Logistic Regression

Basic Model

- use for Binary classification: $y \in \{0, 1\}$, $x \in \mathbb{R}^d$
- $f(x) = w^T x + b, w \in \mathbb{R}^d, b \in \mathbb{R}$
- sigmoid function $\sigma(z) = \frac{1}{1+e^{-z}}$
    - map $\mathbb{R}$ to $[0, 1]$
    - $1 - \sigma(z) = \sigma(-z)$
- $P(y = 1|x) = \sigma(w^T x + b), P(y = 0|x) = 1 - \sigma(w^T x + b)$
    - 用概率表示误差是一种比最小二乘更好的方式
    - y等于0或1只是一种指示，表示这是两种样本，它可以是任意两个不相等的数

Maximum Likelihood Estimation (MLE)

- Likelihood of training data (i.i.d): $\prod_{i=1}^{n} P(y = y_i|x = x_i)$
- 我们希望likelihood尽可能大:

$$\begin{aligned} &\max_{w,b} \prod_{i=1}^{n} P(y = y_i|x = x_i) \\ &= \max_{w,b} \prod_{i=1}^{n} (\sigma(w^T x_i + b))^{y_i} (1 - \sigma(w^T x_i + b))^{1-y_i} \end{aligned}$$

- 但是连乘会导致数字变得非常小(因为都小于1)，所以我们可以使用log:

$$\max_{w,b} \sum_{i=1}^{n} [y_i log(\sigma(w^T x + b)) + (1 - y_i) log(1 - \sigma(w^T x + b))]$$

- so now we have our **loss function** for Logistic Regression:

$$\min_{w,b} - \sum_{i=1}^{n} [y_i log(\sigma(w^T x + b)) + (1 - y_i) log(1 - \sigma(w^T x + b))]$$

    - negative log likelihood = cross entropy loss (交叉熵)

Optimization

- let $\hat{X} = \begin{bmatrix} X \\ 1 \end{bmatrix} \in \mathbb{R}^{d+1}$, $\hat{W} = \begin{bmatrix} w \\ b \end{bmatrix} \in \mathbb{R}^{d+1}$
- Cross Entropy Loss ($L(\hat{W})$):

$$
\begin{aligned}
L(\hat{W}) &= -\sum_{i=1}^{n}[y_i log\frac{1}{1+e^{-\hat{W}^T\hat{X}_i}} + (1-y_i)log(1-\frac{1}{1+e^{-\hat{W}^T\hat{X}_i}})] \\
&= -\sum_{i=1}^{n}[-y_i log(1+e^{-\hat{W}^T\hat{X}_i}) + y_i log(1+e^{\hat{W}^T\hat{X}_i}) - log(1+e^{\hat{W}^T\hat{X}_i})] \\
&= -\sum_{i=1}^{n}[y_i loge^{\hat{W}^T\hat{X}_i} - log(1+e^{\hat{W}^T\hat{X}_i})] \\
&= -\sum_{i=1}^{n}[y_i\hat{W}^T\hat{X}_i - log(1+e^{\hat{W}^T\hat{X}_i})]
\end{aligned}
$$

- 求梯度:

$$
\begin{aligned}
\frac{\partial L(\hat{W})}{\partial \hat{W}} &= -\sum_{i=1}^{n}(y_i\hat{X}_i - \frac{\hat{X}_i e^{\hat{W}^T\hat{X}_i}}{1+e^{\hat{W}^T\hat{X}_i}}) \in \mathbb{R}^{d+1} \\
&= -\sum_{i=1}^{n}(y_i - P(y=1|x_i))\hat{X}_i
\end{aligned}
$$

  - when $y_i = P(y=1|x_i), \forall i$, then $\frac{\partial L(\hat{W})}{\partial \hat{W}} = 0$
    - 这时模型完全能够反映正确的分类，说明此时所有的样本是线性可分(*linearly separable*)的，即可以被模型这个超平面(*hyperplane*)恰好一分为二；但是很显然更多的情况是样本线性不可分，但我们可以保证一定能找到一个全局最优解
- 求Heissan矩阵:

$$
\begin{aligned}
\frac{\partial^2 L(\hat{W})}{\partial \hat{W}\partial \hat{W}^T} &= \sum_{i=1}^{n}\frac{e^{-\hat{W}^T\hat{X}_i}}{(1+e^{-\hat{W}^T\hat{X}_i})^2}\hat{X}_i{\hat{X}_i}^T \\
&= \sum_{i=1}^{n}P(y=1|x_i)(1-P(y=1|x_i))\hat{X}_i{\hat{X}_i}^T
\end{aligned}
$$

  - 我们知道$\hat{X}_i{\hat{X}_i}^T$一定是一个半正定矩阵，那么可以说$L(\hat{W})$一定是一个凸函数，因此通过梯度下降它一定能找到一个全局最优解

标签为{-1,1}的逻辑回归

- $P(y_i=1|x_i) = \sigma(w^Tx_i+b)$
  - $loss(x_i,y_i) = -log\sigma(w^Tx_i+b) = log(1+e^{-y_i(w^Tx_i+b)})$
- $P(y_i=-1|x_i) = \frac{1}{1+e^{w^Tx_i+b}}$
  - $loss(x_i,y_i) = log(1+e^{-y_i(w^Tx_i+b)})$
- 我们发现，无论y_i取-1还是1，损失函数的表达方式是相同的:

$$
L(w,b) = \sum_{i=1}^{n}log(1+e^{-y_i(w^Tx_i+b)})
$$

- 梯度下降为:

$$
\frac{\partial L}{\partial w} = -\sum_{i=1}^{n}\frac{y_i^Tx_i}{1+e^{y_i(w^Tx_i+b)}}
$$

- let $z_i := y_i(w^Tx_i+b)$, then:

$$z_i \begin{cases} > 0 & sign(y_i) = sign(w^T x_i + b) \\ < 0 & sign(y_i) = -sign(w^T x_i + b) \end{cases}$$

  - 可以发现$log(1+e^{z_i})$是一个平滑的单调递减函数，性质很好
  - $\sum_{i=1}^n loss(z_i)$ is the *number* of training point that wrongly classified
  - $\frac{1}{n}\sum_{i=1}^n loss(z_i)$ is the *error rate*
- 0/1 loss function:

$$y = \begin{cases} 0 & x \geq 0 \\ 1 & x < 0 \end{cases}$$

  - not differentiable
  - not continuous at $x = 0$
  - cannot use gradient descent
- cross-entropy loss is an *upper bound* of 0/1 loss
  - *"Substitute loss function"*

Multi-class Classification

- $y \in \{1, 2, \ldots, K\}$, $x \in \mathbb{R}^d$
- **Softmax Regression**
  - 虽然叫回归，但解决的是分类问题
  - Define K linear models $f_k(x) = w_k^T x + b_k,\ k \in \{1, \ldots, K\}$
  - Given (x_i, y_i), find $f_k(x_i) > f_j(x_i),\ \forall j \neq k$, then predict $y_i = k$
- **MLE**
  - $P(y=k|x) = \frac{e^{f_k(x)}}{\sum_{j=1}^K e^{f_j(x)}}$
  - It's a probability distribution:
    - $\sum_{k=1}^K P(y=k|x) = 1$
    - $P(y=k|x) \geq 0,\ \forall k$
  - When $f_k(x) >> f_j(x),\ \forall j \neq k$, then $P(y=k|x) \rightarrow 1$ and $P(y=j|x) \rightarrow 0$
  - MLE log-likelihood:

$$\begin{aligned} Loss &= \min_{\{(w_j, b_j)|j=1,\ldots,K\}} -\sum_{i=1}^n log P(y = y_i | x = x_i) \\ &= -\sum_{i=1}^n log \frac{e^{w_{y_i}^T x_i + b_{y_i}}}{\sum_{j=1}^K e^{w_j^T x_i + b_j}} \end{aligned}$$

- Relation between *Logistic Regression* and *Softmax Regression* with $K = 2$
  - $y = \{1, 2\}$, $x \in \mathbb{R}^d$
  - we define $w := w_1 - w_2$ and $b := b_1 - b_2$
  - then we have:

$$\begin{aligned} P(y=1|x) &= \frac{e^{w_1^T x + b_1}}{e^{w_1^T x + b_1} + e^{w_2^T x + b_2}} \\ &= \frac{1}{1 + e^{(w_2 - w_1)^T x + b_2 - b_1}} \\ &= \frac{1}{1 + e^{-(w^T x + b)}} \\ &= \sigma(w^T x + b) \end{aligned}$$