Logistic Regression

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Logistic Regression (LR)

- LR builds up on a linear model, composed with a sigmoid function

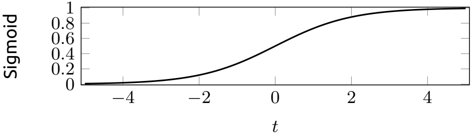
$$p(y \mid \mathbf{w}, \mathbf{x}) = \text{Bernoulli}(\text{sigmoid}(\mathbf{w} \cdot \mathbf{x}))$$

- $Z \sim \text{Bernoulli}(\theta)$

$$Z = \begin{cases} 1 & \text{with probability } \theta \\ 0 & \text{with probability } 1 - \theta \end{cases}$$

- Recall that the sigmoid function is defined by:

$$\text{sigmoid}(t) = \frac{1}{1 + e^{-t}}$$



- As we did in the case of linear models, we assume $x_0 = 1$ for all datapoints, so we do not need to handle the bias term w_0 separately

Prediction Using Logistic Regression

Suppose we have estimated the model parameters $\mathbf{w} \in \mathbb{R}^D$

For a new datapoint $\mathbf{x}_{\text{new}}$, the model gives us the probability

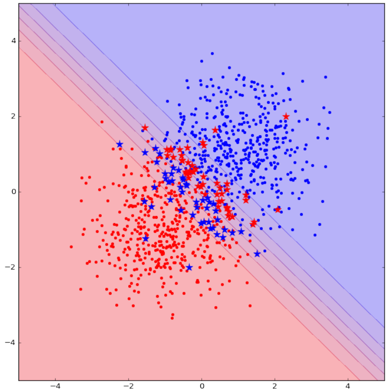
$$p(y_{\text{new}} = 1 \mid \mathbf{x}_{\text{new}}, \mathbf{w}) = \text{sigmoid}(\mathbf{w} \cdot \mathbf{x}_{\text{new}}) = \frac{1}{1 + \exp(-\mathbf{x}_{\text{new}} \cdot \mathbf{w})}$$

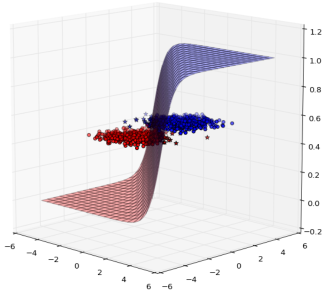
In order to make a prediction we can simply use a threshold at $\frac{1}{2}$

$$\widehat{y}_{\text{new}} = \mathbb{I}(\text{sigmoid}(\mathbf{w} \cdot \mathbf{x}_{\text{new}}) \ \geq \ \frac{1}{2}) = \mathbb{I}(\mathbf{w} \cdot \mathbf{x}_{\text{new}} \geq 0)$$

Class boundary is linear (separating hyperplane)

Prediction Using Logistic Regression





Likelihood of Logistic Regression

Data $\mathcal{D} = \langle(\mathbf{x}_i, y_i)\rangle_{i=1}^N$, where $\mathbf{x}_i \in \mathbb{R}^D$ and $y_i \in \{0, 1\}$.

Let us denote the sigmoid function by σ.

We can write the likelihood of observing the data given model parameters $\mathbf{w}$ as

$$p(\mathbf{y} \mid \mathbf{X}, \mathbf{w}) = \prod_{i=1}^{N} \sigma(\mathbf{w}^\mathsf{T}\mathbf{x}_i)^{y_i} \cdot (1 - \sigma(\mathbf{w}^\mathsf{T}\mathbf{x}_i))^{1-y_i}$$

Let us denote $\mu_i = \sigma(\mathbf{w}^\mathsf{T}\mathbf{x}_i)$.

We can write the negative log-likelihood as

$$\mathrm{NLL}(\mathbf{y} \mid \mathbf{X}, \mathbf{w}) = -\sum_{i=1}^{N}(y_i \log \mu_i + (1 - y_i) \log(1 - \mu_i))$$

Likelihood of Logistic Regression

Recall that $\mu_i = \sigma(\mathbf{w}^\mathsf{T}\mathbf{x}_i)$ and the negative log-likelihood is

$$\mathrm{NLL}(\mathbf{y} \mid \mathbf{X}, \mathbf{w}) = -\sum_{i=1}^{N}(y_i \log \mu_i + (1 - y_i)\log(1 - \mu_i))$$

Let us focus on a single datapoint, the contribution to the negative log-likelihood is

$$\mathrm{NLL}(y_i \mid \mathbf{x}_i, \mathbf{w}) = -(y_i \log \mu_i + (1 - y_i)\log(1 - \mu_i))$$

This is basically the cross-entropy between y_i and μ_i

If $y_i = 1$, then as

- As $\mu_i \to 1$, $\mathrm{NLL}(y_i \mid \mathbf{x}_i, \mathbf{w}) \to 0$
- As $\mu_i \to 0$, $\mathrm{NLL}(y_i \mid \mathbf{x}_i, \mathbf{w}) \to \infty$

Maximum Likelihood Estimate for LR

Recall that $\mu_i = \sigma(\mathbf{w}^\mathsf{T}\mathbf{x}_i)$ and the negative log-likelihood is

$$\mathrm{NLL}(\mathbf{y} \mid \mathbf{X}, \mathbf{w}) = -\sum_{i=1}^{N}(y_i \log \mu_i + (1 - y_i)\log(1 - \mu_i))$$

We can take the gradient with respect to $\mathbf{w}$

$$\nabla_{\mathbf{w}}\mathrm{NLL}(\mathbf{y} \mid \mathbf{X}, \mathbf{w}) = \sum_{i=1}^{N}\mathbf{x}_i(\mu_i - y_i) = \mathbf{X}^\mathsf{T}(\boldsymbol{\mu} - \mathbf{y})$$

And the Hessian is given by,

$$\mathbf{H} = \mathbf{X}^\mathsf{T}\mathbf{S}\mathbf{X}$$

$\mathbf{S}$ is a diagonal matrix where $S_{ii} = \mu_i(1 - \mu_i)$

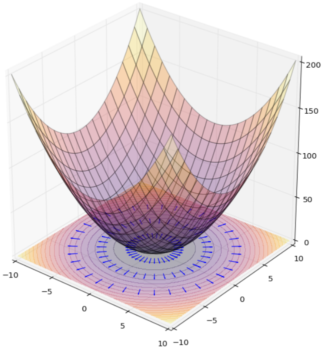
Calculus Background: Gradients

$$z = f(w_1, w_2) = \frac{w_1^2}{a^2} + \frac{w_2^2}{b^2}$$

$$\frac{\partial f}{\partial w_1} = \frac{2w_1}{a^2}$$

$$\frac{\partial f}{\partial w_2} = \frac{2w_2}{b^2}$$

$$\nabla_{\mathbf{w}} f = \begin{bmatrix} \frac{\partial f}{\partial w_1} \\ \frac{\partial f}{\partial w_2} \end{bmatrix} = \begin{bmatrix} \frac{2w_1}{a^2} \\ \frac{2w_2}{b^2} \end{bmatrix}$$



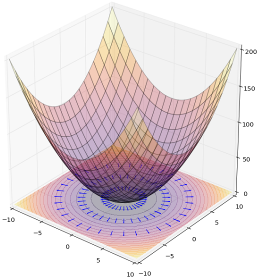
- Gradient vectors are orthogonal to contour curves
- Gradient points in the direction of steepest increase

Calculus Background: Hessians

$$z = f(w_1, w_2) = \frac{w_1^2}{a^2} + \frac{w_2^2}{b^2}$$

$$\nabla_{\mathbf{w}} f = \begin{bmatrix} \frac{\partial f}{\partial w_1} \\ \frac{\partial f}{\partial w_2} \end{bmatrix} = \begin{bmatrix} \frac{2w_1}{a^2} \\ \frac{2w_2}{b^2} \end{bmatrix}$$

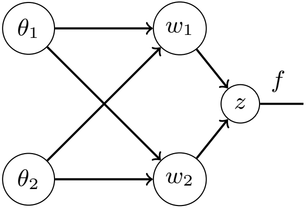
$$\mathbf{H} = \begin{bmatrix} \frac{\partial^2 f}{\partial w_1^2} & \frac{\partial^2 f}{\partial w_1 \partial w_2} \\ \frac{\partial^2 f}{\partial w_2 \partial w_1} & \frac{\partial^2 f}{\partial w_2^2} \end{bmatrix} = \begin{bmatrix} \frac{2}{a^2} & 0 \\ 0 & \frac{2}{b^2} \end{bmatrix}$$



- As long as all second derivates exist, the Hessian H is symmetric
- Hessian captures the curvature of the surface

Calculus Background: Chain Rule

$$z = f(w_1(\theta_1, \theta_2), w_2(\theta_1, \theta_2))$$



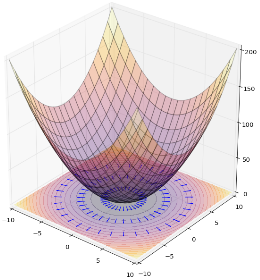
$$\frac{\partial f}{\partial \theta_1} = \frac{\partial f}{\partial w_1} \cdot \frac{\partial w_1}{\partial \theta_1} + \frac{\partial f}{\partial w_2} \cdot \frac{\partial w_2}{\partial \theta_1}$$

We will use this a lot when we study neural networks and back propagation

General Form for Gradient and Hessian

Suppose $\mathbf{w} \in \mathbb{R}^D$ and $f : \mathbb{R}^D \to \mathbb{R}$

The gradient vector contains all first order partial derivatives



$$\nabla_{\mathbf{w}} f(\mathbf{w}) = \begin{bmatrix} \frac{\partial f}{\partial w_1} \\ \frac{\partial f}{\partial w_2} \\ \vdots \\ \frac{\partial f}{\partial w_D} \end{bmatrix}$$

Hessian matrix of f contains all second order partial derivatives.

$$\mathbf{H} = \begin{bmatrix} \frac{\partial^2 f}{\partial w_1^2} & \frac{\partial^2 f}{\partial w_1 \partial w_2} & \cdots & \frac{\partial^2 f}{\partial w_1 \partial w_D} \\ \frac{\partial^2 f}{\partial w_2 \partial w_1} & \frac{\partial^2 f}{\partial w_2^2} & \cdots & \frac{\partial^2 f}{\partial w_2 \partial w_D} \\ \vdots & \vdots & \ddots & \vdots \\ \frac{\partial^2 f}{\partial w_D \partial w_1} & \frac{\partial^2 f}{\partial w_D \partial w_2} & \cdots & \frac{\partial^2 f}{\partial w_D^2} \end{bmatrix}$$

Gradient Descent Algorithm

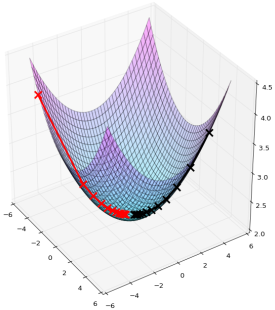
Gradient descent is one of the simplest, but very general algorithm for optimization

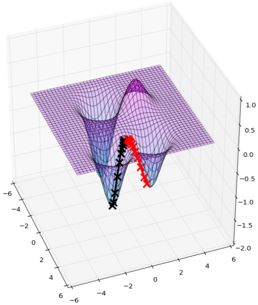
It is an iterative algorithm, producing a new $\mathbf{w}_{t+1}$ at each iteration as

$$\mathbf{w}_{t+1} = \mathbf{w}_t - \eta_t \mathbf{g}_t = \mathbf{w}_t - \eta_t \nabla f(\mathbf{w}_t)$$

We will denote the gradients by $\mathbf{g}_t$

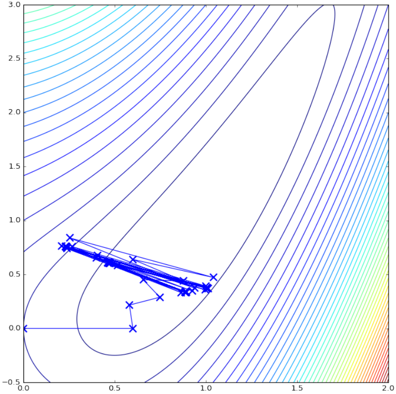
$\eta_t > 0$ is the learning rate or step size

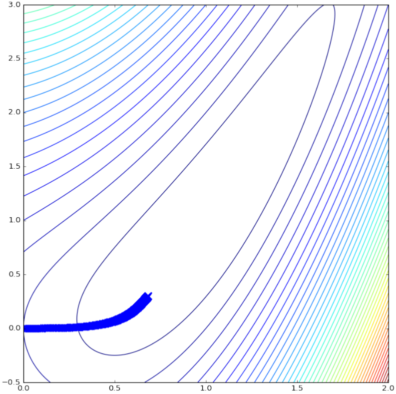




Choosing a Step Size

- Choosing a good step-size is important
- It step size is too large, algorithm may never converge
- If step size is too small, convergence may be very slow
- May want a time-varying step size





Iteratively reweighted least squares

- Gradient descent is a first order optimization method, which means it only uses **first order** gradients to navigate through the loss landscape. This can be slow, especially when some directions of space point steeply downhill, whereas other have a shallower gradient.
- In such problems, it can be much faster to use a **second order** optimization method, that takes the curvature of the space into account.
- The classic second-order method is **Newton's method**.

Iteratively Re-Weighted Least Squares (IRLS)

Depending on the dimension, we can apply Newton's method to estimate $\mathbf{w}$

Let $\mathbf{w}_t$ be the parameters after t Newton steps.

The gradient and Hessian are given by:

$$
\begin{aligned}
\mathbf{g}_t &= \mathbf{X}^\mathsf{T}(\boldsymbol{\mu}_t - \mathbf{y}) = -\mathbf{X}^\mathsf{T}(\mathbf{y} - \boldsymbol{\mu}_t) \\
\mathbf{H}_t &= \mathbf{X}^\mathsf{T}\mathbf{S}_t\mathbf{X}
\end{aligned}
$$

The Newton Update Rule is:

$$
\begin{aligned}
\mathbf{w}_{t+1} &= \mathbf{w}_t - \mathbf{H}_t^{-1}\mathbf{g}_t \\
&= \mathbf{w}_t + (\mathbf{X}^\mathsf{T}\mathbf{S}_t\mathbf{X})^{-1}\mathbf{X}^\mathsf{T}(\mathbf{y} - \boldsymbol{\mu}_t) \\
&= (\mathbf{X}^\mathsf{T}\mathbf{S}_t\mathbf{X})^{-1}\mathbf{X}^\mathsf{T}\mathbf{S}_t(\mathbf{X}\mathbf{w}_t + \mathbf{S}_t^{-1}(\mathbf{y} - \boldsymbol{\mu}_t)) \\
&= (\mathbf{X}^\mathsf{T}\mathbf{S}_t\mathbf{X})^{-1}\mathbf{X}^\mathsf{T}\mathbf{S}_t\mathbf{z}_t
\end{aligned}
$$

Where $\mathbf{z}_t = \mathbf{X}\mathbf{w}_t + \mathbf{S}_t^{-1}(\mathbf{y} - \boldsymbol{\mu}_t)$. Then $\mathbf{w}_{t+1}$ is a solution of the following:

Weighted Least Squares Problem

$$
\text{minimise} \quad \sum_{i=1}^{N} S_{t,ii}(z_{t,i} - \mathbf{w}^\mathsf{T}\mathbf{x}_i)^2
$$

Multiclass Logistic Regression

Multiclass logistic regression is also a discriminative classifier

Let the inputs be $\mathbf{x} \in \mathbb{R}^D$ and $y \in \{1, \ldots, C\}$

There are parameters $\mathbf{w}_c \in \mathbb{R}^D$ for every class $c = 1, \ldots, C$

We'll put this together in a matrix form $\mathbf{W}$ that is $D \times C$

The multiclass logistic model is given by:

$$p(y = c \mid \mathbf{x}, \mathbf{W}) = \frac{\exp(\mathbf{w}_c^\mathsf{T}\mathbf{x})}{\sum_{c'=1}^{C} \exp(\mathbf{w}_{c'}^\mathsf{T}\mathbf{x})}$$

Multiclass Logistic Regression

The multiclass logistic model is given by:

$$p(y = c \mid \mathbf{x}, \mathbf{W}) = \frac{\exp(\mathbf{w}_c^\mathsf{T}\mathbf{x})}{\sum_{c'=1}^{C} \exp(\mathbf{w}_{c'}^\mathsf{T}\mathbf{x})}$$

Recall the softmax function

Softmax

Softmax maps a set of numbers to a probability distribution with mode at the maximum

$$\mathrm{softmax}\left([a_1, \ldots, a_C]^\mathsf{T}\right) = \left[\frac{e^{a_1}}{Z}, \ldots, \frac{e^{a_C}}{Z}\right]^\mathsf{T}$$

where $Z = \sum_{c=1}^{C} e^{a_c}$.

The multiclass logistic model is simply:

$$p(y \mid \mathbf{x}, \mathbf{W}) = \mathrm{softmax}\left(\left[\mathbf{w}_1^\mathsf{T}\mathbf{x}, \ldots, \mathbf{w}_C^\mathsf{T}\mathbf{x}\right]^\mathsf{T}\right)$$

Multiclass Logistic Regression