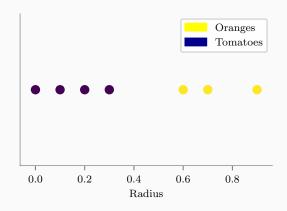
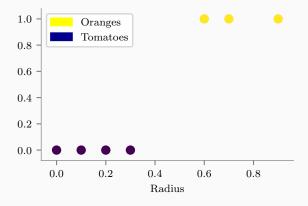
Logistic Regression

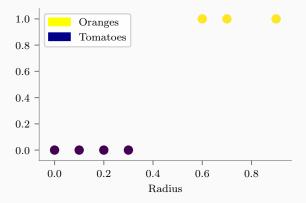
Nipun Batra

February 28, 2023

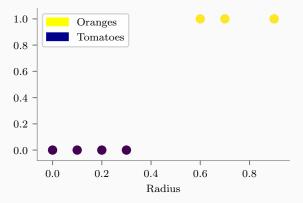
IIT Gandhinagar



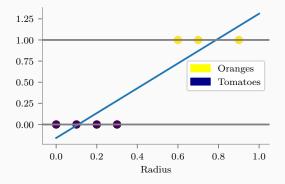




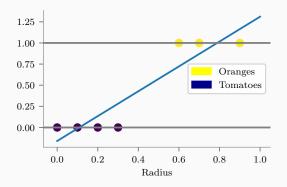
Aim: Probability(Orange | Radius) ? or



Aim: Probability(Orange | Radius) ? or More generally, P(y = 1|X = x)?



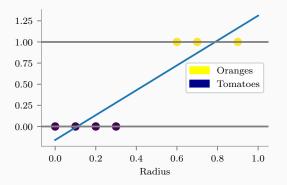
$$P(y = Orange | Radius = r) = \theta_0 + \theta_1 \times r$$



$$P(y = Orange|Radius = r) = \theta_0 + \theta_1 \times r$$

Generally,

$$P(y=1|x) = x^T \theta$$



$$P(y = Orange|Radius = r) = \theta_0 + \theta_1 \times r$$

Generally,

$$P(y=1|x) = x^T \theta$$

For N examples

$$P(\mathbf{y} = 1|X) = X\theta$$

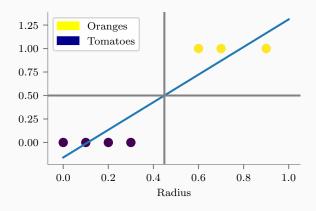
Prediction:

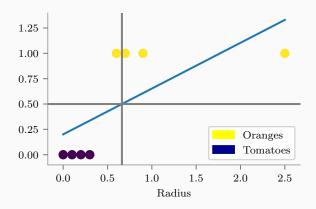
$$\begin{array}{c} \text{If } \theta_0 + \theta_1 \times \textit{Radius} > 0.5 \rightarrow \mathsf{Orange} \\ & \text{Else} \rightarrow \mathsf{Tomato} \end{array}$$

Problem:

Range of
$$X\theta$$
 is $(-\infty, \infty)$

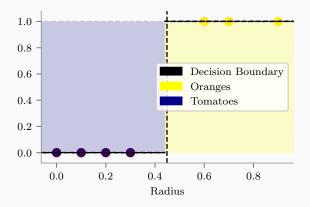
But
$$P(y = 1 | ...) \in [0, 1]$$





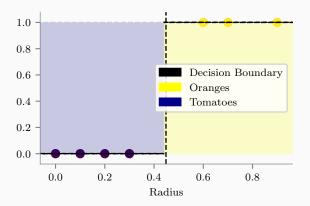
Linear regression for classification gives a poor prediction!

Ideal boundary

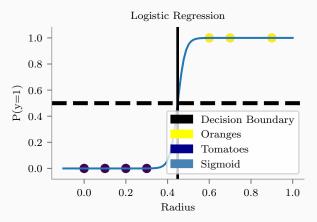


 Have a decision function similar to the above (but not so sharp and discontinuous)

Ideal boundary



- Have a decision function similar to the above (but not so sharp and discontinuous)
- Aim: use linear regression still!



Question. Can we still use Linear Regression? Answer. Yes! Transform $x^T\theta \to [0,1]$

$$x^T\theta \in (-\infty, \infty)$$

$$\phi = \text{Sigmoid / Logistic Function } (\sigma)$$

$$\phi(x^T\theta) \in [0, 1]$$

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

$$0.8 - \frac{1}{0.8} = \frac{1}{0.4}$$

$$0.2 - \frac{1}{0.0} = \frac{1}{0.0}$$

$$0.0 - \frac{1}{0.0} = \frac{1}{0.0}$$

$$0.0 - \frac{1}{0.0} = \frac{1}{0.0}$$



$$z \to \infty$$

 $\sigma(z) \to 1$

$$z \to \infty$$

$$\sigma(z) \to 1$$

$$z \to -\infty$$

$$z \to \infty$$
 $\sigma(z) \to 1$
 $z \to -\infty$
 $\sigma(z) \to 0$

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 $\sigma(z) \to 1$
 $z \to -\infty$
 $\sigma(z) \to 0$
 $z = 0$

$$z \to \infty$$
 $\sigma(z) \to 1$
 $z \to -\infty$
 $\sigma(z) \to 0$
 $z = 0$
 $\sigma(z) = 0.5$

Question. Could you use some other transformation (ϕ) of $x^T\theta$ s.t.

$$\phi(\mathbf{x}^T\theta) \in [0,1]$$

Yes! But Logistic Regression works.

$$P(y = 1|X) = \sigma(X\theta) = \frac{1}{1 + e^{-X\theta}}$$

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$$P(y = 0|X) = 1 - P(y = 1|X) = 1 - \frac{1}{1 + e^{-X\theta}} = \frac{e^{-X\theta}}{1 + e^{-X\theta}}$$

$$P(y = 1|X) = \sigma(X\theta) = \frac{1}{1 + e^{-X\theta}}$$

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$$\therefore \frac{P(y=1|X)}{1-P(y=1|X)} = e^{X\theta} \implies X\theta = \log \frac{P(y=1|X)}{1-P(y=1|X)}$$

Odds (Used in betting)

$$\frac{P(win)}{P(loss)}$$

Here,

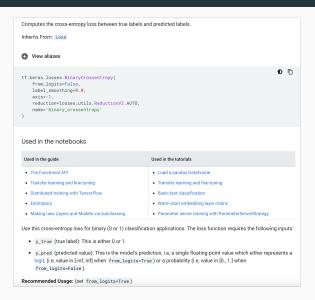
$$Odds = \frac{P(y=1)}{P(y=0)}$$

$$\mathsf{logits} = \mathsf{log\text{-}odds} = \mathsf{log}\,\frac{P(y=1)}{P(y=0)} = X\theta$$

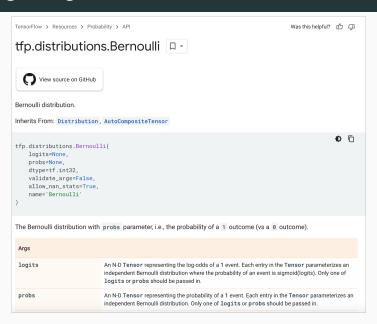
Logits Usage



Logits Usage



Logits Usage



Logistic Regression

 $\ensuremath{\mathsf{Q}}.$ What is decision boundary for Logistic Regression?

Logistic Regression

Q. What is decision boundary for Logistic Regression? Decision Boundary: P(y=1|X)=P(y=0|X) or $\frac{1}{1+e^{-X\theta}}=\frac{e^{-X\theta}}{1+e^{-X\theta}}$ or $e^{X\theta}=1$ or $X\theta=0$

Example with 2 input features

Notebook:

https://nipunbatra.github.io/ml2023/notebooks/posts/logistic.html

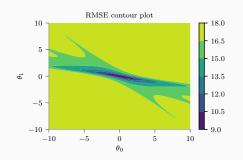
Learning Parameters

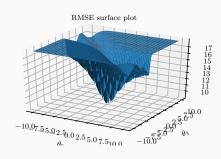
Could we use cost function as:

$$J(\theta) = \sum (y_i - \hat{y}_i)^2$$
$$\hat{y}_i = \sigma(X\theta)$$

Answer: No (Non-Convex)
(See Jupyter Notebook)

Cost function convexity





Learning Parameters

Likelihood =
$$P(D|\theta)$$

 $P(y|X,\theta) = \prod_{i=1}^{n} P(y_i|x_i,\theta)$
where y = 0 or 1

 $\mathsf{Likelihood} = P(D|\theta)$

$$P(y|X,\theta) = \prod_{i=1}^{n} P(y_i|x_i,\theta)$$

$$= \prod_{i=1}^{n} \left\{ \frac{1}{1 + e^{-x_i^T \theta}} \right\}^{y_i} \left\{ 1 - \frac{1}{1 + e^{-x_i^T \theta}} \right\}^{1 - y_i}$$

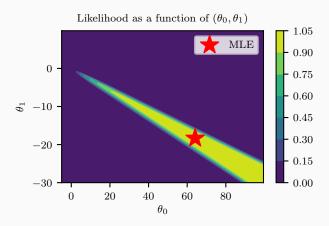
[Above: Similar to $P(D|\theta)$ for Linear Regression;

Difference Bernoulli instead of Gaussian]

$$-\log P(y|X,\theta) = \text{Negative Log Likelihood}$$

= Cost function will be minimising
= $J(\theta)$

Likelihood Visualisation



 Assume you have a coin and flip it ten times and get (H, H, T, T, T, H, H, T, T, T).

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- ullet Idea find MLE estimate for heta

•
$$p(H) = \theta$$
 and $p(T) = 1 - \theta$

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- $\frac{\partial \mathcal{LL}(\theta)}{\partial \theta} = 0 \implies \frac{n_h}{\theta} + \frac{n_t}{1-\theta} = 0 \implies \theta_{MLE} = \frac{n_h}{n_h + n_t}$

$$J(\theta) = -\log\left\{\prod_{i=1}^{n}\left\{\frac{1}{1 + e^{-x_i^T\theta}}\right\}^{y_i}\left\{1 - \frac{1}{1 + e^{-x_i^T\theta}}\right\}^{1 - y_i}\right\}$$

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This cost function is called cross-entropy.

Why?

What is the interpretation of the cost function?

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Let us try to write the cost function for a single example:

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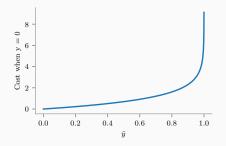
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What is the interpretation of the cost function?

Let us try to write the cost function for a single example:

$$J(\theta) = -y_i \log \hat{y}_i - (1 - y_i) \log(1 - \hat{y}_i)$$

First, assume y_i is 0, then if \hat{y}_i is 0, the loss is 0; but, if \hat{y}_i is 1, the loss tends towards infinity!



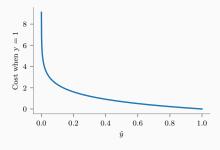
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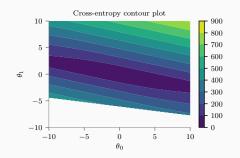
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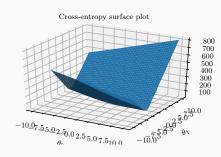
$$J(\theta) = -y_i \log \hat{y}_i - (1 - y_i) \log(1 - \hat{y}_i)$$

Now, assume y_i is 1, then if \hat{y}_i is 0, the loss is huge; but, if \hat{y}_i is 1, the loss is zero!



Cost function convexity





$$\begin{split} \frac{\partial J(\theta)}{\partial \theta_j} &= -\frac{\partial}{\partial \theta_j} \left\{ \sum_{i=1}^n y_i \log(\sigma_{\theta}(x_i)) + (1 - y_i) \log(1 - \sigma_{\theta}(x_i)) \right\} \\ &= -\sum_{i=1}^n \left[y_i \frac{\partial}{\partial \theta_j} \log(\sigma_{\theta}(x_i)) + (1 - y_i) \frac{\partial}{\partial \theta_j} \log(1 - \sigma_{\theta}(x_i)) \right] \end{split}$$

$$\frac{\partial J(\theta)}{\partial \theta_j} = -\sum_{i=1}^n \left[y_i \frac{\partial}{\partial \theta_j} \log(\sigma_{\theta}(x_i)) + (1 - y_i) \frac{\partial}{\partial \theta_j} \log(1 - \sigma_{\theta}(x_i)) \right]$$

$$=-\sum_{i=1}^{n}\left[\frac{y_{i}}{\sigma_{\theta}(x_{i})}\frac{\partial}{\partial\theta_{j}}\sigma_{\theta}(x_{i})+\frac{1-y_{i}}{1-\sigma_{\theta}(x_{i})}\frac{\partial}{\partial\theta_{j}}(1-\sigma_{\theta}(x_{i}))\right] (1)$$

Aside:

$$\begin{split} \frac{\partial}{\partial z} \sigma(z) &= \frac{\partial}{\partial z} \frac{1}{1 + e^{-z}} = -(1 + e^{-z})^{-2} \frac{\partial}{\partial z} (1 + e^{-z}) \\ &= \frac{e^{-z}}{(1 + e^{-z})^2} = \left(\frac{1}{1 + e^{-z}}\right) \left(\frac{e^{-z}}{1 + e^{-z}}\right) = \sigma(z) \left\{\frac{1 + e^{-z}}{1 + e^{-z}} - \frac{1}{1 + e^{-z}}\right\} \\ &= \sigma(z) (1 - \sigma(z)) \end{split}$$

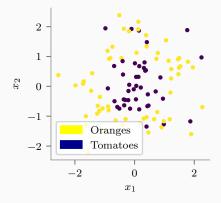
Resuming from (1)

$$\frac{\partial J(\theta)}{\partial \theta_{j}} = -\sum_{i=1}^{n} \left[\frac{y_{i}}{\sigma_{\theta}(x_{i})} \frac{\partial}{\partial \theta_{j}} \sigma_{\theta}(x_{i}) + \frac{1 - y_{i}}{1 - \sigma_{\theta}(x_{i})} \frac{\partial}{\partial \theta_{j}} (1 - \sigma_{\theta}(x_{i})) \right]
= -\sum_{i=1}^{n} \left[\frac{y_{i}\sigma_{\theta}(x_{i})}{\sigma_{\theta}(x_{i})} (1 - \sigma_{\theta}(x_{i})) \frac{\partial}{\partial \theta_{j}} (x_{i}\theta) + \frac{1 - y_{i}}{1 - \sigma_{\theta}(x_{i})} (1 - \sigma_{\theta}(x_{i})) \frac{\partial}{\partial \theta_{j}} (1 - \sigma_{\theta}(x_{i})) \right]
= -\sum_{i=1}^{n} \left[y_{i} (1 - \sigma_{\theta}(x_{i})) x_{i}^{j} - (1 - y_{i}) \sigma_{\theta}(x_{i}) x_{i}^{j} \right]
= -\sum_{i=1}^{n} \left[(y_{i} - y_{i}\sigma_{\theta}(x_{i}) - \sigma_{\theta}(x_{i}) + y_{i}\sigma_{\theta}(x_{i})) x_{i}^{j} \right]
= \sum_{i=1}^{n} \left[\sigma_{\theta}(x_{i}) - y_{i} \right] x_{i}^{j}$$

$$\frac{\partial J(\theta)}{\theta_j} = \sum_{i=1}^{N} \left[\sigma_{\theta}(x_i) - y_i \right] x_i^j$$

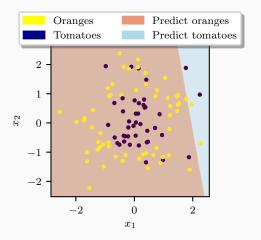
Now, just use Gradient Descent!

Logistic Regression with feature transformation



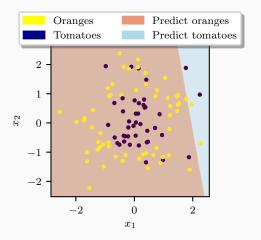
What happens if you apply logistic regression on the above data?

Logistic Regression with feature transformation



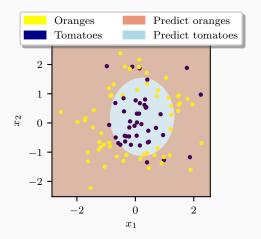
Linear boundary will not be accurate here. What is the technical name of the problem?

Logistic Regression with feature transformation



Linear boundary will not be accurate here. What is the technical name of the problem? Bias!

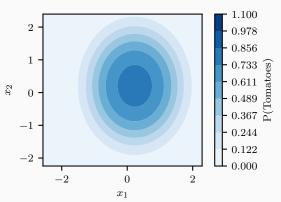
$$\phi(x) = \begin{bmatrix} \phi_0(x) \\ \phi_1(x) \\ \vdots \\ \phi_{K-1}(x) \end{bmatrix} = \begin{bmatrix} 1 \\ x \\ x^2 \\ x^3 \\ \vdots \\ x^{K-1} \end{bmatrix} \in \mathbb{R}^K$$

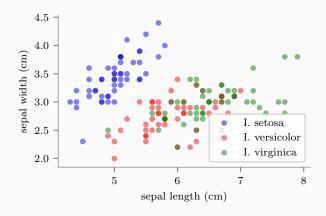


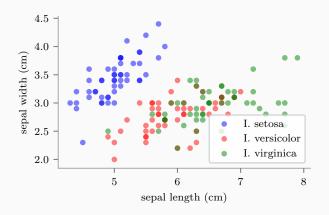
Using x_1^2, x_2^2 as additional features, we are able to learn a more accurate classifier.

How would you expect the probability contours look like?

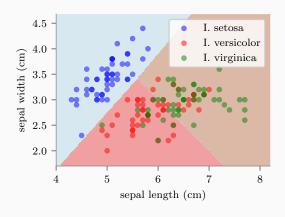
How would you expect the probability contours look like?

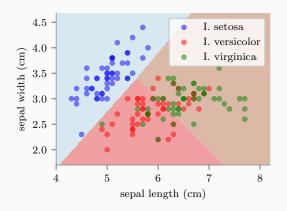




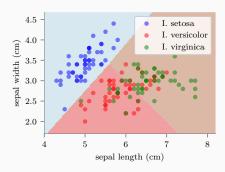


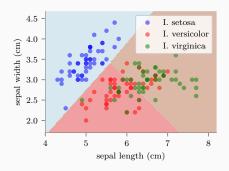
How would you learn a classifier? Or, how would you expect the classifier to learn decision boundaries?



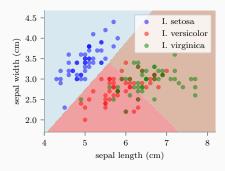


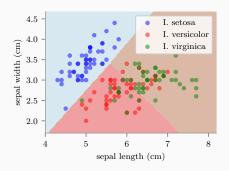
- 1. Use one-vs.-all on Binary Logistic Regression
- 2. Use one-vs.-one on Binary Logistic Regression
- 3. Extend <u>Binary</u> Logistic Regression to <u>Multi-Class</u> Logistic Regression





- 1. Learn P(setosa (class 1)) = $\mathcal{F}(X\theta_1)$
- 2. P(versicolor (class 2)) = $\mathcal{F}(X\theta_2)$
- 3. $P(\text{virginica (class 3)}) = \mathcal{F}(X\theta_3)$
- 4. Goal: Learn $\theta_i \forall i \in \{1, 2, 3\}$
- 5. Question: What could be an \mathcal{F} ?





- 1. Question: What could be an \mathcal{F} ?
- 2. Property: $\sum_{i=1}^{3} \mathcal{F}(X\theta_i) = 1$
- 3. Also $\mathcal{F}(z) \in [0,1]$
- 4. Also, $\mathcal{F}(z)$ has squashing proprties: $R\mapsto [0,1]$

Softmax

$$Z \in \mathbb{R}^d$$
 $\mathcal{F}(z_i) = \frac{e^{z_i}}{\sum_{i=1}^d e^{z_i}}$
 $\therefore \sum \mathcal{F}(z_i) = 1$

 $\mathcal{F}(z_i)$ refers to probability of class <u>i</u>

Softmax for Multi-Class Logistic Regression

$$k = \{1, \dots, k\} \text{classes}$$

$$\theta = \begin{bmatrix} \vdots & \vdots & \vdots & \vdots \\ \theta_1 & \theta_2 & \cdots & \theta_k \\ \vdots & \vdots & \vdots & \vdots \end{bmatrix}$$

$$P(y = k | X, \theta) = \frac{e^{X\theta_k}}{\sum_{k=1}^K e^{X\theta_k}}$$

Softmax for Multi-Class Logistic Regression

For K = 2 classes,

$$P(y = k|X, \theta) = \frac{e^{X\theta_k}}{\sum_{k=1}^{K} e^{X\theta_k}}$$

$$P(y = 0|X, \theta) = \frac{e^{X\theta_0}}{e^{X\theta_0} + e^{X\theta_1}}$$

$$P(y = 1|X, \theta) = \frac{e^{X\theta_1}}{e^{X\theta_0} + e^{X\theta_1}} = \frac{e^{X\theta_1}}{e^{X\theta_1}\{1 + e^{X(\theta_0 - \theta_1)}\}}$$

$$= \frac{1}{1 + e^{-X\theta'}}$$
= Sigmoid!

Assume our prediction and ground truth for the three classes for i^{th} point is:

$$\hat{y}_i = \begin{bmatrix} 0.1\\0.8\\0.1 \end{bmatrix} = \begin{bmatrix} \hat{y}_i^1\\\hat{y}_i^2\\\hat{y}_i^3 \end{bmatrix}$$

$$y_i = \begin{bmatrix} 0 \\ 1 \\ 0 \end{bmatrix} = \begin{bmatrix} y_i^1 \\ y_i^2 \\ y_i^3 \end{bmatrix}$$

meaning the true class is Class #2

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Let us calculate
$$-\sum_{k=1}^{3} y_i^k \log \hat{y}_i^k$$

$$= -(0 \times \log(0.1) + 1 \times \log(0.8) + 0 \times \log(0.1))$$

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Tends to zero

Assume our prediction and ground truth for the three classes for i^{th} point is:

$$\hat{y}_i = \begin{bmatrix} 0.3 \\ 0.4 \\ 0.3 \end{bmatrix} = \begin{bmatrix} \hat{y}_i^1 \\ \hat{y}_i^2 \\ \hat{y}_i^3 \end{bmatrix}$$

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$$= -(0 \times \log(0.1) + 1 \times \log(0.4) + 0 \times \log(0.1))$$

High number! Huge penalty for misclassification!

For 2 class we had:

$$J(\theta) = -\left\{\sum_{i=1}^{n} y_i \log(\sigma_{\theta}(x_i)) + (1 - y_i) \log(1 - \sigma_{\theta}(x_i))\right\}$$

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More generally,

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Extend to K-class:

$$J(\theta) = -\left\{\sum_{i=1}^{n} \sum_{k=1}^{K} y_i^k \log(\hat{y}_i^k)\right\}$$

Now:

$$\frac{\partial J(\theta)}{\partial \theta_k} = \sum_{i=1}^n \left[x_i \left\{ I(y_i = k) - P(y_i = k | x_i, \theta) \right\} \right]$$

Hessian Matrix

The Hessian matrix of f(.) with respect to θ , written $\nabla_{\theta}^2 f(\theta)$ or simply as \mathbb{H} , is the $d \times d$ matrix of partial derivatives,

$$\nabla_{\theta}^{2} f(\theta) = \begin{bmatrix} \frac{\partial^{2} f(\theta)}{\partial \theta_{1}^{2}} & \frac{\partial^{2} f(\theta)}{\partial \theta_{1} \partial \theta_{2}} & \cdots & \frac{\partial^{2} f(\theta)}{\partial \theta_{1} \partial \theta_{n}} \\ \frac{\partial^{2} f(\theta)}{\partial \theta_{2} \partial \theta_{1}} & \frac{\partial^{2} f(\theta)}{\partial \theta_{2}^{2}} & \cdots & \frac{\partial^{2} f(\theta)}{\partial \theta_{2} \partial \theta_{n}} \\ \vdots & \vdots & \ddots & \vdots \\ \frac{\partial^{2} f(\theta)}{\partial \theta_{n} \partial \theta_{1}} & \frac{\partial^{2} f(\theta)}{\partial \theta_{n} \partial \theta_{2}} & \cdots & \frac{\partial^{2} f(\theta)}{\partial \theta_{n}^{2}} \end{bmatrix}$$

Newton's Algorithm

The most basic second-order optimization algorithm is Newton's algorithm, which consists of updates of the form,

$$\theta_{k+1} = \theta_k - \mathbb{H}^1_k g_k$$

where g_k is the gradient at step k. This algorithm is derived by making a second-order Taylor series approximation of $f(\theta)$ around θ_k :

$$f_{quad}(\theta) = f(\theta_k) + g_k^T(\theta - \theta_k) + \frac{1}{2}(\theta - \theta_k)^T \mathbb{H}_k(\theta - \theta_k)$$

differentiating and equating to zero to solve for θ_{k+1} .

Learning Parameters

Now assume:

$$g(\theta) = \sum_{i=1}^{n} \left[\sigma_{\theta}(x_i) - y_i \right] x_i^j = \mathbf{X}^{\mathsf{T}} (\sigma_{\theta}(\mathbf{X}) - \mathbf{y})$$
$$\pi_i = \sigma_{\theta}(x_i)$$

Let \mathbb{H} represent the Hessian of $J(\theta)$

$$\mathbb{H} = \frac{\partial}{\partial \theta} g(\theta) = \frac{\partial}{\partial \theta} \sum_{i=1}^{n} \left[\sigma_{\theta}(x_{i}) - y_{i} \right] x_{i}^{j}$$

$$= \sum_{i=1}^{n} \left[\frac{\partial}{\partial \theta} \sigma_{\theta}(x_{i}) x_{i}^{j} - \frac{\partial}{\partial \theta} y_{i} x_{i}^{j} \right]$$

$$= \sum_{i=1}^{n} \sigma_{\theta}(x_{i}) (1 - \sigma_{\theta}(x_{i})) x_{i} x_{i}^{T}$$

$$= \mathbf{X}^{\mathsf{T}} \operatorname{diag}(\sigma_{\theta}(x_{i}) (1 - \sigma_{\theta}(x_{i}))) \mathbf{X}$$

Iteratively reweighted least squares (IRLS)

For binary logistic regression, recall that the gradient and Hessian of the negative log-likelihood are given by:

$$g(\theta)_k = \mathbf{X}^{\mathsf{T}}(\pi_{\mathbf{k}} - \mathbf{y})$$

$$\mathbf{H}_k = \mathbf{X}^{\mathsf{T}} S_k \mathbf{X}$$

$$\mathbf{S}_k = diag(\pi_{1k}(1 - \pi_{1k}), \dots, \pi_{nk}(1 - \pi_{nk}))$$

$$\pi_{ik} = sigm(\mathbf{x}_i \theta_{\mathbf{k}})$$

The Newton update at iteraion k + 1 for this model is as follows:

$$\theta_{k+1} = \theta_k - \mathbb{H}^{-1} g_k$$

$$= \theta_k + (X^T S_k X)^{-1} X^T (y - \pi_k)$$

$$= (X^T S_k X)^{-1} [(X^T S_k X) \theta_k + X^T (y - \pi_k)]$$

$$= (X^T S_k X)^{-1} X^T [S_k X \theta_k + y - \pi_k]$$

Regularized Logistic Regression

Unregularised:

$$J_1(\theta) = -\left\{\sum_{i=1}^n y_i \log(\sigma_{\theta}(x_i)) + (1 - y_i) \log(1 - \sigma_{\theta}(x_i))\right\}$$

L2 Regularization:

$$J(\theta) = J_1(\theta) + \lambda \theta^T \theta$$

L1 Regularization:

$$J(\theta) = J_1(\theta) + \lambda |\theta|$$