BITS F464: Machine Learning

31 Neural Network

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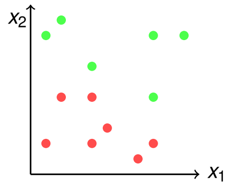
Linear Classification

Consider Following data

x_1	x_2	y
1	9	green
10	9	green
4	7	green
4	5	red
5	3	red
8	9	green
4	2	red
2	5	red
7	1	red
2	10	green
8	5	green
1	2	red
8	2	red

Data is in 2D, so let us visualize

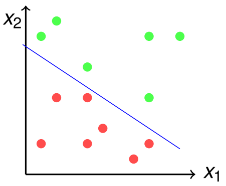


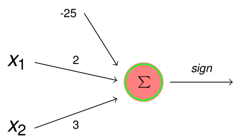
- Data looks linearly separable
- What is the decision boundary?

Many Possibilities, such as
if ($2x_1 + 3x_2 - 25 > 0$) it is green otherwise red

What about this arrangement?

With chosen *decision boundary* $2x_1 + 3x_2 - 25 = 0$





- This illustration is called as **perceptron**
- Provides a graphical way to represent the linear boundary
- Values 3, 2, -25 are its parameters or weights

Given a data
"How to find appropriate parameters?" is an important issue

Perceptron Training Rule

Different algorithms may converge to different acceptable hypotheses

Algorithm 1: Perceptron training rule
1. Begin with random weights w
2. **repeat**
3. **for** *each misclassified example* **do**
4. $w_i = w_i + \eta(t - o)x_i$
5. **until** *all training examples are correctly classified*;
6. **return** w

- **Why would this strategy converge?**
  1. Weight does not change when classification is correct
  2. If perceptron outputs -1 when target is +1: weight increases ↑
  3. If perceptron outputs +1 when target is -1: weight decreases ↓

Conversion with perceptron training rule is subject to linear separability of training example and appropriate η

Example

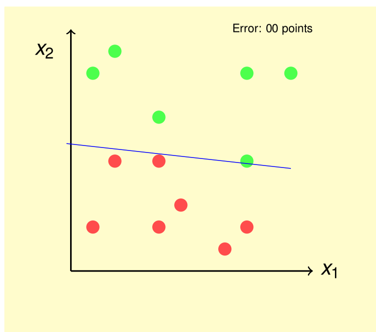
Consider the same data

x_1	x_2	y
1	9	green
10	9	green
4	7	green
4	5	red
5	3	red
8	9	green
4	2	red
2	5	red
7	1	red
2	10	green
8	5	green
1	2	red
8	2	red

$\eta = 0.01$

w0=0.500, w1=0.500, w2=0.500	err=7
w0=0.360, w1=-0.120, w2=0.100	err=6
w0=0.300, w1=-0.180, w2=0.060	err=5
w0=0.240, w1=-0.140, w2=0.140	err=4
w0=0.180, w1=-0.200, w2=0.100	err=5
w0=0.120, w1=-0.160, w2=0.180	err=4
w0=0.080, w1=-0.060, w2=0.180	err=5
w0=0.020, w1=-0.120, w2=0.140	err=4
w0=-0.040, w1=-0.180, w2=0.100	err=5
w0=-0.100, w1=-0.140, w2=0.180	err=4
w0=-0.140, w1=-0.040, w2=0.180	err=5
w0=-0.200, w1=-0.100, w2=0.140	err=3
w0=-0.260, w1=-0.160, w2=0.100	err=4
w0=-0.320, w1=-0.120, w2=0.180	err=3
w0=-0.360, w1=-0.020, w2=0.180	err=3
w0=-0.420, w1=-0.080, w2=0.140	err=2
w0=-0.420, w1=-0.080, w2=0.240	err=2
Fourteen more iterations	
w0=-0.900, w1=-0.020, w2=0.180	err=1
w0=-0.900, w1=-0.020, w2=0.240	err=2
w0=-0.920, w1=0.020, w2=0.220	err=2
w0=-0.960, w1=-0.020, w2=0.220	err=3
w0=-0.980, w1=0.020, w2=0.200	err=2
w0=-1.000, w1=0.060, w2=0.180	err=2
w0=-1.040, w1=0.020, w2=0.180	err=0

Visual Interpretation

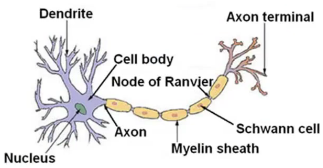


- Conversion is not gradual. (Error is NOT reducing monotonically)
- It is difficult to decide when to stop if data is not linearly separable

Neural Network (NN)

NN is biologically motivated learning model that mimic human brain

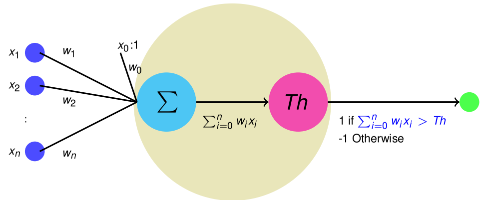
- Started by *W. McCulloch* study on working of neurons in 1943
- MADALINE (1959), an adaptive filter that eliminates echoes on phone lines was the first neural network
- Popularity of Neural Network diminished in 90's but, due to advances in **processing power** and availability of **large data** it again became state-of-the-art



- Cell, Axon, Synopses, Molicules, and Dendrites
- Humans have 10^{11} neurons, each connected to 10^4 others, switches in 10^{-3} sec

A Single Perceptron

Perceptron representation

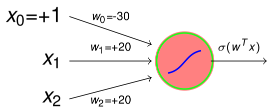


- A single perceptron can represent many boolean functions
- Any *m*-of-*n* function (at least *m* of the *n* inputs must be true) can be represented by perceptron. OR (*m*=1) and AND (*m*=*n*)

Two layer NN can represent any boolean function (Consider SOP)

An Example

Consider a perceptron with output 0/1 as below

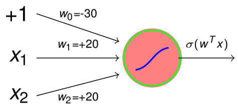


x_1	x_2	Output
0	0	0
0	1	0
1	0	0
1	1	1

This perceptron computes logical AND

- w_0=-10 gives logical OR
- w_0=10, w_1=-20 with single input gives logical NOT
- XOR is not possible

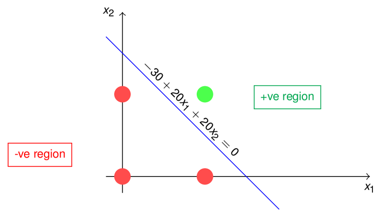
Essentially it Represents A Decision Boundary



Provides positive classification if

$$-30 + 20x_1 + 20x_2 \geq 0$$

Represents a linear decision boundary

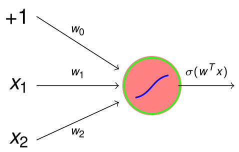


An Example

Design a **perceptron** for

x_1	x_2	Classification
0	0	0
0	1	0
1	0	1
1	1	0

Let us assume following



We have following four equations

$$w_0 + w_1 \times (0) + w_2 \times (0) < 0 \quad (1)$$
$$w_0 + w_1 \times (0) + w_2 \times (1) < 0 \quad (2)$$
$$w_0 + w_1 \times (1) + w_2 \times (0) \geq 0 \quad (3)$$
$$w_0 + w_1 \times (1) + w_2 \times (1) < 0 \quad (4)$$

By (1) $w_0 < 0$ so let $w_0 = -1$
By (2) $w_0+w_2<0$ so let $w_2 = -1$
By (3) $w_0+w_1 \geq 0$ so let $w_1 = 1.5$
By (4) $w_0+w_1+w_2<0$ that is valid

So $(w_0, w_1, w_2) = (-1, -1, 1.5)$

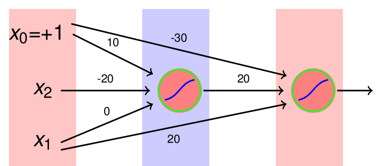
Other possibilities are also there

An Example

Design a **neural network** for

x_1	x_2	Classification
0	0	0
0	1	0
1	0	1
1	1	0

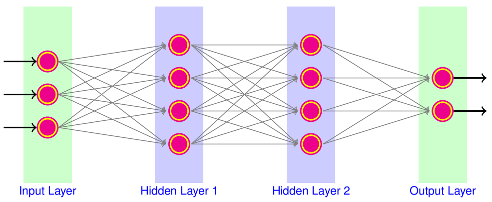
x_1	x_2	$\bar{x}_2$	$(x_1)AND(\bar{x}_2)$
0	0	1	0
0	1	0	0
1	0	1	1
1	1	0	0



This arrangement is mostly avoided, as training is very challenging

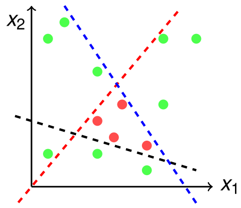
Neural Network

When neurons are interconnected in layers



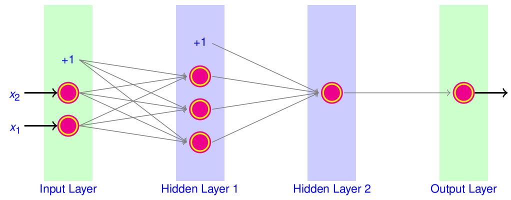
- Number of layers may differ
- Nodes in each intermediate layers may also differ
- Multiple output neurons are used for different class
- **Two levels deep** NN can represent any boolean function

More Example: Design NN for the following data



Whether it is green?

Red-line	Blue-line	Black-line	Color
0	0	0	1
0	0	1	0
0	1	0	1
0	1	1	1
1	0	0	1
1	0	1	1
1	1	0	1
1	1	1	1



Note: Weights and activation in subsequent layers add power to the model in terms of non linearity.

Neural Network Applications

NN is appropriate for problems with the following characteristics:

- Instances are provided by many attribute-value pairs (more data)
- The target function output may be discrete-valued, real-valued, or a vector of several real or discrete valued attributes
- The training examples may contain errors
- Long training times are acceptable
- Fast evaluation of the target function may be required
- The ability of humans to understand the learned target function is not important

Perceptron Training (delta rule)

When data is not linearly-separable, error fluctuates with parameter update so, it becomes difficult to decide when to stop

- Delta rule converges to a best-fit approximation of the target
- Uses gradient descent
- Consider unthresholded perceptron, $o(\vec{x}) = \vec{w}.\vec{x}$
- Training error is defined as

$$E(\vec{w}) = \frac{1}{2}\sum_{d \in D}(t_d - o_d)^2$$

- Gradient would specify direction of steepest increase $\nabla E(\vec{w}) = \left[\frac{\partial E}{\partial w_0}, \frac{\partial E}{\partial w_1}, \ldots, \frac{\partial E}{\partial w_n}\right]$
- Weights can be learned as $w_i = w_i - \eta\frac{\partial E}{\partial w_i}$
- It can be seen that $\frac{\partial E}{\partial w_i} = \sum_{d \in D}(t_d - o_d)(-x_{id})$

Perceptron Training (delta rule)

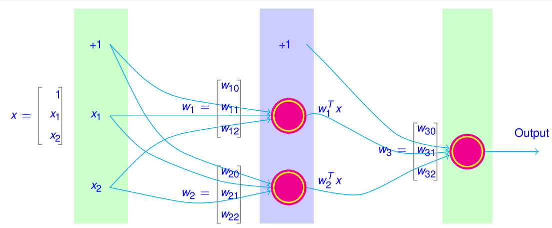
Algorithm 2: Gradient Descent (D, η)

```
Initialize w_i with random weights
repeat
    For each w_i, initialize Δw_i = 0
    for each training example d ∈ D do
        Compute output o using model for d whose target is t
        For each w_i, update Δw_i = Δw_i + η(t−o)x_i
    For each w_i, set w_i = w_i + Δw_i
until termination condition is met;
return w
```

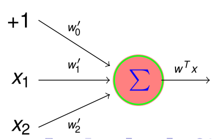
- A date item $d \in D$, is supposed to be multidimensional $d = (x_1, x_2, ..., x_n, t)$
- Algorithm converges toward the minimum error hypothesis.
- Linear programming can also be an approach

Linear Activation is Not Much Interesting

NN with perceptrons have limited capability, even with many layers



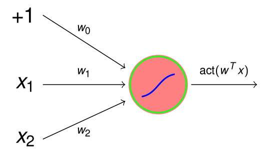
$$\begin{aligned}
Output &= w_{30} \times 1 + w_{31} \times (w_1^T x) + w_{32} \times (w_2^T x) \\
&= w_{30} \times 1 + w_{31} \times [w_{10} \times 1 + w_{11} \times x_1 + w_{12} \times x_2] \\
&\quad + w_{32} \times [w_{20} \times 1 + w_{21} \times x_1 + w_{22} \times x_2] \\
&= (w_{30} + w_{31}w_{10} + w_{32}w_{20}) + (w_{31}w_{11} + w_{32}w_{21}) \times x_1 \\
&\quad + (w_{31}w_{12} + w_{32}w_{22}) \times x_2 \\
&= w_0' + w_1' \times x_1 + w_2' \times x_2
\end{aligned}$$

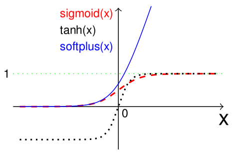


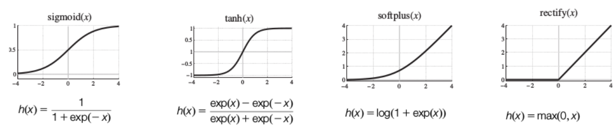
Expression of single perceptron

Neuron

Neuron uses nonlinear activation functions (*sigmoid*, *tanh*, *ReLU*, *softplus etc.*) at the place of thresholding







Multilayer Networks and Backpropagation

- Single perceptron can only express linear decision surface
- We need units whose output is a nonlinear function of its inputs AND is also differentiable (Use Neuron not ~~Perceptron~~)

$$o(\vec{x}) = \sigma(\vec{w}.\vec{x})$$

where $\sigma(y) = \frac{1}{1+e^{-y}}$

- Backpropagation algorithm learns the weights for a fixed set of units and interconnections
- It employs gradient descent to minimize the error between the network output values and the target values for these outputs
- Let Error function is redefined as

$$E(\vec{w}) = \frac{1}{2}\sum_{d\in D}\sum_{k\in outputs}(t_{kd} - o_{kd})^2$$

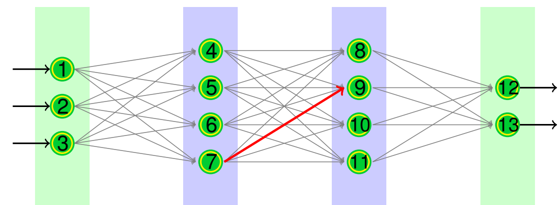
Backpropagation (for 2 layers)

Algorithm 3: Backpropagation(D, η, n_{in}, n_{out}, n_{hidden})

```
Create the feedforward network with n_in, n_out, n_hidden layers
Randomly initialize weights to small values ∈ [−0.05, +0.05]
repeat
    for each <x⃗, t⃗> ∈ D do
        o_u = get output from network ∀ unit u
        δ_k = o_k(1 − o_k)(t_k − o_k) for all output unit k
        δ_h = o_h(1 − o_h) Σ_{k∈outputs}(w_kh δ_k) for all hidden unit h
        w_ji = w_ji + △w_ji      where △w_ji = η δ_j x_ji
until converge;
```

- Recall error function is $E(\vec{w}) = \frac{1}{2}\sum_{d\in D}\sum_{k\in outputs}(t_{kd} - o_{kd})^2$
- For a single training example $E_d(\vec{w}) = \frac{1}{2}\sum_{k\in outputs}(t_k - o_k)^2$
- Weight w_{ji} is updated by adding $\triangle w_{ji} = -\eta\frac{\partial E_d}{\partial w_{ji}}$

Conventions Over The Network



x_{ji}	ith input to unit j (x_{94} is highlighted)
w_{ji}	weight associated with ith input to unit j
net_j	be $\sum_i w_{ji}x_{ji}$ the weighted sum of input for unit j
o_j	output computed by unit j. Consider it as $\sigma(net_j)$
t_j	target output for unit j
outputs	set of units in final layer ($\{12, 13\}$ in our case)
Downstream(j)	units whose immediate input is the output of unit j

We are interested in $\frac{\partial E_d}{\partial w_{ji}}$ it is $\frac{\partial E_d}{\partial net_j} \times \frac{\partial net_j}{\partial w_{ji}}$ and therefore, $\frac{\partial E_d}{\partial net_j} \times x_{ji}$

Value of $\frac{\partial E_d}{\partial net_j}$ for output units

- $\frac{\partial E_d}{\partial net_j} = \frac{\partial E_d}{\partial o_j} \times \frac{\partial o_j}{\partial net_j}$
- $\frac{\partial E_d}{\partial o_j} = \frac{\partial}{\partial o_j}\frac{1}{2}\sum_{k\in outputs}(t_k - o_k)^2 = \frac{\partial}{\partial o_j}\frac{1}{2}(t_j - o_j)^2 = -(t_j - o_j)$
- Note that $o_j = \sigma(net_j)$ therefore $\frac{\partial o_j}{\partial net_j}$ is derivative of sigmoid

$$\begin{aligned}\frac{d}{dx}\sigma(x) &= \frac{d}{dx}\frac{1}{1+e^{-x}} = (-1)(1+e^{-x})^{-2}\frac{d}{dx}(1+e^{-x}) \\ &= (-1)(1+e^{-x})^{-2}(0-e^{-x}) \\ &= \frac{1}{1+e^{-x}} \times \frac{e^{-x}+1-1}{1+e^{-x}} = \sigma(x)(1-\sigma(x))\end{aligned}$$

- As a result $\frac{\partial o_j}{\partial net_j} = \frac{\partial\sigma(net_j)}{\partial net_j} = \sigma(net_j)(1-\sigma(net_j)) = o_j(1-o_j)$
- $\frac{\partial E_d}{\partial net_j} = -(t_j - o_j)o_j(1-o_j)$
- Term $(t_j - o_j)o_j(1-o_j)$ is treated as δ_j

Therefore, $\triangle w_{ji} = -\eta\frac{\partial E_d}{\partial net_j} \times x_{ji} = \boxed{\eta(t_j - o_j)o_j(1-o_j)x_{ji}}$

Value of $\frac{\partial E_d}{\partial net_j}$ for hidden units

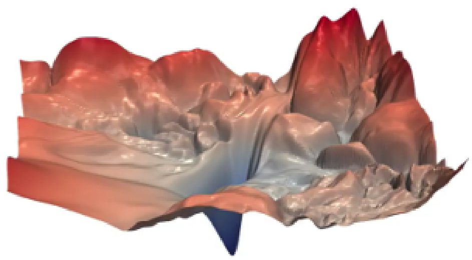
$$\begin{aligned}\frac{\partial E_d}{\partial net_j} &= \sum_{k\in Downstream(j)}\frac{\partial E_d}{\partial net_k} \times \frac{\partial net_k}{\partial net_j} \\ &= \sum_{k\in Downstream(j)} -\delta_k \times \frac{\partial net_k}{\partial net_j} \\ &= \sum_{k\in Downstream(j)} -\delta_k \times \frac{\partial net_k}{\partial o_j} \times \frac{\partial o_j}{\partial net_j} \\ &= \sum_{k\in Downstream(j)} -\delta_k \times w_{kj} \times o_j(1-o_j)\end{aligned}$$

- δ_j being $-\frac{\partial E_d}{\partial net_j} = o_j(1-o_j)\sum_{k\in Downstream(j)}\delta_k \times w_{kj}$

Therefore, $\triangle w_{ji} = \eta\delta_j x_{ji} = \boxed{\eta(o_j(1-o_j)\sum_{k\in Downstream(j)}\delta_k \times w_{kj})x_{ji}}$

Note: $net_k = w_{k1}x_{k1} + w_{k2}x_{k2} + \ldots + w_{kj}x_{kj} + \ldots$; as o_j is input to kth unit so $o_j = x_{kj}$; so $\frac{\partial net_k}{\partial o_j} = w_{kj}$

Loss Landscape [1]



Backpropagation over multilayer networks converge to a local minimum, NOT necessarily to the global minima

[1] Visualizing the Loss Landscape of Neural Nets, Hao Li, Zheng Xu, Gavin Taylor, Christoph Studer, Tom Goldstein, 2018

Backpropagation

- **Adding Momentum:** weight update during n^{th} iteration depend partially on the update that occurred during the $(n-1)^{th}$ iteration

$$\triangle\, w_{ji}(n) = \eta \delta_j x_{ji} + \alpha \triangle\, w_{ji}(n-1)$$

- **Learning in arbitrary acyclic network:** for feed-forward networks of arbitrary depth, δ_r value for a unit in hidden layer is determined as

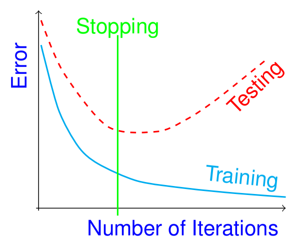
$$\delta_r = o_r(1 - o_r) \sum_{s \in Downstream(r)} w_{sr} \times \delta_s$$

Backpropagation

- Result of Backpropagation over multilayer networks is only guaranteed to converge toward some local minimum and not necessarily to the global minimum error
- No methods are known to predict with certainty when local minima will cause difficulties
- Suggested to use momentum, true gradient descent or multiple networks (initialized with different random weights)
- Any boolean function can precisely be represented by some network having only **two** layers of units (Cybenko 1989; Hornik et al. 1989)
- Every bounded continuous function can be approximated with arbitrarily small error (under a finite norm) by a network with two layers of units
- Any function can be approximated to arbitrary accuracy by a network with three layers of units (Cybenko 1988)

Generalization, Overfitting, and Stopping Criterion

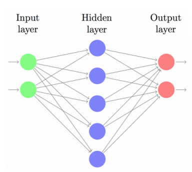
Continue training until the error on the training examples falls below some predetermined threshold could be a poor strategy

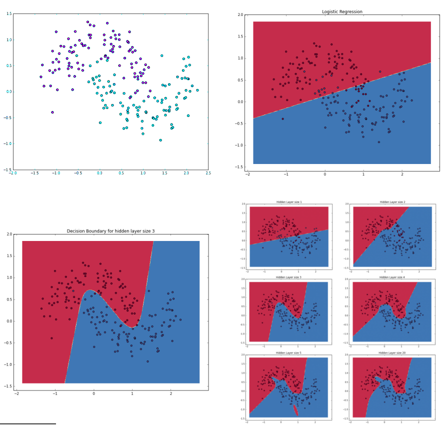


- Weight decay or use of validation set (k-fold ?) is suggested
- Input or output encoding can be used

Coding Example [2]

Consider two class data
Logistic Regression
Neural Network
Decision Boundary
Bigger hidden layer





[2] https://github.com/dennybritz/nn-from-scratch/blob/master/nn-from-scratch.ipynb

An Example Code [1/4] [3]

```
import matplotlib.pyplot as plt
import numpy as np
import sklearn
import sklearn.datasets
import sklearn.linear_model
import matplotlib

matplotlib.rcParams['figure.figsize'] = (10.0, 8.0)
np.random.seed(0)
X, y = sklearn.datasets.make_moons(200, noise=0.20)
plt.scatter(X[:,0], X[:,1], s=40, c=y, cmap=plt.cm.Spectral)

def plot_decision_boundary(pred_func):
    x_min, x_max = X[:, 0].min() - .5, X[:, 0].max() + .5
    y_min, y_max = X[:, 1].min() - .5, X[:, 1].max() + .5
    h = 0.01
    xx, yy = np.meshgrid(np.arange(x_min, x_max, h), np.arange(y_min, y_max, h))
    Z = pred_func(np.c_[xx.ravel(), yy.ravel()])
    Z = Z.reshape(xx.shape)
    plt.contourf(xx, yy, Z, cmap=plt.cm.Spectral)
    plt.scatter(X[:, 0], X[:, 1], c=y, cmap=plt.cm.Spectral)

plot_decision_boundary(lambda x: clf.predict(x))
plt.title("Logistic Regression")
plt.show()
```

[3] https://github.com/dennybritz/nn-from-scratch/blob/master/nn-from-scratch.ipynb

An Example Code [2/4] [4]

```
#### Implementing NN ####
num_examples = len(X) # training set size
nn_input_dim = 2 # input layer dimensionality
nn_output_dim = 2 # output layer dimensionality

epsilon = 0.01 # learning rate for gradient descent
reg_lambda = 0.01 # regularization strength

def calculate_loss(model):
    W1, b1, W2, b2 = model['W1'], model['b1'], model['W2'], model['b2']
    z1 = X.dot(W1) + b1
    a1 = np.tanh(z1)
    z2 = a1.dot(W2) + b2
    exp_scores = np.exp(z2)
    probs = exp_scores / np.sum(exp_scores, axis=1, keepdims=True)
    corect_logprobs = -np.log(probs[range(num_examples), y])
    data_loss = np.sum(corect_logprobs)
    data_loss += reg_lambda/2 * (np.sum(np.square(W1)) + np.sum(np.square(W2)))
    return 1./num_examples * data_loss

def predict(model, x):
    W1, b1, W2, b2 = model['W1'], model['b1'], model['W2'], model['b2']
    z1 = x.dot(W1) + b1
    a1 = np.tanh(z1)
    z2 = a1.dot(W2) + b2
    exp_scores = np.exp(z2)
    probs = exp_scores / np.sum(exp_scores, axis=1, keepdims=True)
    return np.argmax(probs, axis=1)
```

[4] https://github.com/dennybritz/nn-from-scratch/blob/master/nn-from-scratch.ipynb

An Example Code [3/4] [5]

```
def build_model(nn_hdim, num_passes=20000, print_loss=False):
    np.random.seed(0)
    W1 = np.random.randn(nn_input_dim, nn_hdim) / np.sqrt(nn_input_dim)
    b1 = np.zeros((1, nn_hdim))
    W2 = np.random.randn(nn_hdim, nn_output_dim) / np.sqrt(nn_hdim)
    b2 = np.zeros((1, nn_output_dim))
    model = {}
    for i in range(0, num_passes):
        z1 = X.dot(W1) + b1
        a1 = np.tanh(z1)
        z2 = a1.dot(W2) + b2
        exp_scores = np.exp(z2)
        probs = exp_scores / np.sum(exp_scores, axis=1, keepdims=True)
        delta3 = probs
        delta3[range(num_examples), y] -= 1
        dW2 = (a1.T).dot(delta3)
        db2 = np.sum(delta3, axis=0, keepdims=True)
        delta2 = delta3.dot(W2.T) * (1 - np.power(a1, 2))
        dW1 = np.dot(X.T, delta2)
        db1 = np.sum(delta2, axis=0)
        dW2 += reg_lambda * W2
        dW1 += reg_lambda * W1
        W1 += -epsilon * dW1
        b1 += -epsilon * db1
        W2 += -epsilon * dW2
        b2 += -epsilon * db2
        model = { 'W1': W1, 'b1': b1, 'W2': W2, 'b2': b2}
    return model
```

[5] https://github.com/dennybritz/nn-from-scratch/blob/master/nn-from-scratch.ipynb

An Example Code [4/4] [6]

```
# Build a model with a 3-dimensional hidden layer
model = build_model(3, print_loss=True)

# Plot the decision boundary
plot_decision_boundary(lambda x: predict(model, x))
plt.title("Decision Boundary for hidden layer size 3")

plt.show()

######### Varying the number of hidden layers ##########
plt.figure(figsize=(16, 32))
hidden_layer_dimensions = [1, 2, 3, 4, 5, 20, 50]
for i, nn_hdim in enumerate(hidden_layer_dimensions):
    plt.subplot(5, 2, i+1)
    plt.title('Hidden Layer size %d' % nn_hdim)
    model = build_model(nn_hdim)
    plot_decision_boundary(lambda x: predict(model, x))
plt.show()
```

[6] https://github.com/dennybritz/nn-from-scratch/blob/master/nn-from-scratch.ipynb

Thank You!

Thank you very much for your attention!