Introduction to Statistical Machine Learning

Christfried Webers

Statistical Machine Learning Group NICTA and College of Engineering and Computer Science The Australian National University

> Canberra February – June 2013

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

Introduction to Statistical Machine Learning

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Overview

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Linear Classification 1 Linear Classification 2 Neural Networks 1

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Probabilistic Generative Models

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Bayesian Logistic Regression

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Probabilistic Generative Models

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Discriminative Model

Logistic Regression

Least Squares

Laplace Approximation

Bayesian Logistic Regression

In increasing order of complexity

- Find a discriminant function $f(\mathbf{x})$ which maps each input directly onto a class label.
- Discriminative Models
 - ② Solve the inference problem of determining the posterior class probabilities $p(C_k \mid \mathbf{x})$.
 - Use decision theory to assign each new x to one of the classes.

Generative Models

- ② Solve the inference problem of determining the class-conditional probabilities $p(\mathbf{x} \mid C_k)$.
- **②** Also, infer the prior class probabilities $p(C_k)$.
- **③** Use Bayes' theorem to find the posterior $p(C_k \mid \mathbf{x})$.
- **4** Alternatively, model the joint distribution $p(\mathbf{x}, C_k)$ directly.
- Use decision theory to assign each new x to one of the classes.



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Discriminative Model

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Generative approach: model class-conditional densities
 p(x | C_k) and priors p(C_k) to calculate the posterior
 probability for class C₁

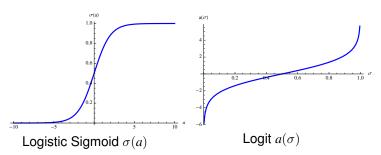
$$p(C_1 \mid \mathbf{x}) = \frac{p(\mathbf{x} \mid C_1)p(C_1)}{p(\mathbf{x} \mid C_1)p(C_1) + p(\mathbf{x} \mid C_2)p(C_2)}$$
$$= \frac{1}{1 + \exp(-a(\mathbf{x}))} = \sigma(a(\mathbf{x}))$$

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

$$a(\mathbf{x}) = \ln \frac{p(\mathbf{x} \mid \mathcal{C}_1) p(\mathcal{C}_1)}{p(\mathbf{x} \mid \mathcal{C}_2) p(\mathcal{C}_2)} = \ln \frac{p(\mathbf{x}, \mathcal{C}_1)}{p(\mathbf{x}, \mathcal{C}_2)}$$
$$\sigma(a) = \frac{1}{1 + \exp(-a)}.$$

- Probabilistic Generative Models

- The logistic sigmoid function $\sigma(a) = \frac{1}{1 + \exp(-a)}$
- "squashing function' because it maps the real axis into a finite interval (0,1)
- $\sigma(-a) = 1 \sigma(a)$
- Derivative $\frac{d}{da}\sigma(a) = \sigma(a)\,\sigma(-a) = \sigma(a)\,(1-\sigma(a))$
- Inverse is called logit function $a(\sigma) = \ln\left(\frac{\sigma}{1-\sigma}\right)$





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Discrete Features

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The normalised exponential is given by

$$p(C_k \mid \mathbf{x}) = \frac{p(\mathbf{x} \mid C_k) p(C_k)}{\sum_j p(\mathbf{x} \mid C_j) p(C_j)} = \frac{\exp(a_k)}{\sum_j \exp(a_j)}$$

where

$$a_k = \ln(p(\mathbf{x} \mid C_k) p(C_k)).$$

- Also called softmax function as it is a smoothed version of the max function.
- Example: If $a_k \gg a_j$ for all $j \neq k$, then $p(C_k \mid \mathbf{x}) \simeq 1$, and $p(C_j \mid \mathbf{x}) \simeq 0$.



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 Assume class-conditional probabilities are Gaussian, all classes share the same covariance. What can we say about the posterior probabilities?

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

where we separated the quadratic term in \mathbf{x} and the linear term.

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

• and $a(\mathbf{x})$ is

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

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

Therefore

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

where

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

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

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Probabilistic Generative Models

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Continuous Input

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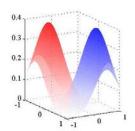
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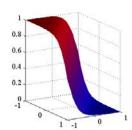
Iterative Reweighted

Laplace Approximation

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Class-conditional densities for two classes (left). Posterior probability $p(C_1 \mid \mathbf{x})$ (right). Note the logistic sigmoid of a linear function of \mathbf{x} .





Use the normalised exponential

$$p(C_k \mid \mathbf{x}) = \frac{p(\mathbf{x} \mid C_k)p(C_k)}{\sum_j p(\mathbf{x} \mid C_j)p(C_j)} = \frac{\exp(a_k)}{\sum_j \exp(a_j)}$$

where

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

• to get a linear function of x

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

where

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

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

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Models

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Probabilistic Discriminative Model.

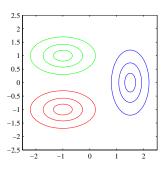
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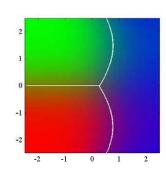
terative Reweighted Least Squares

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- If each class-conditional probability has a different covariance, the quadratic terms $-\frac{1}{2}\mathbf{x}^T\mathbf{\Sigma}^{-1}\mathbf{x}$ do not longer cancel each other out.
- We get a quadratic discriminant.





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Maximum Likelihood Solution

• Given the functional form of the class-conditional densities $p(\mathbf{x} \mid \mathcal{C}_k)$, can we determine the parameters μ and Σ ?

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- Given the functional form of the class-conditional densities $p(\mathbf{x} \mid \mathcal{C}_k)$, can we determine the parameters μ and Σ ?
- Not without data ;-)
- Given also a data set (\mathbf{x}_n, t_n) for n = 1, ..., N. (Using the coding scheme where $t_n = 1$ corresponds to class C_1 and $t_n = 0$ denotes class C_2 .
- Assume the class-conditional densities to be Gaussian with the same covariance, but different mean.
- Denote the prior probability $p(C_1) = \pi$, and therefore $p(C_2) = 1 \pi$.
- Then

$$p(\mathbf{x}_n, C_1) = p(C_1)p(\mathbf{x}_n \mid C_1) = \pi \mathcal{N}(\mathbf{x}_n \mid \boldsymbol{\mu}_1, \boldsymbol{\Sigma})$$

$$p(\mathbf{x}_n, C_2) = p(C_2)p(\mathbf{x}_n \mid C_2) = (1 - \pi) \mathcal{N}(\mathbf{x}_n \mid \boldsymbol{\mu}_2, \boldsymbol{\Sigma})$$

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

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

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

which is maximal for

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

where N_1 is the number of data points in class C_1 .



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• Similarly, we can maximise the log likelihood (and thereby the likelihood $p(\mathbf{t}, \mathbf{X} \,|\, \pi, \boldsymbol{\mu}_1, \boldsymbol{\mu}_2, \boldsymbol{\Sigma})$) depending on the mean $\boldsymbol{\mu}_1$ or $\boldsymbol{\mu}_2$, and get

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

$$\mu_2 = \frac{1}{N_2} \sum_{n=1}^{N} (1 - t_n) \mathbf{x}_n$$

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



Continuous Input

Discrete Feature:

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Iterative Reweighte

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Bayesian Logistic

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

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

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

Discrete Features

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- 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 Naive Bayes assumption is that all features conditioned on the class C_k are independent of each other.

$$p(\mathbf{x} \mid C_k) = \prod_{i=1}^{D} \mu_{k_i}^{x_i} (1 - \mu_{k_i})^{1 - x_i}$$



Discrete Features

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With the naive Bayes

$$p(\mathbf{x} \mid C_k) = \prod_{i=1}^{D} \mu_{k_i}^{x_i} (1 - \mu_{k_i})^{1 - x_i}$$

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

$$p(C_k \mid \mathbf{x}) = \frac{p(\mathbf{x} \mid C_k)p(C_k)}{\sum_j p(\mathbf{x} \mid C_j)p(C_j)} = \frac{\exp(a_k)}{\sum_j \exp(a_j)}$$

as a linear function of the x_i

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



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In increasing order of complexity

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- Generative Models
 - ② Solve the inference problem of determining the class-conditional probabilities $p(\mathbf{x} \mid C_k)$.
 - **②** Also, infer the prior class probabilities $p(C_k)$.
 - **③** Use Bayes' theorem to find the posterior $p(C_k | \mathbf{x})$.
 - **4** Alternatively, model the joint distribution $p(\mathbf{x}, C_k)$ directly.
 - Use decision theory to assign each new x to one of the classes.



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Discriminative Models

Logistic Regression

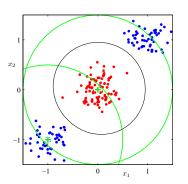
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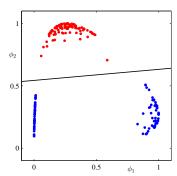
Laplace Approxima

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- Maximise a likelihood function defined through the conditional distribution $p(C_k | \mathbf{x})$ directly.
- Discriminative training
- Typically fewer parameters to be determined.
- As we learn the posteriror $p(\mathcal{C}_k \mid \mathbf{x})$ 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(x) is not modelled.

- Used direct input x until now.
- 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.





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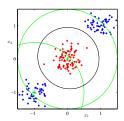
Logistic Regression

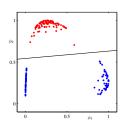
Iterative Reweighted

Laplace Approximation

Bayesian Logistic Regression

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







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Laplace Approximation

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- 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 x from now on.



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Logistic Regression

Least Squares

Laplace Approximation

• Two classes where the posterior of class \mathcal{C}_1 is a logistic sigmoid $\sigma()$ acting on a linear function of the feature vector ϕ

$$p(C_1 | \boldsymbol{\phi}) = y(\boldsymbol{\phi}) = \sigma(\mathbf{w}^T \boldsymbol{\phi})$$

- $p(C_2 | \phi) = 1 p(C_1 | \phi)$
- Model dimension is equal to dimension of the feature space M.
- Compare this to fitting two Gaussians

$$\underbrace{2M}_{\text{means}} + \underbrace{M(M+1)/2}_{\text{shared covariance}} = M(M+5)/2$$

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



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Discriminative Mode

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Laplace Approximation

Bayesian Logist 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 $y_n = p(C_1 \mid \phi_n)$.

 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)\}\$$

Continuous Input

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Discriminative Mode

Logistic Regression

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Bayesian Logistic

• Error function (cross-entropy error)

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

- $y_n = p(C_1 \mid \phi_n) = \sigma(\mathbf{w}^T \phi_n)$
- Gradient of the error function (using $\frac{d\sigma}{da} = \sigma(1-\sigma)$)

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

- gradient does not contain any sigmoid function
- for each data point error is product of deviation $y_n t_n$ and basis function ϕ_n .
- BUT: maximum likelihood solution can exhibit over-fitting even for many data points; should use regularised error or MAP then.





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Discriminative Model

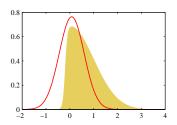
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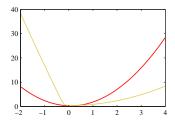
Laplace Approximation

Bayesian Logistic

- 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.



Non-Gaussian (yellow) and Gaussian approximation (red).



Negative log of the Non-Gaussian (yellow) and Gaussian approx. (red).



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Laplace Approximation

Bayesian Logisti Regression

• Assume p(x) can be written as

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

with normalisation $Z = \int f(z) dz$.

- Furthermore, assume Z is unknown!
- 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

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

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Bayesian Logistic

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.

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

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 A is defined as

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

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

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

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Discriminative Models

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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.

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Assume a Gaussian prior because we want a Gaussian posterior.

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

for fixed hyperparameter \mathbf{m}_0 and \mathbf{S}_0 .

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

$$p(\mathbf{w} \mid \mathbf{t}) \propto p(\mathbf{w})p(\mathbf{t} \mid \mathbf{w})$$

where **t** = $(t_1, ..., t_N)^T$.

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Discriminative Model

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Bayesian Logistic Regression

Using our previous result for the cross-entropy 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)\}\$$

we can now calculate the log of the posterior

$$p(\mathbf{w} \mid \mathbf{t}) \propto p(\mathbf{w})p(\mathbf{t} \mid \mathbf{w})$$

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

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

Continuous Input

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• To obtain a Gaussian approximation to

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

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

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



Continuous Input

D....b...b:11:...

Discriminative models

ogistic Regression

Least Squares

Laplace Approximation

Bayesian Logistic Regression

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

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

where

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