DL笔记：深入理解反向传播（BackPropagation）算法

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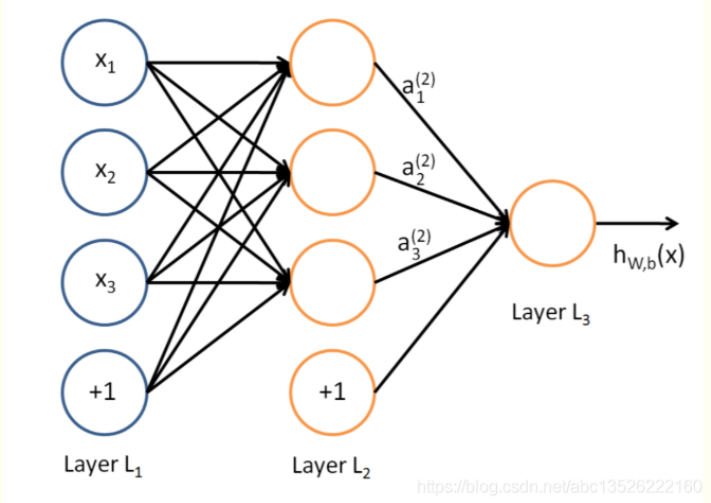
最近在学习深度学习 的东西，一开始看的吴恩达的ML教程，有些不是太理解。反向传播法其实是神经网络的基础了，但是很多人在学的时候总是会遇到一些问题，或者看到大篇的公式觉得好像很难就退缩了，其实不难，就是一个**链式求导法则**反复用。如果不想看公式，可以直接把数值带进去，实际的计算一下，体会一下这个过程之后再来推导公式，这样就会觉得很容易了。

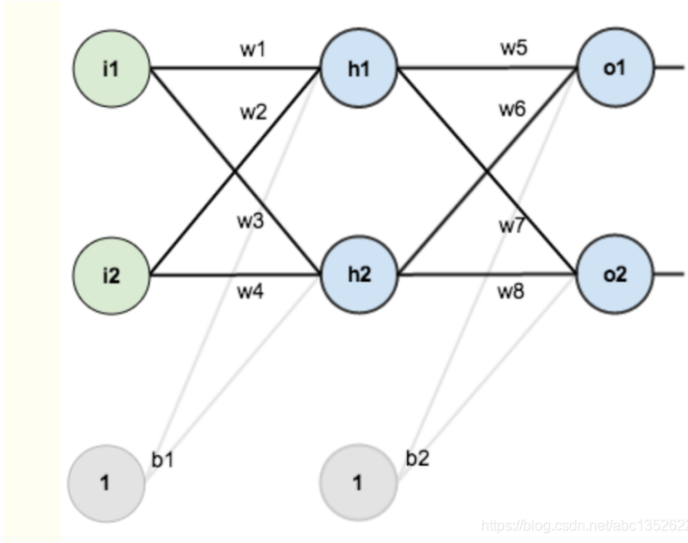
说到神经网络 ，大家看到这个图应该不陌生：



这是典型的三层神经网络的基本构成，Layer L1是输入层，Layer L2是隐含层，Layer L3是输出层，我们现在手里有一堆样本数据{x1,x2,x3,...,xn},输出也是一堆样本数据{y1,y2,y3,...,yn},现在要他们在隐含层做某种变换，让你把数据灌进去后得到你期望的输出。如果你希望你的输出和原始输入一样，那么就是最常见的**自编码模型（Auto-Encoder）**。可能有人会问，为什么要输入输出都一样呢？有什么用啊？其实应用挺广的，在图像识别，文本分类等等都会用到，我会专门再写一篇Auto-Encoder的文章来说明，包括一些变种之类的。如果你的输出和原始输入不一样，那么就是很常见的人工神经网络了，相当于让原始数据通过一个映射来得到我们想要的输出数据，也就是我们今天要讲的话题。

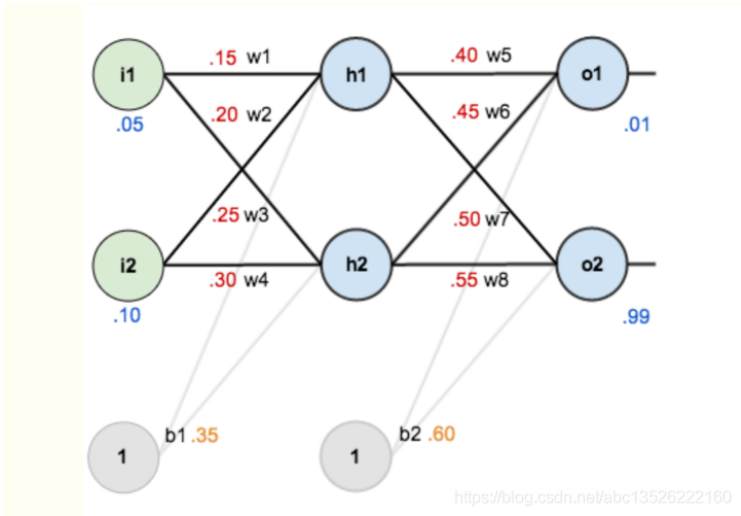
本文直接举一个例子，**带入数值演示反向传播法的过程**，公式的推导等到下次写Auto-Encoder的时候再写，其实也很简单，感兴趣的同学可以自己推导下试试：）（注：本文假设你已经懂得基本的神经网络构成，如果完全不懂，可以参考Poll写的笔记：[Mechine Learning & Algorithm] 神经网络基础）

假设，你有这样一个网络层：



第一层是输入层，包含两个神经元i1，i2，和偏置单元b1；第二层是隐含层，包含两个神经元h1,h2和偏置单元b2，第三层是输出o1,o2，每条线上标的wi是层与层之间连接的权重，激活函数我们默认为sigmoid函数。

现在对他们赋上初值，如下图：



其中，输入数据 i1=0.05，i2=0.10;

输出数据 o1=0.01,o2=0.99;

初始权重 w1=0.15,w2=0.20,w3=0.25,w4=0.30;

w5=0.40,w6=0.45,w7=0.50,w8=0.55

目标：给出输入数据i1,i2(0.05和0.10)，使输出尽可能与原始输出o1,o2(0.01和0.99)接近。

Step 1 前向传播

1.输入层---->隐含层：

计算神经元h1的输入加权和：

$$net_{h1} = w_1 * i_1 + w_2 * i_2 + b_1 * 1$$

$$net_{h1} = 0.15 * 0.05 + 0.2 * 0.1 + 0.35 * 1 = 0.3775$$

神经元h1的输出o1:(此处用到激活函数为sigmoid函数)：

$$out_{h1} = \frac{1}{1+e^{-net_{h1}}} = \frac{1}{1+e^{-0.3775}} = 0.593269992$$

同理，可计算出神经元h2的输出o2：

$$out_{h2} = 0.596884378$$

2.隐含层---->输出层：

计算输出层神经元o1和o2的值：

$$net_{o1} = w_5 * out_{h1} + w_6 * out_{h2} + b_2 * 1$$

$$net_{o1} = 0.4 * 0.593269992 + 0.45 * 0.596884378 + 0.6 * 1 = 1$$

$$out_{o1} = \frac{1}{1+e^{-net_{o1}}} = \frac{1}{1+e^{-1.105905967}} = 0.75136507$$

$$out_{o2} = 0.772928465$$

这样前向传播的过程就结束了，**我们得到输出值为[0.75136079 , 0.772928465]**，与**实际值[0.01 , 0.99]相差还很远**，现在我们对误差进行反向传播 ，更新权值，重新计算输出。

Step 2 反向传播

1.计算总误差

总误差：(square error)

$$E_{total} = \sum \frac{1}{2}(target - output)^2$$

但是有两个输出，所以分别计算o1和o2的误差，总误差为两者之和：

$$E_{o1} = \frac{1}{2}(target_{o1} - out_{o1})^2 = \frac{1}{2}(0.01 - 0.75136507)^2 = 0.274811083$$

$$E_{o2} = 0.023560026$$

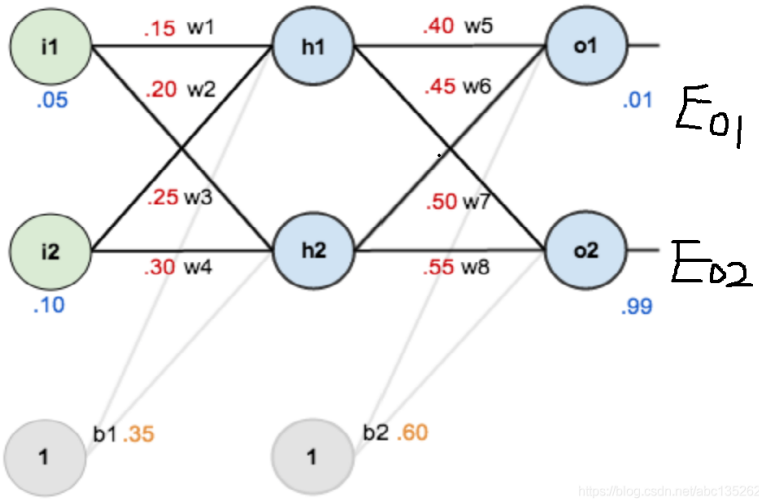
$$E_{total} = E_{o1} + E_{o2} = 0.274811083 + 0.023560026 = 0.298371109$$

2.隐含层---->输出层的权值更新：

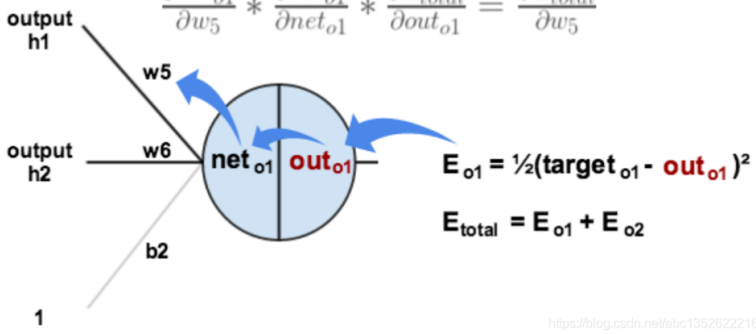
以权重参数w5为例，如果我们想知道w5对整体误差产生了多少影响，可以**用整体误差对w5求偏导求出**：**（链式求导法则）**

$$\frac{\partial E_{total}}{\partial w_5} = \frac{\partial E_{total}}{\partial out_{o1}} * \frac{\partial out_{o1}}{\partial net_{o1}} * \frac{\partial net_{o1}}{\partial w_5}$$

下面的图可以更直观的看清楚误差是怎样反向传播的：



$$\frac{\partial net_{o1}}{\partial w_5} * \frac{\partial out_{o1}}{\partial net_{o1}} * \frac{\partial E_{total}}{\partial out_{o1}} = \frac{\partial E_{total}}{\partial w_5}$$



现在我们来分别计算每个式子的值：

计算： $\frac{\partial E_{total}}{\partial out_{o1}}$ ：

$$E_{total} = \frac{1}{2}(target_{o1} - out_{o1})^2 + \frac{1}{2}(target_{o2} - out_{o2})^2$$

$$\frac{\partial E_{total}}{\partial out_{o1}} = 2 * \frac{1}{2}(target_{o1} - out_{o1})^{2-1} * -1 + 0$$

$$\frac{\partial E_{total}}{\partial out_{o1}} = -(target_{o1} - out_{o1}) = -(0.01 - 0.75136507) = 0.7413650$$

计算： $\frac{\partial out_{o1}}{\partial net_{o1}}$

$$out_{o1} = \frac{1}{1+e^{-net_{o1}}}$$

$$\frac{\partial out_{o1}}{\partial net_{o1}} = out_{o1}(1 - out_{o1}) = 0.75136507(1 - 0.75136507) = 0.186815602$$

(这一步实际上就是对sigmoid函数求导，比较简单，可以自己推导一下)

计算： $\frac{\partial net_{o1}}{\partial w_5}$ ：

$$net_{o1} = w_5 * out_{h1} + w_6 * out_{h2} + b_2 * 1$$

$$\frac{\partial net_{o1}}{\partial w_5} = 1 * out_{h1} * w_5^{(1-1)} + 0 + 0 = out_{h1} = 0.593269992$$

最后三者相乘：

$$\frac{\partial E_{total}}{\partial w_5} = \frac{\partial E_{total}}{\partial out_{o1}} * \frac{\partial out_{o1}}{\partial net_{o1}} * \frac{\partial net_{o1}}{\partial w_5}$$

$$\frac{\partial E_{total}}{\partial w_5} = 0.74136507 * 0.186815602 * 0.593269992 = 0.082167041$$

这样我们就计算出整体误差E(total)对w5的偏导值。

回过头来再看看上面的公式，我们发现：(三个偏导数求出来相乘的)

$$\frac{\partial E_{total}}{\partial w_5} = -(target_{o1} - out_{o1}) * out_{o1}(1 - out_{o1}) * out_{h1}$$

为了表达方便，用 δ_{o1} **来表示输出层的误差：**

$$\delta_{o1} = \frac{\partial E_{total}}{\partial out_{o1}} * \frac{\partial out_{o1}}{\partial net_{o1}} = \frac{\partial E_{total}}{\partial net_{o1}}$$

$$\delta_{o1} = -(target_{o1} - out_{o1}) * out_{o1}(1 - out_{o1})$$

因此，**整体误差E(total)对w5的偏导公式**可以写成：

$$\frac{\partial E_{total}}{\partial w_5} = \delta_{o1} out_{h1}$$

如果输出层误差计为负的话，也可以写成：

$$\frac{\partial E_{total}}{\partial w_5} = -\delta_{o1} out_{h1}$$

最后我们来更新w5的值：

$$w_5^+ = w_5 - \eta * \frac{\partial E_{total}}{\partial w_5} = 0.4 - 0.5 * 0.082167041 = 0.35891648$$

(这里使用的是**梯度下降法**进行更新的，其中 η 为学习率，这里我们取值为0.5)

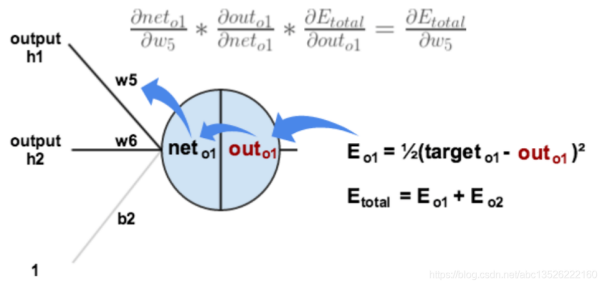
同理，可更新w6,w7,w8:

$$w_6^+ = 0.408666186$$

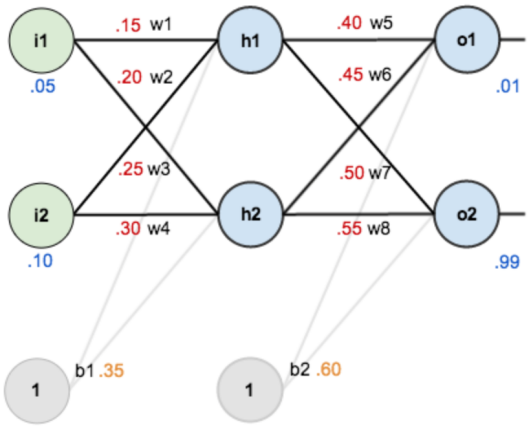
$$w_7^+ = 0.511301270$$

$$w_8^+ = 0.561370121$$

3.隐含层---->隐含层的权值更新：



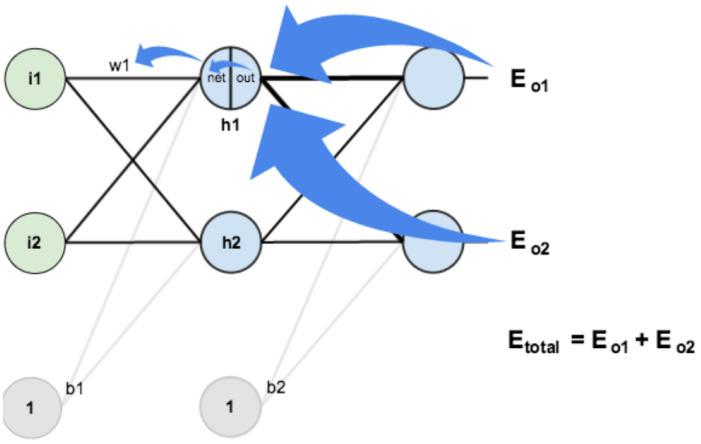
方法其实与上面说的差不多，但是有个地方需要变一下，在**上文计算总误差对w5的偏导时，是从out(o1)---->net(o1)---->w5**,但是在**隐含层之间的权值更新时，是out(h1)---->net(h1)---->w1**,**而out(h1)会接受E(o1)和E(o2)两个地方传来的误差，所以这个地方两个都要计算。**



$$\frac{\partial E_{total}}{\partial w_1} = \frac{\partial E_{total}}{\partial out_{h1}} * \frac{\partial out_{h1}}{\partial net_{h1}} * \frac{\partial net_{h1}}{\partial w_1}$$

$$\downarrow$$

$$\frac{\partial E_{total}}{\partial out_{h1}} = \frac{\partial E_{o1}}{\partial out_{h1}} + \frac{\partial E_{o2}}{\partial out_{h1}}$$



计算 $\frac{\partial E_{total}}{\partial out_{h1}}$ ：

$$\frac{\partial E_{total}}{\partial out_{h1}} = \frac{\partial E_{o1}}{\partial out_{h1}} + \frac{\partial E_{o2}}{\partial out_{h1}}$$

先计算 $\frac{\partial E_{o1}}{\partial out_{h1}}$ ：

$$\frac{\partial E_{o1}}{\partial out_{h1}} = \frac{\partial E_{o1}}{\partial net_{o1}} * \frac{\partial net_{o1}}{\partial out_{h1}}$$

$$\frac{\partial E_{o1}}{\partial net_{o1}} = \frac{\partial E_{o1}}{\partial out_{o1}} * \frac{\partial out_{o1}}{\partial net_{o1}} = 0.74136507 * 0.186815602 = 0.138498562$$

$$net_{o1} = w_5 * out_{h1} + w_6 * out_{h2} + b_2 * 1$$

$$\frac{\partial net_{o1}}{\partial out_{h1}} = w_5 = 0.40$$

$$\frac{\partial E_{o1}}{\partial out_{h1}} = \frac{\partial E_{o1}}{\partial net_{o1}} * \frac{\partial net_{o1}}{\partial out_{h1}} = 0.138498562 * 0.40 = 0.055399425$$

同理，计算出：

$$\frac{\partial E_{o2}}{\partial out_{h1}} = -0.019049119$$

两者相加得到总值：

$$\frac{\partial E_{total}}{\partial out_{h1}} = \frac{\partial E_{o1}}{\partial out_{h1}} + \frac{\partial E_{o2}}{\partial out_{h1}} = 0.055399425 + -0.019049119 = 0.036350306$$

再计算 $\frac{\partial out_{h1}}{\partial net_{h1}}$ ：

$$out_{h1} = \frac{1}{1+e^{-net_{h1}}}$$

$$\frac{\partial out_{h1}}{\partial net_{h1}} = out_{h1}(1 - out_{h1}) = 0.59326999(1 - 0.59326999) = 0.241300709$$

再计算 $\frac{\partial net_{h1}}{\partial w_1}$ ：

$$net_{h1} = w_1 * i_1 + w_2 * i_2 + b_1 * 1$$

$$\frac{\partial net_{h1}}{\partial w_1} = i_1 = 0.05$$

最后，三者相乘：

$$\frac{\partial E_{total}}{\partial w_1} = \frac{\partial E_{total}}{\partial out_{h1}} * \frac{\partial out_{h1}}{\partial net_{h1}} * \frac{\partial net_{h1}}{\partial w_1}$$

$$\frac{\partial E_{total}}{\partial w_1} = 0.036350306 * 0.241300709 * 0.05 = 0.000438568$$

为了简化公式，用sigma(h1)表示隐含层单元h1的误差：

$$\frac{\partial E_{total}}{\partial w_1} = (\sum_o \frac{\partial E_{total}}{\partial out_o} * \frac{\partial out_o}{\partial net_o} * \frac{\partial net_o}{\partial out_{h1}}) * \frac{\partial out_{h1}}{\partial net_{h1}} * \frac{\partial net_{h1}}{\partial w_1}$$

$$\frac{\partial E_{total}}{\partial w_1} = (\sum_o \delta_o * w_{ho}) * out_{h1}(1 - out_{h1}) * i_1$$

$$\frac{\partial E_{total}}{\partial w_1} = \delta_{h1} i_1$$

最后，更新w1的权值：

$$w_1^+ = w_1 - \eta * \frac{\partial E_{total}}{\partial w_1} = 0.15 - 0.5 * 0.000438568 = 0.149780716$$

同理，额可更新w2,w3,w4的权值：

$$w_2^+ = 0.19956143$$

$$w_3^+ = 0.24975114$$

$$w_4^+ = 0.29950229$$

这样误差反向传播法就完成了，最后我们再把更新的权值重新计算，不停地迭代，在这个例子中第一次迭代之后，总误差E(total)由0.298371109下降至0.291027924。迭代10000次后，总误差为0.000035085，输出为[0.015912196,0.984065734](原输入为[0.01,0.99]),证明效果还是不错的。

代码(Python):

```
#coding:utf-8
import random
import math

#
#   参数解释:
#   "pd_" : 偏导的前缀
#   "d_" : 导数的前缀
#   "w_ho" : 隐含层到输出层的权重系数索引
#   "w_ih" : 输入层到隐含层的权重系数的索引

class NeuralNetwork:
    LEARNING_RATE = 0.5

    def __init__(self, num_inputs, num_hidden, num_outputs, hidden_layer_weights = None, hidden_layer_bias = None, output_layer_
        self.num_inputs = num_inputs

        self.hidden_layer = NeuronLayer(num_hidden, hidden_layer_bias)
        self.output_layer = NeuronLayer(num_outputs, output_layer_bias)

        self.init_weights_from_inputs_to_hidden_layer_neurons(hidden_layer_weights)
        self.init_weights_from_hidden_layer_neurons_to_output_layer_neurons(output_layer_weights)

    def init_weights_from_inputs_to_hidden_layer_neurons(self, hidden_layer_weights):
        weight_num = 0
        for h in range(len(self.hidden_layer.neurons)):
            for i in range(self.num_inputs):
                if not hidden_layer_weights:
                    self.hidden_layer.neurons[h].weights.append(random.random())
```

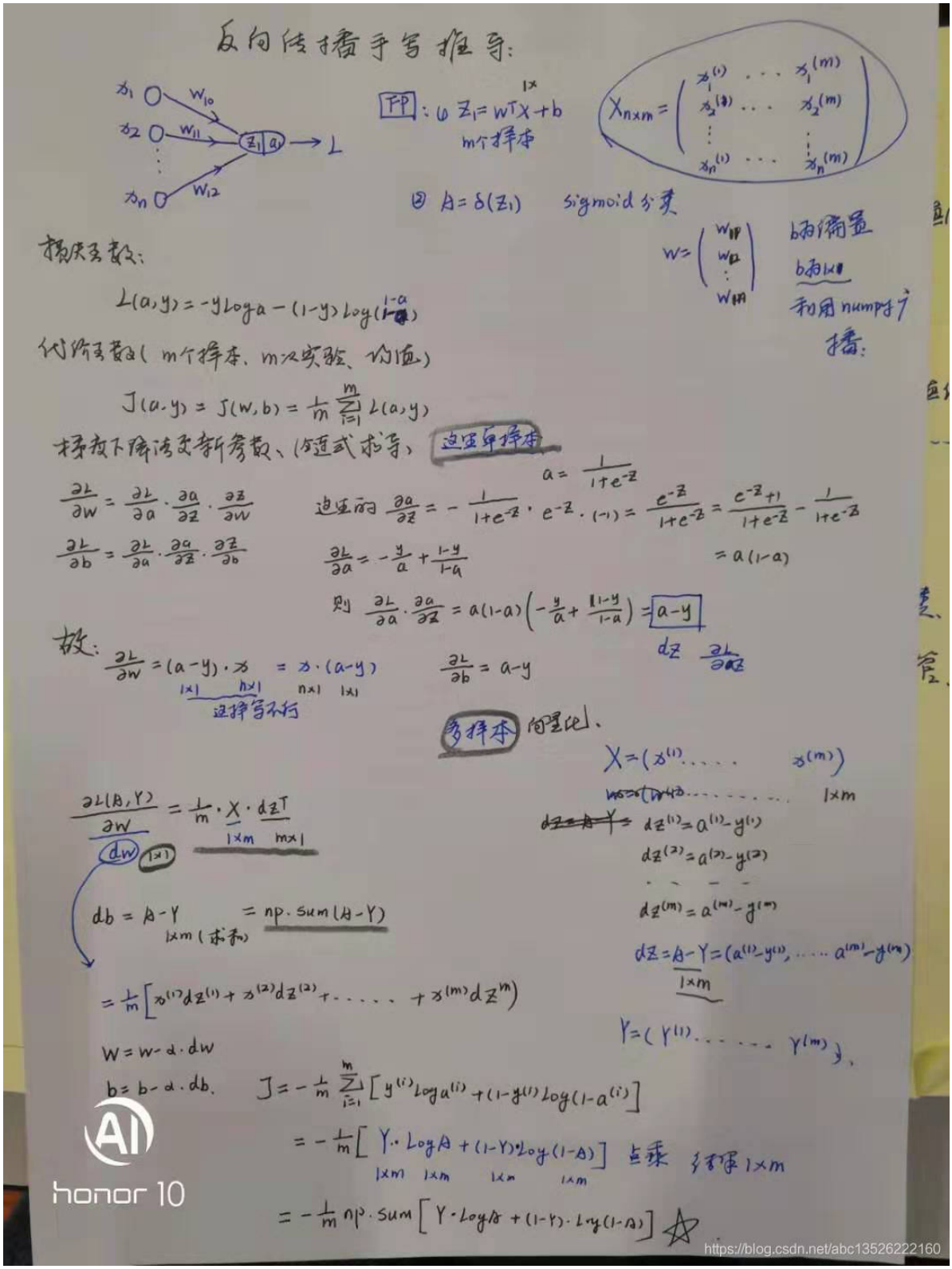
```
                else:                    self.hidden_layer.neurons[h].weights.append(hidden_layer_weights[weight_num])
                weight_num += 1

    def init_weights_from_hidden_layer_neurons_to_output_layer_neurons(self, output_layer_weights):
        weight_num = 0
        for o in range(len(self.output_layer.neurons)):
            for h in range(len(self.hidden_layer.neurons)):
                if not output_layer_weights:
                    self.output_layer.neurons[o].weights.append(random.random())
                else:
                    self.output_layer.neurons[o].weights.append(output_layer_weights[weight_num])
                weight_num += 1

    def inspect(self):
        print('------')
        print('* Inputs: {}'.format(self.num_inputs))
        print('------')
        print('Hidden Layer')
        self.hidden_layer.inspect()
        print('------')
        print('* Output Layer')
        self.output_layer.inspect()
        print('------')

    def feed_forward(self, inputs):
        hidden_layer_outputs = self.hidden_layer.feed_forward(inputs)
        return self.output_layer.feed_forward(hidden_layer_outputs)

    def train(self, training_inputs, training_outputs):
        self.feed_forward(training_inputs)

        # 1. 输出神经元的值
        pd_errors_wrt_output_neuron_total_net_input = [0] * len(self.output_layer.neurons)
        for o in range(len(self.output_layer.neurons)):

            # ∂E/∂z_j
            pd_errors_wrt_output_neuron_total_net_input[o] = self.output_layer.neurons[o].calculate_pd_error_wrt_total_net_input

        # 2. 隐含层神经元的值
        pd_errors_wrt_hidden_neuron_total_net_input = [0] * len(self.hidden_layer.neurons)
        for h in range(len(self.hidden_layer.neurons)):

            # dE/dy_j = Σ ∂E/∂z_j * ∂z/∂y_j = Σ ∂E/∂z_j * w_ij
            d_error_wrt_hidden_neuron_output = 0
            for o in range(len(self.output_layer.neurons)):
                d_error_wrt_hidden_neuron_output += pd_errors_wrt_output_neuron_total_net_input[o] * self.output_layer.neurons[o

            # ∂E/∂z_j = dE/dy_j * ∂z_j/∂
            pd_errors_wrt_hidden_neuron_total_net_input[h] = d_error_wrt_hidden_neuron_output * self.hidden_layer.neurons[h].cal

        # 3. 更新输出层权重系数
        for o in range(len(self.output_layer.neurons)):
            for w_ho in range(len(self.output_layer.neurons[o].weights)):

                # ∂E_j/∂w_ij = ∂E/∂z_j * ∂z_j/∂w_ij
                pd_error_wrt_weight = pd_errors_wrt_output_neuron_total_net_input[o] * self.output_layer.neurons[o].calculate_pd

                # Δw = α * ∂E_j/∂w_i
                self.output_layer.neurons[o].weights[w_ho] -= self.LEARNING_RATE * pd_error_wrt_weight

        # 4. 更新隐含层的权重系数
        for h in range(len(self.hidden_layer.neurons)):
            for w_ih in range(len(self.hidden_layer.neurons[h].weights)):

                # ∂E_j/∂w_i = ∂E/∂z_j * ∂z_j/∂w_i
                pd_error_wrt_weight = pd_errors_wrt_hidden_neuron_total_net_input[h] * self.hidden_layer.neurons[h].calculate_pd
```

```
                # Δw = α * ∂Eⱼ/∂wᵢ
                self.hidden_layer.neurons[h].weights[w_ih] -= self.LEARNING_RATE * pd_error_wrt_weight

    def calculate_total_error(self, training_sets):
        total_error = 0
        for t in range(len(training_sets)):
            training_inputs, training_outputs = training_sets[t]
            self.feed_forward(training_inputs)
            for o in range(len(training_outputs)):
                total_error += self.output_layer.neurons[o].calculate_error(training_outputs[o])
        return total_error

class NeuronLayer:
    def __init__(self, num_neurons, bias):

        # 同一层的神经元共享一个截距项b
        self.bias = bias if bias else random.random()

        self.neurons = []
        for i in range(num_neurons):
            self.neurons.append(Neuron(self.bias))

    def inspect(self):
        print('Neurons:', len(self.neurons))
        for n in range(len(self.neurons)):
            print(' Neuron', n)
            for w in range(len(self.neurons[n].weights)):
                print('  Weight:', self.neurons[n].weights[w])
            print('  Bias:', self.bias)

    def feed_forward(self, inputs):
        outputs = []
        for neuron in self.neurons:
            outputs.append(neuron.calculate_output(inputs))
        return outputs

    def get_outputs(self):
        outputs = []
        for neuron in self.neurons:
            outputs.append(neuron.output)
        return outputs

class Neuron:
    def __init__(self, bias):
        self.bias = bias
        self.weights = []

    def calculate_output(self, inputs):
        self.inputs = inputs
        self.output = self.squash(self.calculate_total_net_input())
        return self.output

    def calculate_total_net_input(self):
        total = 0
        for i in range(len(self.inputs)):
            total += self.inputs[i] * self.weights[i]
        return total + self.bias

    # 激活函数sigmoid
    def squash(self, total_net_input):
        return 1 / (1 + math.exp(-total_net_input))


    def calculate_pd_error_wrt_total_net_input(self, target_output):
        return self.calculate_pd_error_wrt_output(target_output) * self.calculate_pd_total_net_input_wrt_input();
```

```
    # 每一个神经元的误差是由平方差公式计算的
    def calculate_error(self, target_output):
        return 0.5 * (target_output - self.output) ** 2


    def calculate_pd_error_wrt_output(self, target_output):
        return -(target_output - self.output)


    def calculate_pd_total_net_input_wrt_input(self):
        return self.output * (1 - self.output)


    def calculate_pd_total_net_input_wrt_weight(self, index):
        return self.inputs[index]


# 文中的例子:

nn = NeuralNetwork(2, 2, 2, hidden_layer_weights=[0.15, 0.2, 0.25, 0.3], hidden_layer_bias=0.35, output_layer_weights=[0.4, 0.45
for i in range(10000):
    nn.train([0.05, 0.1], [0.01, 0.09])
    print(i, round(nn.calculate_total_error([[[0.05, 0.1], [0.01, 0.09]]]), 9))


#另外一个例子，可以把上面的例子注释掉再运行一下:

# training_sets = [
#     [[0, 0], [0]],
#     [[0, 1], [1]],
#     [[1, 0], [1]],
#     [[1, 1], [0]]
# ]

# nn = NeuralNetwork(len(training_sets[0][0]), 5, len(training_sets[0][1]))
# for i in range(10000):
#     training_inputs, training_outputs = random.choice(training_sets)
#     nn.train(training_inputs, training_outputs)
#     print(i, nn.calculate_total_error(training_sets))
```

最后推荐一个在线演示神经网络变化的网址：http://www.emergentmind.com/neural-network，可以自己填输入输出，然后观看每一次迭代权值的变化，很好玩~

特别感谢作者Charlotte77。 出处：http://www.cnblogs.com/charlotte77/



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