor = plt.scatter(X[50:100,0], X[50:100,1], c='r')
         virginica = plt.scatter(X[100:150,0], X[100:150,1], c='g')
         plt.xlabel("Sepal Length")
         plt.ylabel("Sepal Width")
         plt.legend((setosa, versicolor, virginica), ("Setosa", "Versicolor", "Virginica"))
         sns.despine()
```



It's obvious where the decision boundary should go to separate Setosa from the others, but it's harded to separate Versicolor and Virginica from each other. If you were to write a function yourself, how would you do it? That would be quite challenging.

Let's use the intuition from linear regression to find a way to draw a decision boundary. Obviously, we want to draw some kind of line. It would be better if, instead of just drawing a line, we had some way of saying that a sample fits a certain class in a certain number scale. A very useful scale is probability space: between 0 and 1. That is, can we use the intuitions of linear regression to determine if a sample s belongs to class c with some probability? I.e., $P(C = c|S = s)$. There's already a classifier that can do this for us: logistic regression.

1.1.3 Logistic Regression

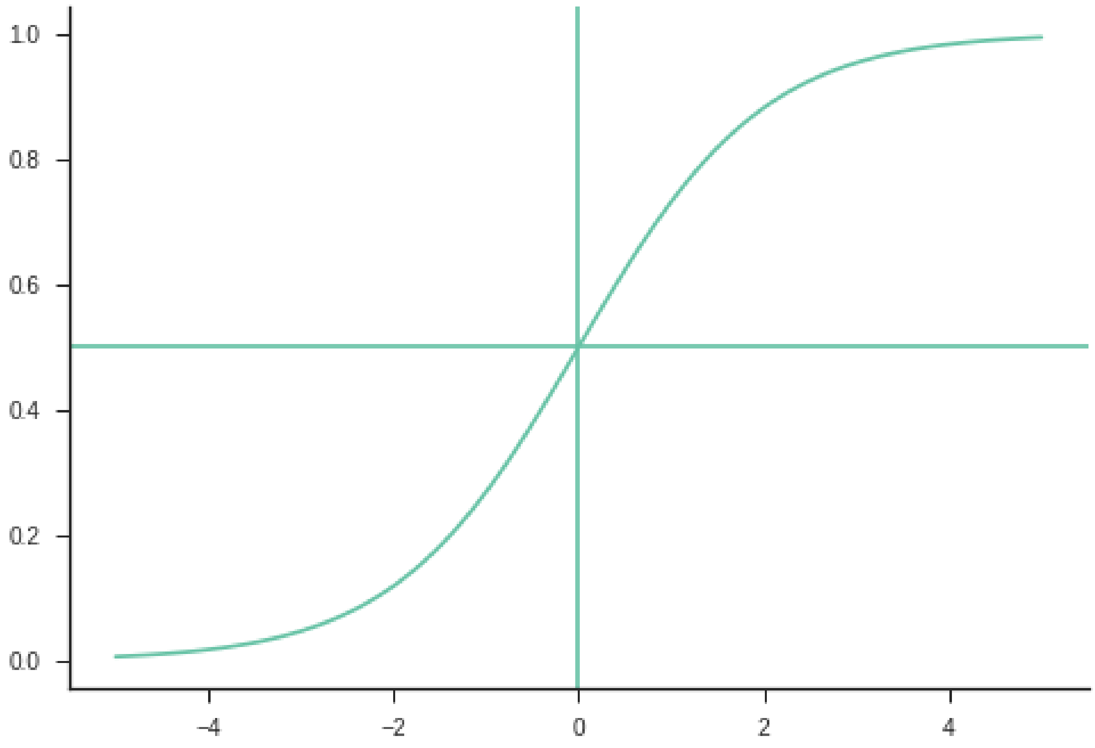
Logistic regression uses the intuitions of linear regression, where we want to fit a line to some data using a cost function and gradient descent, with the added benefit of being able to return a probabiliy.

Instead of fitting line to data, we fit the **logistic function** to the data. Instead of just plotting data points as usual, imagine putting data points from some class c_1 along the 1 line and data points from a different class c_2 along the 0 line.

Here's the logistic function

- Instead of $y = mx + b$, we use this.
- The weights determine where it shifts and how stretched it is.

```
In [129]: x_values = np.linspace(-5, 5, 100)
          y_values = [1 / (1 + math.e**(-x)) for x in x_values]
          plt.plot(x_values, y_values)
          plt.axhline(.5)
          plt.axvline(0)
          sns.despine()
```



```
In [43]: def logistic_func(theta, x):
             return float(1) / (1 + math.e**(-x.dot(theta)))
```

If we want to follow the intuitions of linear regression, we need to initialize some values (i.e., the weights / coefficients), then use gradient descent to minimize the cost function.

```
In [130]: def log_gradient(theta, x, y):
              first_calc = logistic_func(theta, x) - np.squeeze(y)
              final_calc = first_calc.T.dot(x)
              return final_calc

In [131]: def cost_func(theta, x, y):
              '''
              computes the cost function; i.e., (for linear regression) minimize the distance be
              and all of the points
              '''
```

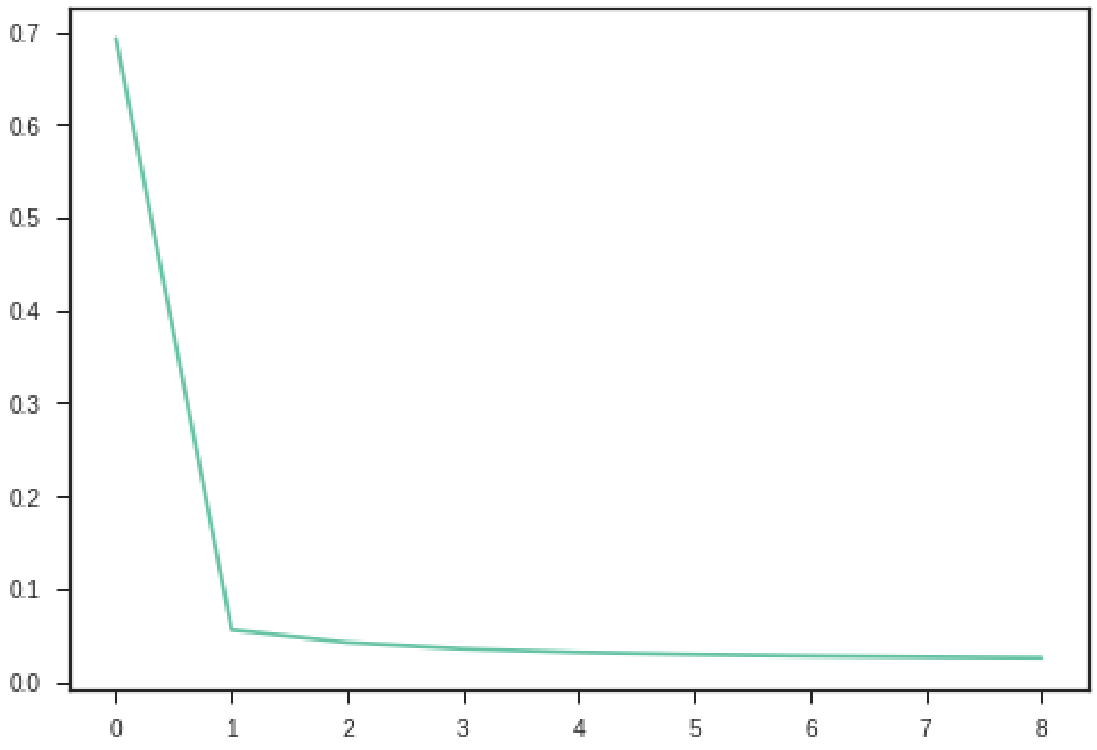
```
        log_func_v = logistic_func(theta,x)
        y = np.squeeze(y)
        step1 = y * np.log(log_func_v)
        step2 = (1-y) * np.log(1 - log_func_v)
        final = -step1 - step2
        return np.mean(final)

    def grad_desc(theta_values, X, y, lr=.001, converge_change=.001):
        '''
        the hard part of learning: gradient descent. Fortunately, the logistic function is
        the derivitive is itself
        '''
        X = (X - np.mean(X, axis=0)) / np.std(X, axis=0) #normalize
        #setup cost iter
        cost_iter = []
        cost = cost_func(theta_values, X, y)
        cost_iter.append([0, cost])
        change_cost = 1 # initialize the change in cost to a high value
        i = 1
        # this actually performs the gradient descent by moving the regression line until
        while(change_cost > converge_change):
            old_cost = cost
            theta_values = theta_values - (lr * log_gradient(theta_values, X, y)) # the co
            cost = cost_func(theta_values, X, y)
            cost_iter.append([i, cost])
            change_cost = old_cost - cost #calculate the change in the cost
            i+=1
        return theta_values, np.array(cost_iter)
```

Now we use our data, applied to the logistic, cost, and gradient descent functions, to learn the weights for the classifier (also knowin as *training*)

```
In [46]: shape = X.shape[1]
         y_flip = np.logical_not(y.reshape(y.shape[0],1)) #flip Setosa to be 1 and Versicolor to
         betas = np.zeros(shape) #start off with zeros for the coefficients
         fitted_values, cost_iter = grad_desc(betas, X, y_flip,  lr=.1)
         fitted_values

Out[46]: array([-3.91547066,  5.42219164, -6.72251116])
```

How well did our cost function work?

```
In [47]: cost_X, cost_y = zip(*cost_iter)
         plt.plot(cost_X, cost_y)

Out[47]: [<matplotlib.lines.Line2D at 0x7f122e383c88>]
```



How well does our classifier perform on the data?

```
In [48]: def pred_values(theta, X, hard=True):
             '''
             predictor values
             '''
             X = (X - np.mean(X, axis=0)) / np.std(X, axis=0) #normalize
             pred_prob = logistic_func(theta, X)
             pred_value = np.where(pred_prob >= .5, 1, 0) # note the threshold of 0.5
             if hard:
                 return pred_value
             return pred_prob

         predicted_y = pred_values(fitted_values, X)
         np.sum(y_flip == predicted_y) / 150.0
```

```
Out[48]: 83.0
```

Logistic regression is a very common classifier for machine learning, but it has some limitations. It's a kind of **linear** classifier because it learns a linear decision boundary between two classes.

What if the problem we are trying to solve isn't linearly separable? One simple example is the XOR problem.

1.2 Learning XOR

XOR, "exclusive or" means we have two bits. When both bits are on/off, it evaluates to zero. When one of the bits are on, then it evaluates to one.

bit 1	bit 2	result
0	0	0
0	1	1
1	0	1
1	1	0

The claim: linear models such as logistic regression cannot learn the xor problem because it's not directly linear separable, but, with enough training data, a 2-layer neural network can. We'll just see about that.

```
In [169]: import pandas as pd
          import numpy as np
          import random
```

let's generate some XOR training data

```
In [182]: m = 10100
          X = []
          y = []
          for i in range(0,m):
              y_i = random.randint(0, 1) # randomly choose a label
              y.append(y_i)
              if y_i == 1: # when y is 1, then pick an input where one of the two bits are on
                  X.append(random.choice([[1,0],[0,1]]))
              else: # otherwise turn both bits on or off
                  X.append(random.choice([[0,0],[1,1]]))

          X[:3], y[:3]

Out[182]: ([[1, 0], [0, 1], [0, 1]], [1, 1, 1])
```

split the test and train data (not that it matters)

```
In [183]: Xtrain, Xtest = np.array(X[:-100]), np.array(X[m-100:])
          ytrain, ytest = np.array(y[:-100]), np.array(y[m-100:])

          Xtrain.shape, ytrain.shape, Xtest.shape, ytest.shape

Out[183]: ((10000, 2), (10000,), (100, 2), (100,))
```

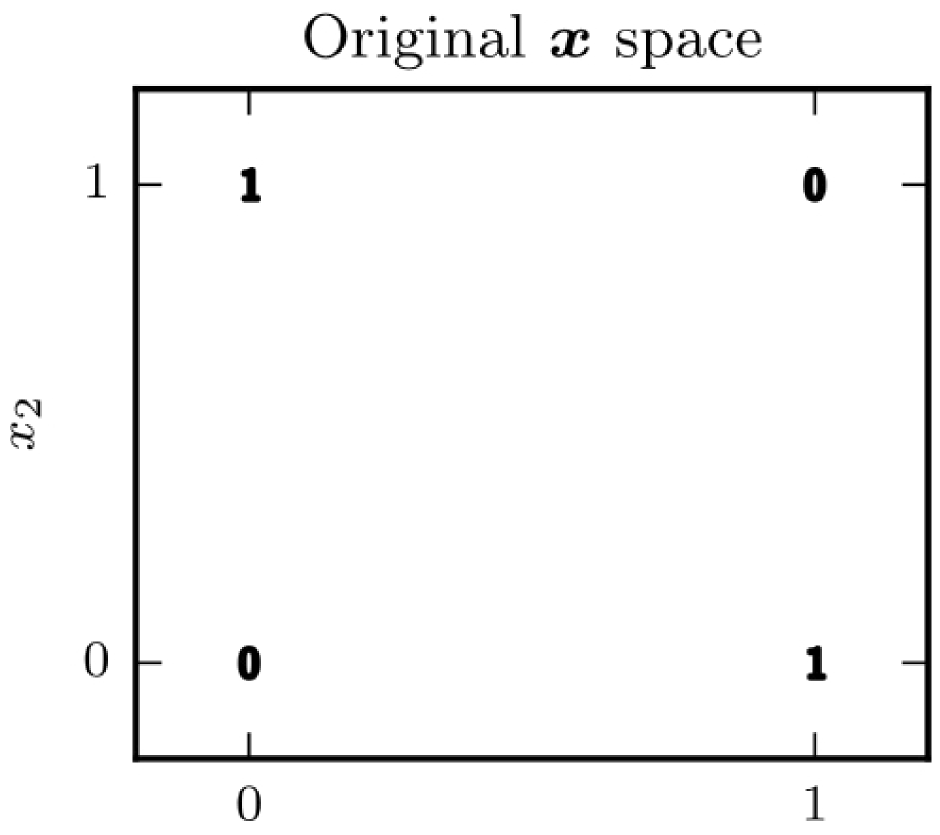
1.2.1 Try Logistic Regression, a linear clasifier

- we'll use scikit-learn's logistic regression classifier

```
In [184]: from sklearn import linear_model
          from sklearn.metrics import accuracy_score


          model = linear_model.LogisticRegression()
          model.fit(Xtrain, ytrain)
          accuracy_score(model.predict(Xtest), ytest)

Out[184]: 0.49
```

What happened? It should have learned the function. The problem: XOR is not linearly separable. Where would a linear classifier like logistic regression draw a line to separate the two classes? It can't.

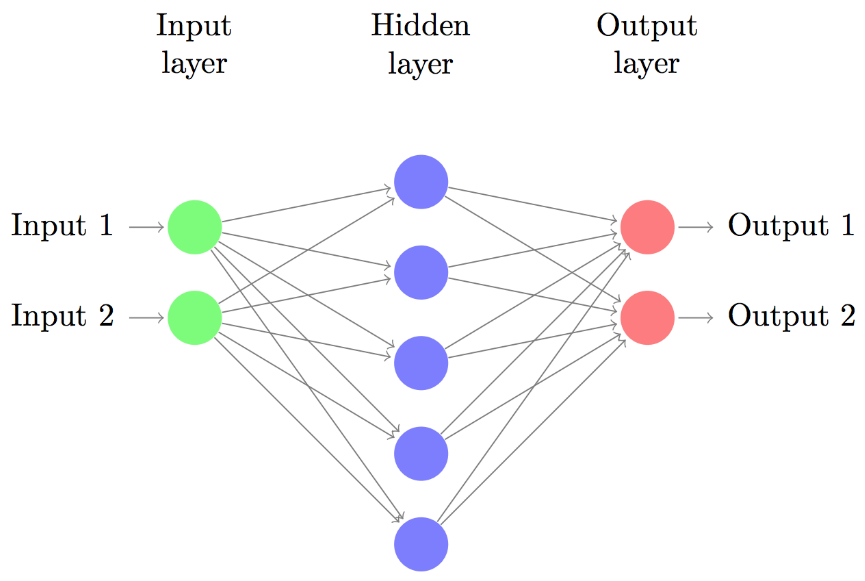
(Image from Goodfellow et al's, Deep Learning book)



xorplot

1.2.2 Try a simple NN with two layers

- Neural networks are similar (at least in this example) to stacking up logistic regression classifiers together.
- You have input, hidden layers (with nodes that have activation functions, like the logistic function) and you have the output



xorplot

- It isn't guaranteed to learn the XOR function the first time. You may have to retrain it multiple times. (Why?)

```
In [188]: from sklearn.neural_network import MLPClassifier
          r = 0
          while r != 1.0:
              model = MLPClassifier(solver='sgd', alpha=1e-5, hidden_layer_sizes=(2, 2))
              model.fit(Xtrain, ytrain)
              r = accuracy_score(model.predict(Xtest), ytest)
              print(r)
```

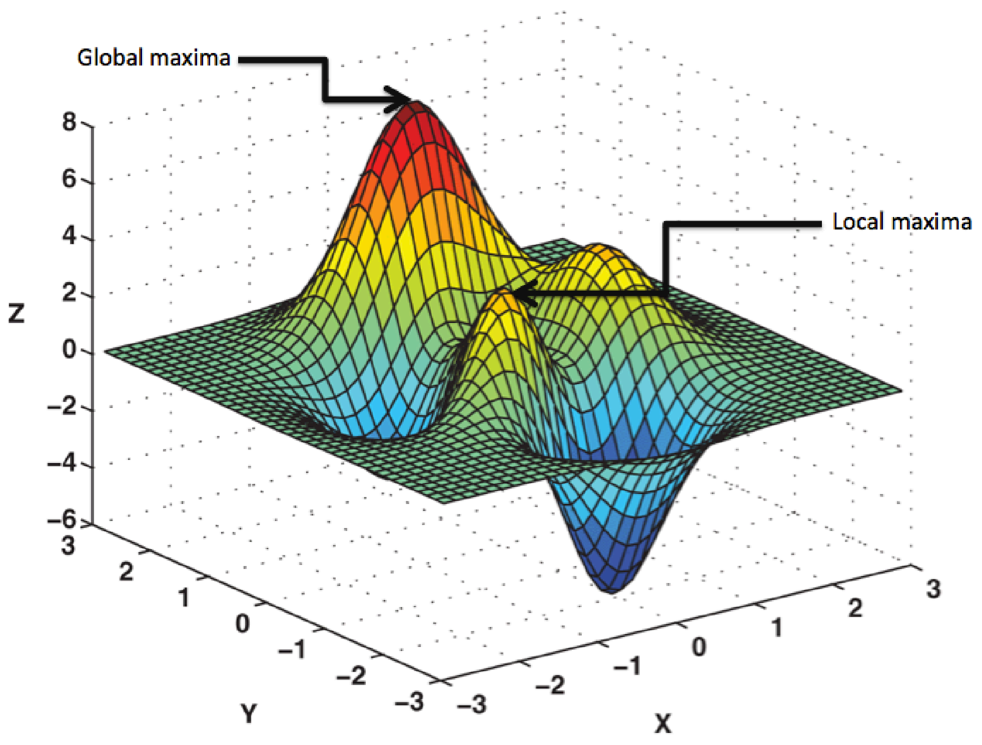
```
0.54
0.46
0.45
0.46
1.0
```

Why does a NN potentially require multiple tries before it gets it right?

Answer: the gradient isn't convex. That is, the gradient of the cost function is not a nice parabola. It has lots of peaks and valleys. Here's an example:

So a tradeoff is that linear classifiers don't have the problem of non-convex gradients, but they also aren't able to solve many problems. Neural networks are able to solve more complicated, non-linear problems, but it means that it has to work harder to traverse the gradient.

```
In [24]: model
```



nonconvex

```
Out[24]: MLPClassifier(activation='relu', alpha=1e-05, batch_size='auto', beta_1=0.9,
                beta_2=0.999, early_stopping=False, epsilon=1e-08,
                hidden_layer_sizes=(2, 2), learning_rate='constant',
                learning_rate_init=0.001, max_iter=200, momentum=0.9,
                nesterovs_momentum=True, power_t=0.5, random_state=None,
                shuffle=True, solver='sgd', tol=0.0001, validation_fraction=0.1,
                verbose=False, warm_start=False)
```

From Page 170 in the Deep Learning book (Goodfellow et al., 2017), we have the following NN that solves the xor problem if we set the weights in the logistic regression classifiers that, put together, make up a NN:

$W = \begin{pmatrix} 1 & 1 \\ 1 & 1 \end{pmatrix}$

$c = \begin{pmatrix} 0 \\ -1 \end{pmatrix}$

$w = \begin{pmatrix} 1 \\ -2 \end{pmatrix}$

Can we test that by setting the weights in some logistic regression classifiers ourselves?

```
In [155]: model_left = linear_model.LogisticRegression() # the bottom left neuron
          model_right = linear_model.LogisticRegression() # the bottom right neuron
          model_top = linear_model.LogisticRegression()   # the top neuron
```

```
In [156]: model_left.coef_ = np.array([[1,1]]) # W
          model_left.intercept_ = np.array([0]) # bias
```

```
         model_left.classes_ = np.array([0,1]) # binary classes
         model_right.coef_ = np.array([[1,1]])  # W
         model_right.intercept_ = np.array([-1]) # bias
         model_right.classes_ = np.array([0,1]) # binary classes
         model_top.coef_ = np.array([[1,-2]]) # W
         model_top.intercept_ = np.array([0])  # bias
         model_top.classes_ = np.array([0,1]) # binary classes
```

```
In [157]: lefts = model_left.predict(Xtest)
          rights = model_right.predict(Xtest)
          accuracy_score(model_top.predict(list(zip(lefts, rights))), ytest)
```

```
Out[157]: 1.0
```

1.2.3 Now let's try to use the logistic function directly without scikit

- (the logistic function is a kind of sigmoid function, meaning it's s-shaped)

```
In [158]: def sigmoid(x):
              return 1/(1 + np.exp(-x))
```

```
In [159]: lefts = sigmoid(np.array([1,1]).dot(Xtest.T) + np.array([0]))
          lefts = 1. * (lefts > 0.5)
          rights = sigmoid(np.array([1,1]).dot(Xtest.T) + np.array([-1]))
          rights = 1. * (rights > 0.5)
          top = sigmoid(np.squeeze(np.array([1,-2]).dot(np.array(list(zip(lefts,rights))).T) + n
          top = 1. * (top > 0.5)

          accuracy_score(top, ytest)
```

```
Out[159]: 1.0
```

So basically, a neural network is a bunch of linear classifiers put together.

1.2.4 Train a simple NN for XOR

- See post

Instead of giving the weights to a simple neural network, let's see how a neural network learns on its own. As before, it will need some kind of model function (in our case, sigmoid), a cost function, and descend the gradient.

```
In [160]: #  XOR.py-A very simple neural network to do exclusive or.
          import numpy as np

          epochs = 60000         # Number of iterations
          inputLayerSize, hiddenLayerSize, outputLayerSize = 2, 2, 1 # 3 neurons

          X = np.array([[0,0], [0,1], [1,0], [1,1]])
          Y = np.array([ [0],   [1],   [1],   [0]])
```

```
        #print(X.shape, Xtrain.shape, ytrain.shape, Y.shape)
        #X=Xtrain
        #Y=ytrain.reshape(ytrain.shape[0],1)

        def sigmoid (x): return 1/(1 + np.exp(-x))      # activation function
        def sigmoid_(x): return x * (1 - x)             # derivative of sigmoid
                                                        # weights on layer inputs
        Wh = np.random.uniform(size=(inputLayerSize, hiddenLayerSize))
        #Wh = np.array([[1,1],[1,1]], dtype=np.float64)
        Wz = np.random.uniform(size=(hiddenLayerSize,outputLayerSize))
        for i in range(epochs):
            # forward propogation
            H = sigmoid(np.dot(X, Wh))                  # hidden layer results
            Z = sigmoid(np.dot(H, Wz))                  # output layer results
            # check for error (cross-entropy)
            E = Y - Z                                   # how much we missed (error) # cost fu
            # backpropogation
            dZ = E * sigmoid_(Z)                        # delta Z
            dH = dZ.dot(Wz.T) * sigmoid_(H)             # delta H
            # update weights
            Wz +=  H.T.dot(dZ)
            Wh +=  X.T.dot(dH)
```

```
In [161]: Z = 1. * (Z > 0.5)
          accuracy_score(Z,Y)
```

```
Out[161]: 1.0
```

1.2.5 The feed-forward part that does the prediction

```
In [162]: def predict(Wh, Wz, X):
              H = sigmoid(np.dot(X, Wh)) # hidden layer
              Z = sigmoid(np.dot(H, Wz)) # top layer
              Z = 1. * (Z > 0.5)
              return Z

          accuracy_score(predict(Wh,Wz,X),Y)
```

```
Out[162]: 1.0
```

```
In [163]: Wh
```

```
Out[163]: array([[0.95607276, 8.44035149],
                 [0.95607267, 8.44025075]])
```

```
In [164]: Wz
```

```
Out[164]: array([[-46.61591534],
                 [ 37.29970264]])
```

1.2.6 Conclusion

NNs are classifiers that can learn a functional mapping f from some input data x to some output a, i.e., $a = f(x)$. They work similarly to other classifiers, except that they can learn functional mappings with data that is non-linear.

```
In [ ]:
```