Statistical Machine Learning

Christian Walder

Machine Learning Research Group
CSIRO Data61

and

College of Engineering and Computer Science
The Australian National University

Canberra
Semester One, 2020.

(Many figures from C. M. Bishop, "Pattern Recognition and Machine Learning")

Outlines

Part VI

Linear Classification 2

Three Models for Decision Problems

In increasing order of complexity

- Find a discriminant function $f(\mathbf{x})$ which maps each input directly onto a class label.
- Discriminative Models
  1. Solve the inference problem of determining the posterior class probabilities $p(\mathcal{C}_k \mid \mathbf{x})$.
  2. Use decision theory to assign each new $\mathbf{x}$ to one of the classes.
- Generative Models
  1. Solve the inference problem of determining the class-conditional probabilities $p(\mathbf{x} \mid \mathcal{C}_k)$.
  2. Also, infer the prior class probabilities $p(\mathcal{C}_k)$.
  3. Use Bayes' theorem to find the posterior $p(\mathcal{C}_k \mid \mathbf{x})$.
  4. Alternatively, model the joint distribution $p(\mathbf{x}, \mathcal{C}_k)$ directly.
  5. Use decision theory to assign each new $\mathbf{x}$ to one of the classes.

Data Generating Process

Given:

- class prior $p(\mathbf{t})$
- class-conditional $p(\mathbf{x} \mid \mathbf{t})$

to generate data from the model we may do the following:

1. Sample the class label from the class prior $p(\mathbf{t})$.
2. Sample the data features from the class-conditional distribution $p(\mathbf{x} \mid \mathbf{t})$.

(more about sampling later — this is called *ancestral* sampling)

Thinking about the data generating process is a useful modelling step, especially when we have more prior knowledge.

- Generative approach: model class-conditional densities $p(\mathbf{x} \mid \mathcal{C}_k)$ and *class* priors (not parameter priors!) $p(\mathcal{C}_k)$ to calculate the posterior probability for class $\mathcal{C}_1$

$$p(\mathcal{C}_1 \mid \mathbf{x}) = \frac{p(\mathbf{x} \mid \mathcal{C}_1)p(\mathcal{C}_1)}{p(\mathbf{x} \mid \mathcal{C}_1)p(\mathcal{C}_1) + p(\mathbf{x} \mid \mathcal{C}_2)p(\mathcal{C}_2)}$$

$$= \frac{1}{1 + \exp(-a(\mathbf{x}))} \equiv \sigma(a(\mathbf{x}))$$

where a and the logistic sigmoid function $\sigma(a)$ are given by

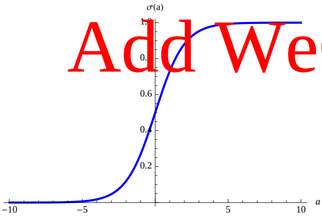
$$a(\mathbf{x}) = \ln \frac{p(\mathbf{x} \mid \mathcal{C}_1)\, p(\mathcal{C}_1)}{p(\mathbf{x} \mid \mathcal{C}_2)\, p(\mathcal{C}_2)} = \ln \frac{p(\mathbf{x}, \mathcal{C}_1)}{p(\mathbf{x}, \mathcal{C}_2)}$$

$$\sigma(a) = \frac{1}{1 + \exp(-a)}.$$

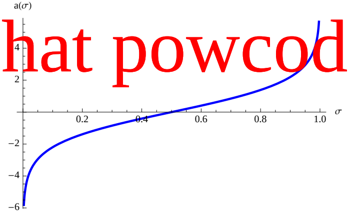
- One point of this re-writing: we may learn $a(\mathbf{x})$ directly as *e.g.* a deep neural network.

Logistic Sigmoid

- The logistic sigmoid function is called a "squashing function" because it squashes the real axis into a finite interval $(0, 1)$.
- Well known properties (derive them):
  - Symmetry: $\sigma(-a) = 1 - \sigma(a)$
  - Derivative: $\frac{\mathrm{d}}{\mathrm{d}a}\sigma(a) = \sigma(a)\,\sigma(-a) = \sigma(a)\,(1 - \sigma(a))$
- Inverse of σ is called the logit function



Sigmoid $\sigma(a) = \frac{1}{1+\exp(-a)}$



Logit $a(\sigma) = \ln\left(\frac{\sigma}{1-\sigma}\right)$

Probabilistic Generative Models - Multiclass

- The normalised exponential is given by

$$p(\mathcal{C}_k \,|\, \mathbf{x}) = \frac{p(\mathbf{x} \,|\, \mathcal{C}_k)\, p(\mathcal{C}_k)}{\sum_j p(\mathbf{x} \,|\, \mathcal{C}_j)\, p(\mathcal{C}_j)} = \frac{\exp(a_k)}{\sum_j \exp(a_j)}$$

where

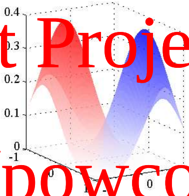
$$a_k = \ln(p(\mathbf{x} \,|\, \mathcal{C}_k)\, p(\mathcal{C}_k)).$$

- Usually called the softmax function as it is a smoothed version of the $\arg\max$ function, in particular:

$$a_k \gg a_j \;\forall j \neq k \Rightarrow \left(p(\mathcal{C}_k \,|\, \mathbf{x}) \approx 1 \wedge p(\mathcal{C}_j \,|\, \mathbf{x}) \approx 0\right)$$

- So, softargmax is a more descriptive though less common name.

- Assume class-conditional probabilities are Gaussian, with the same covariance and different mean:



- Let's characterise the posterior probabilities.
- We may separate the quadratic and linear term in $\mathbf{x}$:

$$p(\mathbf{x} \mid \mathcal{C}_k)$$

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

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

Probabil. Generative Model - Continuous Input

- For two classes

$$p(\mathcal{C}_1 \,|\, \mathbf{x}) = \sigma(a(\mathbf{x}))$$

and $a(\mathbf{x})$ is linear because the quadratic terms in $\mathbf{x}$ cancel (*c.f.* the previous slide):

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

- Therefore

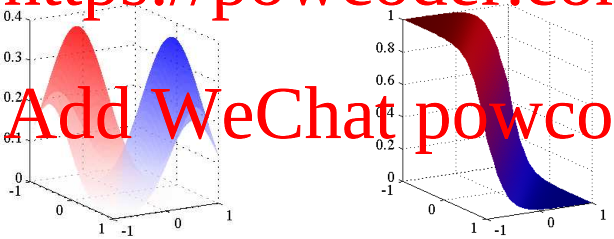
$$p(\mathcal{C}_1 \,|\, \mathbf{x}) = \sigma(\mathbf{w}^T \mathbf{x} + w_0)$$

where

$$\begin{aligned} \mathbf{w} &= \boldsymbol{\Sigma}^{-1}(\boldsymbol{\mu}_1 - \boldsymbol{\mu}_2) \\ w_0 &= -\frac{1}{2}\boldsymbol{\mu}_1^T \,\boldsymbol{\Sigma}^{-1}\boldsymbol{\mu}_1 + \frac{1}{2}\boldsymbol{\mu}_2^T \,\boldsymbol{\Sigma}^{-1}\boldsymbol{\mu}_2 + \ln \frac{p(\mathcal{C}_1)}{p(\mathcal{C}_2)} \end{aligned}$$

Probabil. Generative Model - Continuous Input

Class-conditional densities for two classes (left). Posterior probability $p(\mathcal{C}_1 \mid \mathbf{x})$ (right). Note the logistic sigmoid of a linear function of $\mathbf{x}$.



General Case - K Classes, Shared Covariance

- Use the normalised exponential

$$p(\mathcal{C}_k \mid \mathbf{x}) = \frac{p(\mathbf{x} \mid \mathcal{C}_k)\, p(\mathcal{C}_k)}{\sum_j p(\mathbf{x} \mid \mathcal{C}_j)\, p(\mathcal{C}_j)} = \frac{\exp(a_k)}{\sum_j \exp(a_j)}$$

where

$$a_k = \ln\left(p(\mathbf{x} \mid \mathcal{C}_k)\, p(\mathcal{C}_k)\right).$$

- to get a linear function of $\mathbf{x}$

$$a_k(\mathbf{x}) = \mathbf{w}_k^T \mathbf{x} + w_{k0}.$$

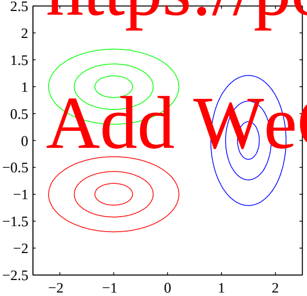
where

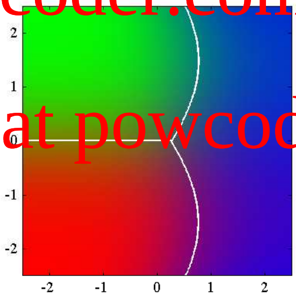
$$\mathbf{w}_k = \mathbf{\Sigma}^{-1} \boldsymbol{\mu}_k$$

$$w_{k0} = -\frac{1}{2} \boldsymbol{\mu}_k^T \mathbf{\Sigma}^{-1} \boldsymbol{\mu}_k + p(\mathcal{C}_k).$$

General Case - K Classes, Different Covariance

- If the class-conditional distributions have different covariances, the quadratic terms $-\frac{1}{2}\mathbf{x}^T\boldsymbol{\Sigma}^{-1}\mathbf{x}$ do not cancel out.
- We get a quadratic discriminant.





Parameter Estimation

- Given the functional form of the class-conditional densities $p(\mathbf{x} \mid \mathcal{C}_k)$, how can we determine the parameters $\boldsymbol{\mu}$ and $\boldsymbol{\Sigma}$ and the class prior?

Parameter Estimation

- Given the functional form of the class-conditional densities $p(\mathbf{x} \,|\, \mathcal{C}_k)$, how can we determine the parameters $\boldsymbol{\mu}$ and $\boldsymbol{\Sigma}$ and the class prior?
- Simplest is maximum likelihood.
- Given also a data set $(\mathbf{x}_n, t_n)$ for $n = 1, \dots, N$. (Using the coding scheme where $t_n = 1$ corresponds to class $\mathcal{C}_1$ and $t_n = 0$ denotes class $\mathcal{C}_2$.
- Assume the class-conditional densities to be Gaussian with the same covariance, but different mean.
- Denote the prior probability $p(\mathcal{C}_1) = \pi$, and therefore $p(\mathcal{C}_2) = 1 - \pi$.
- Then

$$p(\mathbf{x}_n, \mathcal{C}_1) = p(\mathcal{C}_1) p(\mathbf{x}_n \,|\, \mathcal{C}_1) = \pi \, \mathcal{N}(\mathbf{x}_n \,|\, \boldsymbol{\mu}_1, \boldsymbol{\Sigma})$$
$$p(\mathbf{x}_n, \mathcal{C}_2) = p(\mathcal{C}_2) p(\mathbf{x}_n \,|\, \mathcal{C}_2) = (1 - \pi) \, \mathcal{N}(\mathbf{x}_n \,|\, \boldsymbol{\mu}_2, \boldsymbol{\Sigma})$$

Maximum Likelihood Solution

- Thus the likelihood for the whole data set $\mathbf{X}$ and $\mathbf{t}$ is given by

$$p(\mathbf{t}, \mathbf{X} \mid \pi, \boldsymbol{\mu}_1, \boldsymbol{\mu}_2, \boldsymbol{\Sigma})$$
$$= \prod_{n=1}^{N} [\pi \, \mathcal{N}(\mathbf{x}_n \mid \boldsymbol{\mu}_1, \boldsymbol{\Sigma})]^{t_n} \times [(1-\pi) \, \mathcal{N}(\mathbf{x}_n \mid \boldsymbol{\mu}_2, \boldsymbol{\Sigma})]^{1-t_n}$$

- Maximise the log likelihood
- The term depending on π is

$$\sum_{n=1}^{N} (t_n \ln \pi + (1 - t_n) \ln(1 - \pi))$$

- which is maximal for (derive it)

$$\pi = \frac{1}{N} \sum_{n=1}^{N} t_n = \frac{N_1}{N} = \frac{N_1}{N_1 + N_2}$$

where N_1 is the number of data points in class $\mathcal{C}_1$.

Maximum Likelihood Solution

- Similarly, we can maximise the likelihood $p(\mathbf{t}, \mathbf{X} \mid \pi, \boldsymbol{\mu}_1, \boldsymbol{\mu}_2, \boldsymbol{\Sigma})$ w.r.t. the means $\boldsymbol{\mu}_1$ and $\boldsymbol{\mu}_2$, to get

$$\boldsymbol{\mu}_1 = \frac{1}{N_1} \sum_{n=1}^{N} t_n \, \mathbf{x}_n$$

$$\boldsymbol{\mu}_2 = \frac{1}{N_2} \sum_{n=1}^{N} (1 - t_n) \, \mathbf{x}_n$$

- For each class, this are the means of all input vectors assigned to this class.

Maximum Likelihood Solution

- Finally, the log likelihood $\ln p(\mathbf{t}, \mathbf{X} \mid \pi, \boldsymbol{\mu}_1, \boldsymbol{\mu}_2, \boldsymbol{\Sigma})$ can be maximised for the covariance $\boldsymbol{\Sigma}$ resulting in

$$\boldsymbol{\Sigma} = \frac{N_1}{N}\mathbf{S}_1 + \frac{N_2}{N}\mathbf{S}_2$$

$$\mathbf{S}_k = \frac{1}{N_k}\sum_{n \in \mathcal{C}_k}(\mathbf{x}_n - \boldsymbol{\mu}_k)(\mathbf{x}_n - \boldsymbol{\mu}_k)^T$$

Discrete Features - Naïve Bayes

- Assume the input space consists of discrete features, in the simplest case $x_i \in \{0, 1\}$.
- For a D-dimensional input space, a general distribution would be represented by a table with 2^D entries.
- Together with the normalisation constraint, this are $2^D - 1$ independent variables.
- Grows exponentially with the number of features.
- The Naïve Bayes assumption is that, given the class $\mathcal{C}_k$, the features are independent of each other:

$$
\begin{aligned}
p(\mathbf{x} \,|\, \mathcal{C}_k) &= \prod_{i=1}^{D} p(x_i \,|\, \mathcal{C}) \\
&= \prod_{i=1}^{D} \mu_{ki}^{x_i} (1 - \mu_{ki})^{1 - x_i}
\end{aligned}
$$

Discrete Features - Naïve Bayes

Ong & Walder & Webers
Data61 | CSIRO
The Australian National University

- With the naïve Bayes

$$p(\mathbf{x} \mid \mathcal{C}_k) = \prod_{i=1}^{D} \mu_{ki}^{x_i} (1 - \mu_{ki})^{1-x_i}$$

- we can then again find the factors a_k in the normalised exponential

$$p(\mathcal{C}_k \mid \mathbf{x}) = \frac{p(\mathbf{x} \mid \mathcal{C}_k) p(\mathcal{C}_k)}{\sum_j p(\mathbf{x} \mid \mathcal{C}_j) p(\mathcal{C}_j)} = \frac{\exp(a_k)}{\sum_j \exp(a_j)}$$

- as a linear function of the x_i

$$a_k(\mathbf{x}) = \sum_{i=1}^{D} \{x_i \ln \mu_{ki} + (1 - x_i) \ln(1 - \mu_{ki})\} + \ln p(\mathcal{C}_k).$$

Three Models for Decision Problems

In increasing order of complexity

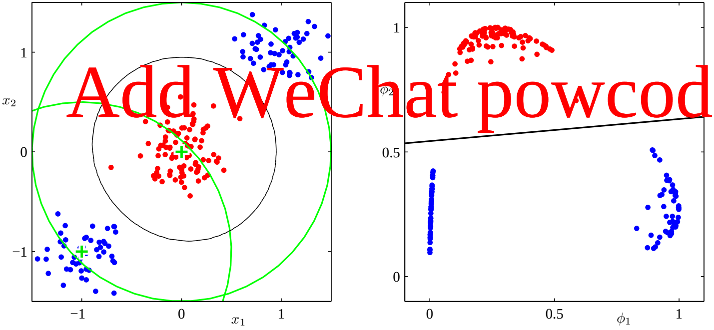
- Find a discriminant function $f(\mathbf{x})$ which maps each input directly onto a class label.
- Discriminative Models
  1. Solve the inference problem of determining the posterior class probabilities $p(\mathcal{C}_k \mid \mathbf{x})$.
  2. Use decision theory to assign each new $\mathbf{x}$ to one of the classes.
- Generative Models
  1. Solve the inference problem of determining the class-conditional probabilities $p(\mathbf{x} \mid \mathcal{C}_k)$.
  2. Also, infer the prior class probabilities $p(\mathcal{C}_k)$.
  3. Use Bayes' theorem to find the posterior $p(\mathcal{C}_k \mid \mathbf{x})$.
  4. Alternatively, model the joint distribution $p(\mathbf{x}, \mathcal{C}_k)$ directly.
  5. Use decision theory to assign each new $\mathbf{x}$ to one of the classes.

Probabilistic Discriminative Models

- Discriminative training: learn only to discriminate between the classes.
- Maximise a likelihood function defined through the conditional distribution $p(\mathcal{C}_k \mid \mathbf{x})$ directly.
- Typically fewer parameters to be determined.
- As we learn the posterior $p(\mathcal{C}_k \mid \mathbf{x})$ directly, prediction may be better than with a generative model where the class-conditional density assumptions $p(\mathbf{x} \mid \mathcal{C}_k)$ poorly approximate the true distributions.
- But: discriminative models can not create synthetic data as $p(\mathbf{x})$ is not modelled.
- As an aside: *certain theoretical analyses show that generative models converge faster to their — albeit worse — asymptotic classification performance and are superior in some regimes.*

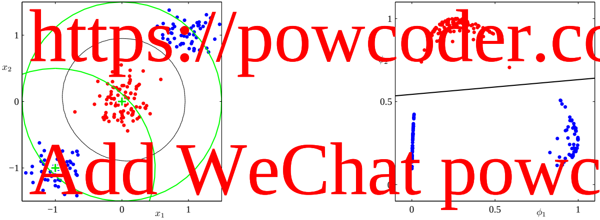
Original Input versus Feature Space

- So far in classification, we used direct input $\mathbf{x}$.
- All classification algorithms work also if we first apply a fixed nonlinear transformation of the inputs using a vector of basis functions $\phi(\mathbf{x})$.
- Example: Use two Gaussian basis functions centered at the green crosses in the input space.



Original Input versus Feature Space

- Linear decision boundaries in the feature space generally correspond to nonlinear boundaries in the input space.
- Classes which are NOT linearly separable in the input space may become linearly separable in the feature space:



- If classes overlap in input space, they will also overlap in feature space — nonlinear features $\phi(\mathbf{x})$ can not remove the overlap; but they may increase it.

Original Input versus Feature Space

- Fixed basis functions do not adapt to the data and therefore have important limitations (see discussion in Linear Regression).
- Understanding of more advanced algorithms becomes easier if we introduce the feature space now and use it instead of the original input space.
- Some applications use fixed features successfully by avoiding the limitations.
- We will therefore use ϕ instead of $\mathbf{x}$ from now on.

Logistic Regression

- Two classes where the posterior of class $\mathcal{C}_1$ is a logistic sigmoid $\sigma()$ acting on a linear function of the input:

$$p(\mathcal{C}_1 \mid \phi) = y(\phi) = \sigma(\mathbf{w}^T \phi)$$

- $p(\mathcal{C}_2 \mid \phi) = 1 - p(\mathcal{C}_1 \mid \phi)$
- Model dimension is equal to dimension of the feature space M.
- Compare this to fitting two Gaussians, which has a quadratic number of parameters in M:

$$\underbrace{2M}_{\text{means}} + \underbrace{M(M+1)/2}_{\text{shared covariance}}$$

- For larger M, the logistic regression model has a clear advantage.

Logistic Regression

- Determine the parameter via maximum likelihood for data (ϕ_n, t_n), $n = 1, \dots, N$, where $\phi_n = \phi(\mathbf{x}_n)$. The class membership is coded as $t_n \in \{0, 1\}$.
- Likelihood function

$$p(\mathbf{t} \mid \mathbf{w}) = \prod_{n=1}^{N} y_n^{t_n} (1 - y_n)^{1 - t_n}$$

where $y_n = p(\mathcal{C}_1 \mid \phi_n)$.

- Error function: negative log likelihood resulting in the cross-entropy error function

$$E(\mathbf{w}) = -\ln p(\mathbf{t} \mid \mathbf{w}) = -\sum_{n=1}^{N} \{t_n \ln y_n + (1 - t_n) \ln(1 - y_n)\}$$

- Error function (cross-entropy loss)

$$E(\mathbf{w}) = -\sum_{n=1}^{N} \{t_n \ln y_n + (1 - t_n) \ln(1 - y_n)\}$$

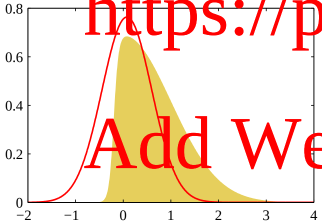
- $y_n = p(\mathcal{C}_1 \mid \phi_n) = \sigma(\mathbf{w}^T \phi_n)$
- We obtain the gradient of the error function using the chain rule and the sigmoid result $\frac{d\sigma}{da} = \sigma(1 - \sigma)$ (derive it).

$$\nabla E(\mathbf{w}) = \sum_{n=1}^{N} (y_n - t_n) \phi_n$$

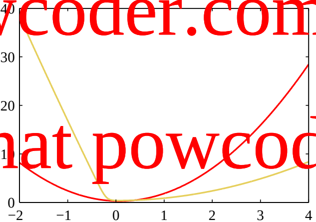
- for each data point error is product of deviation $y_n - t_n$ and basis function ϕ_n.
- We can now use gradient descent.
- We may easily modify this to reduce over-fitting by using regularised error or MAP (how?).

Laplace Approximation

- Given a continous distribution $p(x)$ which is not Gaussian, can we approximate it by a Gaussian $q(x)$?
- Need to find a mode of $p(x)$. Try to find a Gaussian with the same mode:



p.d.f. of :
Non-Gaussian (yellow) and
Gaussian approximation (red).



negative log p.d.f. of :
Non-Gaussian (yellow) and
Gaussian approxmation. (red).

Ong & Walder & Webers
Data61 | CSIRO
The Australian National University

Laplace Approximation

- Cheap and nasty but sometimes effective.
- Assume $p(x)$ can be written as

$$p(z) = \frac{1}{Z} f(z)$$

  with normalisation $Z = \int f(z) \, \mathrm{d}z$.
- We do not even need to know Z to find the Laplace approximation.
- A mode of $p(z)$ is at a point z_0 where $p'(z_0) = 0$.
- Taylor expansion of $\ln f(z)$ at z_0

$$\ln f(z) \simeq \ln f(z_0) - \frac{1}{2} A (z - z_0)^2$$

  where

$$A = -\frac{d^2}{dz^2} \ln f(z) \mid_{z=z_0}$$

- Exponentiating

$$\ln f(z) \simeq \ln f(z_0) - \frac{1}{2} A (z - z_0)^2$$

- we get

$$f(z) \simeq f(z_0) \exp\{-\frac{A}{2}(z - z_0)^2\}.$$

- And after normalisation we get the Laplace approximation

$$q(z) = \left(\frac{A}{2\pi}\right)^{1/2} \exp\{-\frac{A}{2}(z - z_0)^2\}.$$

- Only defined for precision $A > 0$ as only then $p(z)$ has a maximum.

Laplace Approximation - Vector Space

- Approximate p($\mathbf{z}$) for $z \in \mathbb{R}^M$

$$p(\mathbf{z}) = \frac{1}{Z} f(\mathbf{z})$$

- we get the Taylor expansion

$$\ln f(\mathbf{z}) \simeq \ln f(\mathbf{z}_0) - \frac{1}{2}(\mathbf{z} - \mathbf{z}_0)^T \mathbf{A} (\mathbf{z} - \mathbf{z}_0)$$

- where the Hessian $\mathbf{A}$ is defined as

$$\mathbf{A} = -\nabla\nabla \ln f(\mathbf{z}) \,|_{\mathbf{z}=\mathbf{z}_0}.$$

- The Laplace approximation of $p(\mathbf{z})$ is then

$$q(\mathbf{z}) \propto \exp\left\{-\frac{1}{2}(\mathbf{z} - \mathbf{z}_0)^T \mathbf{A} (\mathbf{z} - \mathbf{z}_0)\right\}$$
$$\Rightarrow q(\mathbf{z}) = \mathcal{N}(\mathbf{z} \,|\, \mathbf{z}_0, \mathbf{A}^{-1})$$

Bayesian Logistic Regression

- Exact Bayesian inference for the logistic regression is intractable.
- Why? Need to normalise a product of prior probabilities and likelihoods which itself are a product of logistic sigmoid functions, one for each data point.
- Evaluation of the predictive distribution also intractable.
- Therefore we will use the Laplace approximation.
- The predictive distribution remains intractable even under the Laplace approximation to the posterior distribution, but it can be approximated.

Bayesian Logistic Regression

- Assume a Gaussian prior:

$$p(\mathbf{w}) = \mathcal{N}(\mathbf{w} \,|\, \mathbf{m}_0, \mathbf{S}_0)$$

for fixed hyperparameters $\mathbf{m}_0$ and $\mathbf{S}_0$.

- Hyperparameters are parameters of a prior distribution. In contrast to the model parameters $\mathbf{w}$, they are not learned.
- For a set of training data $(\mathbf{x}_n, t_n)$, where $n = 1, \ldots, N$, the posterior is given by

$$p(\mathbf{w} \,|\, \mathbf{t}) \propto p(\mathbf{w}) p(\mathbf{t} \,|\, \mathbf{w})$$

where $\mathbf{t} = (t_1, \ldots, t_N)^T$.

Bayesian Logistic Regression

- Using our previous result for the cross-entropy function

$$E(\mathbf{w}) = -\ln p(\mathbf{t} \,|\, \mathbf{w}) = -\sum_{n=1}^{N} \{t_n \ln y_n + (1 - t_n) \ln(1 - y_n)\}$$

we can now calculate the log of the posterior

$$p(\mathbf{w} \,|\, \mathbf{t}) \propto p(\mathbf{w}) p(\mathbf{t} \,|\, \mathbf{w})$$

using the notation $y_n = \sigma(\mathbf{w}^T \boldsymbol{\phi}_n)$ as

$$\ln p(\mathbf{w} \,|\, \mathbf{t}) = -\frac{1}{2} (\mathbf{w} - \mathbf{m}_0)^T \mathbf{S}_0^{-1} (\mathbf{w} - \mathbf{m}_0) + \sum_{n=1}^{N} \{t_n \ln y_n + (1 - t_n) \ln(1 - y_n)\}$$

Bayesian Logistic Regression

- To obtain a Gaussian approximation to

$$\ln p(\mathbf{w}\,|\,\mathbf{t})$$

$$= -\frac{1}{2}(\mathbf{w}-\mathbf{m}_0)^T \mathbf{S}_0^{-1}(\mathbf{w}-\mathbf{m}_0) + \sum_{n=1}^{N} \{t_n \ln y_n + (1-t_n)\ln(1-y_n)\}$$

1. Find $\mathbf{w}_{MAP}$ which maximises $\ln p(\mathbf{w}\,|\,\mathbf{t})$. This defines the mean of the Gaussian approximation. (Note: This is a nonlinear function in $\mathbf{w}$ because $y_n = \sigma(\mathbf{w}^T \boldsymbol{\phi}_n)$.)
2. Calculate the second derivative of the negative log likelihood to get the inverse covariance of the Laplace approximation

$$\mathbf{S}_N = -\nabla\nabla \ln p(\mathbf{w}\,|\,\mathbf{t}) = \mathbf{S}_0^{-1} + \sum_{n=1}^{N} y_n(1-y_n)\boldsymbol{\phi}_n\boldsymbol{\phi}_n^T.$$

Nowadays the gradient and Hessian would be computed with automatic differentiation; one need only implement $\ln p(\mathbf{w}\,|\,\mathbf{t})$.

Bayesian Logistic Regression

- The approximated Gaussian (via Laplace approximation) of the posterior distribution is now

$$q(\mathbf{w} \mid \phi) = \mathcal{N}(\mathbf{w} \mid \mathbf{w}_{MAP}, \mathbf{S}_N)$$

where

$$\mathbf{S}_N = -\nabla\nabla \ln p(\mathbf{w} \mid \mathbf{t}) = \mathbf{S}_0^{-1} + \sum_{n=1}^{N} y_n(1 - y_n)\phi_n\phi_n^T$$