Logistic regression

Machine Learning (CSCI 5770G)

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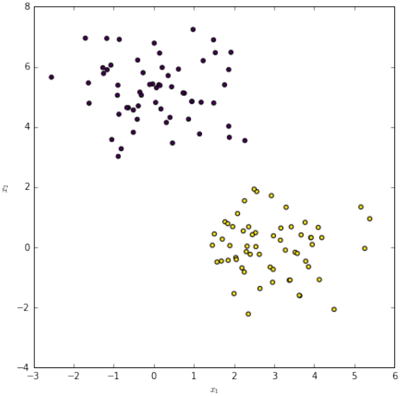
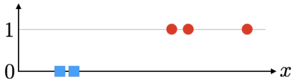
Logistic regression

- Logistic regression is for binary classification
- The target variable y takes on values in $\{0, 1\}$





Binary classification

The goal of binary classification is to learn $h_\theta(\mathbf{x})$, which can be used to assign a label $y \in \{0, 1\}$ to the input $\mathbf{x}$. Label y takes values in $\{0, 1\}$, so we can use Bernoulli distribution to specify its probability distribution. Specifically

$$\mathrm{Pr}(y = 1) = h_\theta(\mathbf{x})$$
$$\mathrm{Pr}(y = 0) = 1 - h_\theta(\mathbf{x})$$

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$$\Pr(y = 1) = h_\theta(\mathbf{x})$$
$$\Pr(y = 0) = 1 - h_\theta(\mathbf{x})$$

Or more succinctly

$$\Pr(y) = h_\theta(\mathbf{x})^y \left(1 - h_\theta(\mathbf{x})\right)^{1-y}$$

Bernoulli distribution

A Bernoulli random variable X takes values in $\{0, 1\}$

$$\begin{aligned}\Pr(X|\theta) &= \begin{cases}\theta & \text{if } X = 1\\ 1-\theta & \text{otherwise}\end{cases}\\ &= \theta^X(1-\theta)^{1-X}\end{aligned}$$

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Example usage

Bernoulli distribution $\mathrm{Ber}(X|\theta)$ can be used to model coin tosses.

Likelihood for binary classification

Under the assumption that data is independant and identically distributed (i.e., i.i.d.) the likelihood for the entire data is

$$\Pr(y|\mathbf{X}, \theta) = \prod_{i=1}^{N} h_\theta(\mathbf{x}^{(i)})^{y^{(i)}} \left(1 - h_\theta(\mathbf{x}^{(i)})\right)^{1-y^{(i)}}$$

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What form should $h_\theta(.)$ take?

Entropy

- Average level of information in a random variable.
- Given a discrete random variable X, which takes values in the alphabet $\mathcal{X}$ and is distributed according to $p : \mathcal{X} \to [0, 1]$:

$$H(X) = -\sum_{x \in \mathcal{X}} p(x) \log p(x) = \mathbb{E}_{x \sim p(x)}[-\log p(x)]$$

- Choice of base for $\log$ varies with applications
  - Base 2 gives the unit of bits or shannons
  - Base e gives units of nats
  - Base 10 gives units of dits, bans, or hartley

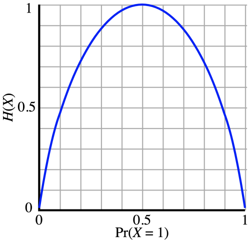


Figure from https://en.wikipedia.org/wiki/Entropy

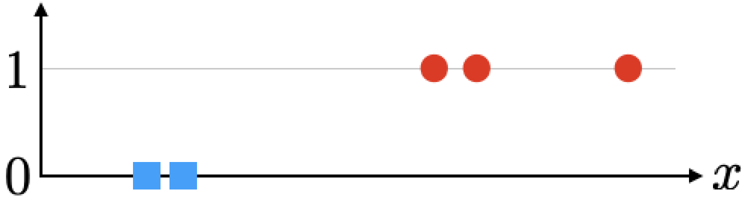
Cross entropy

- Cross-entropy beween two distributions p and q is a measure of the average number of bits needed to identify an event from a set $\mathcal{X}$ with true distribution p when the coding scheme used for the set is optimized for an estimated probability distribution q

$$H(p,q) = -\sum_{x \in \mathcal{X}} p(x) \log q(x) = -\mathbb{E}_{x \sim p(x)}[\log q(x)]$$

= - 0.2 * log 0.5 - 0.8 log 0.5

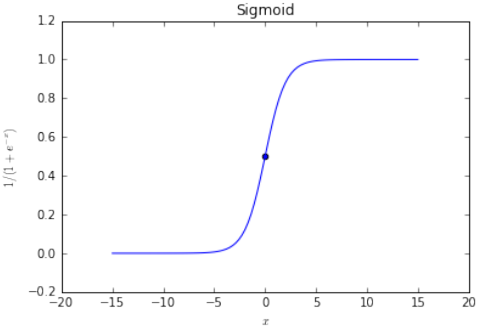
Lets consider a simple 1D case for binary classification



Sigmoid function

$\mathrm{sigm}(x)$ refers to a *sigmoid* function, also known as the *logistic* or *logit* function.

$$\mathrm{sigm}(x) = \frac{1}{1+e^{-x}} = \frac{e^x}{e^x+1}$$



Logistic regression

For logistic regression, we set $h_\theta(\mathbf{x}) = \mathrm{sigm}(\mathbf{x}^T\theta)$. So

$$\Pr(y|\mathbf{X},\theta) = \prod_{i=1}^{N} \left[\frac{1}{1+e^{-\mathbf{x}^{(i)T}\theta}}\right]^{y^{(i)}} \left[1 - \frac{1}{1+e^{-\mathbf{x}^{(i)T}\theta}}\right]^{1-y^{(i)}}$$

where

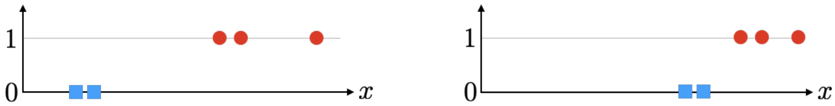
$$\mathbf{x}^T\theta = \theta_0 + \sum_{i=1}^{M} \theta_i \mathbf{x}_i$$

.

Sigmoid function

$$\Pr(y|x,\theta) = \left[\frac{1}{1+e^{-(\theta_0+\theta_1 x)}}\right]^y \left[1 - \frac{1}{1+e^{-(\theta_0+\theta_1 x)}}\right]^{1-y}$$

- $\theta = (\theta_0, \theta_1)$ are model parameters.
- θ_0 controls the shift.
- θ_1 controls the scale (how steep is the slope of the sigmoid function).



MLE for logistic regression (1)

Likelihood

$$L(\theta) = \Pr(y|\mathbf{X}, \theta)$$

Negative log-likelihood

$$\begin{aligned} l(\theta) &= -\log L(\theta) \\ &= -\sum_{i=1}^{N} y^{(i)} \log h_\theta(\mathbf{x}^{(i)}) + (1 - y^{(i)}) \log(1 - h_\theta(\mathbf{x}^{(i)})) \end{aligned}$$

We prefer to work in the log domain for mathematical convenience. Plus there are numerical advantages of working in the log domain.

MLE for logistic regression (2)

Goal

Our goal is to find parameters θ that maximize the likelihood (or minimize the negative log-likelihood).

$$\theta^* = \arg\min_{\theta} l(\theta)$$

Derivative of sigmoid

$$
\begin{aligned}
\frac{d}{dx}\mathrm{sigm}(x) &= \frac{d}{dx}\frac{1}{1+e^{-x}} \\
&= \frac{-(-1)e^{-x}}{(1+e^{-x})^2} \\
&= \left(\frac{e^{-x}}{1+e^{-x}}\right)\left(\frac{1}{1+e^{-x}}\right) \\
&= \left(\frac{1-1+e^{-x}}{1+e^{-x}}\right)\left(\frac{1}{1+e^{-x}}\right) \\
&= \left(1-\frac{1}{1+e^{-x}}\right)\left(\frac{1}{1+e^{-x}}\right) \\
&= (1-\mathrm{sigm}(x))\,\mathrm{sigm}(x)
\end{aligned}
$$

Gradient of a sigmoid w.r.t. θ

We know that

$$\frac{d}{dx}\mathrm{sigm}(x) = (1 - \mathrm{sigm}(x))\,\mathrm{sigm}(x)$$

It follows

$$\frac{d}{d\theta}\mathrm{sigm}(\mathbf{x}^T\theta) = \Big(1 - \mathrm{sigm}(\mathbf{x}^T\theta)\Big)\,\mathrm{sigm}(\mathbf{x}^T\theta)\mathbf{x}$$

MLE for logistic regression

Negative log likelihood contribution by sample i

$$
\begin{aligned}
l^{(i)}(\theta) = & - y^{(i)} \log h_\theta(\mathbf{x}^{(i)}) \\
& - (1 - y^{(i)}) \log(1 - h_\theta(\mathbf{x}^{(i)}))
\end{aligned}
$$

MLE for logistic regression

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Gradient of $l^{(i)}(\theta)$:

$$\nabla_\theta l^{(i)} = ?$$

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Gradient of $l^{(i)}(\theta)$:

$$\nabla_\theta l^{(i)} = ?$$

MLE for logistic regression

Notation change

- Replacing $\mathrm{sigm}(\mathbf{x}^{(i)^T})$ with s
- Replacing $y^{(i)}$ with y
- Replacing $\mathbf{x}^{(i)}$ with $\mathbf{x}$

$$\nabla_\theta l^{(i)} = \nabla_\theta \left[-y \log s - (1-y)\log(1-s) \right]$$

MLE for logistic regression

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$$\begin{aligned}\nabla_\theta l^{(i)} =& \nabla_\theta \left[-y \log s - (1-y)\log(1-s)\right] \\ =& -y\frac{s(1-s)\mathbf{x}}{s} - (1-y)\frac{s(1-s)\mathbf{x}}{1-s}\end{aligned}$$

MLE for logistic regression

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=& -y\frac{s(1-s)\mathbf{x}}{s} - (1-y)\frac{s(1-s)\mathbf{x}}{1-s} \\
=& -y\mathbf{x} + ys\mathbf{x} - s\mathbf{x} - ys\mathbf{x}
\end{aligned}
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MLE for logistic regression

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=& -y\mathbf{x} - s\mathbf{x} \\
=& -\mathbf{x}(y-s)
\end{aligned}
$$

Therefore (after fixing the notation),

$$\nabla_\theta l^{(i)} = -\mathbf{x}^{(i)}(y^{(i)} - h_\theta(\mathbf{x}^{(i)}))$$

MLE for logistic regression

Gradient of $l(\theta)$ for ith example

$$\nabla_\theta l^{(i)} = -\mathbf{x}^{(i)}(y^{(i)} - h_\theta(\mathbf{x}^{(i)}))$$

Stochastic gradient descent rule

$$\theta^{(k+1)} = \theta^{(k)} - \eta \nabla l^{(i)}(\theta)$$

MLE for logistic regression

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MLE for logistic regression

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&= \theta^{(k)} + \eta \mathbf{x}^{(i)}(y^{(i)} - h_\theta(\mathbf{x}^{(i)})) \\
&= \theta^{(k)} + \eta \mathbf{x}^{(i)}(y^{(i)} - \mathrm{sigm}({\mathbf{x}^{(i)}}^T \theta)),
\end{aligned}$$

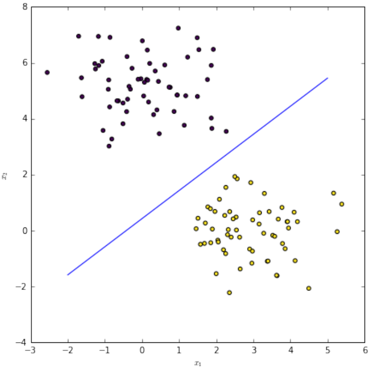
where η is the learning rate and k refers the the gradient descent iteration (step).

Logistic regression for binary classification

Given a point $\mathbf{x}^{(*)}$, classify using the following rule

$$y^{(*)} = \begin{cases} 1 & \text{if } \Pr(y|\mathbf{x}^{(*)}, \theta) \geq 0.5 \\ 0 & \text{otherwise} \end{cases}$$

The decision boundary is $\mathbf{x}^T\theta = 0$. Recall that this is where the sigmoid function is 0.5.



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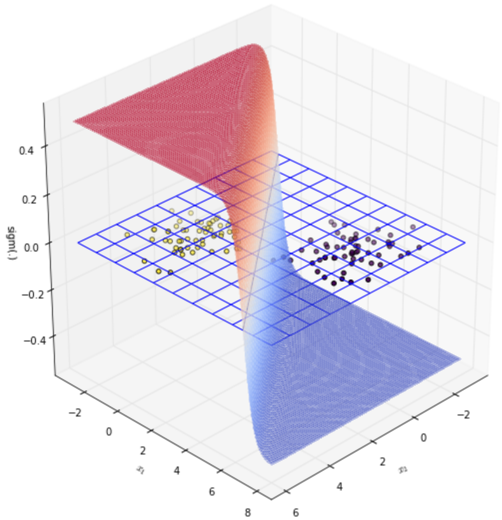
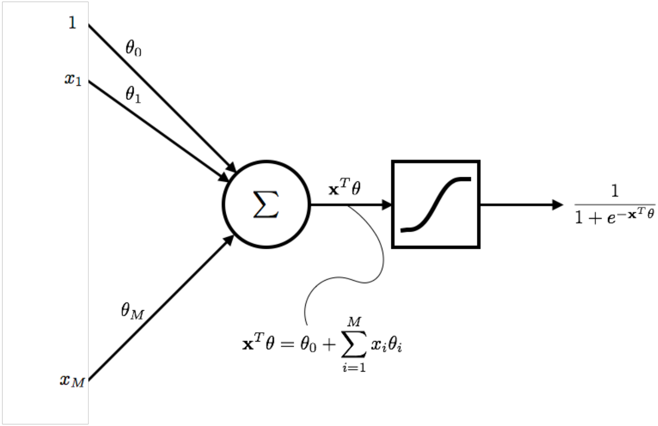


Network view of logisitc regression

- By changing the activation function to sigmoid and using the cross-entropy loss instead the least-squares loss that we use for linear regression, we are able to perform binary classification.



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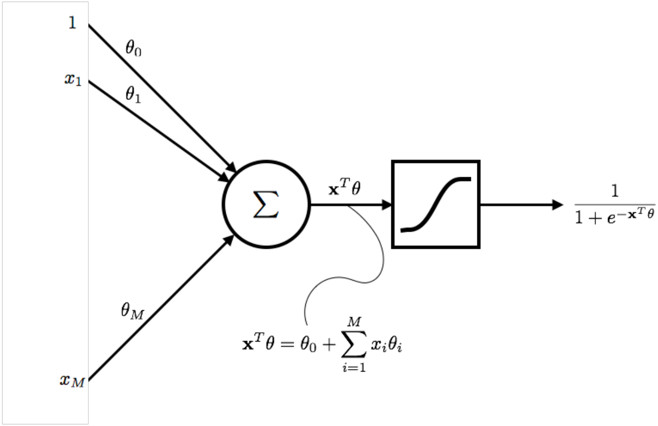

Artificial neuron

Summary

- We looked at logisitc regression, a binary classifier.
- Bernoulli distribution

Summary

- We looked at logisitc regression, a binary classifier.
- Bernoulli distribution
- Linear regression and logistic regression topics provide an excellent opportunity to study and understand the concepts underpinning neural networks

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