Probabilistic classification

Course of Machine Learning
Master Degree in Computer Science
University of Rome "Tor Vergata"
a.a. 2019-2020

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Naive Bayes classifiers recap

A *language model* is a (categorical) probability distribution on a vocabulary of terms (possibly, all words which occur in a large collection of documents).

Use

A language model can be applied to predict (generate) the next term occurring in a text. The probability of occurrence of a term is related to its information content and is at the basis of a number of information retrieval techniques.

Hypothesis

It is assumed that the probability of occurrence of a term is independent from the preceding terms in a text (*bag of words* model).

Bayesian classifiers

A language model can be applied to derive document classifiers into two or more classes through Bayes' rule.

- given two classes C_1, C_2, assume that, for any document d, the probabilities $p(C_1|d)$ and $p(C_2|d)$ are known: then, d can be assigned to the class with higher probability
- how to derive $p(C_k|d)$ for any document, given a collection $\mathcal{C}_1$ of documents known to belong to C_1 and a similar collection $\mathcal{C}_2$ for C_2? Apply Bayes' rule:

  $$p(C_k|d) \propto p(d|C_k)p(C_k)$$

  the evidence $p(d)$ is the same for both classes, and can be ignored.
- we have still the problem of computing $p(C_k)$ and $p(d|C_k)$ from $\mathcal{C}_1$ and $\mathcal{C}_2$

Bayesian classifiers

Computing $p(C_k)$

The prior probabilities $p(C_k)$ $(k = 1, 2)$ can be easily estimated from $\mathcal{C}_1, \mathcal{C}_2$: for example, by applying ML, we obtain

$$p(C_k) = \frac{|\mathcal{C}_1|}{|\mathcal{C}_1| + |\mathcal{C}_2|}$$

Naive bayes classifiers

Computing $p(d|C_k)$

For what concerns the likelihoods $p(d|C_k)$ $(k = 1, 2)$, we observe that d can be seen, according to the bag of words assumption, as a multiset of n_d terms

$$d = \{\bar{t}_1, \bar{t}_2, \ldots, \bar{t}_{n_d}\}$$

By applying the product rule, it results

$$
\begin{aligned}
p(d|C_k) &= p(\bar{t}_1, \ldots, \bar{t}_{n_d}|C_k) \\
&= p(\bar{t}_1|C_k)p(\bar{t}_2|\bar{t}_1, C_k)\cdots p(\bar{t}_{n_d}|\bar{t}_1, \ldots, \bar{t}_{n_d-1}, C_k)
\end{aligned}
$$

Naive bayes classifiers

The naive Bayes assumption

Computing $p(d|C_k)$ is much easier if we assume that terms are pairwise conditionally independent, given the class C_k, that is, for $i, j = 1 \ldots, n_d$ and $k = 1, 2$,

$$
p(\bar{t}_i, \bar{t}_j|C_k) = p(\bar{t}_i|C_k)p(\bar{t}_2|C_k)
$$

as, a consequence,

$$
p(d|C_k) = \prod_{j=1}^{n_d} p(\bar{t}_j|C_k)
$$

that is, we model the document as a set of samples from a categorical distribution (the language model): ML is applied to select the best categorical distribution (class)

Language models and NB classifiers

The categorical distributions $p(\bar{t}_j|C_k)$ have been derived for C_1 and C_2, respectively from documents in $\mathcal{C}_1$ and $\mathcal{C}_2$.

Generative models

- Classes are modeled by suitable conditional distributions $p(\mathbf{x}|C_k)$ (language models in the previous case): it is possible to sample from such distributions to generate random documents statistically equivalent to the documents in the collection used to derive the model.
- Bayes' rule allows to derive $p(C_k|\mathbf{x})$ given such models (and the prior distributions $p(C_k)$ of classes)
- We may derive the parameters of $p(\mathbf{x}|C_k)$ and $p(C_k)$ from the dataset, for example through maximum likelihood estimation
- Classification is performed by comparing $p(C_k|\mathbf{x})$ for all classes

Deriving posterior probabilities

- Let us consider the binary classification case and observe that

$$
p(C_1|\mathbf{x}) = \frac{p(\mathbf{x}|C_1)p(C_1)}{p(\mathbf{x}|C_1)p(C_1) + p(\mathbf{x}|C_2)p(C_2)} = \frac{1}{1 + \frac{p(\mathbf{x}|C_2)p(C_2)}{p(\mathbf{x}|C_1)p(C_1)}}
$$

- Let us define

$$
a = \log \frac{p(\mathbf{x}|C_1)p(C_1)}{p(\mathbf{x}|C_2)p(C_2)} = \log \frac{p(C_1|\mathbf{x})}{p(C_2|\mathbf{x})}
$$

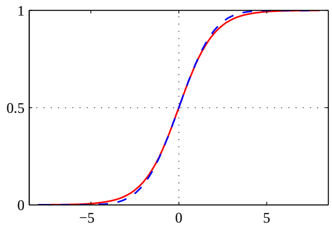
  that is, a is the log of the ratio between the posterior probabilities (*log odds*)

- We obtain that

$$
p(C_1|\mathbf{x}) = \frac{1}{1 + e^{-a}} = \sigma(a) \qquad p(C_2|\mathbf{x}) = 1 - \frac{1}{1 + e^{-a}} = \frac{1}{1 + e^{a}}
$$

- $\sigma(x)$ is the *logistic function* or (*sigmoid*)

Sigmoid



Useful properties of the sigmoid

- $\sigma(-x) = 1 - \sigma(x)$
- $\dfrac{d\sigma(x)}{dx} = \sigma(x)(1-\sigma(x))$

Deriving posterior probabilities

- In the case $K > 2$, the general formula holds

$$p(C_k|\mathbf{x}) = \frac{p(\mathbf{x}|C_k)p(C_k)}{\sum_j p(\mathbf{x}|C_j)p(C_j)}$$

- Let us define, for each $k = 1, \ldots, K$

$$a_k(\mathbf{x}) = \log(p(\mathbf{x}|C_k)p(C_k)) = \log p(C_k|\mathbf{x}) + \log p(C_k)$$

- Then, we may write

$$p(C_k|\mathbf{x}) = \frac{e^{a_k}}{\sum_j e^{a_j}} = s(a_k)$$

- $s(\mathbf{x})$ is the *softmax* function (or *normalized exponential*) and it can be seen as an extension of the sigmoid to the case $K > 2$
- $s(\mathbf{x})$ can be seen as a smoothed version of the maximum:
  if $a_k \gg a_j$ for all $j \neq k$, then $s(a_k) \simeq 1$ and $s(a_j) \simeq 0$ for all $j \neq k$

Gaussian discriminant analysis

In Gaussian discriminant analysis (GDA) all class conditional distributions $p(\mathbf{x}|C_k)$ are assumed gaussians. This implies that the corresponding posterior distributions $p(C_k|\mathbf{x})$ can be easily derived.

Hypothesis

All distributions $p(\mathbf{x}|C_k)$ have same covariance matrix $\mathbf{\Sigma}$, of size $D \times D$. Then,

$$p(\mathbf{x}|C_k) = \frac{1}{(2\pi)^{d/2}|\mathbf{\Sigma}|^{1/2}} \exp\left(-\frac{1}{2}(\mathbf{x}-\boldsymbol{\mu}_k)^T\mathbf{\Sigma}^{-1}(\mathbf{x}-\boldsymbol{\mu}_k)\right)$$

Binary case

If $K = 2$,

$$p(C_1|\mathbf{x}) = \sigma(a(\mathbf{x}))$$

where

$$
\begin{aligned}
a(\mathbf{x}) &= \log \frac{p(\mathbf{x}|C_1)p(C_1)}{p(\mathbf{x}|C_2)p(C_2)} \\
&= \log \frac{\frac{1}{(2\pi)^{d/2}|\mathbf{\Sigma}|^{1/2}} exp\left(-\frac{1}{2}(\mathbf{x}-\boldsymbol{\mu}_1)^T\mathbf{\Sigma}^{-1}(\mathbf{x}-\boldsymbol{\mu}_1)\right)p(C_1)}{\frac{1}{(2\pi)^{d/2}|\mathbf{\Sigma}|^{1/2}} exp\left(-\frac{1}{2}(\mathbf{x}-\boldsymbol{\mu}_2)^T\mathbf{\Sigma}^{-1}(\mathbf{x}-\boldsymbol{\mu}_2)\right)p(C_2)} \\
&= \frac{1}{2}(\boldsymbol{\mu}_2^T\mathbf{\Sigma}^{-1}\boldsymbol{\mu}_2 - \mathbf{x}^T\mathbf{\Sigma}^{-1}\boldsymbol{\mu}_2 - \boldsymbol{\mu}_2^T\mathbf{\Sigma}^{-1}\mathbf{x}) - \\
&\quad - \frac{1}{2}(\boldsymbol{\mu}_1^T\mathbf{\Sigma}^{-1}\boldsymbol{\mu}_1 - \mathbf{x}^T\mathbf{\Sigma}^{-1}\boldsymbol{\mu}_1 - \boldsymbol{\mu}_1^T\mathbf{\Sigma}^{-1}\mathbf{x}) + \log \frac{p(C_1)}{p(C_2)}
\end{aligned}
$$

Binary case

Observe that the results of all products involving $\mathbf{\Sigma}^{-1}$ are scalar, hence, in particular

$$
\begin{aligned}
\mathbf{x}^T\mathbf{\Sigma}^{-1}\boldsymbol{\mu}_1 &= \boldsymbol{\mu}_1^T\mathbf{\Sigma}^{-1}\mathbf{x} \\
\mathbf{x}^T\mathbf{\Sigma}^{-1}\boldsymbol{\mu}_2 &= \boldsymbol{\mu}_2^T\mathbf{\Sigma}^{-1}\mathbf{x}
\end{aligned}
$$

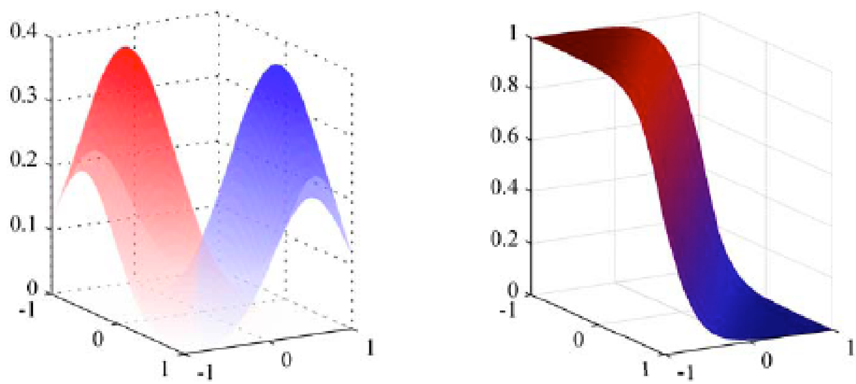
Then,

$$
a(\mathbf{x}) = \frac{1}{2}(\boldsymbol{\mu}_2^T\mathbf{\Sigma}^{-1}\boldsymbol{\mu}_2 - \boldsymbol{\mu}_1^T\mathbf{\Sigma}^{-1}\boldsymbol{\mu}_1) + (\boldsymbol{\mu}_1^T\mathbf{\Sigma}^{-1} - \boldsymbol{\mu}_2^T\mathbf{\Sigma}^{-1})\mathbf{x} + \log \frac{p(C_1)}{p(C_2)} = \mathbf{w}^T\mathbf{x} + w_0
$$

with

$$
\begin{aligned}
\mathbf{w} &= \mathbf{\Sigma}^{-1}(\boldsymbol{\mu}_1 - \boldsymbol{\mu}_2) \\
w_0 &= \frac{1}{2}(\boldsymbol{\mu}_2^T\mathbf{\Sigma}^{-1}\boldsymbol{\mu}_2 - \boldsymbol{\mu}_1^T\mathbf{\Sigma}^{-1}\boldsymbol{\mu}_1) + \log \frac{p(C_1)}{p(C_2)}
\end{aligned}
$$

Example



Left, the class conditional distributions $p(\mathbf{x}|C_1), p(\mathbf{x}|C_2)$, gaussians with $D = 2$. Right the posterior distribution of C_1, $p(C_1|\mathbf{x})$ with sigmoidal slope.

Discriminant function

The discriminant function can be obtained by the condition $p(C_1|\mathbf{x}) = p(C_2|\mathbf{x})$, that is, $\sigma(a(\mathbf{x})) = \sigma(-a(\mathbf{x}))$.

This is equivalent to $a(\mathbf{x}) = -a(\mathbf{x})$ and to $a(\mathbf{x}) = 0$. As a consequence, it results

$$
\mathbf{w}^T\mathbf{x} + w_0 = 0
$$

or

$$
\mathbf{\Sigma}^{-1}(\boldsymbol{\mu}_1 - \boldsymbol{\mu}_2)\mathbf{x} + \frac{1}{2}(\boldsymbol{\mu}_2^T\mathbf{\Sigma}^{-1}\boldsymbol{\mu}_2 - \boldsymbol{\mu}_1^T\mathbf{\Sigma}^{-1}\boldsymbol{\mu}_1) + \log \frac{p(C_2)}{p(C_1)} = 0
$$

Simple case: $\mathbf{\Sigma} = \lambda\mathbf{I}$ (that is, $\sigma_{ii} = \lambda$ for $i = 1, \ldots, d$). In this case, the discriminant function is

$$2(\boldsymbol{\mu}_2 - \boldsymbol{\mu}_1)\mathbf{x} + ||\boldsymbol{\mu}_1||^2 - ||\boldsymbol{\mu}_2||^2 + 2\lambda \log \frac{p(C_2)}{p(C_1)} = 0$$

Multiple classes

In this case, we refer to the softmax function:

$$p(C_k|\mathbf{x}) = s(a_k(\mathbf{x}))$$

where $a_k(\mathbf{x}) = \log(p(\mathbf{x}|C_k)p(C_k))$.

By the above considerations, it easily turns out that

$$a_k(\mathbf{x}) = \frac{1}{2}\left(\boldsymbol{\mu}_k^T\mathbf{\Sigma}^{-1}\mathbf{x} - \boldsymbol{\mu}_k^T\mathbf{\Sigma}^{-1}\boldsymbol{\mu}_k\right) + \log p(C_k) - \frac{d}{2}\log(2\pi) - \frac{1}{2}\log|\mathbf{\Sigma}| = \mathbf{w}_k^T\mathbf{x} + w_{0k}$$

Multiple classes

Decision boundaries corresponding to the case when there are two classes C_j, C_k such that the corresponding posterior probabilities are equal, and larger than the probability of any other class. That is,

$$p(C_k|\mathbf{x}) = p(C_j|\mathbf{x}) \qquad p(C_i|\mathbf{x}) < p(C_k|\mathbf{x}) \quad i \neq j,k$$

hence

$$e^{a_k(\mathbf{x})} = e^{a_j(\mathbf{x})} \qquad e^{a_i(\mathbf{x})} < e^{a^k(\mathbf{x})} \quad i \neq j,k$$

that is,

$$a_k(\mathbf{x}) = a_j(\mathbf{x}) \qquad a_i(\mathbf{x}) < a^k(\mathbf{x}) \quad i \neq j,k$$

As shown, this implies that boundaries are linear.

General covariance matrices, binary case

The class conditional distributions $p(\mathbf{x}|C_k)$ are gaussians with different covariance matrices

$$\begin{aligned}
a(\mathbf{x}) &= \log\frac{p(\mathbf{x}|C_1)p(C_1)}{p(\mathbf{x}|C_2)p(C_2)} \\
&= \log\frac{exp\left(-\frac{1}{2}(\mathbf{x}-\boldsymbol{\mu}_1)^T\mathbf{\Sigma}_1^{-1}(\mathbf{x}-\boldsymbol{\mu}_1)\right)}{exp\left(-\frac{1}{2}(\mathbf{x}-\boldsymbol{\mu}_2)^T\mathbf{\Sigma}_2^{-1}(\mathbf{x}-\boldsymbol{\mu}_2)\right)} + \frac{1}{2}\log\frac{|\mathbf{\Sigma}_2|}{|\mathbf{\Sigma}_1|} + \log\frac{p(C_1)}{p(C_2)} \\
&= \frac{1}{2}\left((\mathbf{x}-\boldsymbol{\mu}_2)^T\mathbf{\Sigma}_2^{-1}(\mathbf{x}-\boldsymbol{\mu}_2) - (\mathbf{x}-\boldsymbol{\mu}_1)^T\mathbf{\Sigma}_1^{-1}(\mathbf{x}-\boldsymbol{\mu}_1)\right) + \frac{1}{2}\log\frac{|\mathbf{\Sigma}_2|}{|\mathbf{\Sigma}_1|} + \log\frac{p(C_1)}{p(C_2)}
\end{aligned}$$

General covariance matrices, binary case

By applying the same considerations, the decision boundary turns out to be

$$\left((\mathbf{x}-\boldsymbol{\mu}_2)^T\mathbf{\Sigma}_2^{-1}(\mathbf{x}-\boldsymbol{\mu}_2) - (\mathbf{x}-\boldsymbol{\mu}_1)^T\mathbf{\Sigma}_1^{-1}(\mathbf{x}-\boldsymbol{\mu}_1)\right) + \log\frac{|\mathbf{\Sigma}_2|}{|\mathbf{\Sigma}_1|} + 2\log\frac{p(C_1)}{p(C_2)} = 0$$

Classes are separated by a (at most) quadratic surface.

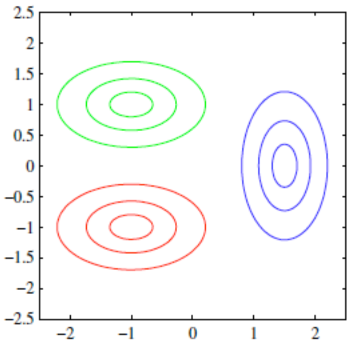
General covariance, multiple classe

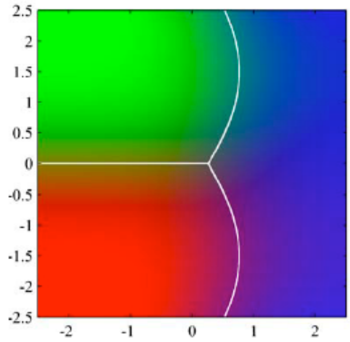
It can be proved that boundary surfaces are at most quadratic.

Example

Left: 3 classes, modeled by gaussians with different covariance matrices.

Right: posterior distribution of classes, with boundary surfaces.





GDA and maximum likelihood

The class conditional distributions $p(\mathbf{x}|C_k)$ can be derived from the training set by maximum likelihood estimation.

For the sake of simplicity, assume $K = 2$ and both classes share the same $\mathbf{\Sigma}$.

It is then necessary to estimate $\boldsymbol{\mu}_1, \boldsymbol{\mu}_2$, $\mathbf{\Sigma}$, and $\pi = p(C_1)$ (clearly, $p(C_2) = 1 - \pi$).

GDA and maximum likelihood

Training set $\mathcal{T}$: includes n elements $(\mathbf{x}_i, t_i)$, with

$$t_i = \begin{cases} 0 & \text{se } \mathbf{x}_i \in C_2 \\ 1 & \text{se } \mathbf{x}_i \in C_1 \end{cases}$$

If $\mathbf{x} \in C_1$, then $p(\mathbf{x}, C_1) = p(\mathbf{x}|C_1)p(C_1) = \pi \cdot \mathcal{N}(\mathbf{x}|\boldsymbol{\mu}_1, \mathbf{\Sigma})$

If $\mathbf{x} \in C_2$, $p(\mathbf{x}, C_2) = p(\mathbf{x}|C_2)p(C_2) = (1 - \pi) \cdot \mathcal{N}(\mathbf{x}|\boldsymbol{\mu}_2, \mathbf{\Sigma})$

The likelihood of the training set $\mathcal{T}$ is

$$L(\pi, \boldsymbol{\mu}_1, \boldsymbol{\mu}_2, \mathbf{\Sigma}|\mathcal{T}) = \prod_{i=1}^{n} (\pi \cdot \mathcal{N}(\mathbf{x}_i|\boldsymbol{\mu}_1, \mathbf{\Sigma}))^{t_i} ((1 - \pi) \cdot \mathcal{N}(\mathbf{x}_i|\boldsymbol{\mu}_2, \mathbf{\Sigma}))^{1-t_i}$$

GDA and maximum likelihood

The corresponding log likelihood is

$$\begin{aligned} l(\pi, \boldsymbol{\mu}_1, \boldsymbol{\mu}_2, \mathbf{\Sigma}|\mathcal{T}) = &\sum_{i=1}^{n} (t_i \log \pi + t_i \log(\mathcal{N}(\mathbf{x}_i|\boldsymbol{\mu}_1, \mathbf{\Sigma}))) + \\ &+ \sum_{i=1}^{n} ((1 - t_i) \log(1 - \pi) + (1 - t_i) \log(\mathcal{N}(\mathbf{x}_i|\boldsymbol{\mu}_2, \mathbf{\Sigma}))) \end{aligned}$$

Its derivative wrt π is

$$\frac{\partial l}{\partial \pi} = \frac{\partial}{\partial \pi} \sum_{i=1}^{n} (t_i \log \pi + (1 - t_i) \log(1 - \pi)) = \sum_{i=1}^{n} \left(\frac{t_i}{\pi} - \frac{(1 - t_i)}{1 - \pi} \right) = \frac{n_1}{\pi} - \frac{n_2}{1 - \pi}$$

which is equal to 0 for

$$\pi = \frac{n_1}{n}$$

GDA and maximum likelihood

The maximum wrt $\boldsymbol{\mu}_1$ (and $\boldsymbol{\mu}_2$) is obtained by computing the gradient

$$\frac{\partial l}{\partial \boldsymbol{\mu}_1} = \frac{\partial}{\partial \boldsymbol{\mu}_1} \sum_{i=1}^{n} t_i \log(\mathcal{N}(\mathbf{x}_i|\boldsymbol{\mu}_1, \mathbf{\Sigma})) = \cdots = \mathbf{\Sigma}^{-1} \sum_{i=1}^{n} t_i(\mathbf{x}_i - \boldsymbol{\mu}_1)$$

As a consequence, we have $\frac{\partial l}{\partial \boldsymbol{\mu}_1} = 0$ for

$$\sum_{i=1}^n t_i \mathbf{x}_i = \sum_{i=1}^n t_i \boldsymbol{\mu}_1$$

hence, for

$$\boldsymbol{\mu}_1 = \frac{1}{n_1} \sum_{\mathbf{x}_i \in C_1} \mathbf{x}_i$$

GDA and maximum likelihood

Similarly, $\frac{\partial l}{\partial \boldsymbol{\mu}_2} = 0$ for

$$\boldsymbol{\mu}_2 = \frac{1}{n_2} \sum_{\mathbf{x}_i \in C_2} \mathbf{x}_i$$

GDA and maximum likelihood

Maximizing the log-likelihood wrt $\boldsymbol{\Sigma}$ provides

$$\boldsymbol{\Sigma} = \frac{n_1}{n}\mathbf{S}_1 + \frac{n_2}{n}\mathbf{S}_2$$

where

$$\mathbf{S}_1 = \frac{1}{n_1} \sum_{\mathbf{x}_i \in C_1} (\mathbf{x}_i - \boldsymbol{\mu}_1)(\mathbf{x}_i - \boldsymbol{\mu}_1)^T$$

$$\mathbf{S}_2 = \frac{1}{n_2} \sum_{\mathbf{x}_i \in C_2} (\mathbf{x}_i - \boldsymbol{\mu}_2)(\mathbf{x}_i - \boldsymbol{\mu}_2)^T$$

and let

$$\mathbf{S} = \frac{n_1}{n}\mathbf{S}_1 + \frac{n_2}{n}\mathbf{S}_2$$

GDA: discrete features

- In the case of d discrete (for example, binary) features we may apply the Naive Bayes hypothesis (independence of features, given the class)
- Then, we may assume that, for any class C_k, the value of the i-th feature is sampled from a Bernoulli distribution of parameter p_{ki}; by the conditional independence hypothesis, it results into

  $$p(\mathbf{x}|C_k) = \prod_{i=1}^d p_{ki}^{x_i}(1 - p_{ki})^{1-x_i}$$

  where $p_{ki} = p(x_i = 1|C_k)$ could be estimated by ML, as in the case of language models
- Functions $a_k(\mathbf{x})$ can then be defined as:

  $$a_k(\mathbf{x}) = \log(p(\mathbf{x}|C_k)p(C_k)) = \sum_{i=1}^D (x_i \log p_{ki} + (1 - x_i)\log(1 - p_{ki})) + \log p(C_k)$$

  These are still linear functions on $\mathbf{x}$.

- The same considerations can be done in the case of non binary features, where, for any class C_k, we may assume the value of the i-th feature is sampled from a distribution on a suitable domain (e.g. Poisson in the case of count data)

Generative models and the exponential family

The property that $p(C_k|\mathbf{x})$ is a generalized linear model with sigmoid (for the binary case) and softmax (for the multiclass case) activation function holds more in general than assuming a gaussian or bernoulli class conditional distribution $p(\mathbf{x}|C_k)$.

Indeed, let the class conditional probability wrt C_k belong to the exponential family, that is it may be written in the form

$$p(\mathbf{x}|\boldsymbol{\theta}_k) = g(\boldsymbol{\theta}_k)f(\mathbf{x})e^{\boldsymbol{\phi}(\boldsymbol{\theta}_k)^T\mathbf{x}}$$

Generative models and the exponential family

In the case of binary classification, we check that $a(\mathbf{x})$ is a linear function

$$\begin{aligned} a(\mathbf{x}) &= \log\frac{p(\mathbf{x}|\boldsymbol{\theta}_1)p(\boldsymbol{\theta}_1)}{p(\mathbf{x}|\boldsymbol{\theta}_2)p(\boldsymbol{\theta}_2)} = \log\frac{g(\boldsymbol{\theta}_1)e^{\frac{1}{s}\boldsymbol{\phi}(\boldsymbol{\theta}_1)^T\mathbf{x}}p(\boldsymbol{\theta}_1)}{g(\boldsymbol{\theta}_2)e^{\frac{1}{s}\boldsymbol{\phi}(\boldsymbol{\theta}_2)^T\mathbf{x}}p(\boldsymbol{\theta}_2)} \\ &= (\boldsymbol{\phi}(\boldsymbol{\theta}_1) - \boldsymbol{\phi}(\boldsymbol{\theta}_2))^T\,\mathbf{x} + \log g(\boldsymbol{\theta}_1) - \log g(\boldsymbol{\theta}_2) + \log p(\boldsymbol{\theta}_1) - \log p(\boldsymbol{\theta}_2) \end{aligned}$$

Similarly, for multiclass classification, we may easily derive that

$$a_k(\mathbf{x}) = \boldsymbol{\phi}(\boldsymbol{\theta}_k)^T\mathbf{x} + \log g(\boldsymbol{\theta}_k) + p(\boldsymbol{\theta}_k)$$

for all k.

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 a instances of *generalized linear models*

GLM

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

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

where f 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

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

   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, $\boldsymbol{\theta}(\mathbf{x}) = \mathbf{w}^T\overline{\mathbf{x}}$

GLM and normal distribution

1. $y \in \mathbb{R}$, and $p(y|\mathbf{x}) = \frac{1}{\sqrt{2\pi}\sigma}e^{-\left(\frac{y-\mu(\mathbf{x})}{\sigma}\right)^2}$ 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 $me\mathbf{u}(y)|\mathbf{x}$ 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 $\theta_1(\mathbf{x}) = \mathbf{w}_1^T\overline{\mathbf{x}}$

Then, a linear regression results

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

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 $\theta(\mathbf{x}) = \mathbf{w}^T\overline{\mathbf{x}}$

Then, a logistic regression derives

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

GLM and categorical distribution

1. $y \in \{1,\ldots,K\}$, and $p(y|\mathbf{x}) = \prod_1^K \pi_i(\mathbf{x})^{y_i}$ (where $y_i = 1$ if $y = i$ and $y = 0$ otherwise) is a categorical distribution with probabilities $\pi_1(\mathbf{x}),\ldots,\pi_K(\mathbf{x})$): the natural parameter is then $\boldsymbol{\theta}(\mathbf{x}) = (\theta_1(\mathbf{x}),\ldots,\theta_K(\mathbf{x}))^T$, 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 $\mathbf{u}(y) = (y_1,\ldots,y_K)^T$ 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 $\sum_{i=1}^K \pi_i(\mathbf{x}) = 1$, it derives

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

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

GLM and categorical distribution

Then, a softmax regression results, with

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

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 $\theta(\mathbf{x}) = \mathbf{w}^T\overline{\mathbf{x}}$

Then, a Poisson regression derives

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

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 $\theta(\mathbf{x}) = \mathbf{w}^T\overline{\mathbf{x}}$

Then, an exponential regression derives

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

Discriminative approach

Alternative idea

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

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

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 $\boldsymbol{\mu}_1, \boldsymbol{\mu}_2$,
  - 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

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

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

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

- it results,

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

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

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

Maximum likelihood estimation

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

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

Newton-Raphson method

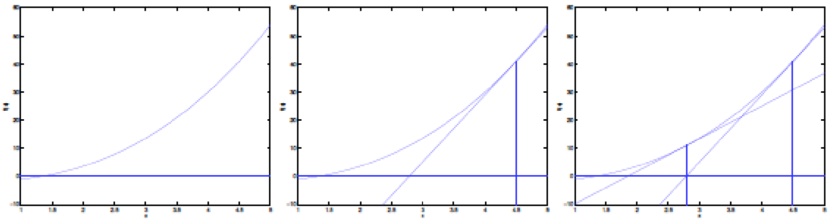
- Maximization of $l(\mathbf{w}|\mathbf{X},\mathbf{t})$ through the well-known Newton-Raphson algorithm to compute the roots of a given function
- Given f : R $\mapsto$ R, the algorithm finds $z \in$ R such that $f(z) = 0$ through a sequence of iterations, starting from an initial value z_0 and performing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

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

Newton-Raphson and linear regression

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

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

- Then,

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

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

- At each iteration, the update is

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

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

Newton-Raphson and logistic regression

Here, we have

$$E(\mathbf{w}) = -l(\mathbf{w}|\mathbf{X}, \mathbf{t}) = -\sum_{i=1}^{n} \left(t_i \ln \sigma(\mathbf{w}^T\overline{\mathbf{x}}_i) + (1-t_i)\ln(1-\sigma(\mathbf{w}^T\overline{\mathbf{x}}_i))\right)$$

(this is called *cross-entropy function*). Hence,

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

$$\mathbf{H} = \frac{\partial}{\partial \mathbf{w}}\frac{\partial E}{\partial \mathbf{w}} = \sum_{i=1}^{n}\sigma(\mathbf{w}^T\overline{\mathbf{x}}_i)(1-\sigma(\mathbf{w}^T\overline{\mathbf{x}}_i))\overline{\mathbf{x}}_i\overline{\mathbf{x}}_i^T = \overline{\mathbf{X}}^T\mathbf{R}_{\mathbf{w}}\overline{\mathbf{X}}$$

where

- $\mathbf{s}_{\mathbf{w}}$ is a vector of size n such that $\mathbf{s}_{\mathbf{w}i} = y(\mathbf{x}_i) = \sigma(\mathbf{w}^T\overline{\mathbf{x}}_i)$ for $i = 1, \ldots, n$
- $\mathbf{R}_{\mathbf{w}}$ is a $n \times n$ diagonal matrix such that

$$\mathbf{R}_{\mathbf{w}ii} = y(\mathbf{x}_i)(1-y(\mathbf{x}_i)) = \sigma(\mathbf{w}^T\overline{\mathbf{x}}_i)(1-\sigma(\mathbf{w}^T\overline{\mathbf{x}}_i)) = \mathbf{s}_{\mathbf{w}i}(1-\mathbf{s}_{\mathbf{w}i})$$

Newton-Raphson and logistic regression

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

$$\begin{aligned}\mathbf{w}^{(i+1)} &= \mathbf{w}^{(i)} - (\overline{\mathbf{X}}^T\mathbf{R}_{\mathbf{w}^{(i)}}\overline{\mathbf{X}})^{-1}\overline{\mathbf{X}}^T(\mathbf{s}_{\mathbf{w}^{(i)}} - \mathbf{t})\\ &= (\overline{\mathbf{X}}^T\mathbf{R}_{\mathbf{w}^{(i)}}\overline{\mathbf{X}})^{-1}((\overline{\mathbf{X}}^T\mathbf{R}_{\mathbf{w}^{(i)}}\overline{\mathbf{X}})\mathbf{w}^{(i)} - \overline{\mathbf{X}}^T(\mathbf{s}_{\mathbf{w}^{(i)}} - \mathbf{t}))\\ &= (\overline{\mathbf{X}}^T\mathbf{R}_{\mathbf{w}^{(i)}}\overline{\mathbf{X}})^{-1}\overline{\mathbf{X}}^T\mathbf{R}_{\mathbf{w}^{(i)}}\mathbf{z}_{\mathbf{w}^{(i)}}\end{aligned}$$

  where $\mathbf{z}_{\mathbf{w}^{(i)}}$ is a vector of size n defined as

$$\mathbf{z}_{\mathbf{w}^{(i)}} = \overline{\mathbf{X}}\mathbf{w}^{(i)} - \mathbf{R}_{\mathbf{w}^{(i)}}^{-1}(\mathbf{s}_{\mathbf{w}^{(i)}} - \mathbf{t})$$

  As it can be seen, $\mathbf{z}_{\mathbf{w}^{(i)}}$ 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

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

  for given weights $\psi_1, \ldots, \psi_n$. Clearly, the least squares problems corresponds to the case $\psi_i = 1$ for $i = 1, \ldots, n$

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

$$\mathbf{w} = (\overline{\mathbf{X}}^T\mathbf{\Psi}\overline{\mathbf{X}})^{-1}\overline{\mathbf{X}}^T\mathbf{\Psi}\mathbf{t}$$

  where $\mathbf{\Psi}$ is a diagonal matrix such that $\mathbf{\Psi}_{ii} = \psi_i$

Iterated reweighted least squares

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

$$\mathbf{w}^{(k+1)} = (\overline{\mathbf{X}}^T\mathbf{R}_{\mathbf{w}^{(k)}}\overline{\mathbf{X}})^{-1}\overline{\mathbf{X}}^T\mathbf{R}_{\mathbf{w}^{(k)}}\mathbf{z}_{\mathbf{w}^{(k)}}$$

- This corresponds to optimizing the weighted least squares cost function for feature matrix $\mathbf{X}$, target vector $\tilde{\mathbf{t}} = \overline{\mathbf{X}}\mathbf{w}^{(i)} - \mathbf{R}^{-1}_{\mathbf{w}^{(i)}}(\mathbf{s}_{\mathbf{w}^{(i)}} - \mathbf{t})$, and weights $\psi_k = \sigma((\mathbf{w}^{(k)})^T\overline{\mathbf{x}}_i)(1-\sigma((\mathbf{w}^{(k)})\overline{\mathbf{x}}_i))$

- 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 $\mathbf{\Psi} = \mathbf{R}_{\mathbf{w}^{(i+1)}}$ and $\tilde{t} = \mathbf{z}_{\mathbf{w}^{(i+1)}}$.

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 $\mathbf{\Sigma}$ 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 vector $\mathbf{w} = (\mathbf{w}_1, \ldots, \mathbf{w}_K)$ of model coefficients, of size $(d+1)K$, where the j-th block of $\mathbf{w}$ ($j = 1, \ldots, K$) corresponds to the vector $\mathbf{w}_j$ of the $d+1$ coefficients for class C_j.
- In this case, the likelihood is defined as

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

where $\mathbf{X}$ is the usual matrix of features and $\mathbf{T}$ is an $n \times K$ matrix such that the i-th row of $\mathbf{T}$ 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

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

The gradient is the vector of size $(d+1)K$ defined as

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

ML and softmax regression

- To derive $\dfrac{\partial l(\mathbf{w})}{\partial \mathbf{w}_j}$ let

$$y_{ik} = \frac{e^{a_{ik}}}{\sum_{r=1}^{K} e^{a_{ir}}} \qquad \text{with} \qquad a_{ik} = \mathbf{w}_k^T \overline{\mathbf{x}}_i$$

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

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

- For each $i = 1, \ldots, n$, $j = 0, \ldots, d$, $k = 1, \ldots, K$,

$$\frac{\partial a_{ik}}{\partial w_{kj}} = \frac{\partial}{\partial w_{kj}} \mathbf{w}_k^T \overline{\mathbf{x}}_i = x_{ik} \qquad \frac{\partial y_{ik}}{\partial a_{ik}} = y_{ik}(1 - y_{ik}) \qquad \frac{\partial y_{ik}}{\partial a_{ir}} = -y_{ir} y_{ik} \qquad \text{if } r \neq k$$

ML and softmax regression

Hence,

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

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

$$\begin{aligned}
p(\mathcal{C}_1 | \mathbf{x}, \mathbf{X}, \mathbf{t}) &= \int p(\mathcal{C}_1 | \mathbf{x}, \mathbf{w}) p(\mathbf{w} | \mathbf{X}, \mathbf{t}) d\mathbf{w} \\
&= \int \sigma(\mathbf{w}^T \boldsymbol{\phi}(\mathbf{x})) p(\mathbf{w} | \mathbf{X}, \mathbf{t}) d\mathbf{w}
\end{aligned}$$

- 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

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

Posterior distribution of coefficients

That is,

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

and

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

with the normalization factor

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

Predictive distribution intractability

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

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

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)