Logistic Regression and Softmax Regression

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Content

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Linear Classification and Regression

The linear signal:

$$s = \mathbf{w}^\top \mathbf{x}$$

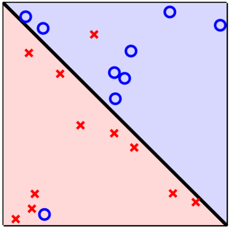


Figure: Linear Classification

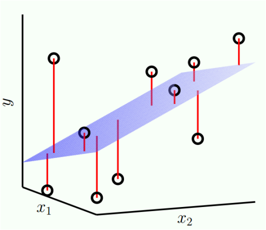


Figure: Linear Regression

Predicting a Probability

Will someone have a heart attack over the next year?

age	62 years
gender	male
blood sugar	120 mg/dL40,000
HDL	50
LDL	120
Mass	190 lbs
Height	5′ 10″
...	...

Classification: Yes/No
Logistic Regression: Likelihood of heart attack

$$h_{\mathbf{w}}(\mathbf{x}) = g\left(\sum_{i=1}^{m} w_i x_i\right) = g(\mathbf{w}^\top \mathbf{x})$$

Logistic function

Definition

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

- The function is a continuous function.
- If $z \to +\infty$, then $g\left(z\right) \to 1$; If $z \to -\infty$, then $g\left(z\right) \to 0$.

Logistic function
Definition

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

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

The Data is Still Binary

$$\mathcal{D} = \{(\mathbf{x}_1, y_1 = \pm 1), ..., (\mathbf{x}_n, y_n = \pm 1)\}$$

- $\mathbf{x}_n \leftarrow$ a persons health information.
- $y_n = \pm 1 \leftarrow$ did they have a heart attack or not.
- We cannot measure a probability.
- We can only see the occurence of an event and try to infer a probability.

The Target Function is Inherently Noisy

$$h_{\mathbf{w}}(\mathbf{x}) = \mathbb{P}[y = +1|\mathbf{x}]$$

The data is generated from a noisy target function:

$$P(y|\mathbf{x}) = \begin{cases} h_{\mathbf{w}}(\mathbf{x}) & y = 1 \\ 1 - h_{\mathbf{w}}(\mathbf{x}) & y = -1 \end{cases}$$

What Makes an h Good?

Fitting the data means finding a good h

$$\text{h is good if: } \begin{cases} h_{\mathbf{w}}(\mathbf{x}) \approx 1 & y = 1 \\ h_{\mathbf{w}}(\mathbf{x}) \approx 0 & y = -1 \end{cases}$$

A simple error measure that captures this:

$$\mathbf{E}_{in}(h) = \frac{1}{n} \sum_{i-1}^{n} \left(h_{\mathbf{w}}(\mathbf{x}_i) - \frac{1}{2}(1 + y_i)\right)^2$$

Not very convenient (hard to minimize).

The Cross Entropy Error Measure

$$\mathbf{E}_{in}(\mathbf{w}) = \frac{1}{n}\sum_{i=1}^{n}\log(1 + e^{-y_n \cdot \mathbf{w}^\top \mathbf{x}})$$

- It is based on an intuitive probabilistic interpretation of h.
- It is very convenient and mathematically friendly (easy to minimize).

The Probabilistic Interpretation

Suppose that $h_{\mathbf{w}}(\mathbf{x}) = g(\mathbf{w}^\top \mathbf{x})$ closely captures $\mathbb{P}[+1|\mathbf{x}]$:

$$P(y|\mathbf{x}) = \begin{cases} g(\mathbf{w}^\top \mathbf{x}) & y = 1 \\ 1 - g(\mathbf{w}^\top \mathbf{x}) & y = -1 \end{cases}$$

The Probabilistic Interpretation

So, if $h_{\mathbf{w}}(\mathbf{x}) = g(\mathbf{w}^\top \mathbf{x})$ closely captures $\mathbb{P}[+1|\mathbf{x}]$:

$$P(y|\mathbf{x}) = \begin{cases} g(\mathbf{w}^\top \mathbf{x}) & y = 1 \\ 1 - g(\mathbf{w}^\top \mathbf{x}) = g(-\mathbf{w}^\top \mathbf{x}) & y = -1 \end{cases}$$

...or, more compactly,

$$P(y|\mathbf{x}) = g(y \cdot \mathbf{w}^\top \mathbf{x})$$

The Likelihood

$$P(y|\mathbf{x}) = g(y \cdot \mathbf{w}^\top \mathbf{x})$$

Recall: $(\mathbf{x}_1, y_1), ..., (\mathbf{x}_n, y_n)$ are independently generated.

Likelihood:

The probability of getting the $y_1, ..., y_n$ in $\mathcal{D}$ from the corresponding $\mathbf{x}_1, ..., \mathbf{x}_n$:

$$P(y_1, ..., y_n | \mathbf{x}_1, ..., \mathbf{x}_n) = \prod_{i=1}^{n} P(y_i | \mathbf{x}_i)$$

Maximizing The Likelihood

$$
\begin{aligned}
\max \prod_{i=1}^{n} P(y_i|\mathbf{x}_i) &\Leftrightarrow \max \log \left(\prod_{i=1}^{n} P(y_i|\mathbf{x}_i) \right) \\
&\equiv \max \sum_{i=1}^{n} \log P(y_i|\mathbf{x}_i) \\
&\Leftrightarrow \min -\frac{1}{n} \sum_{i=1}^{n} \log P(y_i|\mathbf{x}_i) \\
&\equiv \min \frac{1}{n} \sum_{i=1}^{n} \log \frac{1}{P(y_i|\mathbf{x}_i)} \\
&\equiv \min \frac{1}{n} \sum_{i=1}^{n} \log \frac{1}{g(y_i \cdot \mathbf{w}^\top \mathbf{x}_i)} \\
&\equiv \min \frac{1}{n} \sum_{i=1}^{n} \log(1 + e^{-y_i \cdot \mathbf{w}^\top \mathbf{x}_i}) = \min E_{in}(\mathbf{w})
\end{aligned}
$$

Regularization

$$J(\mathbf{w}) = \frac{1}{n}\sum_{i=1}^{n}\log(1 + e^{-y_i \cdot \mathbf{w}^\top \mathbf{x}_i}) + \frac{\lambda}{2}||\mathbf{w}||_2^2$$

Small values for parameters $w_0, w_1, ..., w_{m-1}$

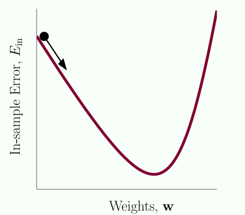
- "Simpler" model
- Less prone to overfitting

Regularization parameter λ

- Trade off between fitting the training set well and keeping the model relatively simple

Finding The Best Weights

Use the Gradient Descent



Minimize $E_{in}(\mathbf{w})$ by repeated gradient steps:

- Compute gradient of loss with respect to parameters $\frac{\partial J(\mathbf{w})}{\partial \mathbf{w}}$
- Update parameters with rate η

$$\mathbf{w}' \to \mathbf{w} - \eta \frac{\partial J(\mathbf{w})}{\partial \mathbf{w}} = (1-\eta\lambda)\mathbf{w} + \eta \frac{1}{n} \sum_{i=1}^{n} \frac{y_i \mathbf{x}_i}{1+e^{y_i \cdot \mathbf{w}^\top \mathbf{x}_i}}$$

Logistic Regression: $y_i \in \{0, 1\}$

Assume that the labels are binary: $y_i \in \{0, 1\}$

$$h_{\mathbf{w}}(\mathbf{x}) = g(\mathbf{w}^\top \mathbf{x}) = \frac{1}{1 + e^{-\mathbf{w}^\top \mathbf{x}}}$$

Probability:

$$p = \begin{cases} h_{\mathbf{w}}(\mathbf{x}_i) & y_i = 1 \\ 1 - h_{\mathbf{w}}(\mathbf{x}_i) & y_i = 0 \end{cases}$$

Log-likehood loss function:

$$\begin{aligned}
\max \prod_{i=1}^{n} P(y_i|\mathbf{x}_i) &\Leftrightarrow \max \log \left(\prod_{i=1}^{n} P(y_i|\mathbf{x}_i) \right) \\
&\equiv \max \sum_{i=1}^{n} \log P(y_i|\mathbf{x}_i) \\
&\Leftrightarrow \min -\frac{1}{n} \sum_{i=1}^{n} \log P(y_i|\mathbf{x}_i)
\end{aligned}$$

$$P(y_i|\mathbf{x}_i) = h_{\mathbf{w}}(\mathbf{x}_i)^{y_i} \cdot (1 - h_{\mathbf{w}}(\mathbf{x}_i))^{(1-y_i)}$$

$$J(\mathbf{w}) = -\frac{1}{n} \left[\sum_{i=1}^{n} y_i \log\, h_{\mathbf{w}}(\mathbf{x}_i) + (1 - y_i) \log\, (1 - h_{\mathbf{w}}(\mathbf{x}_i)) \right]$$

The Gradient of The Loss Function

For a sample:

$$\begin{aligned}\frac{\partial J(\mathbf{w})}{\partial \mathbf{w}} &= -\frac{1}{\partial \mathbf{w}} \cdot \partial \left[y \cdot \log\, h_{\mathbf{w}}(\mathbf{x}) + (1-y)\log\,(1-h_{\mathbf{w}}(\mathbf{x}))\right] \\ &= -y \cdot \frac{1}{h_{\mathbf{w}}(\mathbf{x})} \cdot \frac{\partial h_{\mathbf{w}}(\mathbf{x})}{\partial \mathbf{w}} + (1-y) \cdot \frac{1}{1-h_{\mathbf{w}}(\mathbf{x})} \frac{\partial h_{\mathbf{w}}(\mathbf{x})}{\partial \mathbf{w}}\end{aligned}$$

Note:

$$g(z) = \frac{1}{1+e^{-z}},\;\; g'(z) = \frac{e^{-z}}{(1+e^{-z})^2} = g(z)\left[1-g(z)\right]$$

The Gradient of The Loss Function

For a sample:

$$
\begin{aligned}
\frac{\partial J(\mathbf{w})}{\partial \mathbf{w}} &= -y \cdot \frac{1}{h_{\mathbf{w}}(\mathbf{x})} \cdot \frac{\partial h_{\mathbf{w}}(\mathbf{x})}{\partial \mathbf{w}} + (1-y) \cdot \frac{1}{1-h_{\mathbf{w}}(\mathbf{x})} \frac{\partial h_{\mathbf{w}}(\mathbf{x})}{\partial \mathbf{w}} \\
&= -y \cdot \frac{1}{h_{\mathbf{w}}(\mathbf{x})} \cdot \frac{\partial g\left(\mathbf{w}^\top \mathbf{x}\right)}{\partial \mathbf{w}} + (1-y) \cdot \frac{1}{1-h_{\mathbf{w}}(\mathbf{x})} \frac{\partial g\left(\mathbf{w}^\top \mathbf{x}\right)}{\partial \mathbf{w}} \\
&= \left(-\frac{\mathbf{x}y}{h_{\mathbf{w}}(\mathbf{x})} + \frac{\mathbf{x}(1-y)}{1-h_{\mathbf{w}}(\mathbf{x})}\right) \cdot g\left(\mathbf{w}^\top \mathbf{x}\right) \cdot \left[1-g\left(\mathbf{w}^\top \mathbf{x}\right)\right] \\
&= \left(h_{\mathbf{w}}(\mathbf{x}) - y\right) \mathbf{x}
\end{aligned}
$$

Use The Gradient Descent to Get $\mathbf{w}$

For a sample:

$$\frac{\partial J(\mathbf{w})}{\partial \mathbf{w}} = (h_{\mathbf{w}}(\mathbf{x}) - y)\,\mathbf{x}$$

$$\mathbf{w} := \mathbf{w} - \alpha\,(h_{\mathbf{w}}(\mathbf{x}) - y)\,\mathbf{x}$$

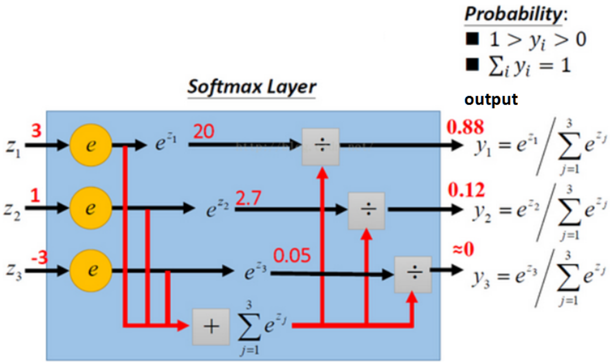
For all samples:

$$\frac{\partial J(\mathbf{w})}{\partial \mathbf{w}} = \frac{1}{n}\sum_{i=1}^{n}(h_{\mathbf{w}}(\mathbf{x}_i) - y)\,\mathbf{x}_i$$

$$\mathbf{w} := \mathbf{w} - \frac{1}{n}\sum_{i=1}^{n}\alpha\,(h_{\mathbf{w}}(\mathbf{x}_i) - y_i)\,\mathbf{x}_i$$

Contents

Softmax Regression
Multi-class classification



$$p\left(y_i = j \mid \mathbf{x}_i; \mathbf{w}\right) = \frac{e^{\mathbf{w}_j^\top \mathbf{x}_i}}{\sum_{l=1}^{k} e^{\mathbf{w}_l^\top \mathbf{x}_i}}$$

Softmax Regression

Multi-class classification

$$h_{\mathbf{w}}(\mathbf{x}) = \begin{bmatrix} p(y_i = 1|\mathbf{x}_i; \mathbf{w}) \\ p(y_i = 2|\mathbf{x}_i; \mathbf{w}) \\ \vdots \\ p(y_i = k|\mathbf{x}_i; \mathbf{w}) \end{bmatrix} = \frac{1}{\sum_{j=1}^{k} e^{\mathbf{w}_j^\top \mathbf{x}_i}} \begin{bmatrix} e^{\mathbf{w}_1^\top \mathbf{x}_i} \\ e^{\mathbf{w}_2^\top \mathbf{x}_i} \\ \vdots \\ e^{\mathbf{w}_k^\top \mathbf{x}_i} \end{bmatrix}$$

- Multi-class classification: $y \in \{1, 2, ..., k\}$.
- $p\left(y = j \mid \mathbf{x}\right)$ represents the probability of the class label.
- The term $\frac{1}{\sum_{j=1}^{k} e^{\mathbf{w}_j^\top \mathbf{x}^{(i)}}}$ normalizes the distribution, so the elements sum to 1.

Softmax function

Logistic function vs Softmax function

When the number of the classes is two:

$$\begin{aligned}
h_{\mathbf{w}}(\mathbf{x}) &= \begin{bmatrix} p\left(y=0 \mid \mathbf{x};\mathbf{w}\right) \\ p\left(y=1 \mid \mathbf{x};\mathbf{w}\right) \end{bmatrix} \\
&= \frac{1}{e^{\mathbf{w}_0^\top \mathbf{x}} + e^{\mathbf{w}_1^\top \mathbf{x}}} \begin{bmatrix} e^{\mathbf{w}_0^\top \mathbf{x}} \\ e^{\mathbf{w}_1^\top \mathbf{x}} \end{bmatrix} \\
&= \frac{1}{e^{(\mathbf{w}_0-\mathbf{w}_1)^\top \mathbf{x}} + e^{(\mathbf{w}_1-\mathbf{w}_1)^\top \mathbf{x}}} \begin{bmatrix} e^{(\mathbf{w}_0-\mathbf{w}_1)^\top \mathbf{x}} \\ e^{(\mathbf{w}_1-\mathbf{w}_1)^\top \mathbf{x}} \end{bmatrix} \\
&= \frac{1}{e^{(\mathbf{w}_0-\mathbf{w}_1)^\top \mathbf{x}} + e^{(\mathbf{0})^\top \mathbf{x}}} \begin{bmatrix} e^{(\mathbf{w}_0-\mathbf{w}_1)^\top \mathbf{x}} \\ e^{(\mathbf{0})^\top \mathbf{x}} \end{bmatrix}
\end{aligned}$$

Let $-\mathbf{w} = \mathbf{w}_0 - \mathbf{w}_1$

Softmax function

Logistic function vs Softmax function

$$h_{\mathbf{w}}(\mathbf{x}) = \frac{1}{1+e^{-\mathbf{w}^\top \mathbf{x}}} \begin{bmatrix} e^{-\mathbf{w}^\top \mathbf{x}} \\ 1 \end{bmatrix}$$

$$= \begin{bmatrix} 1 - \frac{1}{1+e^{-\mathbf{w}^\top \mathbf{x}}} \\ \\ \frac{1}{1+e^{-\mathbf{w}^\top \mathbf{x}}} \end{bmatrix}$$

- Softmax regression is a generalization of logistic regression.

Softmax function
Cost function

Represent $\mathbf{w} = \begin{bmatrix} \mathbf{w}_1 & \mathbf{w}_2 & \dots & \mathbf{w}_k \end{bmatrix}$, the softmax cost function

$$J(\mathbf{w}) = -\frac{1}{n}\left[\sum_{i=1}^{n}\sum_{j=1}^{k}\mathbb{I}\left\{y_i = j\right\}\log\frac{e^{\mathbf{w}_j^\top \mathbf{x}_i}}{\sum_{l=1}^{k} e^{\mathbf{w}_l^\top \mathbf{x}_i}}\right]$$

- $\mathbb{I}\left\{\cdot\right\}$ is the indicator function.
- $\mathbb{I}${a true statement}=1.
- $\mathbb{I}${a false statement}=0.

The logistic regression cost function could also have been written:

$$
\begin{aligned}
J(\mathbf{w}) &= -\frac{1}{n}\left[\sum_{i=1}^{n} y_i \log\, h_{\mathbf{w}}(\mathbf{x}_i) + (1-y_i)\log\,(1-h_{\mathbf{w}}(\mathbf{x}_i))\right] \\
&= -\frac{1}{n}\left[\sum_{i=1}^{n}\sum_{j=0}^{1}\mathbb{I}\{y_i = j\}\log P(y_i = j|\mathbf{x}_i;\mathbf{w})\right]
\end{aligned}
$$

Softmax function

Derivation

For $\mathbf{w}_j \ (j = 1, ..., k)$

$$\frac{\partial J(\mathbf{w})}{\partial \mathbf{w}_j} = \frac{\partial \left\{ -\frac{1}{n} \cdot \left[\sum_{i=1}^{n} \sum_{j=1}^{k} \mathbb{I}\{y_i = j\} \, log \frac{e^{\mathbf{w}_j^\top \mathbf{x}_i}}{\sum_{l=1}^{k} e^{\mathbf{w}_l^\top \mathbf{x}_i}} \right] \right\}}{\partial \mathbf{w}_j}$$

$$= -\frac{1}{n} \sum_{i=1}^{n} \frac{\partial \sum_{j=1}^{k} \mathbb{I}\{y_i = j\} \left(\log e^{\mathbf{w}_j^\top \mathbf{x}_i} - \log \sum_{l=1}^{k} e^{\mathbf{w}_l^\top \mathbf{x}_i} \right)}{\partial \mathbf{w}_j}$$

$$= -\frac{1}{n} \sum_{i=1}^{n} \left[\mathbb{I}\{y_i = j\} \mathbf{x}_i - \frac{1}{\sum_{l=1}^{k} e^{\mathbf{w}_l^\top \mathbf{x}_i}} \cdot \frac{\partial \sum_{l=1}^{k} e^{\mathbf{w}_l^\top \mathbf{x}_i}}{\partial \mathbf{w}_j} \right]$$

$$= -\frac{1}{n} \sum_{i=1}^{n} \left[\mathbb{I}\{y_i = j\} \mathbf{x}_i - \frac{\mathbf{x}_i \cdot e^{\mathbf{w}_j^\top \mathbf{x}_i}}{\sum_{l=1}^{k} e^{\mathbf{w}_l^\top \mathbf{x}_i}} \right]$$

$$= \frac{1}{n} \sum_{i=1}^{n} \left(p(y_i = j \mid \mathbf{x}_i; \mathbf{w}) - \mathbb{I}\{y_i = j\} \right) \mathbf{x}_i$$

Softmax function
Properties

Softmax function has a redundant set of parameters.

$$p\left(y_i = j \mid \mathbf{x}_i; \mathbf{w}\right) = \frac{e^{\mathbf{w}_j^\top \mathbf{x}_i}}{\sum_{l=1}^{k} e^{\mathbf{w}_l^\top \mathbf{x}_i}}$$

$$= \frac{e^{\mathbf{w}_j^\top \mathbf{x}_i} \div e^{\varphi^\top \mathbf{x}_i}}{\sum_{l=1}^{k} \left(e^{\mathbf{w}_l^\top \mathbf{x}_i} \div e^{\varphi^\top \mathbf{x}_i}\right)}$$

$$= \frac{e^{\left(\mathbf{w}_j - \varphi\right)^\top \mathbf{x}_i}}{\sum_{l=1}^{k} e^{\left(\mathbf{w}_l - \varphi\right)^\top \mathbf{x}_i}}$$

- Subtract φ from every $\mathbf{w}_j$ does not affect the hypothesis predictions

Softmax function

Cost function

The cost function $J(\mathbf{w})$ is minimized by some setting of the parameters $(\mathbf{w}_1, \mathbf{w}_2, \ldots \mathbf{w}_k)$, then it is also minimized by $(\mathbf{w}_1 - \varphi, \mathbf{w}_2 - \varphi, \ldots \mathbf{w}_k - \varphi)$ for any value of φ.

- However using the weight decay method, the minimizer of $J(\mathbf{w})$ is unique.

$$J(\mathbf{w}) = -\frac{1}{n}\left[\sum_{i=1}^{n}\sum_{j=1}^{k}\mathbb{I}\{y_i = j\}\log\frac{e^{\mathbf{w}_j^\top \mathbf{x}_i}}{\sum_{l=1}^{k} e^{\mathbf{w}_l^\top \mathbf{x}_i}}\right] + \frac{\lambda}{2}||\mathbf{w}||_2^2$$

$$\frac{\partial J(\mathbf{w})}{\partial \mathbf{w}_j} = \frac{1}{n}\sum_{i=1}^{n}\left[\mathbf{x}_i\left(p\left(y_i = j \mid \mathbf{x}_i; \mathbf{w}\right) - \mathbb{I}\{y_i = j\}\right)\right] + \lambda\mathbf{w}_j$$

THANK YOU!