PRML学习笔记——第四章

Linear Models for Classification

Datasets如果能被linear decision surface确切separate,就被称为*linear separable*.

4.1. Discriminant Functions

4.1.1 Two classes

最简单的linear discriminator function可以是:

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

原点到decision surface的距离为:

$$\frac{\mathbf{w}^{\mathrm{T}}\mathbf{x}}{\|\mathbf{w}\|} = -\frac{w_0}{\|\mathbf{w}\|}$$

空间中任一点到surface的距离为:

$$\frac{y(\mathbf{x})}{\|\mathbf{w}\|}$$

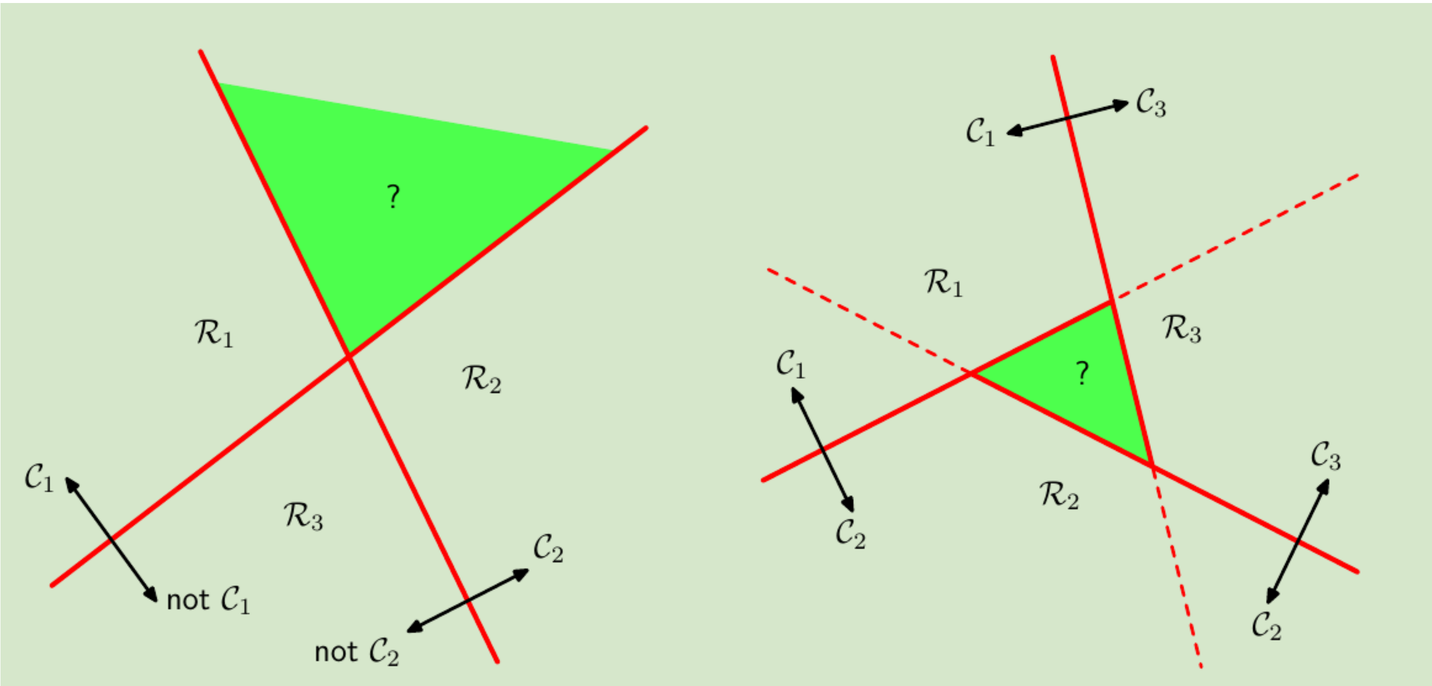
4.1.2 Multiple classes

对于一个K分类问题,我们定义K个linear function:

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

当$y_k(x) > y_j(x)$ for all $j \neq k$,就assign class k.并且$\mathcal{C}_k$和$\mathcal{C}_j$的decision boundary是

$$(\mathbf{w}_k - \mathbf{w}_j)^{\mathrm{T}}\mathbf{x} + (w_{k0} - w_{j0}) = 0$$



左图简单使用$K-1$个二分类器(one-versus-the-rest)会产生ambiguous region,右图使用$K(K-1)/2$个二分类器(one-versus-one)仍然会出现ambiguous region.

4.1.3 Least squares for classification

对于每一个类,都有一个linear model:

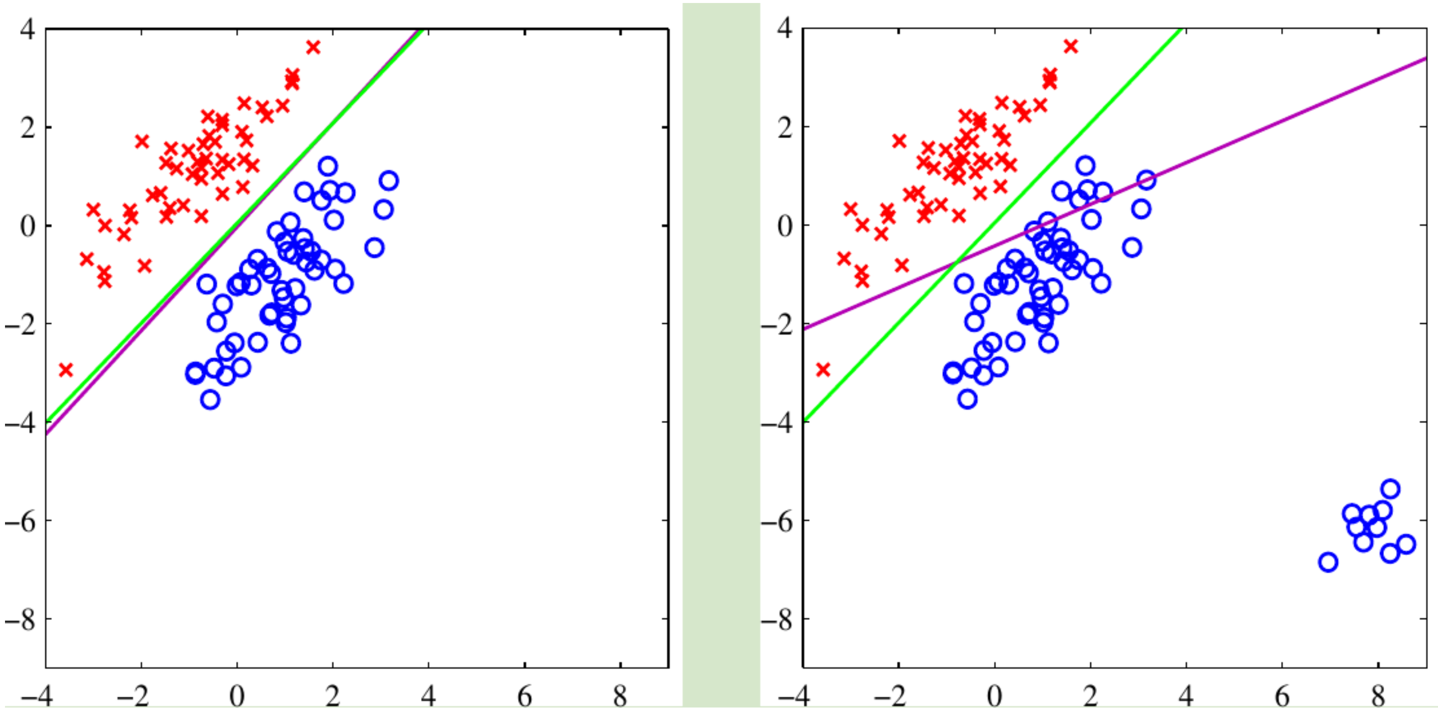
$$y_k(\mathbf{x}) = \mathbf{w}_k^{\mathrm{T}}\mathbf{x} + w_{k0}$$

group 起来就可以写成:$\mathbf{y}(\mathbf{x}) = \widetilde{\mathbf{W}}^{\mathrm{T}}\widetilde{\mathbf{x}}$
优化目标是sum-of-square error:

$$E_D(\widetilde{\mathbf{W}}) = \frac{1}{2}\mathrm{Tr}\left\{(\widetilde{\mathbf{X}}\widetilde{\mathbf{W}} - \mathbf{T})^{\mathrm{T}}(\widetilde{\mathbf{X}}\widetilde{\mathbf{W}} - \mathbf{T})\right\}$$

可以解出:

$$\widetilde{\mathbf{W}} = \left(\widetilde{\mathbf{X}}^{\mathrm{T}}\widetilde{\mathbf{X}}\right)^{-1}\widetilde{\mathbf{X}}^{\mathrm{T}}\mathbf{T} = \widetilde{\mathbf{X}}^{\dagger}\mathbf{T}$$



这样的模型很大的问题就是no robustness,如图上的紫色线受右下角蓝色data point影响.

4.1.4 Fisher's linear discriminant

一种以dimensionality reduction为视角的linear discriminator model:

$$y = \mathbf{w}^{\mathrm{T}}\mathbf{x}$$

y是个scalar,只要设定个threshold就能用来classify.
基本思想是让两个class的mean在投影到一维空间后尽可能靠的远(between-class),并且两类投影后各自的covariance尽可能小(within-class).于是maximize:

$$J(\mathbf{w})=\frac{\mathbf{w}^{\mathrm{T}}\mathbf{S}_{\mathrm{B}}\mathbf{w}}{\mathbf{w}^{\mathrm{T}}\mathbf{S}_{\mathrm{W}}\mathbf{w}}$$

其中:$\mathbf{S}_{\mathrm{B}}=\left(\mathbf{m}_{2}-\mathbf{m}_{1}\right)\left(\mathbf{m}_{2}-\mathbf{m}_{1}\right)^{\mathrm{T}}$,
$\mathbf{S}_{\mathbf{W}}=\sum_{n\in\mathcal{C}_{1}}\left(\mathbf{x}_{n}-\mathbf{m}_{1}\right)\left(\mathbf{x}_{n}-\mathbf{m}_{1}\right)^{\mathrm{T}}+\sum_{n\in\mathcal{C}_{2}}\left(\mathbf{x}_{n}-\mathbf{m}_{2}\right)\left(\mathbf{x}_{n}-\mathbf{m}_{2}\right)^{\mathrm{T}}$..对$\mathbf{w}$求微分:

$$\left(\mathbf{w}^{\mathrm{T}}\mathbf{S}_{\mathrm{B}}\mathbf{w}\right)\mathbf{S}_{\mathbf{W}}\mathbf{w}=\left(\mathbf{w}^{\mathrm{T}}\mathbf{S}_{\mathbf{W}}\mathbf{w}\right)\mathbf{S}_{\mathrm{B}}\mathbf{w}$$

又括号内是scalar,$\mathbf{S}_{\mathbf{W}}$与$(\mathbf{m_{2}}-\mathbf{m_{1}})$同向,所以:

$$\mathbf{w}\propto\mathbf{S}_{\mathrm{W}}^{-1}\left(\mathbf{m}_{2}-\mathbf{m}_{1}\right)$$

4.1.5 Relation to least squares

在least-squares的方法中,将$\mathcal{C}_1$的target设为N/N_1,$\mathcal{C}_2$的target设为$-N/N_2$,得到的解与Fisher solution一样.

4.1.6 Fisher’s discriminant for multiple classes

考虑有$K>2$个类,可以将input space投影到$K-1$维的空间.

$$\mathbf{y}=\mathbf{W}^{\mathrm{T}}\mathbf{x}$$

类似二分类的想法,使用between-class covariance最大,within-class covariance最小的目标:

$$J(\mathbf{W})=\operatorname{Tr}\left\{\left(\mathbf{W}^{\mathrm{T}}\mathbf{S}_{\mathrm{W}}\mathbf{W}\right)^{-1}\left(\mathbf{W}^{\mathrm{T}}\mathbf{S}_{\mathrm{B}}\mathbf{W}\right)\right\}$$

其中

$$\mathbf{S}_{\mathrm{W}}=\sum_{k=1}^{K}\sum_{n\in\mathcal{C}_{k}}\left(\mathbf{y}_{n}-\boldsymbol{\mu}_{k}\right)\left(\mathbf{y}_{n}-\boldsymbol{\mu}_{k}\right)^{\mathrm{T}}$$
$$\mathbf{S}_{\mathrm{B}}=\sum_{k=1}^{K}N_{k}\left(\boldsymbol{\mu}_{k}-\boldsymbol{\mu}\right)\left(\boldsymbol{\mu}_{k}-\boldsymbol{\mu}\right)^{\mathrm{T}}$$

4.1.7 The perceptron algorithm

perceptron 是个仅用于二分类的算法,discriminator function是

$$y(\mathbf{x})=f\left(\mathbf{w}^{\mathrm{T}}\boldsymbol{\phi}(\mathbf{x})\right)$$

这里的$f(\cdot)$是一个step function:

$$f(a)=\begin{cases}+1, & a \geqslant 0 \\ -1, & a<0\end{cases}$$

$\boldsymbol{\phi}(\boldsymbol{x})$是basis function.通过minimize一个error function优化$\mathbf{w}$:

$$E_{\mathrm{P}}(\mathbf{w})=-\sum_{n \in \mathcal{M}} \mathbf{w}^{\mathrm{T}} \boldsymbol{\phi}_{n} t_{n}$$

使用stochastic gradient descent去优化这个function:

$$\mathbf{w}^{(\tau+1)}=\mathbf{w}^{(\tau)}-\eta \nabla E_{\mathrm{P}}(\mathbf{w})=\mathbf{w}^{(\tau)}+\eta \boldsymbol{\phi}_{n} t_{n}$$

4.2. Probabilistic Generative Models

现在我们来考虑二分类的posterior:

$$\begin{aligned} p\left(\mathcal{C}_{1} \mid \mathbf{x}\right) &=\frac{p\left(\mathbf{x} \mid \mathcal{C}_{1}\right) p\left(\mathcal{C}_{1}\right)}{p\left(\mathbf{x} \mid \mathcal{C}_{1}\right) p\left(\mathcal{C}_{1}\right)+p\left(\mathbf{x} \mid \mathcal{C}_{2}\right) p\left(\mathcal{C}_{2}\right)} \\ &=\frac{1}{1+\exp (-a)}=\sigma(a) \end{aligned}$$

其中$a=\ln \frac{p\left(\mathbf{x} \mid \mathcal{C}_{1}\right) p\left(\mathcal{C}_{1}\right)}{p\left(\mathbf{x} \mid \mathcal{C}_{2}\right) p\left(\mathcal{C}_{2}\right)}$,$\sigma(a)$被称为*logistic sigmoid*.

但多分类的时候:

$$\begin{aligned} p\left(\mathcal{C}_{k} \mid \mathbf{x}\right) &=\frac{p\left(\mathbf{x} \mid \mathcal{C}_{k}\right) p\left(\mathcal{C}_{k}\right)}{\sum_{j} p\left(\mathbf{x} \mid \mathcal{C}_{j}\right) p\left(\mathcal{C}_{j}\right)} \\ &=\frac{\exp \left(a_{k}\right)}{\sum_{j} \exp \left(a_{j}\right)} \end{aligned}$$

其中$a_{k}=\ln p\left(\mathbf{x} \mid \mathcal{C}_{k}\right) p\left(\mathcal{C}_{k}\right)$.式中的normalized exponential也被称为*softmax function*.

4.2.1 Continuous inputs

假设input variable服从同covariance的Gaussian:

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

posterior是:

$$p\left(\mathcal{C}_1 \mid \mathbf{x}\right)=\sigma\left(\mathbf{w}^{\mathrm{T}} \mathbf{x}+w_0\right)$$

其中

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

观察到quadratic消失了,也就意味着decision boundary是linear的.若不假设不同class covariance一致,那么得到的decision boundary是曲面.

4.2.2 Maximum likelihood solution

仍然假设data关于类别服从共covariance的Gaussian.二分类为例,$t_n=1$是$\mathcal{C}_1$,$t_n=0$是$\mathcal{C}_2$,设prior是$p(\mathcal{C}_1)=\pi$,$p(\mathcal{C}_2)=1-\pi$,则posterior:

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

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

可以计算likelihood:

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

MLE的结果:

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

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

$$\begin{aligned} &-\tfrac{1}{2} \textstyle\sum_{n=1}^N t_n \ln |\boldsymbol{\Sigma}|-\tfrac{1}{2} \textstyle\sum_{n=1}^N t_n\left(\mathbf{x}_n-\boldsymbol{\mu}_1\right)^{\mathrm{T}} \boldsymbol{\Sigma}^{-1}\left(\mathbf{x}_n-\boldsymbol{\mu}_1\right) \\ &-\tfrac{1}{2} \textstyle\sum_{n=1}^N\left(1-t_n\right) \ln |\boldsymbol{\Sigma}|-\tfrac{1}{2} \textstyle\sum_{n=1}^N\left(1-t_n\right)\left(\mathbf{x}_n-\boldsymbol{\mu}_2\right)^{\mathrm{T}} \boldsymbol{\Sigma}^{-1}\left(\mathbf{x}_n-\boldsymbol{\mu}_2\right) \\ &=-\tfrac{N}{2} \ln |\boldsymbol{\Sigma}|-\tfrac{N}{2} \operatorname{Tr}\left\{\boldsymbol{\Sigma}^{-1} \mathbf{S}\right\} \end{aligned}$$

其中

$$
\begin{aligned}
\mathbf{S} &= \frac{N_1}{N}\mathbf{S}_1 + \frac{N_2}{N}\mathbf{S}_2 \\
\mathbf{S}_1 &= \frac{1}{N_1}\sum_{n\in\mathcal{C}_1}\left(\mathbf{x}_n-\boldsymbol{\mu}_1\right)\left(\mathbf{x}_n-\boldsymbol{\mu}_1\right)^{\mathrm{T}} \\
\mathbf{S}_2 &= \frac{1}{N_2}\sum_{n\in\mathcal{C}_2}\left(\mathbf{x}_n-\boldsymbol{\mu}_2\right)\left(\mathbf{x}_n-\boldsymbol{\mu}_2\right)^{\mathrm{T}}.
\end{aligned}
$$

最终$\mathbf{\Sigma}=\mathbf{S}$.也就是两类的weighted average of covariance.

4.2.3 Discrete features

当input是discrete时,考虑变量是binary,做*naive bayes*假设:所有变量都是independent,所以class-conditional distribution:

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

4.3. Probabilistic Discriminative Models

4.3.1 Fixed basis functions

目前的model都是关于parameter是linear的,但由于basis function(可以是nonlinear)的存在,尽管decision boundary在feature space中是linear,关于input space可以是nonlinear.

4.3.2 Logistic regression

考虑二分类的情况,sigmoid有个微分性质:

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

设$t_n\in\{0,1\}$,likelihood function可写成:

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

通过取negative logarithm of the likelihood(NLL/cross entropy error):

$$E(\mathbf{w})=-\ln p(\mathbf{t} \mid \mathbf{w})=-\sum_{n=1}^{N}\left\{t_{n} \ln y_{n}+\left(1-t_{n}\right) \ln \left(1-y_{n}\right)\right\}$$

求gradient:

$$\nabla E(\mathbf{w})=\sum_{n=1}^{N}\left(y_{n}-t_{n}\right) \phi_{n}$$

如此可以用gradient descent来解.

`note:` 由于logistic regression实际是MLE,所以不可避免会引入over-fit,通过加入regularization或者求MAP最大可以解决.

4.3.3 Iterative reweighted least squares

logistic regression的cross entropy error无法得到closed-form solution是因为一阶导中包含了非线性(sigmoid)的求和.利用*Newton-Raphson* iterative optimization scheme,我们可以更efficient求解:

$$\mathbf{w}^{(\text {new })}=\mathbf{w}^{(\text {old })}-\mathbf{H}^{-1} \nabla E(\mathbf{w})$$

首先求出cross entropy的一阶导和hessian matrix:

$$\begin{aligned}
\nabla E(\mathbf{w}) &=\sum_{n=1}^{N}\left(y_{n}-t_{n}\right) \phi_{n}=\mathbf{\Phi}^{\mathrm{T}}(\mathbf{y}-\mathbf{t}) \\
\mathbf{H}=\nabla \nabla E(\mathbf{w}) &=\sum_{n=1}^{N} y_{n}\left(1-y_{n}\right) \boldsymbol{\phi}_{n} \boldsymbol{\phi}_{n}^{\mathrm{T}}=\mathbf{\Phi}^{\mathrm{T}} \mathbf{R} \mathbf{\Phi}
\end{aligned}$$

其中的$\mathbf{R}$是$n \times n$的diagonal matrix,对角元素为:

$$R_{n n}=y_{n}\left(1-y_{n}\right)$$

由于$1>y_{n}>0$,所以$\mathbf{H}$是正定的,也就说明logistic regression有global minimum solution.
IRLS:

$$\begin{aligned}
\mathbf{w}^{(\text {new })} &=\mathbf{w}^{(\text {old })}-\left(\mathbf{\Phi}^{\mathrm{T}} \mathbf{R} \Phi\right)^{-1} \mathbf{\Phi}^{\mathrm{T}}(\mathbf{y}-\mathbf{t}) \\
&=\left(\mathbf{\Phi}^{\mathrm{T}} \mathbf{R} \mathbf{\Phi}\right)^{-1}\left\{\mathbf{\Phi}^{\mathrm{T}} \mathbf{R} \Phi \mathbf{w}^{(\text {old })}-\mathbf{\Phi}^{\mathrm{T}}(\mathbf{y}-\mathbf{t})\right\} \\
&=\left(\mathbf{\Phi}^{\mathrm{T}} \mathbf{R} \mathbf{\Phi}\right)^{-1} \mathbf{\Phi}^{\mathrm{T}} \mathbf{R} \mathbf{z}
\end{aligned}$$

4.3.4 Multiclass logistic regression

多分类的posterior为:

$$p\left(\mathcal{C}_k \mid \boldsymbol{\phi}\right)=y_k(\boldsymbol{\phi})=\frac{\exp \left(a_k\right)}{\sum_j \exp \left(a_j\right)}$$

其中$a_k=\mathbf{w}_k^{\mathrm{T}} \boldsymbol{\phi}$.

softmax的derivation也有性质:

$$\frac{\partial y_k}{\partial a_j}=y_k\left(I_{kj}-y_j\right)$$

使用likelihood:

$$p\left(\mathbf{T} \mid \mathbf{w}_1, \ldots, \mathbf{w}_K\right)=\prod_{n=1}^N \prod_{k=1}^K p\left(\mathcal{C}_k \mid \phi_n\right)^{t_{nk}}=\prod_{n=1}^N \prod_{k=1}^K y_{nk}^{t_{nk}}$$

NLL为:

$$E\left(\mathbf{w}_1, \ldots, \mathbf{w}_K\right)=-\ln p\left(\mathbf{T} \mid \mathbf{w}_1, \ldots, \mathbf{w}_K\right)=-\sum_{n=1}^N \sum_{k=1}^K t_{nk} \ln y_{nk}$$

类似于二分类的logistic regression,多分类有类似的优化形式:

$$\begin{aligned}
\nabla_{\mathbf{w}_j} E\left(\mathbf{w}_1, \ldots, \mathbf{w}_K\right) &= \sum_{n=1}^N\left(y_{nj}-t_{nj}\right) \phi_n \\
\nabla_{\mathbf{w}_k} \nabla_{\mathbf{w}_j} E\left(\mathbf{w}_1, \ldots, \mathbf{w}_K\right) &= -\sum_{n=1}^N y_{nk}\left(I_{kj}-y_{nj}\right) \phi_n \boldsymbol{\phi}_n^{\mathrm{T}}
\end{aligned}$$

4.3.5 Probit regression

posterior被描述为linear combination of feature后的activation输出.$p(t=1 \mid a)=f(a)$,这里的$f(\cdot)$即为activation.通过设置阈值θ来给出target类别:

$$\begin{cases}t_n=1 & \text{if } a_n \geqslant \theta \\ t_n=0 & \text{otherwise}\end{cases}$$

现在把θ看成从一个从$p(\theta)$的distribution里抽取得到的,那么activation function可以这样给出

$$f(a)=\int_{-\infty}^{a} p(\theta) \mathrm{d} \theta$$

当θ取标准正态分布的时候:

$$\Phi(a)=\int_{-\infty}^{a} \mathcal{N}(\theta \mid 0,1) \mathrm{d} \theta$$

被称为*probit function*.使用了这个函数作为activation function时的GLM(generalize linear model)被称为*probit regression*.

`note:` 由于probit带有二次项,所以比logistic regresion更易收outliers影响.

4.4 The Laplace Approximation

由于sigmoid等一些非线性activation function的存在,无法进行解析积分$p(z)$.Laplace approximation是使用Gaussian的$q(z)$去approximate$p(z)$,来解决这个问题.设要被近似的概率为$p(z)=\frac{1}{Z} f(z)$.其中Z用作normalization.我们使用概率的众数z_0点:

$$\left.\frac{d f(z)}{d z}\right|_{z=z_{0}}=0$$

在z_0使用Taylor展开:

$$\ln f(z) \simeq \ln f\left(z_{0}\right)-\frac{1}{2} A\left(z-z_{0}\right)^{2}$$

其中$A=-\left.\frac{d^{2}}{d z^{2}} \ln f(z)\right|_{z=z_{0}}$.如此可以用Gaussian去近似$p(z)$:

$$q(z)=\left(\frac{A}{2 \pi}\right)^{1 / 2} \exp \left\{-\frac{A}{2}\left(z-z_{0}\right)^{2}\right\}$$

4.5. Bayesian Logistic Regression

4.5.1 Laplace approximation

prior用Gaussian:

$$p(\mathbf{w})=\mathcal{N}\left(\mathbf{w} \mid \mathbf{m}_{0}, \mathbf{S}_{0}\right)$$

likelihood用laplace approximate,并利用bayes' theorem $p(\mathbf{w} \mid \mathbf{t}) \propto p(\mathbf{w}) p(\mathbf{t} \mid \mathbf{w})$求posterior最大:

$$
\begin{aligned}
\ln p(\mathbf{w} \mid \mathbf{t})=&-\frac{1}{2}\left(\mathbf{w}-\mathbf{m}_0\right)^{\mathrm{T}} \mathbf{S}_0^{-1}\left(\mathbf{w}-\mathbf{m}_0\right) \\
&+\sum_{n=1}^N\left\{t_n \ln y_n+\left(1-t_n\right) \ln \left(1-y_n\right)\right\}+\text { const }
\end{aligned}
$$

这样得到的解是MAP解:

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

4.5.2 Predictive distribution

现在考虑marginalize这一步:

$$
p\left(\mathcal{C}_1 \mid \boldsymbol{\phi}, \mathbf{t}\right)=\int p\left(\mathcal{C}_1 \mid \boldsymbol{\phi}, \mathbf{w}\right) p(\mathbf{w} \mid \mathbf{t}) \mathrm{d} \mathbf{w} \simeq \int \sigma\left(\mathbf{w}^{\mathrm{T}} \boldsymbol{\phi}\right) q(\mathbf{w}) \mathrm{d} \mathbf{w}
$$

引入δ函数:

$$
\sigma\left(\mathbf{w}^{\mathrm{T}} \boldsymbol{\phi}\right)=\int \delta\left(a-\mathbf{w}^{\mathrm{T}} \boldsymbol{\phi}\right) \sigma(a) \mathrm{d} a
$$

最后predictive function:

$$
p\left(\mathcal{C}_1 \mid \mathbf{t}\right)=\int \sigma(a) p(a) \mathrm{d} a=\int \sigma(a) \mathcal{N}\left(a \mid \mu_a, \sigma_a^2\right) \mathrm{d} a
$$