Machine Learning - Waseda University
Logistic Regression

AD

June 2011

Introduction

- Assume you are given some training data $\left\{\mathbf{x}^i, y^i\right\}_{i=1}^N$ where $\mathbf{x}^i \in \mathbb{R}^d$ and y^i can take C different values.
- Given an input test data $\mathbf{x}$, you want to predict/estimate the output y associated to $\mathbf{x}$.
- A common approach consists of using

$$p\left(y=k \mid \mathbf{x}\right)=\frac{p\left(\mathbf{x} \mid y=k\right) p\left(y=k\right)}{\sum_{j=0}^{C-1} p\left(\mathbf{x} \mid y=j\right) p\left(y=j\right)}.$$

- This requires modelling and learning the parameters of the class conditional density of features $p\left(\mathbf{x} \mid y=k\right)$.
- This can be tedious for complicated problems.

Logistic Regression

- Discriminative model: we model and learn directly $p(y = k|\mathbf{x})$ and bypassing the introduction of $p(\mathbf{x}|y = k)$.
- Consider the following model for $C = 2$ (binary classification)

$$\begin{aligned} p(y = 1|\mathbf{x}, \mathbf{w}) &= 1 - p(y = 0|\mathbf{x}, \mathbf{w}) \\ &= g\left(\mathbf{w}^{\mathsf{T}}\mathbf{x}\right) \end{aligned}$$

where $\mathbf{w} = (w_0 \ \cdots \ w_d)^{\mathsf{T}}$, $\mathbf{x} = (x_0 \ \cdots \ x_d)^{\mathsf{T}}$ so

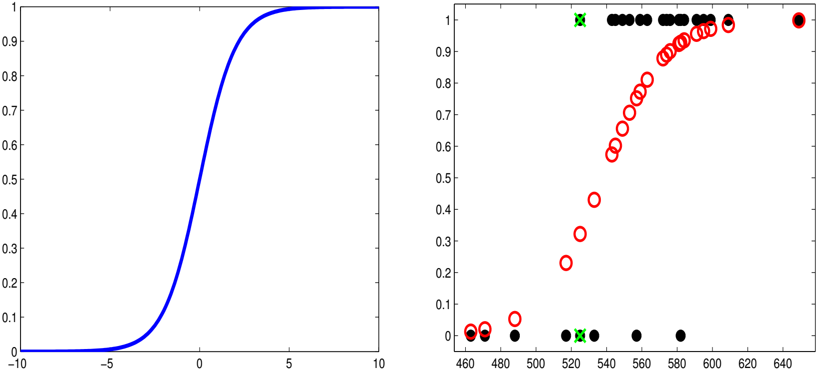
$$z = \mathbf{w}^{\mathsf{T}}\mathbf{x} = w_0 + \sum_{j=1}^{d} w_j x_j$$

and g is a "squashing" function: $g : \mathbb{R} \to [0, 1]$.

- Logistic regression corresponds to

$$g(z) = \frac{1}{1 + \exp(-z)} = \frac{\exp(z)}{1 + \exp(z)}.$$

Logistic Function



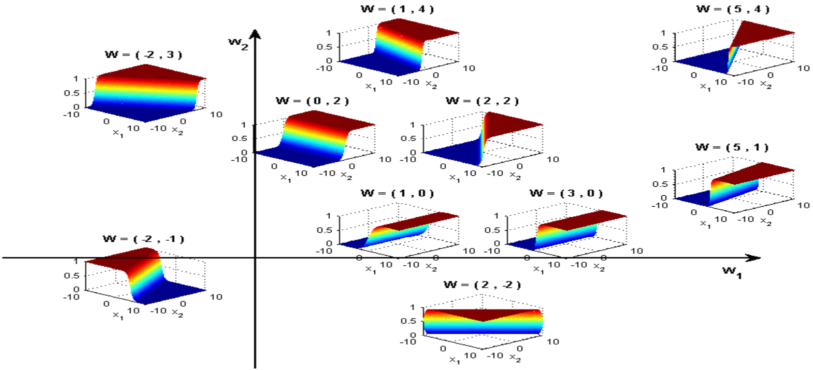
(Left) logistic or sigmoid function (Right) logistic regression for x=SAT score and y=pass/fail class (solid black dots are the data), open red circles are predicted probabilities.

Logistic Regression

- The log odds ratio satisfies

$$LOR(\mathbf{x}) = \log \frac{p(y=1|\mathbf{x},\mathbf{w})}{p(y=0|\mathbf{x},\mathbf{w})} = \mathbf{w}^{\mathsf{T}}\mathbf{x}$$

  so the logistic parameters are easily interpretable.
- If $w_j > 0$, then increasing x_j makes $y = 1$ more likely while decreasing x_j makes $y = 0$ more likely (and opposite if $w_j = 0$). $w_j = 0$ means x_j has no impact on the outcome.
- Logistic regression partitions the input space into two regions whose decision boundary is $\{\mathbf{x} : LOR(\mathbf{x}) = 0\} = \{\mathbf{x} : \mathbf{w}^{\mathsf{T}}\mathbf{x} = 0\}$
- Simple model of a neuron: it forms a weighted sum of its inputs and the "fires" an output pulse if this sum exceeds a threshold. Logistic regression mimics this as you can sort of think of it as a process which "fires" if $p(y=1|\mathbf{x},\mathbf{w}) > p(y=0|\mathbf{x},\mathbf{w})$ equivalently if $LOR(\mathbf{x}) > 0$.



Plots of $p\left(y=1 | w_1 x_1 + w_2 x_2\right)$. Here $\mathbf{w} = (w_1, w_2)$ define the normal to the decision boundary. Points to the right have $\mathbf{w}^T\mathbf{x} > 0$ and to the left have $\mathbf{w}^T\mathbf{x} < 0$.

Using Basis Functions for Logistic Regression

- Similarly to regression, we can use basis functions; i.e.

$$p\left(y=1|\,\mathbf{x},\mathbf{w}\right)=g\left(\mathbf{w}^{\mathsf{T}}\Phi\left(\mathbf{x}\right)\right)$$

where $\mathbf{w}=\left(w_1 \;\; \cdots \;\; w_m\right)^{\mathsf{T}}$, $\Phi\left(\mathbf{x}\right)=\left(\Phi_1\left(\mathbf{x}\right) \;\; \cdots \;\; \Phi_m\left(\mathbf{x}\right)\right)^{\mathsf{T}}$.

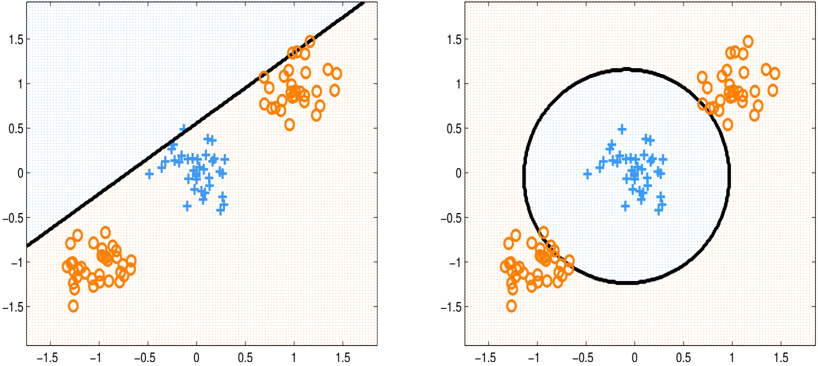
- For example, if $\mathbf{x}\in\mathbb{R}$ then we can pick

$$\Phi\left(\mathbf{x}\right)=\left(1,x,\ldots,x^m\right)$$

- For $\mathbf{x}\in\mathbb{R}^d$, we can pick some radial basis functions

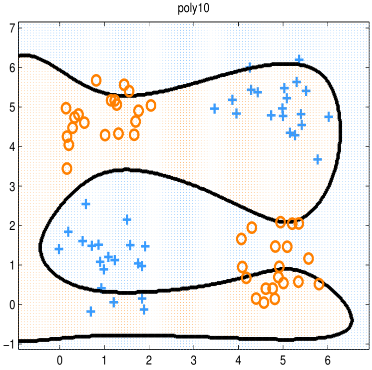
$$\Phi_j\left(\mathbf{x}\right)=\exp\left(-\frac{\left(\mathbf{x}-\boldsymbol{\mu}_j\right)^{\mathsf{T}}\left(\mathbf{x}-\boldsymbol{\mu}_j\right)}{2\sigma^2}\right).$$

Example



(left) Logistic regression in the original feature space $\mathbf{x} = (x_1, x_2)$. (right) Logistic regression obtained after performing a 2nd degree poly expansion $\Phi(\mathbf{x}) = \left(1, x_1, x_2, x_1^2, x_2^2\right)$.

Example



(left) Logistic regression for $\Phi(\mathbf{x}) = \left(1, x_1, x_2, ..., x_1^{10}, x_2^{10}\right)$. (right) Logistic regression using 4 radial basis functions with centers $\boldsymbol{\mu}_j$ specified by black crosses.

MLE Parameter Learning for Logistic Regression

- To learn the parameters $\mathbf{w}$, we can maximize w.r.t $\mathbf{w}$ the (conditional) log-likelihood function

$$l(\mathbf{w}) = \log \ p\left(\left\{ y^i \right\}_{i=1}^N \middle| \left\{ \mathbf{x}^i \right\}_{i=1}^N, \mathbf{w} \right) = \log \prod_{i=1}^N p\left(y^i \middle| \mathbf{x}^i, \mathbf{w} \right)$$

$$= \sum_{i=1}^N \log p\left(y^i \middle| \mathbf{x}^i, \mathbf{w} \right)$$

- We have

$$l(\mathbf{w}) = \sum_{i=1}^N y^i \log p\left(y^i = 1 \middle| \mathbf{x}^i, \mathbf{w} \right) + \left(1 - y^i\right) \log p\left(y^i = 0 \middle| \mathbf{x}^i, \mathbf{w} \right)$$

$$= -\sum_{i=1}^N \left(1 - y^i\right) \mathbf{w}^{\mathsf{T}} \Phi\left(\mathbf{x}^i\right) - \sum_{i=1}^N \log\left(1 + \exp\left(-\mathbf{w}^{\mathsf{T}} \Phi\left(\mathbf{x}^i\right)\right)\right)$$

- **Good news**: $l(\mathbf{w})$ is concave so there is no local maxima.
- **Bad news:** there is no-closed form solution for $\widehat{\mathbf{w}}_{\mathsf{MLE}}$.

Gradient Ascent

- Gradient ascent is one of the most basic method to maximize a function.
- It is an iterative procedure such that at iteration t :

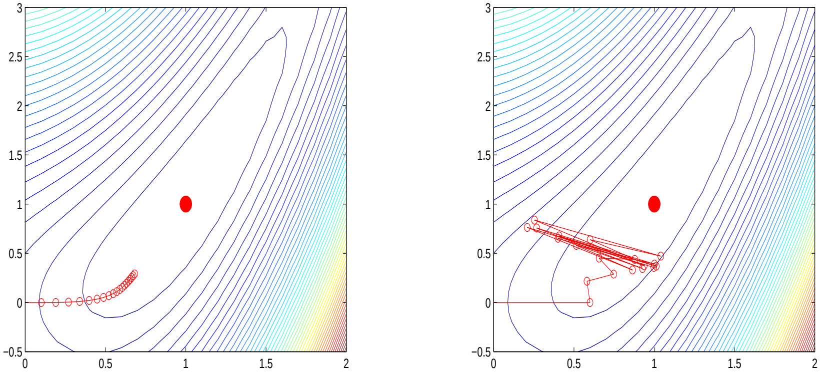
$$\mathbf{w}^{(t)} = \mathbf{w}^{(t-1)} + \eta \ \ \nabla_{\mathbf{w}} l\left(\mathbf{w}\right)\Big|_{\mathbf{w}^{(t-1)}}$$

where the gradient is

$$\nabla_{\mathbf{w}} l\left(\mathbf{w}\right) = \left[\begin{array}{ccc} \frac{\partial l(\mathbf{w})}{\partial w_1} & \cdots & \frac{\partial l(\mathbf{w})}{\partial w_m} \end{array}\right]^{\mathsf{T}}$$

and $\eta > 0$ is the learning rate.

Gradient Descent Example



Gradient descent on a simple function, starting from (0,0) for 20 steps using $\eta = 0.1$ (left) and $\eta = 0.6$ (right)

Gradient Ascent for Logistic Regression

- We have

$$\nabla l\left(\mathbf{w}\right)=\sum_{i=1}^{N}\left(y^{i}-g\left(\mathbf{w}^{\mathsf{T}}\Phi\left(\mathbf{x}^{i}\right)\right)\right)\Phi\left(\mathbf{x}^{i}\right)=\Phi^{\mathsf{T}}\left(\mathbf{y}-\boldsymbol{\mu}\right)$$

  where $[\Phi]_{i,j}=\Phi_j\left(\mathbf{x}^i\right)$, $\mathbf{y}=\left(y^1\ \cdots\ y^N\right)^{\mathsf{T}}$ and $\boldsymbol{\mu}=\left(g\left(\mathbf{w}^{\mathsf{T}}\Phi\left(\mathbf{x}^1\right)\right)\ \cdots\ g\left(\mathbf{w}^{\mathsf{T}}\Phi\left(\mathbf{x}^N\right)\right)\right)^{\mathsf{T}}$.
- So in vector-form, we will do

$$\begin{aligned}\mathbf{w}^{(t)} &= \mathbf{w}^{(t-1)}+\eta\ \left.\nabla_{\mathbf{w}} l\left(\mathbf{w}\right)\right|_{\mathbf{w}^{(t-1)}} \\ &= \mathbf{w}^{(t-1)}+\eta\ \Phi^{\mathsf{T}}\left(\mathbf{y}-\boldsymbol{\mu}^{(t-1)}\right)\end{aligned}$$

  where $\boldsymbol{\mu}^{(t-1)}$ corresponds to $\boldsymbol{\mu}$ computed using $\mathbf{w}^{(t-1)}$.

Iterative Reweighted Least Squares

- Newton's method is a generic (second order) optimization algorithm which converges faster than the simple gradient algorithm. It proceeds as follows at iteration t

$$\mathbf{w}^{(t)} = \mathbf{w}^{(t-1)} - \left[\nabla^2 l\left(\mathbf{w}^{(t-1)}\right)\right]^{-1} \nabla l\left(\mathbf{w}^{(t-1)}\right).$$

- We have

$$\nabla^2 l(\mathbf{w}) = -\Phi^{\mathsf{T}} U \Phi$$

with U a diagonal matrix with diagonal element

$$[U]_{i,i} = g\left(\mathbf{w}^{\mathsf{T}} \Phi\left(\mathbf{x}^i\right)\right)\left[1 - g\left(\mathbf{w}^{\mathsf{T}} \Phi\left(\mathbf{x}^i\right)\right)\right].$$

- It can be written as

$$\begin{aligned}\mathbf{w}^{(t)} &= \left(\Phi^{\mathsf{T}} U^{(t-1)} \Phi\right)^{-1} \Phi^{\mathsf{T}} U^{(t-1)} \\ &\times \left(\Phi \mathbf{w}^{(t-1)} + \left[U^{(t-1)}\right]^{-1}\left(\mathbf{y} - \boldsymbol{\mu}^{(t-1)}\right)\right)\end{aligned}$$

where $U^{(t-1)}$ and $\boldsymbol{\mu}^{(t-1)}$ corresponds to U and $\boldsymbol{\mu}$ with $\mathbf{w}^{(t-1)}$.

Regularized Logistic Regression via Gaussian Prior

- Similarly to regression, we can regularize the solution by assigning a Gaussian prior to **w**

$$p(\mathbf{w}) = \prod_{k=1}^{m} p(w_k) = \prod_{k=1}^{m} \mathcal{N}(w_k; 0, \lambda)$$

- This pushes the parameters **w** towards zero and can prevent overfitting. In this case, we have

$$\begin{aligned} \mathbf{w}_{MAP} &= \arg\max \ p\left(\mathbf{w} | \left\{\mathbf{x}^i, y^i\right\}_{i=1}^{N}\right) \\ &= \arg\max \ l(\mathbf{w}) - \frac{\mathbf{w}^{\mathsf{T}}\mathbf{w}}{2\lambda}. \end{aligned}$$

- $\mathbf{w}_{MAP}$ can be computed iteratively using

$$\mathbf{w}^{(t-1)} + \eta \ \left\{-\lambda^{-1}\mathbf{w}^{(t-1)} + \Phi^{\mathsf{T}}\left(\mathbf{y} - \boldsymbol{\mu}^{(t-1)}\right)\right\}$$

- Regularization parameter can be estimated using cross-validation or by maximizing marginal likelihood.

Regularized Logistic Regression via Laplace Prior

- Similarly to regression, we can regularize the solution by assigning a Gaussian prior to $\mathbf{w}$

$$p(\mathbf{w}) = \prod_{k=1}^{m} p(w_k) = \prod_{k=1}^{m} \frac{1}{2\lambda} \exp\left(-\frac{|w_k|}{\lambda}\right)$$

- This pushes the parameters $\mathbf{w}$ towards zero and can prevent overfitting. In this case, we have

$$\begin{aligned} \mathbf{w}_{MAP} &= \arg\max \ p\left(\mathbf{w} | \left\{\mathbf{x}^i, y^i\right\}_{i=1}^{N}\right) \\ &= \arg\max \ l(\mathbf{w}) - \frac{1}{2\lambda} \sum_{k=1}^{m} |w_k| . \end{aligned}$$

- The objective function is convex and efficient procedures have been developed to compute $\mathbf{w}_{MAP}$. Similarly to the regression case, this can lead to sparse solution; e.g. you can have $w_{k,MAP} = 0$ exactly.
- Regularization parameter can be estimated using cross-validation or by maximizing marginal likelihood.

Multinomial Logistic Regression

- Consider now the case where $C > 2$. We could consider the following generalization

$$p\left(y = c|\, \mathbf{x}, \{\mathbf{w}_c\}_{c=1}^{C}\right) = \frac{\exp\left(\mathbf{w}_c^{\mathsf{T}} \Phi\left(\mathbf{x}\right)\right)}{\sum_{k=1}^{C} \exp\left(\mathbf{w}_k^{\mathsf{T}} \Phi\left(\mathbf{x}\right)\right)} \text{ for } c = 1, ..., C$$

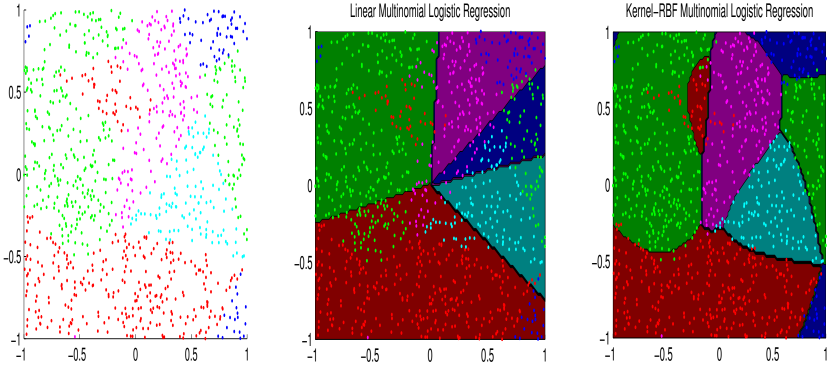
  but this is not identifiable as
  $p\left(y = c|\, \mathbf{x}, \{\mathbf{w}_c + \mathbf{w}'\}_{c=1}^{C}\right) = p\left(y = c|\, \mathbf{x}, \{\mathbf{w}_c\}_{c=1}^{C}\right)$.

- Hence we set $\mathbf{w}_C = \begin{pmatrix} 0 & \cdots & 0 \end{pmatrix}^{\mathsf{T}}$ to obtain

$$\begin{aligned} p\left(y = c|\, \mathbf{x}, \{\mathbf{w}_c\}_{c=1}^{C-1}\right) &= \frac{\exp\left(\mathbf{w}_c^{\mathsf{T}} \Phi\left(\mathbf{x}\right)\right)}{1 + \sum_{k=1}^{C-1} \exp\left(\mathbf{w}_k^{\mathsf{T}} \Phi\left(\mathbf{x}\right)\right)} \text{ for } c = 1, ..., C \\ p\left(y = C|\, \mathbf{x}, \{\mathbf{w}_c\}_{c=1}^{C-1}\right) &= \frac{1}{1 + \sum_{k=1}^{C-1} \exp\left(\mathbf{w}_k^{\mathsf{T}} \Phi\left(\mathbf{x}\right)\right)}. \end{aligned}$$

- The (conditional) log-likelihood is concave w.r.t $\{\mathbf{w}_c\}_{c=1}^{C-1}$ so MLE estimates can be computed using gradient.

Example



(left) Some 5 class data in 2d (center) Multinomial logistic regression in the original feature space $\mathbf{x} = (x_1, x_2)$ (right) RBF basis functions with bandwidth 1 using $m = 1 + N$. We use all the data points as centers.

Full Bayesian Analysis of Logistic Regression

- Even for Gaussian priors on $\mathbf{w}$, one cannot compute

$$p\left(\left\{y^i\right\}_{i=1}^N \middle| \left\{\mathbf{x}^i\right\}_{i=1}^N, \boldsymbol{\lambda}\right) = \frac{p\left(\left\{y^i\right\}_{i=1}^N \middle| \left\{\mathbf{x}^i\right\}_{i=1}^N, \mathbf{w}\right) p\left(\mathbf{w} \middle| \boldsymbol{\lambda}\right)}{p\left(\left\{y^i\right\}_{i=1}^N \middle| \left\{\mathbf{x}^i\right\}_{i=1}^N, \boldsymbol{\lambda}\right)}$$

where

$$p\left(\left\{y^i\right\}_{i=1}^N \middle| \left\{\mathbf{x}^i\right\}_{i=1}^N, \boldsymbol{\lambda}\right) = \int p\left(\left\{y^i\right\}_{i=1}^N \middle| \left\{\mathbf{x}^i\right\}_{i=1}^N, \mathbf{w}\right) p\left(\mathbf{w} \middle| \boldsymbol{\lambda}\right) d\mathbf{w}$$

- Contrary to regression, there is no closed form Bayesian analysis possible.
- If you want to do Bayesian inference, then approximations are necessary.