

Probabilistic classification - discriminative models

Course of Machine Learning
Master Degree in Computer Science
University of Rome "Tor Vergata"
a.a. 2021-2022

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Generalized linear models

In the cases considered above, the posterior class distributions $p(C_k|\mathbf{x})$ are sigmoidal or softmax with argument given by a linear combination of features in \mathbf{x} , i.e., they are instances of *generalized linear models*

A *generalized linear model* (GLM) is a function

$$y(\mathbf{x}) = f(\mathbf{w}^T \mathbf{x} + w_0)$$

where f (usually called the *response function*) is in general a non linear function.

Each iso-surface of $y(\mathbf{x})$, such that by definition $y(\mathbf{x}) = c$ (for some constant c), is such that

$$f(\mathbf{w}^T \mathbf{x} + w_0) = c$$

and

$$\mathbf{w}^T \mathbf{x} + w_0 = f^{-1}(y) = c'$$

(c' constant).

Hence, iso-surfaces of a GLM are hyper-planes, thus implying that boundaries are hyperplanes themselves.

Exponential families and GLM

Let us assume we wish to predict a random variable y as a function of a different set of random variables \mathbf{x} . By definition, a prediction model for this task is a GLM if the following hypotheses hold:

1. the conditional distribution of y given \mathbf{x} , $p(y|\mathbf{x})$ belongs to the exponential family: that is, we may write it as

$$p(y|\mathbf{x}) = \frac{1}{s} g(\boldsymbol{\theta}(\mathbf{x})) f\left(\frac{y}{s}\right) e^{\frac{1}{s} \boldsymbol{\theta}(\mathbf{x})^T \mathbf{u}(y)}$$

for suitable $g, \boldsymbol{\theta}, \mathbf{u}$

2. for any \mathbf{x} , we wish to predict the expected value of $\mathbf{u}(y)$ given \mathbf{x} , that is $E[\mathbf{u}(y)|\mathbf{x}]$
3. $\boldsymbol{\theta}(\mathbf{x})$ (the *natural parameter*) is a linear combination of the features, $\boldsymbol{\theta}(\mathbf{x}) = \mathbf{w}^T \bar{\mathbf{x}}$

GLM and normal distribution

1. $y \in \mathbf{R}$, and $p(y|\mathbf{x}) = \frac{1}{\sqrt{2\pi}\sigma} e^{-\frac{(y-\mu(\mathbf{x}))^2}{2\sigma^2}}$ is a normal distribution with mean $\mu(\mathbf{x})$ and constant variance σ^2 : it is easy to verify that

$$\boldsymbol{\theta}(\mathbf{x}) = \begin{pmatrix} \theta_1(\mathbf{x}) \\ \theta_2 \end{pmatrix} = \begin{pmatrix} \mu(\mathbf{x})/\sigma^2 \\ -1/2\sigma^2 \end{pmatrix}$$

and $\mathbf{u}(y) = y$

2. we wish to predict the value of $E[\mathbf{u}(y)|\mathbf{x}]$ as $y(\mathbf{x}) = E[y|\mathbf{x}]$, then

$$y(\mathbf{x}) = \mu(\mathbf{x}) = \sigma^2 \theta_1(\mathbf{x})$$

3. we assume there exists \mathbf{w} such that $\theta_1(\mathbf{x}) = \mathbf{w}_1^T \bar{\mathbf{x}}$

Then, a linear regression results

$$y(\mathbf{x}) = \mathbf{w}_1^T \bar{\mathbf{x}}$$

GLM and Bernoulli distribution

1. $y \in \{0, 1\}$, and $p(y|\mathbf{x}) = \pi(\mathbf{x})^y (1 - \pi(\mathbf{x}))^{1-y}$ is a Bernoulli distribution with parameter $\pi(\mathbf{x})$: then, the natural parameter $\theta(\mathbf{x})$ is

$$\theta(\mathbf{x}) = \log \frac{\pi(\mathbf{x})}{1 - \pi(\mathbf{x})}$$

and $\mathbf{u}(y) = y$

2. we wish to predict the value of $E[\mathbf{u}(y)|\mathbf{x}]$ as $y(\mathbf{x}) = E[y|\mathbf{x}] = p(y = 1|\mathbf{x})$, then

$$p(y = 1|\mathbf{x}) = \pi(\mathbf{x}) = \frac{1}{1 + e^{-\theta(\mathbf{x})}}$$

3. we assume there exists \mathbf{w} such that $\theta(\mathbf{x}) = \mathbf{w}^T \bar{\mathbf{x}}$

Then, a logistic regression derives

$$y(\mathbf{x}) = \frac{1}{1 + e^{-\mathbf{w}^T \bar{\mathbf{x}}}}$$

GLM and categorical distribution

1. $y \in \{1, \dots, K\}$, and $p(y|\mathbf{x}) = \prod_{i=1}^K \pi_i(\mathbf{x})^{y_i}$ (where $y_i = 1$ if $y = i$ and $y = 0$ otherwise) is a categorical distribution with probabilities $\pi_1(\mathbf{x}), \dots, \pi_K(\mathbf{x})$ (where $\sum_{i=1}^K \pi_i(\mathbf{x}) = 1$): the natural parameter is then $\theta(\mathbf{x}) = (\theta_1(\mathbf{x}), \dots, \theta_K(\mathbf{x}))^T$, with

$$\theta_i(\mathbf{x}) = \log \frac{\pi_i(\mathbf{x})}{\pi_K(\mathbf{x})} = \log \frac{\pi_i(\mathbf{x})}{1 - \sum_{j=1}^{K-1} \pi_j(\mathbf{x})}$$

and $\mathbf{u}(y) = (y_1, \dots, y_K)^T$ is the 1-to- K representation of y

2. we wish to predict the expectations $y_i(\mathbf{x}) = E[u_i(y)|\mathbf{x}] = p(y = i|\mathbf{x})$ as

$$p(y = i|\mathbf{x}) = E[u_i(y)|\mathbf{x}] = \pi_i(\mathbf{x}) = \pi_K(\mathbf{x}) e^{\theta_i(\mathbf{x})}$$

Since $1 = \sum_{i=1}^K \pi_i(\mathbf{x}) = \pi_K(\mathbf{x}) \sum_{i=1}^K e^{\theta_i(\mathbf{x})}$, it derives

$$\pi_K(\mathbf{x}) = \frac{1}{\sum_{i=1}^K e^{\theta_i(\mathbf{x})}} \quad \text{and} \quad \pi_i(\mathbf{x}) = \frac{e^{\theta_i(\mathbf{x})}}{\sum_{i=1}^K e^{\theta_i(\mathbf{x})}}$$

3. we assume there exist $\mathbf{w}_1, \dots, \mathbf{w}_K$ such that $\theta_i(\mathbf{x}) = \mathbf{w}_i^T \bar{\mathbf{x}}$

GLM and categorical distribution

Then, a softmax regression results, with

$$y_i(\mathbf{x}) = \frac{e^{\mathbf{w}_i^T \bar{\mathbf{x}}}}{\sum_{j=1}^K e^{\mathbf{w}_j^T \bar{\mathbf{x}}}} \quad \text{if } i \neq K$$

$$y_K(\mathbf{x}) = \frac{1}{\sum_{j=1}^K e^{\mathbf{w}_j^T \bar{\mathbf{x}}}}$$

GLM and additional regressions

Other regression types can be defined by considering different models for $p(y|\mathbf{x})$. For example,

1. Assume $y \in \{0, \dots\}$ is a non negative integer (for example we are interested to count data), and $p(y|\mathbf{x}) = \frac{\lambda(\mathbf{x})^y}{y!} e^{-\lambda(\mathbf{x})}$ is a Poisson distribution with parameter $\lambda(\mathbf{x})$: then, the natural parameter $\theta(\mathbf{x})$ is

$$\theta(\mathbf{x}) = \log \lambda(\mathbf{x})$$

and $\mathbf{u}(y) = y$

2. we wish to predict the value of $E[\mathbf{u}(y)|\mathbf{x}]$ as $y(\mathbf{x}) = E[y|\mathbf{x}]$, then

$$y(\mathbf{x}) = \lambda(\mathbf{x}) = e^{\theta(\mathbf{x})}$$

3. we assume there exists \mathbf{w} such that $\theta(\mathbf{x}) = \mathbf{w}^T \bar{\mathbf{x}}$

Then, a Poisson regression derives

$$y(\mathbf{x}) = e^{\mathbf{w}^T \bar{\mathbf{x}}}$$

GLM and additional regressions

1. Assume $y \in [0, \infty)$ is a non negative real (for example we are interested to time intervals), and $p(y|\mathbf{x}) = \lambda(\mathbf{x}) e^{-\lambda(\mathbf{x}) y}$ is an exponential distribution with parameter $\lambda(\mathbf{x})$: then, the natural parameter $\theta(\mathbf{x})$ is

$$\theta(\mathbf{x}) = -\lambda(\mathbf{x})$$

and $\mathbf{u}(y) = y$

2. we wish to predict the value of $E[\mathbf{u}(y)|\mathbf{x}]$ as $y(\mathbf{x}) = E[y|\mathbf{x}]$, then

$$y(\mathbf{x}) = \frac{1}{\lambda(\mathbf{x})} = -\frac{1}{\theta(\mathbf{x})}$$

3. we assume there exists \mathbf{w} such that $\theta(\mathbf{x}) = \mathbf{w}^T \bar{\mathbf{x}}$

Then, an exponential regression derives

$$y(\mathbf{x}) = -\frac{1}{\mathbf{w}^T \bar{\mathbf{x}}}$$

Discriminative approach

We could directly assume that $p(C_k|\mathbf{x})$ is a GLM and derive its coefficients (for example through ML estimation).

Comparison wrt the generative approach:

- Less information derived (we do not know $p(\mathbf{x}|C_k)$, thus we are not able to generate new data)

- Simpler method, usually a smaller set of parameters to be derived
- Better predictions, if the assumptions done with respect to $p(\mathbf{x}|C_k)$ are poor.

Logistic regression

Logistic regression is a GLM deriving from the hypothesis of a Bernoulli distribution of y , which results into

$$p(C_1|\mathbf{x}) = \sigma(\mathbf{w}^T \mathbf{x}) = \frac{1}{1 + e^{-\mathbf{w}^T \mathbf{x}}}$$

where base functions could also be applied.

The model is equivalent, for the binary classification case, to linear regression for the regression case.

Degrees of freedom

- In the case of d features, logistic regression requires $d + 1$ coefficients w_0, \dots, w_d to be derived from a training set
- A generative approach with gaussian distributions requires:
 - $2d$ coefficients for the means μ_1, μ_2 ,
 - for each covariance matrix

$$\sum_{i=1}^d i = d(d+1)/2 \quad \text{coefficients}$$

– one prior cla probability $p(C_1)$

- As a total, it results into $d(d+1) + 2d + 1 = d(d+3) + 1$ coefficients (if a unique covariance matrix is assumed $d(d+1)/2 + 2d + 1 = d(d+5)/2 + 1$ coefficients)

Maximum likelihood estimation

Let us assume that targets of elements of the training set can be conditionally (with respect to model coefficients) modeled through a Bernoulli distribution. That is, assume

$$p(t_i|\mathbf{x}_i, \mathbf{w}) = p_i^{t_i} (1 - p_i)^{1-t_i}$$

where $p_i = p(C_1|\mathbf{x}_i) = \sigma(\mathbf{w}^T \mathbf{x}_i)$.

Then, the likelihood of the training set targets \mathbf{t} given \mathbf{X} is

$$p(\mathbf{t}|\mathbf{X}, \mathbf{w}) = L(\mathbf{w}|\mathbf{X}, \mathbf{t}) = \prod_{i=1}^n p(t_i|\mathbf{x}_i, \mathbf{w}) = \prod_{i=1}^n p_i^{t_i} (1 - p_i)^{1-t_i}$$

and the log-likelihood is

$$l(\mathbf{w}|\mathbf{X}, \mathbf{t}) = \log L(\mathbf{w}|\mathbf{X}, \mathbf{t}) = \sum_{i=1}^n (t_i \log p_i + (1 - t_i) \log(1 - p_i))$$

Maximum likelihood estimation

- Since

$$\frac{\partial l(\mathbf{w}|\mathbf{X}, \mathbf{t})}{\partial \mathbf{w}} = \sum_{i=1}^n \frac{\partial l(\mathbf{w}|\mathbf{X}, \mathbf{t})}{\partial p_i} \frac{\partial p_i}{\partial a_i} \frac{\partial a_i}{\partial \mathbf{w}} \frac{\partial l(\mathbf{w}|\mathbf{X}, \mathbf{t})}{\partial p_i} = \frac{t_i}{p_i} - \frac{1 - t_i}{1 - p_i} = \frac{t_i - p_i}{p_i(1 - p_i)}$$

$$\frac{\partial p_i}{\partial a_i} = \frac{\partial \sigma(a_i)}{\partial a_i} = \sigma(a_i)(1 - \sigma(a_i)) = p_i(1 - p_i)$$

$$\frac{\partial a_i}{\partial \mathbf{w}} = \mathbf{x}_i$$

- it results,

$$\frac{\partial l(\mathbf{w}|\mathbf{X}, \mathbf{t})}{\partial \mathbf{w}} = \sum_{i=1}^n (t_i - p_i) \bar{\mathbf{x}}_i = \sum_{i=1}^n (t_i - \sigma(\mathbf{w}^T \bar{\mathbf{x}}_i)) \bar{\mathbf{x}}_i$$

Maximum likelihood estimation

To maximize the likelihood, we could apply a gradient ascent algorithm, where at each iteration the following update of the currently estimated \mathbf{w} is performed

$$\begin{aligned} \mathbf{w}^{(j+1)} &= \mathbf{w}^{(j)} + \alpha \frac{\partial l(\mathbf{w}|\mathbf{X}, \mathbf{t})}{\partial \mathbf{w}} \Big|_{\mathbf{w}^{(j)}} \\ &= \mathbf{w}^{(j)} + \alpha \sum_{i=1}^n (t_i - \sigma((\mathbf{w}^{(j)})^T \bar{\mathbf{x}}_i)) \bar{\mathbf{x}}_i \\ &= \mathbf{w}^{(j)} + \alpha \sum_{i=1}^n (t_i - y(\mathbf{x}_i)) \bar{\mathbf{x}}_i \end{aligned}$$

Maximum likelihood estimation

As a possible alternative, at each iteration only one coefficient in \mathbf{w} is updated

$$\begin{aligned} w_k^{(j+1)} &= w_k^{(j)} + \alpha \frac{\partial l(\mathbf{w}|\mathbf{X}, \mathbf{t})}{\partial w_k} \Big|_{\mathbf{w}^{(j)}} \\ &= w_k^{(j+1)} + \alpha \sum_{i=1}^n (t_i - \sigma((\mathbf{w}^{(j)})^T \bar{\mathbf{x}}_i)) x_{ik} \\ &= w_k^{(j+1)} + \alpha \sum_{i=1}^n (t_i - y(\mathbf{x}_i)) x_{ik} \end{aligned}$$

Newton-Raphson method

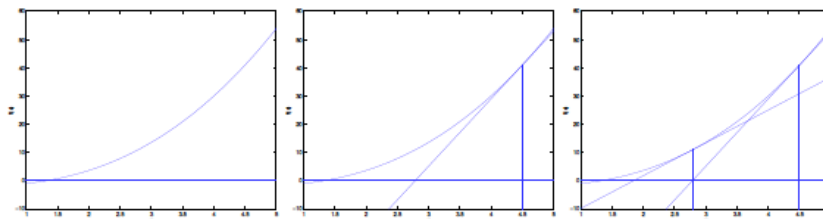
- Maximization of $l(\mathbf{w}|\mathbf{X}, \mathbf{t})$ through the well-known Newton-Raphson algorithm to compute the roots of a given function
- Given $f : \mathbf{R} \mapsto \mathbf{R}$, the algorithm finds $z \in \mathbf{R}$ such that $f(z) = 0$ through a sequence of iterations, starting from an initial value z_0 and performing the following update

$$z_{i+1} = z_i - \frac{f(z_i)}{f'(z_i)}$$

- At each iteration, the algorithm approximates f by a line tangent to f in $(z_i, f(z_i))$, and defines z_{i+1} as the value where the line intersects the x axis

Newton-Raphson method

- Example of application of the method



- Newton-Raphson method can be also applied to compute maximum and minimum points for a function by finding zeros of the first derivative: this corresponds to applying the following update

$$z_{i+1} = z_i - \frac{f'(z_i)}{f''(z_i)}$$

Newton-Raphson and multivariate functions

- To apply Newton-Raphson to logistic regression we have to extend it to the case of a vector variable, since the maximization has to be performed with respect to the vector \mathbf{w} of coefficients
- In a multivariate framework, the first derivative is substituted by the gradient $\frac{\partial}{\partial \mathbf{w}}$, while the second derivative corresponds to the *Hessian matrix* \mathbf{H} , defined as follows

$$\mathbf{H}_{ij}(f) = \frac{\partial^2 f}{\partial w_i \partial w_j}$$

- The update operation turns out to be

$$\mathbf{w}^{(i+1)} = \mathbf{w}^{(i)} - (\mathbf{H}(f)|_{\mathbf{w}^{(i)}})^{-1} \frac{\partial f}{\partial \mathbf{w}}|_{\mathbf{w}^{(i)}}$$

Newton-Raphson and linear regression

- In the case of linear regression, the error function to be minimized is

$$E(\mathbf{w}) = \frac{1}{2} \sum_{i=1}^n (y_i - t_i)^2 = \frac{1}{2} \sum_{i=1}^n (\mathbf{w}^T \bar{\mathbf{x}}_i - t_i)^2$$

- Then,

$$\frac{\partial E}{\partial \mathbf{w}} = \sum_{i=1}^n (y_i - t_i) \bar{\mathbf{x}}_i = \bar{\mathbf{x}}^T (\mathbf{y} - \mathbf{t}) = \bar{\mathbf{x}}^T \mathbf{y} - \bar{\mathbf{x}}^T \mathbf{t} = \bar{\mathbf{x}}^T \bar{\mathbf{x}} \mathbf{w} - \bar{\mathbf{x}}^T \mathbf{t}$$

since $\mathbf{y} = \bar{\mathbf{x}} \mathbf{w}$, and

$$\mathbf{H} = \frac{\partial}{\partial \mathbf{w}} \frac{\partial E}{\partial \mathbf{w}} = \sum_{i=1}^n \bar{\mathbf{x}}_i \bar{\mathbf{x}}_i^T = \bar{\mathbf{x}}^T \bar{\mathbf{x}}$$

- At each iteration, the update is

$$\mathbf{w}^{(i+1)} = \mathbf{w}^{(i)} - (\bar{\mathbf{x}}^T \bar{\mathbf{x}})^{-1} (\bar{\mathbf{x}}^T \bar{\mathbf{x}} \mathbf{w}^{(i)} - \bar{\mathbf{x}}^T \mathbf{t}) = (\bar{\mathbf{x}}^T \bar{\mathbf{x}})^{-1} \bar{\mathbf{x}}^T \mathbf{t}$$

- We get the well-known solution, which is obtained in a single iteration.

Newton-Raphson and logistic regression

Here, we have the cross-entropy loss function

$$E(\mathbf{w}) = -l(\mathbf{w}|\mathbf{X}, \mathbf{t}) = - \sum_{i=1}^n (t_i \log y_i + (1 - t_i) \log(1 - y_i))$$

with $y_i = \sigma(a_i)$ and $a_i = \mathbf{w}^T \bar{\mathbf{x}}_i$. Hence,

$$\frac{\partial E}{\partial \mathbf{w}} = - \frac{\partial l(\mathbf{w}|\mathbf{X}, \mathbf{t})}{\partial \mathbf{w}} = \sum_{i=1}^n (y_i - t_i) \bar{\mathbf{x}}_i = \bar{\mathbf{x}}^T (\mathbf{y} - \mathbf{t})$$

$$\mathbf{H} = \frac{\partial}{\partial \mathbf{w}} \frac{\partial E}{\partial \mathbf{w}} = \sum_{i=1}^n y_i (1 - y_i) \bar{\mathbf{x}}_i \bar{\mathbf{x}}_i^T = \bar{\mathbf{x}}^T \mathbf{Y} \bar{\mathbf{x}}$$

where

- \mathbf{y} is the vector of predictions $y_i = \sigma(a_i) = \sigma(\mathbf{w}^T \bar{\mathbf{x}}_i)$ for $i = 1, \dots, n$
- \mathbf{Y} is a $n \times n$ diagonal matrix such that

$$Y_{ii} = y_i(1 - y_i)$$

Newton-Raphson and logistic regression

- In the case of logistic regression, the update is then

$$\mathbf{w}^{(i+1)} = \mathbf{w}^{(i)} - (\bar{\mathbf{x}}^T \mathbf{Y}^{(i)} \bar{\mathbf{x}})^{-1} \bar{\mathbf{x}}^T (\mathbf{y}^{(i)} - \mathbf{t})$$

where both \mathbf{y} and \mathbf{Y} are dependent from $\mathbf{w}^{(i)}$, hence from i . Then,

$$\begin{aligned} \mathbf{w}^{(i+1)} &= (\bar{\mathbf{x}}^T \mathbf{Y}^{(i)} \bar{\mathbf{x}})^{-1} ((\bar{\mathbf{x}}^T \mathbf{Y}^{(i)} \bar{\mathbf{x}}) \mathbf{w}^{(i)} - \bar{\mathbf{x}}^T (\mathbf{y}^{(i)} - \mathbf{t})) \\ &= (\bar{\mathbf{x}}^T \mathbf{Y}^{(i)} \bar{\mathbf{x}})^{-1} \bar{\mathbf{x}}^T \mathbf{Y}^{(i)} \mathbf{z}^{(i)} \end{aligned}$$

where

$$\mathbf{z}^{(i)} = \bar{\mathbf{x}} \mathbf{w}^{(i)} - \mathbf{Y}^{(i)-1} (\mathbf{y}^{(i)} - \mathbf{t}) = \mathbf{a}^{(i)} - \mathbf{Y}^{(i)-1} (\mathbf{y}^{(i)} - \mathbf{t})$$

Clearly, $\mathbf{z}^{(i)}$ is a function of $\mathbf{w}^{(i)}$, hence of the step i .

Iterated reweighted least squares

- Let us consider the weighted extension of the least squares cost function, denoted as *weighted least squares* cost function, defined as

$$\sum_{i=1}^n \psi_i (\mathbf{y}_i - t_i)^2 = \sum_{i=1}^n \psi_i (\mathbf{w}^T \bar{\mathbf{x}}_i - t_i)^2$$

for given weights ψ_1, \dots, ψ_n . Clearly, the least squares problems corresponds to the case $\psi_i = 1$ for $i = 1, \dots, n$

- It can be proved that, for this problem, the optimum is

$$\mathbf{w} = (\bar{\mathbf{x}}^T \mathbf{\Psi} \bar{\mathbf{x}})^{-1} \bar{\mathbf{x}}^T \mathbf{\Psi} \mathbf{t}$$

where the weight matrix $\mathbf{\Psi}$ is a diagonal matrix with $\Psi_{ii} = \psi_i$

Iterated reweighted least squares

- Let us remind that, at each step of NR algorithm applied to logistic regression, the following update is performed

$$\mathbf{w}^{(i+1)} = (\bar{\mathbf{x}}^T \mathbf{Y}^{(i)} \bar{\mathbf{x}})^{-1} \bar{\mathbf{x}}^T \mathbf{Y}^{(i)} \mathbf{z}^{(i)}$$

- This corresponds to optimizing the weighted least squares cost function for feature matrix \mathbf{X} , target vector $\tilde{\mathbf{t}} = \mathbf{z}^{(i)}$, and weights $\psi_k = y_k^{(i)}(1 - y_k^{(i)})$
- The update of $\mathbf{w}^{(i)}$ performed at each iteration can then be computed by solving a new instance of the weighted least square problem, setting $\mathbf{w}^{(i+1)}$ to the solution obtained, and deriving the new values of $\mathbf{\Psi} = \mathbf{Y}^{(i+1)}$ and $\tilde{\mathbf{t}} = \mathbf{z}^{(i+1)}$.

Logistic regression and GDA

- Observe that assuming $p(\mathbf{x}|C_1)$ are $p(\mathbf{x}|C_2)$ as multivariate normal distributions with same covariance matrix Σ results into a logistic $p(C_1|\mathbf{x})$.
- The opposite, however, is not true in general: in fact, GDA relies on stronger assumptions than logistic regression.
- The more the normality hypothesis of class conditional distributions with same covariance is verified, the more GDA will tend to provide the best models for $p(C_1|\mathbf{x})$

Logistic regression and GDA

- Logistic regression relies on weaker assumptions than GDA: it is then less sensible from a limited correctness of such assumptions, thus resulting in a more robust technique
- Since $p(C_i|\mathbf{x})$ is logistic under a wide set of hypotheses about $p(\mathbf{x}|C_i)$, it will usually provide better solutions (models) in all such cases, while GDA will provide poorer models as far as the normality hypotheses is less verified.

Softmax regression

- In order to extend the logistic regression approach to the case $K > 2$, let us consider the matrix $\mathbf{W} = (\mathbf{w}_1, \dots, \mathbf{w}_K)$ of model coefficients, of size $(d+1) \times K$, where \mathbf{w}_j is the $d+1$ -dimensional vector of coefficients for class C_j .
- In this case, the likelihood is defined as

$$p(\mathbf{T}|\mathbf{X}, \mathbf{W}) = \prod_{i=1}^n \prod_{k=1}^K p(C_k|\mathbf{x}_i)^{t_{ik}} = \prod_{i=1}^n \prod_{k=1}^K \left(\frac{e^{\mathbf{w}_k^T \bar{\mathbf{x}}_i}}{\sum_{r=1}^K e^{\mathbf{w}_r^T \bar{\mathbf{x}}_i}} \right)^{t_{ik}}$$

where \mathbf{X} is the usual matrix of features and \mathbf{T} is the $n \times K$ matrix where row i is the 1-to- K coding of t_i . That is, if $\mathbf{x}_i \in C_k$ then $t_{ik} = 1$ and $t_{ir} = 0$ for $r \neq k$.

ML and softmax regression

The log-likelihood is then defined as

$$l(\mathbf{W}) = \sum_{i=1}^n \sum_{k=1}^K t_{ik} \log \left(\frac{e^{\mathbf{w}_k^T \bar{\mathbf{x}}_i}}{\sum_{r=1}^K e^{\mathbf{w}_r^T \bar{\mathbf{x}}_i}} \right)$$

And the gradient is defined as

$$\frac{\partial l(\mathbf{W})}{\partial \mathbf{W}} = \left(\frac{\partial l(\mathbf{W})}{\partial \mathbf{w}_1}, \dots, \frac{\partial l(\mathbf{W})}{\partial \mathbf{w}_K} \right)$$

ML and softmax regression

- To derive $\frac{\partial l(\mathbf{W})}{\partial \mathbf{w}_j}$ let , observe that we may write

$$l(\mathbf{W}) = \sum_{i=1}^n \sum_{k=1}^K t_{ik} \log y_{ik}$$

with

$$y_{ik} = \frac{e^{a_{ik}}}{\sum_{r=1}^K e^{a_{ir}}} \quad \text{and} \quad a_{ik} = \mathbf{w}_k^T \bar{\mathbf{x}}_i$$

for $k = 1, \dots, K$ and $i = 1, \dots, n$.

ML and softmax regression

- Observe now that, for each $i = 1, \dots, n$, $j, k = 1, \dots, K$,

$$\frac{\partial a_{ik}}{\partial \mathbf{w}_j} = \frac{\partial \mathbf{w}_k^T \bar{\mathbf{x}}_i}{\partial \mathbf{w}_j} = \begin{cases} \bar{\mathbf{x}}_i & \text{if } j = k \\ \mathbf{0} & \text{if } j \neq k \end{cases}$$

$$\frac{\partial y_{ik}}{\partial a_{ij}} = \begin{cases} y_{ik}(1 - y_{ik}) & \text{if } j = k \\ -y_{ij}y_{ik} & \text{if } j \neq k \end{cases}$$

$$\frac{\partial y_{ik}}{\partial \mathbf{w}_j} = \sum_r \frac{\partial y_{ik}}{\partial a_{ir}} \frac{\partial a_{ir}}{\partial \mathbf{w}_j} = \frac{\partial y_{ik}}{\partial a_{ij}} \frac{\partial a_{ij}}{\partial \mathbf{w}_j} = \frac{\partial y_{ik}}{\partial a_{ij}} \bar{\mathbf{x}}_i = \begin{cases} y_{ik}(1 - y_{ik})\bar{\mathbf{x}}_i & \text{if } j = k \\ -y_{ij}y_{ik}\bar{\mathbf{x}}_i & \text{if } j \neq k \end{cases}$$

ML and softmax regression

Hence

$$\begin{aligned} \frac{\partial l(\mathbf{w})}{\partial \mathbf{w}_j} &= \frac{\partial}{\partial \mathbf{w}_j} \sum_{k=1}^K \sum_{i=1}^n t_{ik} \log y_{ik} = \frac{\partial}{\partial \mathbf{w}_j} \sum_{i=1}^n t_{ij} \log y_{ij} + \frac{\partial}{\partial \mathbf{w}_j} \sum_{k \neq j} \sum_{i=1}^n t_{ik} \log y_{ik} \\ &= \sum_{i=1}^n t_{ij} \frac{1}{y_{ij}} \frac{\partial y_{ij}}{\partial \mathbf{w}_j} + \sum_{k \neq j} \sum_{i=1}^n t_{ik} \frac{1}{y_{ik}} \frac{\partial y_{ik}}{\partial \mathbf{w}_j} \\ &= \sum_{i=1}^n t_{ij} \frac{1}{y_{ij}} y_{ij}(1 - y_{ij})\bar{\mathbf{x}}_i - \sum_{k \neq j} \sum_{i=1}^n t_{ik} \frac{1}{y_{ik}} y_{ik}y_{ij}\bar{\mathbf{x}}_i \\ &= \left(\sum_{i=1}^n t_{ij} - \sum_{i=1}^n y_{ij} \sum_{k=1}^K t_{ik} \right) \bar{\mathbf{x}}_i = \left(\sum_{i=1}^n t_{ij} - \sum_{i=1}^n y_{ij} \right) \bar{\mathbf{x}}_i = \sum_{i=1}^n (t_{ij} - y_{ij}) \bar{\mathbf{x}}_i \end{aligned}$$

Observe that the gradient has the same structure than in the case of linear regression and logistic regression.

ML and softmax regression: gradient ascent method

- Applying a gradient method to maximize the log-likelihood $l(\mathbf{w})$ requires using the gradient $\frac{\partial l}{\partial \mathbf{w}}$ to explore the dK -dimensional space of model coefficient values
- As an alternative, on-line gradient descent: at each iteration the ascent is performed only wrt to a cyclically selected coefficient \mathbf{w}_k , evaluating only the gradient $\frac{\partial l}{\partial \mathbf{w}_k}$ in a space of dimension d

ML and softmax regression: Newton-Raphson

- The alternative approach of applying Newton-Raphson method requires computing the Hessian matrix $\mathbf{H}(\mathbf{w})$, of size $dK \times dK$
- $\mathbf{H}(\mathbf{w})$ is structured in blocks of size $d \times d$, where block (j, k) provides the coefficients of

$$\frac{\partial^2 l(\mathbf{w})}{\partial \mathbf{w}_j \partial \mathbf{w}_k} = - \sum_{i=1}^n y_{ik} (I_{kj} - y_{kj}) \bar{\mathbf{x}}_i \bar{\mathbf{x}}_i^T$$

where $I_{ii} = 1$, and $I_{ij} = 0$ if $i \neq j$.

Probit regression

- In a GLM, $p(C_1|\mathbf{x}) = f(\mathbf{w}^T \bar{\mathbf{x}})$ where f is the activation function (a sigmoid in the case of logistic regression)
- In probit regression a *stochastic threshold model* is applied for classification, as follows:
 - Assume a probability distribution $\pi(\theta)$ is given, and let $\Pi(\theta)$ be the corresponding cumulative distribution: that is, $\Pi(z) = \pi(\theta < z)$
 - Let \mathbf{w} be the model coefficients. In order to classify \mathbf{x} , the linear combination $a_i = \mathbf{w}^T \bar{\mathbf{x}}$ is computed
 - By definition, $p(C_1|\mathbf{x}) = \Pi(\mathbf{w}^T \bar{\mathbf{x}})$: that is, $p(C_1|\mathbf{x})$ corresponds to the probability that a value sampled from $\pi(\theta)$ is less than $\mathbf{w}^T \bar{\mathbf{x}}$
 - A threshold value θ is sampled from a given distribution $p(\theta)$
 - \mathbf{x}_i is classified in C_1 if $a_i \geq \theta$, otherwise it is classified in C_0 .
- That is, the activation function, i.e. the probability that \mathbf{x} is classified in C_1 , is given by the cumulative function

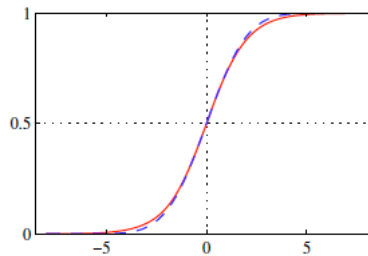
$$f(a) = \int_{-\infty}^{\mathbf{w}^T \bar{\mathbf{x}}} \pi(\theta) d\theta$$

Probit regression

- A relevant case is the one of a gaussian $\pi(\theta)$ with zero mean and unitary variance, which results into a *probit* activation function

$$\Phi(a) = \int_{-\infty}^a \frac{1}{\sqrt{2\pi}} e^{-\frac{\theta^2}{2}} d\theta$$

- observe that $\Phi(a)$ is monotonically increasing, with $0 < \Phi(a) < 1$



- Usually, similar to logistic regression

Bayesian logistic regression

- Used to overcome the overfitting problem by assuming a prior distribution
- The aim is to estimate the posterior class (predictive) distribution, that is the expectation of the model prediction wrt to the distribution of model coefficients,

$$\begin{aligned} p(C_1|\mathbf{x}, \mathbf{X}, \mathbf{t}) &= \int p(C_1|\mathbf{x}, \mathbf{w}) p(\mathbf{w}|\mathbf{X}, \mathbf{t}) d\mathbf{w} \\ &= \int \sigma(\mathbf{w}^T \bar{\mathbf{x}}) p(\mathbf{w}|\mathbf{X}, \mathbf{t}) d\mathbf{w} \end{aligned}$$

- we need some way to evaluate the posterior distribution of coefficients $p(\mathbf{w}|\mathbf{X}, \mathbf{t})$ for any \mathbf{w}

Posterior distribution of coefficients

By Bayes' rule,

$$p(\mathbf{w}|\mathbf{X}, \mathbf{t}) = \frac{p(\mathbf{t}|\mathbf{X}, \mathbf{w})p(\mathbf{w})}{p(\mathbf{t}|\mathbf{X})} = \frac{p(\mathbf{t}|\mathbf{X}, \mathbf{w})p(\mathbf{w})}{\int p(\mathbf{t}|\mathbf{X}, \mathbf{w}')p(\mathbf{w}')d\mathbf{w}'}$$

where the likelihood is $p(\mathbf{t}|\mathbf{X}, \mathbf{w}) = \prod_{i=1}^n p(t_i|\mathbf{x}_i, \mathbf{w})$, with

$$p(t_i|\mathbf{x}_i, \mathbf{w}) = \begin{cases} \sigma(\mathbf{w}^T \bar{\mathbf{x}}) & \text{if } t_i = 1 \\ 1 - \sigma(\mathbf{w}^T \bar{\mathbf{x}}) & \text{if } t_i = 0 \end{cases}$$

Posterior distribution of coefficients

That is,

$$p(\mathbf{t}|\mathbf{X}, \mathbf{w}) = \prod_{i=1}^n \sigma(\mathbf{w}^T \bar{\mathbf{x}})^{t_i} (1 - \sigma(\mathbf{w}^T \bar{\mathbf{x}}))^{1-t_i}$$

and

$$p(\mathbf{w}|\mathbf{X}, \mathbf{t}) = \frac{p(\mathbf{w}) \prod_{i=1}^n \sigma(\mathbf{w}^T \bar{\mathbf{x}})^{t_i} (1 - \sigma(\mathbf{w}^T \bar{\mathbf{x}}))^{1-t_i}}{Z}$$

with the normalization factor

$$Z = \int p(\mathbf{w}) \prod_{i=1}^n \sigma(\mathbf{w}^T \bar{\mathbf{x}})^{t_i} (1 - \sigma(\mathbf{w}^T \bar{\mathbf{x}}))^{1-t_i} d\mathbf{w}$$

Predictive distribution intractability

Z is hard to compute: we are only able to evaluate the numerator

$$g(\mathbf{w}; \mathbf{X}, \mathbf{t}) = p(\mathbf{w}) \prod_{i=1}^n \sigma(\mathbf{w}^T \bar{\mathbf{x}})^{t_i} (1 - \sigma(\mathbf{w}^T \bar{\mathbf{x}}))^{1-t_i}$$

which is proportional to $p(\mathbf{w}|\mathbf{X}, \mathbf{t})$ through an unknown proportionality coefficient.

Predictive distribution intractability

Possible options:

1. find a single value of \mathbf{w} which maximizes $p(\mathbf{w}|\mathbf{X}, \mathbf{t})$: this corresponds to the value which maximizes $g(\mathbf{w}; \mathbf{X}, \mathbf{t})$ (this is the usual MAP approach)
2. approximate $p(\mathbf{w}|\mathbf{X}, \mathbf{t})$ with some other probability density which can be treated analytically (*variational approach*)
3. sample from $p(\mathbf{w}|\mathbf{X}, \mathbf{t})$, knowing only $g(\mathbf{w}; \mathbf{X}, \mathbf{t})$ (*Montecarlo approach*)