

Neural Network

倒数第一层Softmax函数 倒数第二层输出Logit值

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Softmax Function

2 Logit Model

Introduction



Loss Function

损失函数: 定义在single样本上, 计算单个样本误差

Cost Function

代价函数: 定义在the whole训练集上, 计算Loss function的期望

Object Function

目标函数:最优化问题(maximize/minimize)对应的函数。

Object Function

- = Empirical Risk + Structural Risk (经验风险+结构风险)
- = Cost Function + Regularization (代价函数+正则化)



目标:用 $f_1(x)$ 或 $f_2(x)$ 或 $f_3(x)$ 来拟合Price

分析:

经验风险:训练集all样本的平均Loss >

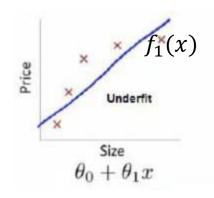
 $\min Empirical Risk = \min \frac{1}{N} (\sum_{i=1}^{N} L(y_i, f(x_i)))$

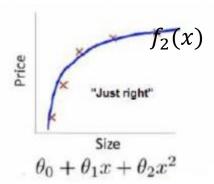
$$f_1(x) > f_2(x) > f_3(x)$$

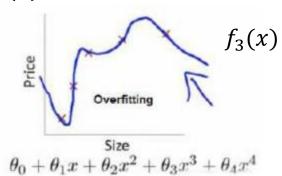
结构风险: 度量f(x)的复杂度(即正则化) \rightarrow

$$J(f) = L_1 norm \ \vec{\boxtimes} J(f) = L_2 norm$$

$$f_1(x) < f_2(x) < f_3(x)$$









1 Softmax Function

2 Logit Model

https://www.cnblogs.com/zongfa/p/8971213.html

https://www.cnblogs.com/eczhou/p/7860483.html



Softmax Function计算公式

Function: Output of Neurons \rightarrow map Probability in [0,1]

Vector: $Z = (Z_1, Z_2, ..., Z_i)$ 称 Network原始输出Z为置信度

$$Softmax(Z_i) = S_i = \frac{e^i}{\sum_i e^j} \qquad (e \approx 2.718)$$

Eg. Z = (3, 1, -3)

 $(e^{Z_1}, e^{Z_2}, e^{Z_3}) = (e^3, e^1, e^{-3}) \approx (20, 2.7, 0.05)$

 $\sum_{j} e^{j} = \sum_{j=1}^{3} e^{Z_{j}} = e^{Z_{1}} + e^{Z_{2}} + e^{Z_{3}} = 22.75$

$$(S_{1}, S_{2}, S_{3}) = \left(\frac{e^{Z_{1}}}{\sum_{j} e^{j}}, \frac{e^{Z_{2}}}{\sum_{j} e^{j}}, \frac{e^{Z_{3}}}{\sum_{j} e^{j}}\right)$$

$$= \left(\frac{e^{Z_{1}}}{e^{Z_{1}} + e^{Z_{2}} + e^{Z_{3}}}, \frac{e^{Z_{2}}}{e^{Z_{1}} + e^{Z_{2}} + e^{Z_{3}}}, \frac{e^{Z_{3}}}{e^{Z_{1}} + e^{Z_{2}} + e^{Z_{3}}}\right)$$

$$= \left(\frac{20}{22.75}, \frac{2.7}{22.75}, \frac{0.05}{22.75}\right)$$

$$\approx (0.88, 0.12, 0.00)$$

Neural Network: 最后一层选取输出预测label时,就选取概率最大的节点作为预测值输出。如果是多分类问题,需要选取n个节点输出时,就找概率最大的前n个值输出。



Softmax Function计算实例

Eg.

$$V = (3, 1, -3)$$

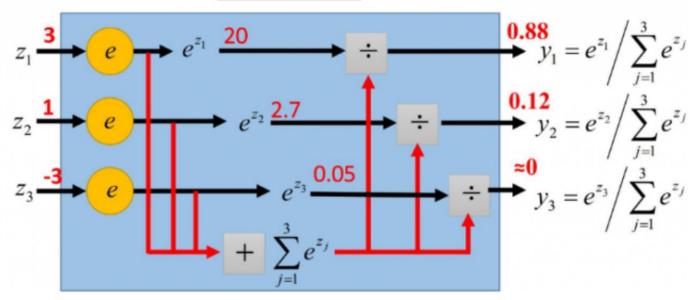
 $(S_1, S_2, S_3) \approx (0.88, 0.12, 0.00)$

Softmax layer as the output layer

Probability:

- $1 > y_i > 0$
- $\blacksquare \sum_i y_i = 1$

Softmax Layer





Softmax Function 求导

- (1) Softmax作为神经网络的last layer,输出一组概率值,而Softmax层实际上不是神经元层,它不具有网络参数。
- (2) Neural Network每一层的权重矩阵W的更新过程: 首先明确,权重更新是一个倒推链式过程! last layer → first layer,逐层用 Loss Function对各节点的权重求偏导,执行更新。
- Step 1 倒数第二层weight update 用整个模型的Loss Function对倒数第二层权重矩阵的每一个节点权重求偏导数, $\partial(Loss)$

 $w_k' = w_k - \lambda \cdot \frac{\partial(Loss)}{\partial(w_k)}$

Step 2 链式法则
$$\frac{\partial(Loss)}{\partial(w_k)} = \frac{\partial(Loss)}{\partial(y)} \cdot \frac{\partial(y)}{\partial(w_k)}$$

由倒数第二层的权重矩阵倒推更新倒数第三层的权重矩阵。

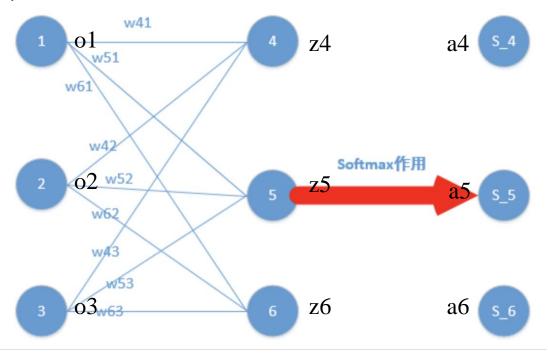
(3)为什么要用loss对每个权重矩阵求偏导数? 在用梯度下降法对Loss进行改善时,每次优化一个步长的梯度,就需要进行梯度求导。





Softmax Function 相关求导案例

Step 1 倒数第三层→倒数第二层 已知节点输出o1、o2、o3,模型参数: W₄₁, W₄₂, W₄₃, W₅₁, W₅₂, W₅₃, W₆₁, W₆₂, W₆₃ 求z4、z5、z6?



Step 2 倒数第二层 \rightarrow 倒数第一层(Softmax) $Softmax(z_4, z_5, z_6) = (a_4, a_5, a_6)$

$$z4 = w41*o1+w42*o2+w43*o3$$

$$z5 = w51*o1+w52*o2+w53*o3$$

$$z6 = w61*o1+w62*o2+w63*o3$$

$$a_4 = rac{e^{z4}}{z^{z4} + z^{z5} + z^{z6}}$$

$$a_5=rac{e^{z5}}{z^{z4}+z^{z5}+z^{z6}}$$

$$a_6=rac{e^{z6}}{z^{z4}+z^{z5}+z^{z6}}$$



Softmax Function 相关求导案例

Step 3 使用交叉熵作为Loss Function

计算预测的概率分布和真实答案的概率分布之间的距离

i: 节点标号。 y_i : 真实值。 a_i : Softmax值。

$$Softmax(z_4, z_5, z_6) = (a_4, a_5, a_6)$$

$$Loss = -\sum_{i} y_{i} lna_{i} = -(y_{4} lna_{4} + y_{5} lna_{5} + y_{6} lna_{6})$$

Step 4 二分类问题,只预测一个结果, (a_4, a_5, a_6) 中只有一个元素 a_j 真实值 y_i 为1,其余都为0

设
$$a_j = 1, j = 4,5,6$$
中的一个

则
$$Loss = -y_j lna_j = -lna_j$$

Step 5 设目标:对权重 w_{41} 求偏导数

a.损失函数求偏导数传到节点i = 4: $\frac{\partial(Loss)}{\partial(a_A)}$

b.链式法则对权重 w_{41} 求偏导数:

$$\frac{\partial(Loss)}{\partial(w_{41})} = \frac{\partial(Loss)}{\partial(a_j)} \cdot \frac{\partial(a_j)}{\partial(z_4)} \cdot \frac{\partial(z_4)}{\partial(w_{41})} = -\left(\frac{1}{a_j}\right) \cdot \frac{\partial(a_j)}{\partial(z_4)} \cdot o1$$

$$o1$$
已知,关键在求 $\frac{\partial(a_j)}{\partial(z_4)}$!





w41

Softmax Function 相关求导案例

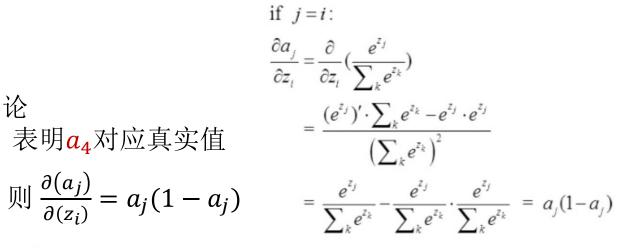
Step 6

目标: 求
$$\frac{\partial(a_j)}{\partial(z_4)}$$

解答:分情况讨论

(1) i = i = 4,表明 α_4 对应真实值

则
$$\frac{\partial(a_j)}{\partial(z_i)} = a_j(1 - a_j)$$



Step 7 权重梯度

$$\frac{\partial (Loss)}{\partial (w_{41})} = -\left(\frac{1}{a_j}\right) \cdot \frac{\partial (a_j)}{\partial (z_i)} \cdot o1$$

$$= -\left(\frac{1}{a_j}\right) \cdot \frac{\partial (a_j)}{\partial (z_4)} \cdot o1$$

$$= -\left(\frac{1}{a_j}\right) \cdot \frac{\partial (a_j)}{\partial (z_4)} \cdot o1$$

$$= -\left(\frac{1}{a_j}\right) \cdot a_j (1 - a_j) \cdot o1$$

$$= (a_j - 1) \cdot o1 = (a_4 - 1) \cdot o1$$





Softmax Function 相关求导案例

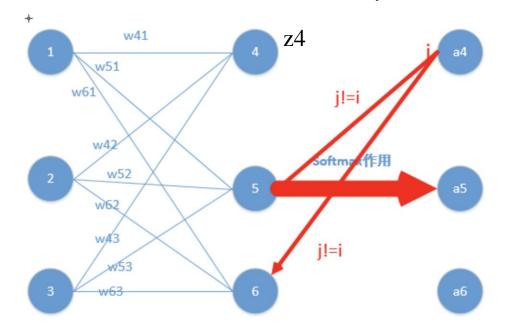
Step 6

目标: 求
$$\frac{\partial(a_j)}{\partial(z_4)}$$

解答: 分情况讨论

(2) $j \neq i = 4$,表明 α_4 不对应真实值

则
$$\frac{\partial(a_j)}{\partial(z_i)} = -a_j a_i$$



if
$$j \neq i$$
:

$$\frac{\partial a_j}{\partial z_i} = \frac{\partial}{\partial z_i} \left(\frac{e^{z_j}}{\sum_k e^{z_k}} \right)$$

$$= \frac{0 \cdot \sum_k e^{z_k} - e^{z_j} \cdot e^{z_i}}{\left(\sum_k e^{z_k} \right)^2}$$

$$= -\frac{e^{z_j}}{\sum_k e^{z_k}} \cdot \frac{e^{z_i}}{\sum_k e^{z_k}} = -a_j a_i$$

Step 7 权重梯度

$$\frac{\partial(Loss)}{\partial(w_{41})} = -\left(\frac{1}{a_j}\right) \cdot \frac{\partial(a_j)}{\partial(z_i)} \cdot o1$$

$$= -\left(\frac{1}{a_j}\right) \cdot \frac{\partial(a_j)}{\partial(z_4)} \cdot o1$$

$$= -\left(\frac{1}{a_j}\right) \cdot (-a_j a_i) \cdot o1$$

$$= -\left(\frac{1}{a_j}\right) \cdot (-a_j a_4) \cdot o1 = a_4 \cdot o_{12}$$



Softmax Function 求导计算举例

已知:某个训练样本的分类分数向量,该样本的真实分类是第二个

$$V = (z_1, z_2, z_3) = (2,3,4)$$

求偏导数?

解:

Softmax(
$$z_1, z_2, z_3$$
)
= (a_1, a_2, a_3)
= $(\frac{e^{Z_1}}{e^{Z_1} + e^{Z_2} + e^{Z_3}}, \frac{e^{Z_2}}{e^{Z_1} + e^{Z_2} + e^{Z_3}}, \frac{e^{Z_3}}{e^{Z_1} + e^{Z_2} + e^{Z_3}})$
= $(0.0903, 0.2447, 0.665)$

则偏导数可快速求得:

$$\begin{pmatrix}
\frac{\partial(Loss)}{\partial(a_1)}, \frac{\partial(Loss)}{\partial(a_2)}, \frac{\partial(Loss)}{\partial(a_3)} \\
= (a_1, a_2 - 1, a_3) \\
= (0.0903, 0.2447 - 1, 0.665) \\
= (0.0903, -0.7553, 0.665)$$



Apply Softmax Function in Neural Network

解决多分类问题方法: 设置n个(类别数目)输出节点

Neural Network Input: 样例

Neural Network output: n维数组(每一维度表示一个类别)

(1) 前向传播算法得到每个维度值

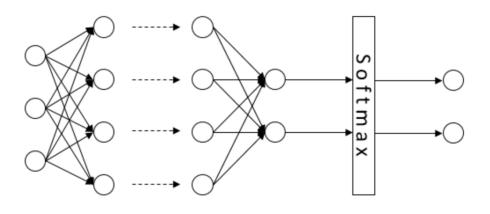
维度值含义: 样例属于该类别的概率大小。

 \sum_n 维度值=1

- (2) 概率事件:一个样例属于某一个类别,则样例的分类符合一个概率分布。
- (3) n维分类→Softmax回归→概率分布

 輸入层
 原始
 原始
 Softmax层
 最终

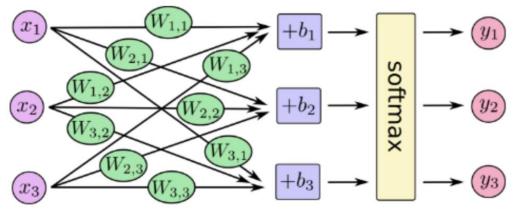
 輸出层
 輸出层





Softmax回归的图解

Step 1 Softmax在Network中的功能位置



Step 2 过程抽象成等式

Step 3 等式向量化,加速计算

$$\begin{bmatrix} y_1 \\ y_2 \\ y_3 \end{bmatrix} = \begin{array}{cccc} \text{softmax} & \begin{bmatrix} W_{1,1} & W_{1,2} & W_{1,3} \\ W_{2,1} & W_{2,2} & W_{2,3} \\ W_{3,1} & W_{3,2} & W_{3,3} \end{bmatrix} \cdot \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} + \begin{bmatrix} b_1 \\ b_2 \\ b_3 \end{bmatrix}$$



Softmax Function

2 Logit Model

https://www.jianshu.com/p/96f762d317b9

https://www.jianshu.com/p/498f7bf488a2

https://www.jianshu.com/p/d93dec4f4a46



一、线性回归Model的局限性

Requirement: 因变量是定量变量,如定距vector、定比vector;不能是定性变量,如定序vector、定类vector。

二、实际情况

Real World: 经常出现因变量是定性变量,比如分类变量。

三、一元线性回归

假设神经元数目: 1 神经元output: 0或1

神经元learning problem → Binary Logistic Regression(二值逻辑回归)

Logit Model



三、一元线性回归

一元线性回归的数学模型抽象:

Step 1 Number of data point: m

Step 2 Data point: $(x^{(1)}, y^{(1)})(x^{(2)}, y^{(2)}) \dots (x^{(m)}, y^{(m)})$ 即 $(x^{(i)}, y^{(i)})$, 整数 $i \in [1, m]$

Step 3 目标: 找出一条直线 $y = \theta x + b$,即求得一对 (θ, b) ,满足all data points到该线的距离和最小。



三、一元线性回归

一元线性回归的数学模型抽象:

Step 4 代价函数(Cost Function):

$$J(\theta,b) = \frac{1}{2} \sum_{1}^{m} (\hat{\pi}i \wedge \hat{\eta}) = \frac{1}{2} \sum_{1}^{m} (\hat{\pi}i \wedge \hat{\eta}) = \frac{1}{2} \sum_{1}^{m} ((\theta x^{(i)} + b) - y^{(i)})^{2}$$

$$= \frac{((\theta x^{(1)} + b) - y^{(1)})^{2} + ((\theta x^{(2)} + b) - y^{(2)})^{2} + \dots + ((\theta x^{(m)} + b) - y^{(m)})^{2}}{2}$$

一元线性回归→最优化问题(找到一条最优直线)

Step 5 求达到 $min J(\theta, b)$ 的 θ 和b值

方法(1):建立 $J(\theta,b)$ 关于变量 θ 和b的方程组

方法 (2): 梯度下降法求最佳 θ 和b

$$\begin{cases} \frac{\partial J(\theta, b)}{\partial \theta} = 0\\ \frac{\partial J(\theta, b)}{\partial b} = 0 \end{cases}$$



三、一元线性回归

一元线性回归的数学模型抽象:

梯度下降法求最佳θ和b

Step 1 设定初始值 θ_0 , b_0 , 学习率 α

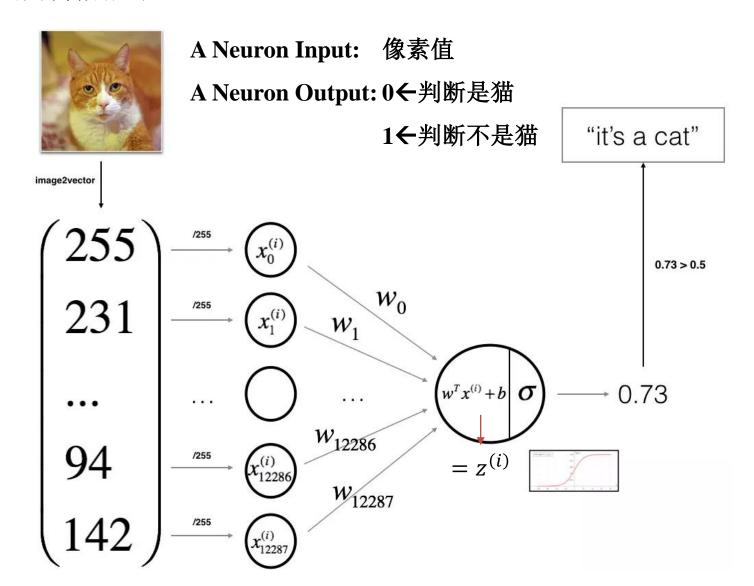
Step 2 开始递归

$$\theta_{\text{update}} = \theta - \alpha \cdot \frac{\partial J(\theta, b)}{\partial \theta}$$

$$b_{\text{update}} = b - \alpha \cdot \frac{\partial J(\theta, b)}{\partial b}$$

Step n 递归结束, return 最佳点 (θ, b)







前向传播公式: How to compute cost function

Input: $x^{(i)} = (x_0^{(i)}, x_1^{(i)}, \dots, x_{12887}^{(i)})^T$ | $\boxed{12888}$ pixels

目标: 找到训练参数 $w = (w_0, w_1, ..., w_{12887})^T$ (多维) 和b

多元线性回归→最优化问题(找到一个最优超平面)

Output:

Step 1 多元线性回归(神经网络节点的前半段计算)

$$\begin{aligned} \mathbf{z}^{(i)} &= \mathbf{w}^T \mathbf{x}^{(i)} + \mathbf{b} \\ &= \begin{bmatrix} w_0 & w_1 & \dots & w_{12887} \end{bmatrix} \begin{bmatrix} x_0^{(i)} \\ x_1^{(i)} \\ \dots \\ x_{12887}^{(i)} \end{bmatrix} + \mathbf{b} \\ &= w_0 x_0^{(i)} + w_1 x_1^{(i)} + \dots + w_{12887} x_{12887}^{(i)} + \mathbf{b} \end{aligned}$$





前向传播公式: How to compute cost function

Output:

Step 2 将
$$z^{(i)}$$
变换到(0,1)

$$\hat{y}^{(i)} = a^{(i)} = sigmoid(z^{(i)})$$

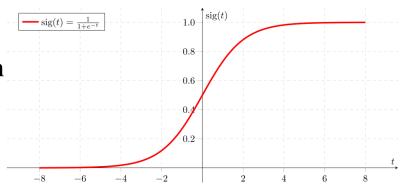
注: ŷ(cap)表示y上有一条折线,是回归估计的预测值。

$$a^{(i)} = sigmoid(z^{(i)}) = \frac{1}{1 + e^{-z^{(i)}}} = \frac{1}{1 + e^{-(w_0 x_0^{(i)} + w_1 x_1^{(i)} + \dots + w_{12887} x_{12887}^{(i)} + b)}}$$

Step 3 计算m个样本的总代价函数(即 J(w,b))

Loss函数:
$$L(a^{(i)}, y^{(i)}) = -[y^{(i)} \log a^{(i)}] - [(1 - y^{(i)}) \log(1 - a^{(i)})]$$

Cost函数:
$$J(w,b) = \frac{1}{m} \sum_{1}^{m} L(预测值向量, 真实值向量) = \frac{1}{m} \sum_{1}^{m} L(a^{(i)}, y^{(i)})$$





反向传播公式:即对cost function的变量求偏异,用链式求导。

已知:
$$J(w,b) = \frac{1}{m} \sum_{1}^{m} L(a^{(i)}, y^{(i)}) \quad \text{求导数} = \frac{1}{a^{(i)}} ?$$

$$L(a^{(i)}, y^{(i)}) = -(y^{(i)} \log a^{(i)}) - (1 - y^{(i)}) \log(1 - a^{(i)})$$

$$\hat{y}^{(i)} = a^{(i)} = sigmoid(z^{(i)}) = \frac{1}{1 + e^{-z^{(i)}}}$$

$$z^{(i)} = w^{T} x^{(i)} + b$$

求解:

$$\begin{cases} \frac{\partial J}{\partial w} = \frac{\partial J}{\partial z} \cdot \frac{\partial z}{\partial w} \\ \frac{\partial J}{\partial b} = \frac{\partial J}{\partial z} \cdot \frac{\partial z}{\partial w} \end{cases}$$



求解:

Step 1
$$\frac{\partial z}{\partial w} = x^{(i)}$$
 $\frac{\partial z}{\partial b} = 1$
Step 2 $\frac{\partial J}{\partial z} = \frac{\partial J}{\partial L} \cdot \frac{\partial L}{\partial a} \cdot \frac{\partial a}{\partial z} = \left(\frac{1}{m} \sum_{i=1}^{m} \frac{\partial L}{\partial a}\right) \cdot \frac{\partial a}{\partial z}$
 $\frac{\partial L}{\partial a} = ? = -\frac{y^{(i)}}{a^{(i)}} + \frac{1 - y^{(i)}}{1 - a^{(i)}}$
 $\frac{\partial a}{\partial z} = ? = \frac{1}{1 + e^{-z^{(i)}}} \cdot \left(1 - \frac{1}{1 + e^{-z^{(i)}}}\right)$

sigmod function:

$$f(z) = \frac{1}{1 + e^{-z}}$$

$$\frac{\partial f(z)}{\partial z} = \frac{1}{1 + e^{-z}} \cdot \left(1 - \frac{1}{1 + e^{-z}}\right) = f(z)(1 - f(z))$$



求解:

Step 1
$$\frac{\partial z}{\partial w} = x^{(i)}$$
 $\frac{\partial z}{\partial b} = 1$
Step 2 $\frac{\partial J}{\partial z} = \frac{\partial J}{\partial L} \cdot \frac{\partial L}{\partial a} \cdot \frac{\partial a}{\partial z} = \left(\frac{1}{m} \sum_{1}^{m} \frac{\partial L}{\partial a}\right) \cdot \frac{\partial a}{\partial z}$
 $\frac{\partial J}{\partial z} = \left(\frac{1}{m} \sum_{1}^{m} -\frac{y^{(i)}}{a^{(i)}} + \frac{1 - y^{(i)}}{1 - a^{(i)}}\right) \cdot \frac{1}{1 + e^{-z^{(i)}}} \cdot \left(1 - \frac{1}{1 + e^{-z^{(i)}}}\right)$

$$= \left(\frac{1}{m} \sum_{1}^{m} -\frac{y^{(i)}}{a^{(i)}} + \frac{1 - y^{(i)}}{1 - a^{(i)}}\right) \cdot \frac{1}{1 + e^{-z^{(i)}}} \cdot \left(1 - \frac{1}{1 + e^{-z^{(i)}}}\right)$$

$$= \left(\frac{1}{m} \sum_{1}^{m} -\frac{y^{(i)}}{a^{(i)}} + \frac{1 - y^{(i)}}{1 - a^{(i)}}\right) \cdot a^{(i)} \cdot \left(1 - a^{(i)}\right)$$

$$= \frac{1}{m} \sum_{1}^{m} \frac{1 - y^{(i)}}{a^{(i)}} - \frac{y^{(i)}}{1 - a^{(i)}} = \frac{1}{m} \sum_{1}^{m} \left(a^{(i)} - y^{(i)}\right)$$
?



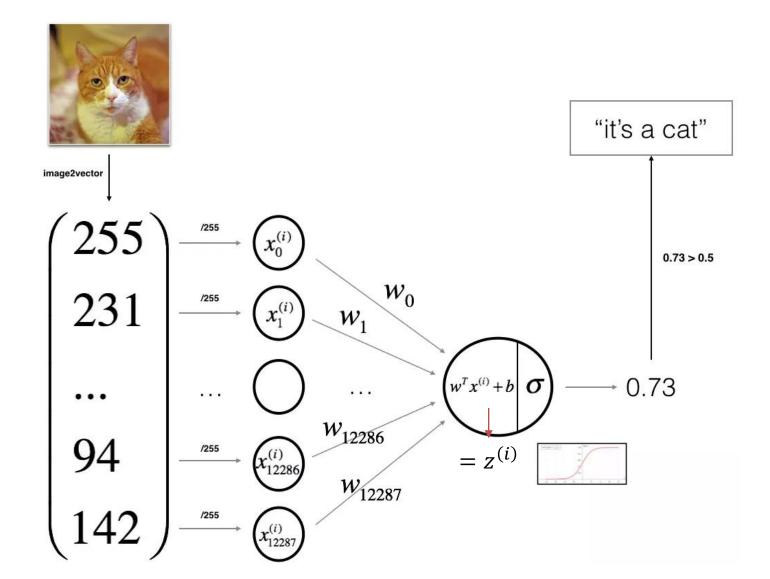
求解:

Step 1
$$\frac{\partial z}{\partial w} = x^{(i)}$$
 $\frac{\partial z}{\partial b} = 1$
Step 2 $\frac{\partial J}{\partial z} = \frac{1}{m} \sum_{1}^{m} (a^{(i)} - y^{(i)})$
Step 3 $\frac{\partial J}{\partial w} = \frac{\partial J}{\partial z} \cdot \frac{\partial z}{\partial w} = \frac{1}{m} \sum_{1}^{m} (a^{(i)} - y^{(i)}) \cdot x^{(i)} = \frac{1}{m} X (A - Y)^{T} ?$
 $\frac{\partial J}{\partial b} = \frac{\partial J}{\partial z} \cdot \frac{\partial z}{\partial w} = \frac{1}{m} \sum_{1}^{m} (a^{(i)} - y^{(i)})$

可以看出,J(w,b)对w,b求的偏导也是各样本点平均值的形式



五、损失函数推导





五、损失函数推导

Sigmod Function 值域:
$$\hat{y}^{(i)} = sigmoid(z^{(i)}) \in (0,1)$$

构建伯努利概率分布

Logistic Regression output: 0或1

如何构建伯努利概率分布:

Step 1 简写
$$\hat{y}^{(i)}$$

$$z^{(i)} = w^T x^{(i)} + b \qquad \qquad \hat{y} = \emptyset(w^T x + b)$$
 $\hat{y}^{(i)} = a^{(i)} = sigmoid(z^{(i)})$

Step 2 约定 \hat{y} 的概率含义

$$\hat{y} = p(y = 1|x)$$
 |给定样本 x 时, y 属于类别1的概率 $1 - \hat{y} = p(y = 0|x)$ |给定样本 x 时, y 属于类别0的概率

五、损失函数推导

Sigmod Function 值域: $\hat{y}^{(i)} = sigmoid(z^{(i)}) \in (0,1)$

构建伯努利概率分布

Logistic Regression output: 0或1

如何构建伯努利概率分布:

Step 3 整合成条件概率公式Pr(y|x)

$$\begin{cases} \Pr(y|x) = \hat{y} & \text{, If } y = 1 \\ \Pr(y|x) = 1 - \hat{y}, \text{If } y = 0 \end{cases}$$

Step 4 合并

$$Pr(y|x) = \hat{y}^y (1 - \hat{y})^{1-y}$$



六、支持处理分类变量的统计分析法

- (1) 判别分析
- (2) Probit分析(离散选择模型)这是什么?
- (3) Logistic回归分析: 1) 二元Logistic回归分析: vector只有1/0两种取值
 - 2) 多元Logistic回归分析: vector有多种取值(后文说

Logistic Regression要求output只有1或0。Which right?)

(4) 对数线性Model

七、Logit Model性质

(1) 首个离散选择模型 (1959 Luce推导出)

- (2) Logit模型与最大效用理论一致 (1960 Marschark证明)
- (3)极值分布→可以推出Logit形式的模型 (1965 Marley证明)
- (4) Logit形式的模型效用非确定项→服从极值分布(1974 McFadden证明)
- (5) 亮点:选择枝的减少/增加不影响各选择枝之间被选概率的比值!





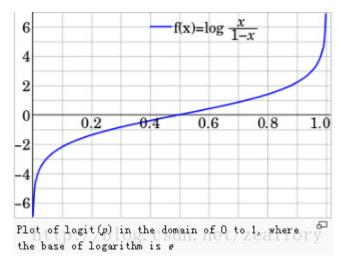
Logit Model(分类评定模型) = Logistic Regression(逻辑回归)

求Logit值的相关参数定义:

(1) 优势比:
$$odds = \frac{P(y=1)}{P(y=0)}$$

(2) 效用值: logit = log(odds)

$$logit(p) = log(\frac{p}{1-p}), p \in (0,1)$$



$$= \log(p) - \log(1 - p) = -\log()$$

The logit function is the inverse of the sigmoidal "logistic" function. When the function's variable represents a probability p, the logit function gives the logodds, or the logarithm of the odds p/(1-p).



Thanks





