Probabilistic classification

Course of Machine Learning Master Degree in Computer Science University of Rome "Tor Vergata"

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Some general considerations

Observe that, in general, it is possible to write, in the binary classification case,

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

if we define

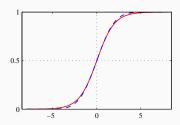
$$a = \log \frac{p(\mathbf{x}|C_1)p(C_1)}{p(\mathbf{x}|C_2)p(C_2)} = \log \frac{p(C_1|\mathbf{x})}{p(C_2|\mathbf{x})}$$

that is, if a is the log of the ratio between the posterior probabilities (log odds), we obtain that

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

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

Sigmoid



Useful properties of the sigmoid

$$\cdot \ \sigma(-x) = 1 - \sigma(x)$$

$$\cdot \ \sigma(-x) = 1 - \sigma(x)$$

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

In the case K > 2, the general formula holds

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

If we define, for each $k = 1, \dots, K$

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

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

Definition

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 Σ , of size $D \times D$. Then,

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

If
$$K=2$$
,
$$p(C_1|\mathbf{x}) = \sigma(a(\mathbf{x}))$$

where

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

Binary case

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

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

Then,

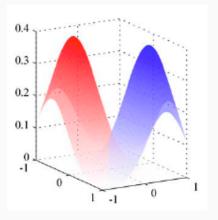
$$a(\mathbf{x}) = \frac{1}{2} (\mu_2^T \Sigma^{-1} \mu_2 - \mu_1^T \Sigma^{-1} \mu_1) + (\mu_1^T \Sigma^{-1} - \mu_2^T \Sigma^{-1}) \mathbf{x} + \log \frac{p(C_1)}{p(C_2)}$$
$$= \mathbf{w}^T \mathbf{x} + w_0$$

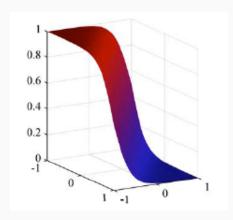
with

$$\mathbf{w} = \mathbf{\Sigma}^{-1}(\boldsymbol{\mu}_1 - \boldsymbol{\mu}_2)$$

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

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

$$\Sigma^{-1}(\mu_1 - \mu_2)\mathbf{x} + \frac{1}{2}(\mu_2^T \Sigma^{-1} \mu_2 - \mu_1^T \Sigma^{-1} \mu_1) + \log \frac{p(C_2)}{p(C_1)} = 0$$

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

$$2(\mu_2 - \mu_1)\mathbf{x} + ||\mu_1||^2 - ||\mu_2||^2 + 2\lambda \log \frac{p(C_2)}{p(C_1)} = 0$$

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

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

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,

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

hence

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

that is,

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

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

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

General covariance matrices, binary case

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

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

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

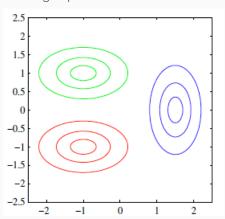
General covariance, multiple classe

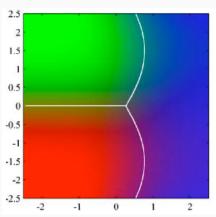
It can be proved that boundary surfaces are at most quadratic.

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 ${\bf \Sigma}.$

It is then necessary to estimate μ_1, μ_2, Σ , 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 $p(\mathbf{x}, C_1) = p(\mathbf{x}|C_1)p(C_1) = \pi \cdot \mathcal{N}(\mathbf{x}|\boldsymbol{\mu}_1, \boldsymbol{\Sigma})$

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

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

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

The corresponding log likelihood is

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

$$+ \sum_{i=1}^n \left((1 - t_i) \log(1 - \pi) + (1 - t_i) \log(\mathcal{N}(\mathbf{x}_i | \boldsymbol{\mu}_2, \boldsymbol{\Sigma})) \right)$$

Its derivative wrt π is

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

which is equal to 0 for

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

The maximum wrt μ_1 (and μ_2) is obtained by computing the gradient

$$\frac{\partial l}{\partial \boldsymbol{\mu}_1} = \frac{\partial}{\partial \boldsymbol{\mu}_1} \sum_{i=1}^n t_i \log(\mathcal{N}(\mathbf{x}_i | \boldsymbol{\mu}_1, \boldsymbol{\Sigma})) = -\frac{1}{2} \frac{\partial}{\partial \boldsymbol{\mu}_1} \sum_{i=1}^n t_i (\mathbf{x}_i - \boldsymbol{\mu}_1)^T \boldsymbol{\Sigma}^{-1} (\mathbf{x}_i - \boldsymbol{\mu}_1)$$

Let $\boldsymbol{\xi}_i = (\mathbf{x}_i - \boldsymbol{\mu}_1)$, then, by the chain rule of derivatives,

$$\frac{\partial l}{\partial \boldsymbol{\mu}_{1}} = -\frac{1}{2} \sum_{i=1}^{n} t_{i} \frac{\partial}{\partial \boldsymbol{\mu}_{1}} \left(\boldsymbol{\xi}_{i}^{T} \boldsymbol{\Sigma}^{-1} \boldsymbol{\xi}_{i} \right) = -\frac{1}{2} \sum_{i=1}^{n} t_{i} \frac{\partial \boldsymbol{\xi}_{i}}{\partial \boldsymbol{\mu}_{1}} \frac{\partial}{\partial \boldsymbol{\xi}_{i}} \left(\boldsymbol{\xi}_{i}^{T} \boldsymbol{\Sigma}^{-1} \boldsymbol{\xi}_{i} \right)
= \frac{1}{2} \sum_{i=1}^{n} t_{i} \left(\boldsymbol{\Sigma}^{-1} + (\boldsymbol{\Sigma}^{-1})^{T} \right) \boldsymbol{\xi}_{i} = \boldsymbol{\Sigma}^{-1} \sum_{i=1}^{n} t_{i} (\mathbf{x}_{i} - \boldsymbol{\mu}_{1})$$

since in general

$$\frac{\partial}{\partial \mathbf{a}} \left(\mathbf{a}^T \mathbf{A} \mathbf{a} \right) = (\mathbf{A} + \mathbf{A}^T) \mathbf{a}$$

and $\mathbf{\Sigma}^{-1} = (\mathbf{\Sigma}^{-1})^T$ by the symmetry of the covariance matrix.

GDA and maximum likelihood

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

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

hence, for

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

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

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

To maximize the log-likelihood wrt Σ , derive the corresponding gradient

$$\begin{split} \frac{\partial l}{\partial \boldsymbol{\Sigma}} &= \sum_{i=1}^{n} t_{i} \frac{\partial}{\partial \boldsymbol{\Sigma}} \log(\mathcal{N}(\mathbf{x}_{i} | \boldsymbol{\mu}_{1}, \boldsymbol{\Sigma})) + \sum_{i=1}^{n} (1 - t_{i}) \frac{\partial}{\partial \boldsymbol{\Sigma}} \log(\mathcal{N}(\mathbf{x}_{i} | \boldsymbol{\mu}_{2}, \boldsymbol{\Sigma})) \\ &= \sum_{i=1}^{n} t_{i} \frac{\partial}{\partial \boldsymbol{\Sigma}} \log |\boldsymbol{\Sigma}|^{-\frac{1}{2}} + \frac{\partial}{\partial \boldsymbol{\Sigma}} \left((\mathbf{x}_{i} - \boldsymbol{\mu}_{1})^{T} \boldsymbol{\Sigma}^{-1} (\mathbf{x}_{i} - \boldsymbol{\mu}_{1}) \right) \\ &+ \sum_{i=1}^{n} (1 - t_{i}) \frac{\partial}{\partial \boldsymbol{\Sigma}} \log |\boldsymbol{\Sigma}|^{-\frac{1}{2}} + \frac{\partial}{\partial \boldsymbol{\Sigma}} \left((\mathbf{x}_{i} - \boldsymbol{\mu}_{2})^{T} \boldsymbol{\Sigma}^{-1} (\mathbf{x}_{i} - \boldsymbol{\mu}_{2}) \right) \\ &= -\frac{n}{2} \frac{\partial}{\partial \boldsymbol{\Sigma}} \log |\boldsymbol{\Sigma}| - \frac{1}{2} \frac{\partial}{\partial \boldsymbol{\Sigma}} \sum_{\mathbf{x}_{i} \in C_{1}} \left((\mathbf{x}_{i} - \boldsymbol{\mu}_{1})^{T} \boldsymbol{\Sigma}^{-1} (\mathbf{x}_{i} - \boldsymbol{\mu}_{1}) \right) \\ &- \frac{1}{2} \frac{\partial}{\partial \boldsymbol{\Sigma}} \sum_{\mathbf{x}_{i} \in C_{2}} \left((\mathbf{x}_{i} - \boldsymbol{\mu}_{2})^{T} \boldsymbol{\Sigma}^{-1} (\mathbf{x}_{i} - \boldsymbol{\mu}_{2}) \right) \end{split}$$

GDA and maximum likelihood

Observe now that $\mathbf{x}^T \mathbf{A} \mathbf{x}$ is a scalar, hence $\mathbf{x}^T \mathbf{A} \mathbf{x} = tr(\mathbf{x}^T \mathbf{A} \mathbf{x})$; moreover, in general

$$tr(ABC) = tr(CAB) = tr(BCA)$$

As a consequence, $\mathbf{x}^T \mathbf{A} \mathbf{x} = \operatorname{tr} \left(\mathbf{A} \mathbf{x} \mathbf{x}^T \right)$ and

$$\frac{\partial l}{\partial \Sigma} = -\frac{n}{2} \frac{\partial}{\partial \Sigma} \log |\Sigma| - \frac{1}{2} \frac{\partial}{\partial \Sigma} \sum_{\mathbf{x}_i \in C_1} \operatorname{tr} \left((\mathbf{x}_i - \boldsymbol{\mu}_1) (\mathbf{x}_i - \boldsymbol{\mu}_1)^T \Sigma^{-1} \right)$$
$$- \frac{1}{2} \frac{\partial}{\partial \Sigma} \sum_{\mathbf{x}_i \in C_2} \operatorname{tr} \left((\mathbf{x}_i - \boldsymbol{\mu}_2) (\mathbf{x}_i - \boldsymbol{\mu}_2)^T \Sigma^{-1} \right)$$

Let us now define the following matrices

$$\begin{aligned} \mathbf{S}_1 &= \frac{1}{n_1} \sum_{\mathbf{x}_i \in C_1} (\mathbf{x}_i - \boldsymbol{\mu}_1) (\mathbf{x}_i - \boldsymbol{\mu}_1)^T \\ \mathbf{S}_2 &= \frac{1}{n_2} \sum_{\mathbf{x}_i \in C_2} (\mathbf{x}_i - \boldsymbol{\mu}_2) (\mathbf{x}_i - \boldsymbol{\mu}_2)^T \end{aligned}$$

and let

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

By applying these definitions, we obtain

$$\begin{split} \frac{\partial l}{\partial \mathbf{\Sigma}} &= -\frac{n}{2} \frac{\partial}{\partial \mathbf{\Sigma}} \log |\mathbf{\Sigma}| - \frac{n}{2} \frac{\partial}{\partial \mathbf{\Sigma}} \mathrm{tr} \left(\mathbf{S} \mathbf{\Sigma}^{-1} \right) \\ &= -\frac{n}{2} \left(\mathbf{\Sigma}^{-1} \right)^T - \frac{n}{2} \frac{\partial \mathbf{\Sigma}^{-1}}{\partial \mathbf{\Sigma}} \frac{\partial}{\partial \mathbf{\Sigma}^{-1}} \mathrm{tr} \left(\mathbf{\Sigma}^{-1} \mathbf{S} \right) \\ &= -\frac{n}{2} \mathbf{\Sigma}^{-1} + \frac{n}{2} (\mathbf{\Sigma}^{-1} \mathbf{\Sigma}^{-1}) \mathbf{S}^T \\ &= \frac{n}{2} \mathbf{\Sigma}^{-1} \left(-\mathbf{I} + \mathbf{\Sigma}^{-1} \mathbf{S} \right) \end{split}$$

since in general

$$\frac{\partial}{\partial \mathbf{A}} \log |\mathbf{A}| = \mathbf{A}^{-1}$$
 $\frac{\partial}{\partial \mathbf{A}} \operatorname{tr}(\mathbf{B}\mathbf{A}) = \mathbf{B}^{T}$ $\frac{\partial \mathbf{A}^{-1}}{\partial \mathbf{A}} = \mathbf{A}^{-1} \mathbf{A}^{-1}$

This results into $\frac{\partial l}{\partial \mathbf{\Sigma}} = \mathbf{0}$ iff $\mathbf{\Sigma} = \mathbf{S}$

GDA: discrete features

In the case of discrete (for example, binary) features we may simplify the model by assuming features are conditionally independent, given the class (naive Bayes hypothesis). Then,

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

where $p_{ki} = p(x_i = 1|C_k)$.

Functions $a_k(\mathbf{x})$ can then be defined as in the softmax model:

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

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

These are still linear functions on x.

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 \mathcal{C}_k belong to the exponential family, that is it has the form

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

with the additional constraint that ${\bf u}$ is the identity function, that is ${\bf u}({\bf x})={\bf x}.$

Generative models and the exponential family

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

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

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.

Probabilistic discriminative models

Generative models

For a large set of distributions type for $p(\mathbf{x}|C_k)$ the posterior class distributions $p(C_k|\mathbf{x})$ are sigmoidal (in the binary case) or softmax (for more classes): in both cases, with argument given by a linear combination of features in \mathbf{x} .

We may derive both the parameters of $p(\mathbf{x}|C_k)$ and the prior class probabilities $p(C_k)$ through maximum likelihood estimation, and next apply Bayes' rule to derive $p(C_k|\mathbf{x})$, at least up to a normalization factor.

Discriminative approach

Alternative idea

We could directly assume that $p(C_k|\mathbf{x})$ is sigmoidal (indeed a generalized linear model with sigmoidal non linear function) and derive it (for example through ML estimation of its parameters).

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.

Generalized linear models

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.

Logistic regression

Logistic regression is a GLM such that

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

where the use of basis functions is explicitly considered.

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,\ldots,w_d to be derived from a training set
- A generative approach with gaussian distributions requires:
 - \cdot $\,2d$ coefficients for the means $oldsymbol{\mu}_1,oldsymbol{\mu}_2$,
 - · 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)

 \cdot Training set \mathbf{X}, \mathbf{t} . The likelihood is

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

where
$$p_i = p(C_1|\phi(\mathbf{x}_i)) = \sigma(a_i)$$
, with $a_i = \mathbf{w}^T \phi(\mathbf{x}_i)$

· The log-likelihood is then

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

· Note that

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

and

$$\frac{\partial l(\mathbf{w}|\mathbf{X}, \mathbf{t})}{\partial p_i} = \frac{t_i}{p_i} - \frac{1 - t_i}{1 - p_i} = \frac{t_i - p_i}{p_i(1 - p_i)}$$
$$\frac{\partial p_i}{\partial a_i} = \frac{\partial \sigma(a_i)}{\partial a_i} = \sigma(a_i)(1 - \sigma(a_i)) = p_i(1 - p_i)$$
$$\frac{\partial a_i}{\partial \mathbf{w}} = \phi(\mathbf{x}_i)$$

· Hence,

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

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

$$\mathbf{w}^{(j+1)} = \mathbf{w}^{(j)} + \alpha \frac{\partial l(\mathbf{w}|\mathbf{X}, \mathbf{t})}{\partial \mathbf{w}}|_{\mathbf{w}^{(j)}}$$

$$= \mathbf{w}^{(j)} + \alpha \sum_{i=1}^{n} (t_i - \sigma((\mathbf{w}^{(j)})^T \phi(\mathbf{x}_i))) \phi(\mathbf{x}_i)$$

$$= \mathbf{w}^{(j)} + \alpha \sum_{i=1}^{n} (t_i - y(\mathbf{x}_i)) \phi(\mathbf{x}_i)$$

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

$$w_k^{(j+1)} = w_k^{(j)} + \alpha \frac{\partial l(\mathbf{w}|\mathbf{X}, \mathbf{t})}{\partial w_k} \Big|_{\mathbf{w}^{(j)}}$$

$$= w_k^{(j+1)} + \alpha \sum_{i=1}^n (t_i - \sigma((\mathbf{w}^{(j)})^T \phi(\mathbf{x}_i))) \phi_k(\mathbf{x}_i)$$

$$= w_k^{(j+1)} + \alpha \sum_{i=1}^n (t_i - y(\mathbf{x}_i)) \phi_k(\mathbf{x}_i)$$

Newton-Raphson method

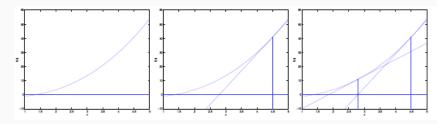
- Maximization of $l(\mathbf{w}|\mathbf{X},\mathbf{t})$ through the well-known Newton-Raphson algorithm to compute the roots of a given function
- Given $f: \mathbb{R} \mapsto \mathbb{R}$, the algorithm finds $z \in \mathbb{R}$ such that f(z) = 0 through a sequence of iterations, starting from an initial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

· The error function, to be minimized, is

$$E(\mathbf{w}) = \frac{1}{2} \sum_{i=1}^{n} (\mathbf{w}^{T} \boldsymbol{\phi}(\mathbf{x}_{i}) - t_{i})^{2}$$

· Then,

$$\frac{\partial E}{\partial \mathbf{w}} = \sum_{i=1}^{n} (\mathbf{w}^{T} \boldsymbol{\phi}(\mathbf{x}_{i}) - t_{i}) \boldsymbol{\phi}(\mathbf{x}_{i}) = \boldsymbol{\Phi}^{T} \boldsymbol{\Phi} \mathbf{w} - \boldsymbol{\Phi}^{T} \mathbf{t}$$

$$\mathbf{H} = \frac{\partial}{\partial \mathbf{w}} \frac{\partial E}{\partial \mathbf{w}} = \sum_{i=1}^{n} \phi(\mathbf{x}_i) \phi(\mathbf{x}_i)^T = \mathbf{\Phi}^T \mathbf{\Phi}$$

· At each iteration, the update is

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

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

Here, we have

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

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

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

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

where

- $\mathbf{s}_{\mathbf{w}}$ is a vector such that $\mathbf{s}_{\mathbf{w}i} = \sigma(\mathbf{w}^T \boldsymbol{\phi}(\mathbf{x}_i))$ for $i = 1, \dots, n$
- \cdot $\mathbf{R}_{\mathbf{w}}$ is a diagonal matrix such that

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

Newton-Raphson and logistic regression

In the case of logistic regression, the update is then

$$\begin{split} \mathbf{w}^{(i+1)} &= \mathbf{w}^{(i)} - (\boldsymbol{\Phi}^T \mathbf{R}_{\mathbf{w}^{(i)}} \boldsymbol{\Phi})^{-1} \boldsymbol{\Phi}^T (\mathbf{s}_{\mathbf{w}^{(i)}} - \mathbf{t}) \\ &= (\boldsymbol{\Phi}^T \mathbf{R}_{\mathbf{w}^{(i)}} \boldsymbol{\Phi})^{-1} ((\boldsymbol{\Phi}^T \mathbf{R}_{\mathbf{w}^{(i)}} \boldsymbol{\Phi}) \mathbf{w}^{(i)} - \boldsymbol{\Phi}^T (\mathbf{s}_{\mathbf{w}^{(i)}} - \mathbf{t})) \\ &= (\boldsymbol{\Phi}^T \mathbf{R}_{\mathbf{w}^{(i)}} \boldsymbol{\Phi})^{-1} \boldsymbol{\Phi}^T \mathbf{R}_{\mathbf{w}^{(i)}} \mathbf{z}_{\mathbf{w}^{(i)}} \end{split}$$

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

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

As can be seen, $\mathbf{z}_{\mathbf{w}^{(i)}}$ is a function of $\mathbf{w}^{(i)}$, hence of i.

Iterated reweighted least squares

• The value $(\Phi^T \mathbf{R}_{\mathbf{w}^{(i)}} \Phi)^{-1} \Phi^T \mathbf{R}_{\mathbf{w}^{(i)}} \mathbf{z}_{\mathbf{w}^{(i)}}$ can be seen as the solution of a suitable instance of the weighted least squares problem defined as the minimization of

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

for given weights ψ_1, \ldots, ψ_n

· For this problem, the optimum is

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

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

- · In our case $\Psi = \mathbf{R}_{\mathbf{w}^{(i)}}$ and $\mathbf{t} = \mathbf{z}_{\mathbf{w}^{(i)}} = \Phi \mathbf{w}^{(i)} \mathbf{R}_{\mathbf{w}^{(i)}}^{-1} (\mathbf{s}_{\mathbf{w}^{(i)}} \mathbf{t})$: both of them are functions of i
- The update of $\mathbf{w}^{(i)}$ performed at each iteration implies solving a new instance of the weighted least square problem, setting $\mathbf{w}^{(i+1)}$ to the solution obtained, and deriving the new values $\mathbf{R}_{\mathbf{w}^{(i+1)}}$ and $\mathbf{z}_{\mathbf{w}^{(i+1)}}$.

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 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 vector \mathbf{w} of model coefficients, of size dK, where the k-th block of \mathbf{w} $(k=1,\ldots,K)$ corresponds to the vector \mathbf{w}_k of coefficients for class C_k .
- · In this case, the likelihood is defined as

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

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

ML and softmax regression

The log-likelihood is then defined as

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

The gradient $\frac{\partial l(\mathbf{w})}{\partial \mathbf{w}}$ is a vector of size dK, where its j-th block $(j=1,\ldots,K)$ corresponds to $\frac{\partial l(\mathbf{w})}{\partial \mathbf{w}_j}$.

ML and softmax regression

• To derive $\frac{\partial l(\mathbf{w})}{\partial \mathbf{w}_j}$ let

$$y_{ik} = \frac{e^{a_{ik}}}{\sum_{r=1}^{K} e^{a_{ir}}}$$
 with $a_{ik} = \mathbf{w}_k^T \phi(\mathbf{x}_i)$

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

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

• For each
$$i=1,\ldots,n,\,j=1,\ldots,M,\,k=1,\ldots,K,$$

$$\frac{\partial a_{ik}}{\partial w_{kj}} = \frac{\partial}{\partial w_{kj}} \mathbf{w}_k^T \boldsymbol{\phi}(\mathbf{x}_i) = \phi_j(\mathbf{x}_i)$$

$$\frac{\partial y_{ik}}{\partial a_{ik}} = y_{ik}(1-y_{ik})$$

$$\frac{\partial y_{ik}}{\partial a_{ir}} = -y_{ir}y_{ik} \quad \text{if } r \neq k$$

Hence,

$$\frac{\partial l(\mathbf{w})}{\partial \mathbf{w}_{j}} = \frac{\partial}{\partial \mathbf{w}_{j}} \sum_{k=1}^{K} \sum_{i=1}^{n} t_{ik} \log y_{ik} = \frac{\partial l}{\partial \mathbf{w}_{j}} \sum_{i=1}^{n} t_{ij} \log y_{ij} + \frac{\partial l}{\partial \mathbf{w}_{j}} \sum_{k \neq j}^{n} \sum_{i=1}^{n} t_{ik} \log y_{ik}$$

$$= \sum_{i=1}^{n} t_{ij} \frac{1}{y_{ij}} \frac{\partial y_{ij}}{\partial a_{ij}} \frac{\partial a_{ij}}{\partial \mathbf{w}_{j}} + \sum_{k \neq j} \sum_{i=1}^{n} t_{ik} \frac{1}{y_{ik}} \frac{\partial y_{ik}}{\partial a_{ik}} \frac{\partial a_{ik}}{\partial \mathbf{w}_{j}}$$

$$= \sum_{i=1}^{n} t_{ij} \frac{1}{y_{ij}} y_{ij} (1 - y_{ij}) \phi(\mathbf{x}_{i}) - \sum_{k \neq j} \sum_{i=1}^{n} t_{ik} \frac{1}{y_{ik}} y_{ik} y_{ij} \phi(\mathbf{x}_{i})$$

$$= \left(\sum_{i=1}^{n} t_{ij} - \sum_{i=1}^{n} y_{ij} \sum_{k=1}^{K} t_{ik}\right) \phi(\mathbf{x}_{i})$$

$$= \left(\sum_{i=1}^{n} t_{ij} - \sum_{i=1}^{n} y_{ij}\right) \phi(\mathbf{x}_{i}) = \sum_{i=1}^{n} (t_{ij} - y_{ij}) \phi(\mathbf{x}_{i})$$

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

Bayesian logistic regression

Bayesian logistic regression

- Used to overcome the overfitting problem by assuming a prior distribution
- The aim is to estimate the posterior class distribution

$$p(C_1|\mathbf{x}, \mathbf{X}, \mathbf{t}) = \int p(C_1|\mathbf{x}, \mathbf{w}) p(\mathbf{w}|\mathbf{X}, \mathbf{t}) d\mathbf{w}$$
$$= \int \sigma(\mathbf{w}^T \phi(\mathbf{x})) p(\mathbf{w}|\mathbf{X}, \mathbf{t}) d\mathbf{w}$$

• Thus, we need to derive the posterior distribution of coefficients $p(\mathbf{w}|\mathbf{X},\mathbf{t})$: this is in general intractable

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

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

that is,

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

and

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

with

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

Predictive distribution intractability

Since the predictive distribution is the expectation of the model prediction wrt to the distribution of model coefficients,

$$p(C_1|\mathbf{x}, \mathbf{X}, \mathbf{t}) = \int \sigma(\mathbf{w}^T \boldsymbol{\phi}(\mathbf{x})) p(\mathbf{w}|\mathbf{X}, \mathbf{t}) d\mathbf{w}$$

we need some way to evaluate $p(\mathbf{w}|\mathbf{X}, \mathbf{t})$ for any \mathbf{w} . Unfortunately, since Z is hard to compute, we are only able to evaluate

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

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
- 3. sample from $p(\mathbf{w}|\mathbf{X}, \mathbf{t})$, knowing only $g(\mathbf{w}; \mathbf{X}, \mathbf{t})$