

# Probabilistic classification

Course of Machine Learning  
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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

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

By applying the product rule, it results

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

# 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  $i, j = 1 \dots, n_d$  and  $k = 1, 2$ ,

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

as, a consequence,

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

## Language models and NB classifiers

The probabilities  $p(\bar{t}_j | C_k)$  are available for all terms if language models have been derived for  $C_1$  and  $C_2$ , respectively from documents in  $\mathcal{C}_1$  and  $\mathcal{C}_2$ .

## Generative models

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Given a language model, it is possible to sample from the distribution to generate random documents statistically equivalent to the documents in the collection used to derive the model.

## 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  $\Sigma$ , of size  $D \times D$ . Then,

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



## Binary case

If  $K = 2$ ,

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

where

$$\begin{aligned} a(\mathbf{x}) &= \log \frac{p(\mathbf{x}|C_1)p(C_1)}{p(\mathbf{x}|C_2)p(C_2)} \\ &= \log \frac{\frac{1}{(2\pi)^{d/2}|\Sigma|^{1/2}} \exp\left(-\frac{1}{2}(\mathbf{x} - \mu_1)^T \Sigma^{-1}(\mathbf{x} - \mu_1)\right) p(C_1)}{\frac{1}{(2\pi)^{d/2}|\Sigma|^{1/2}} \exp\left(-\frac{1}{2}(\mathbf{x} - \mu_2)^T \Sigma^{-1}(\mathbf{x} - \mu_2)\right) p(C_2)} \\ &= \frac{1}{2}(\mu_2^T \Sigma^{-1} \mu_2 - \mathbf{x}^T \Sigma^{-1} \mu_2 - \mu_2^T \Sigma^{-1} \mathbf{x}) - \\ &\quad - \frac{1}{2}(\mu_1^T \Sigma^{-1} \mu_1 - \mathbf{x}^T \Sigma^{-1} \mu_1 - \mu_1^T \Sigma^{-1} \mathbf{x}) + \log \frac{p(C_1)}{p(C_2)} \end{aligned}$$

## Binary case

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

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

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

Then,

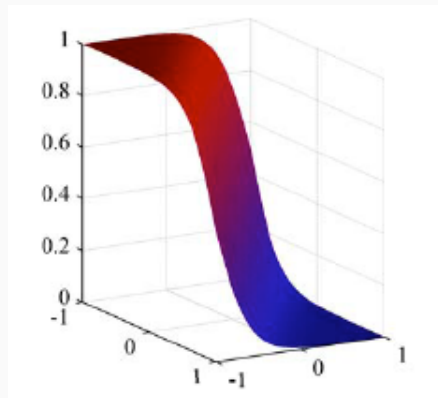
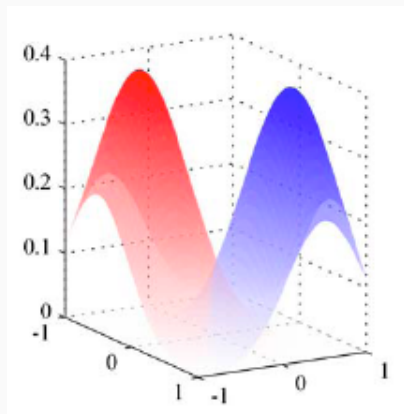
$$a(\mathbf{x}) = \frac{1}{2}(\boldsymbol{\mu}_2^T \Sigma^{-1} \boldsymbol{\mu}_2 - \boldsymbol{\mu}_1^T \Sigma^{-1} \boldsymbol{\mu}_1) + (\boldsymbol{\mu}_1^T \Sigma^{-1} - \boldsymbol{\mu}_2^T \Sigma^{-1})\mathbf{x} + \log \frac{p(C_1)}{p(C_2)} = \mathbf{w}^T \mathbf{x} + w_0$$

with

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

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

## 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

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

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

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

## 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

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

## General covariance matrices, binary case

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

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

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



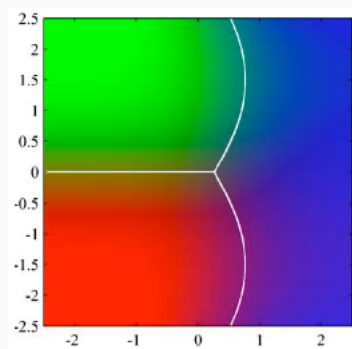
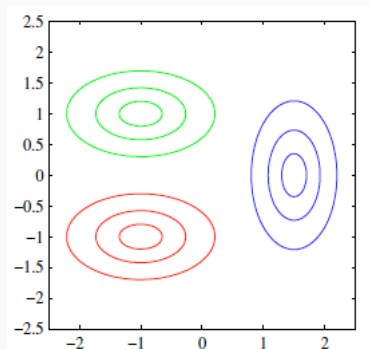
## General covariance, multiple classe

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  $\Sigma$ .

It is then necessary to estimate  $\mu_1, \mu_2, \Sigma$ , 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  $p(\mathbf{x}, C_1) = p(\mathbf{x}|C_1)p(C_1) = \pi \cdot \mathcal{N}(\mathbf{x}|\boldsymbol{\mu}_1, \boldsymbol{\Sigma})$

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

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

## GDA and maximum likelihood

The corresponding log likelihood is

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

Its derivative wrt  $\pi$  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  $\mu_1$  (and  $\mu_2$ ) is obtained by computing the gradient

$$\frac{\partial l}{\partial \mu_1} = \frac{\partial}{\partial \mu_1} \sum_{i=1}^n t_i \log(\mathcal{N}(\mathbf{x}_i | \mu_1, \Sigma)) = \dots = \Sigma^{-1} \sum_{i=1}^n t_i (\mathbf{x}_i - \mu_1)$$

As a consequence, we have  $\frac{\partial l}{\partial \mu_1} = 0$  for

$$\sum_{i=1}^n t_i \mathbf{x}_i = \sum_{i=1}^n t_i \mu_1$$

hence, for

$$\mu_1 = \frac{1}{n_1} \sum_{\mathbf{x}_i \in C_1} \mathbf{x}_i$$

## GDA and maximum likelihood

Similarly,  $\frac{\partial l}{\partial \mu_2} = 0$  for

$$\mu_2 = \frac{1}{n_2} \sum_{\mathbf{x}_i \in C_2} \mathbf{x}_i$$

## GDA and maximum likelihood

Maximizing the log-likelihood wrt  $\Sigma$  provides

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

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

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

## 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.



## 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

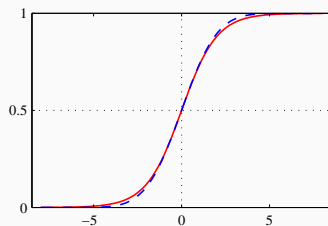
$$a = \log \frac{p(\mathbf{x}|C_1)p(C_1)}{p(\mathbf{x}|C_2)p(C_2)} = \log \frac{p(C_1|\mathbf{x})}{p(C_2|\mathbf{x})} = \log$$

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

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

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

# Sigmoid



Useful properties of the sigmoid

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

# Softmax

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  $k = 1, \dots, K$

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

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  $j \neq k$

## 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.

# 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

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

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

# Generative models and the exponential family

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

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

Similarly, for multiclass classification, we may easily derive that

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

for all  $k$ .

## 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.

# Logistic regression

Logistic regression is a GLM such that

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

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  $w_0, \dots, w_d$  to be derived from a training set
- A generative approach with gaussian distributions requires:
  - $2d$  coefficients for the means  $\mu_1, \mu_2$ ,
  - 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

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

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

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

■ 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

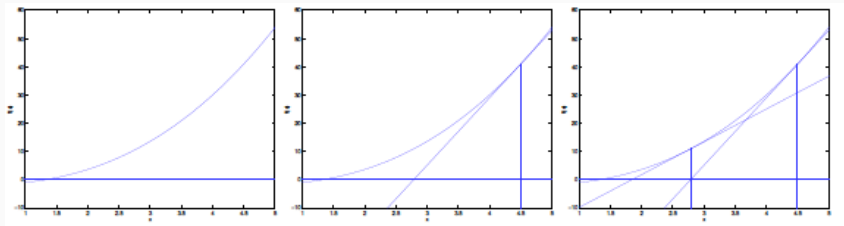
- Maximization of  $l(\mathbf{w}|\mathbf{X}, \mathbf{t})$  through the well-known Newton-Raphson algorithm to compute the roots of a given function
- Given  $f : \mathbb{R} \mapsto \mathbb{R}$ , the algorithm finds  $z \in \mathbb{R}$  such that  $f(z) = 0$  through a sequence of iterations, starting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

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

- Then,

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

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

- 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

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

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

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

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

where

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

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

# Newton-Raphson and logistic regression

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

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

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

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

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

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

for given weights  $\psi_1, \dots, \psi_n$ . 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

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

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

# 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  $\tilde{\mathbf{t}} = \overline{\mathbf{X}}\mathbf{w}^{(i)} - \mathbf{R}_{\mathbf{w}^{(i)}}^{-1}(\mathbf{s}_{\mathbf{w}^{(i)}} - \mathbf{t})$ , and weights  $\psi_k = \sigma((\mathbf{w}^{(k)})^T \overline{\mathbf{x}}_i)(1 - \sigma((\mathbf{w}^{(k)})^T \overline{\mathbf{x}}_i))$
- 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  $\Psi = \mathbf{R}_{\mathbf{w}^{(i+1)}}$  and  $\tilde{\mathbf{t}} = \mathbf{z}_{\mathbf{w}^{(i+1)}}$ .

## Logistic regression and GDA

- Observe that assuming  $p(\mathbf{x}|C_1)$  and  $p(\mathbf{x}|C_2)$  as multivariate normal distributions with same covariance matrix  $\Sigma$  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  $\mathbf{w} = (\mathbf{w}_1, \dots, \mathbf{w}_K)$  of model coefficients, of size  $(d+1)K$ , where the  $j$ -th block of  $\mathbf{w}$  ( $j = 1, \dots, K$ ) corresponds to the vector  $\mathbf{w}_j$  of the  $d+1$  coefficients for class  $C_j$ .
- In this case, the likelihood is defined as

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

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

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

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

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

## ML and softmax regression

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

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

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  $i = 1, \dots, n$ ,  $j = 0, \dots, d$ ,  $k = 1, \dots, K$ ,

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

# ML and softmax regression

Hence,

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

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

# 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,

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

- 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

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

## Posterior distribution of coefficients

That is,

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

and

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

with the normalization factor

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

## Predictive distribution intractability

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

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

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)