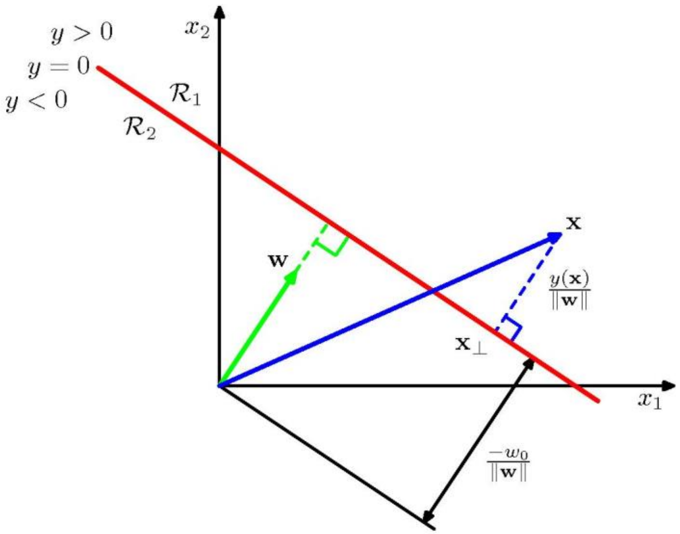
PATTERN RECOGNITION AND MACHINE LEARNING

CHAPTER 4: LINEAR MODELS FOR CLASSIFICATION

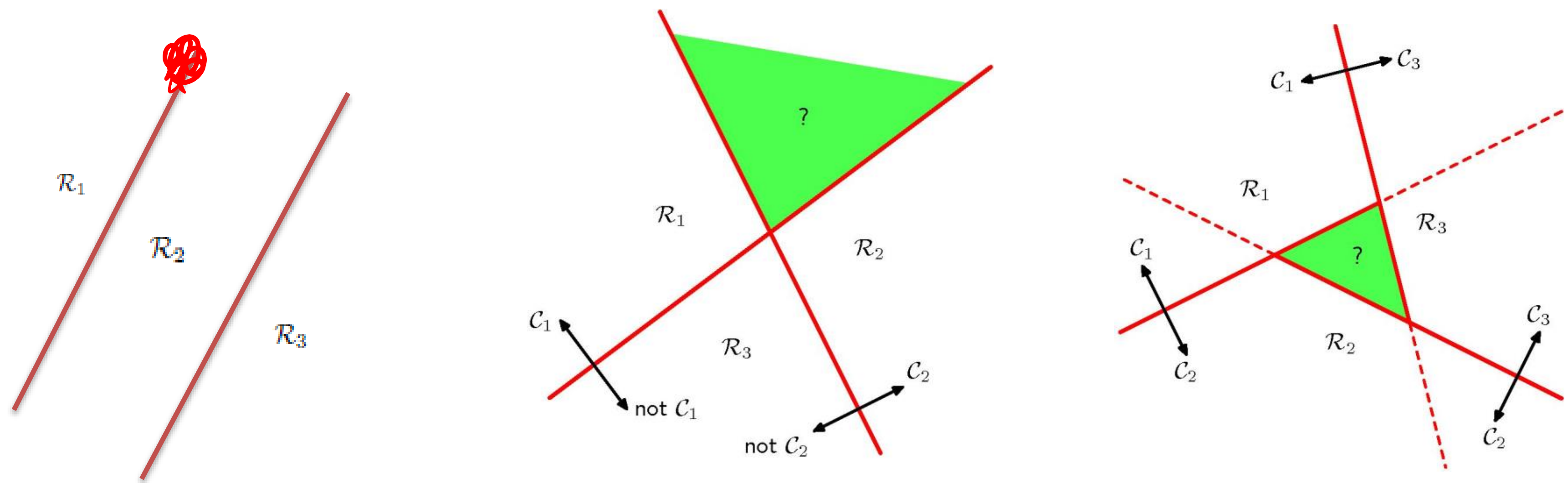
Discriminant Functions – Two Classes



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

Discriminant Functions – Multiple Classes

Can we construct a K (>2)-class classifier using a set of two class discriminants?



Least Squares for Classification

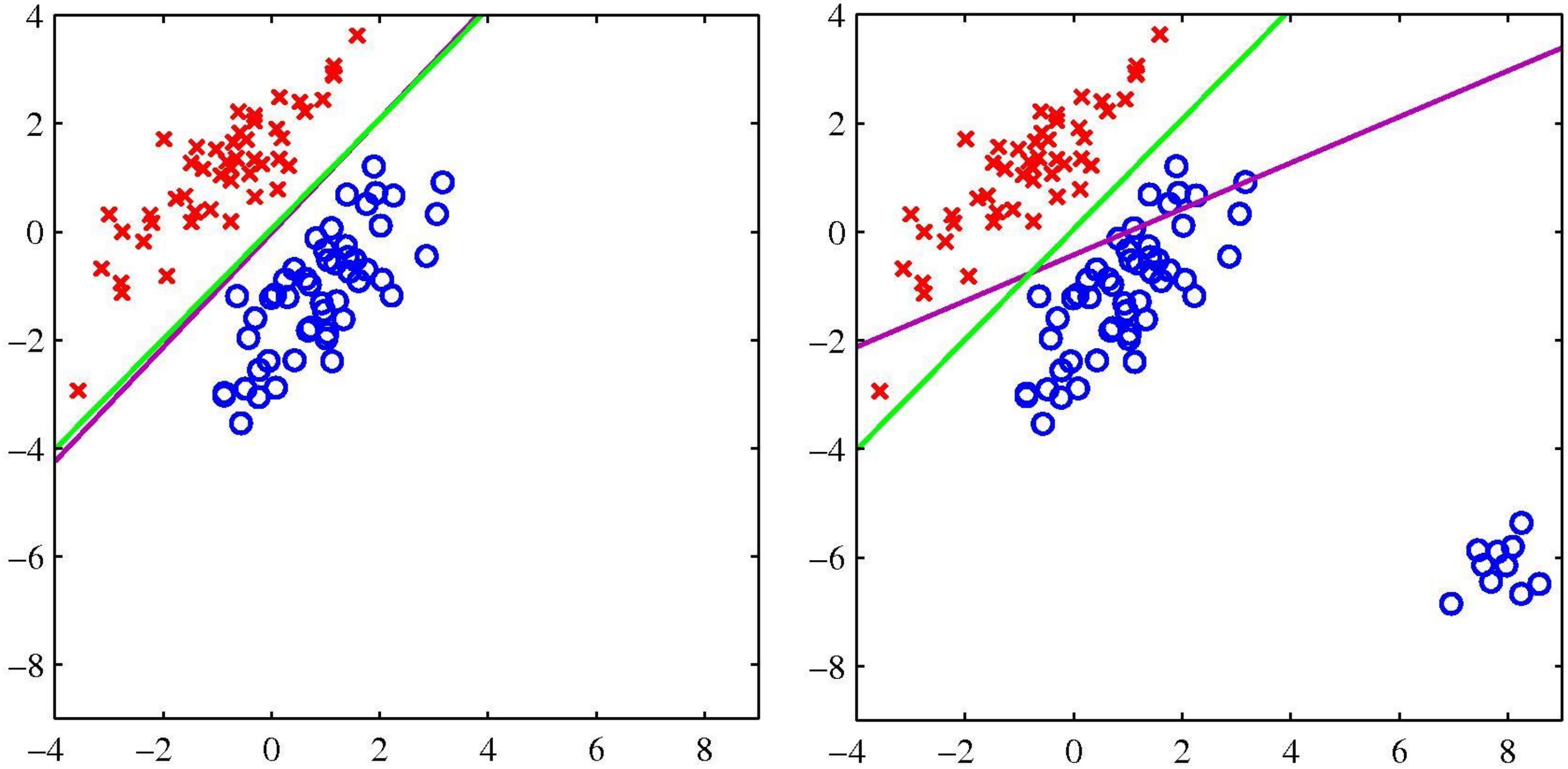
$$y_k(\mathbf{x}) = \mathbf{w}_k^{\mathrm{T}}\mathbf{x} + w_{k0}$$

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

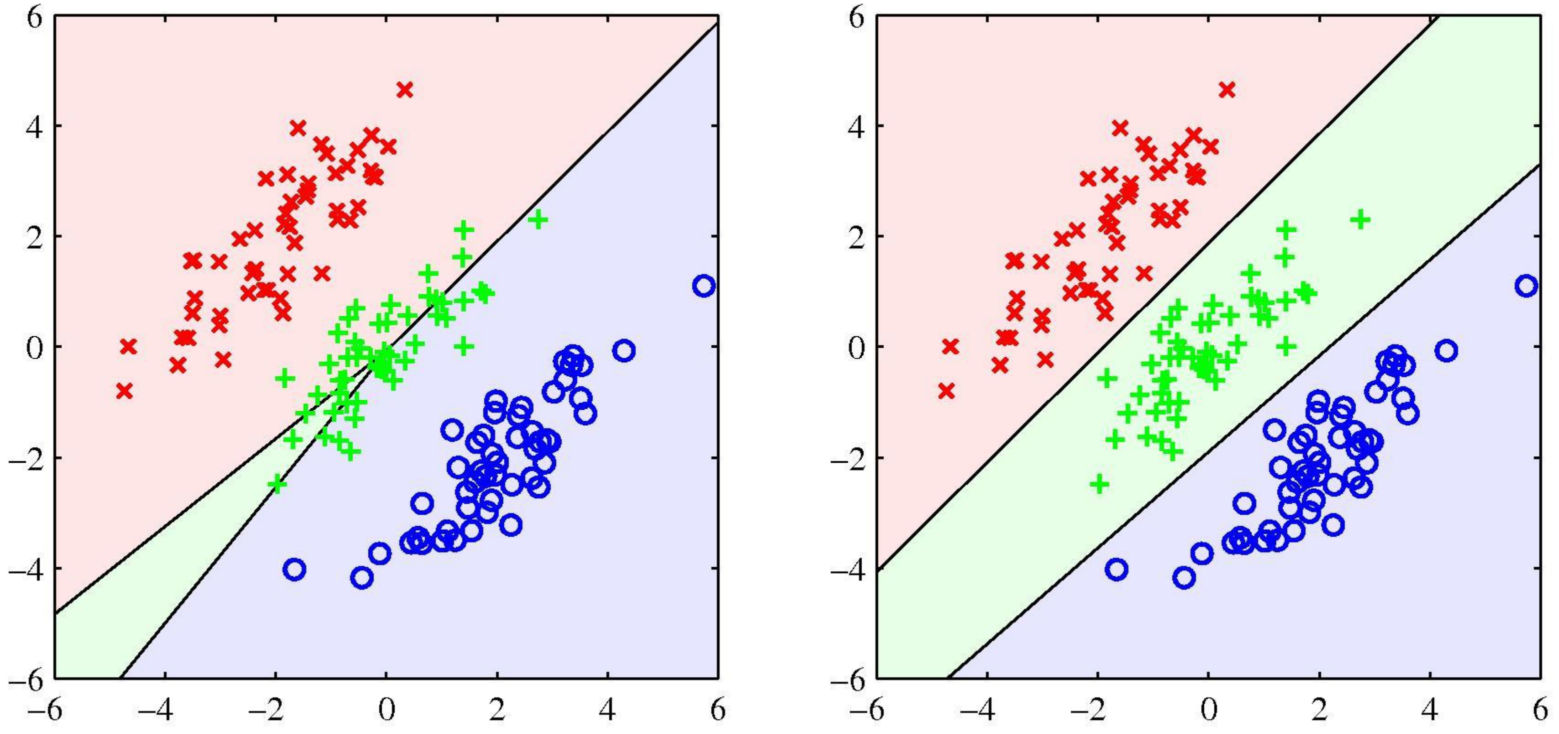
$$E_D(\widetilde{\mathbf{W}}) = \frac{1}{2}\mathrm{Tr}\left\{(\widetilde{\mathbf{X}}\widetilde{\mathbf{W}} - \mathbf{T})^{\mathrm{T}}(\widetilde{\mathbf{X}}\widetilde{\mathbf{W}} - \mathbf{T})\right\}$$

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

Least Squares for Classification



Least Squares for Classification



Fisher's linear discriminant

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

$$\mathbf{m}_1 = \frac{1}{N_1}\sum_{n \in \mathcal{C}_1} \mathbf{x}_n, \qquad \mathbf{m}_2 = \frac{1}{N_2}\sum_{n \in \mathcal{C}_2} \mathbf{x}_n$$

$$m_2 - m_1 = \mathbf{w}^{\mathrm{T}}(\mathbf{m}_2 - \mathbf{m}_1) \qquad m_k = \mathbf{w}^{\mathrm{T}}\mathbf{m}_k \qquad s_k^2 = \sum_{n\in\mathcal{C}_k} (y_n - m_k)^2$$

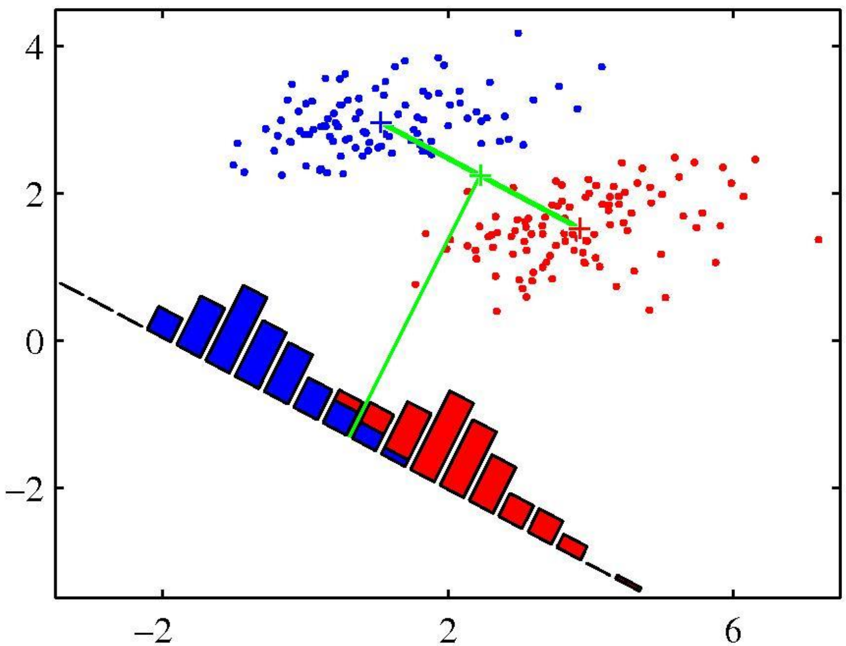
$$J(\mathbf{w}) = \frac{(m_2 - m_1)^2}{s_1^2 + s_2^2} \qquad J(\mathbf{w}) = \frac{\mathbf{w}^{\mathrm{T}}\mathbf{S}_{\mathrm{B}}\mathbf{w}}{\mathbf{w}^{\mathrm{T}}\mathbf{S}_{\mathrm{W}}\mathbf{w}}$$

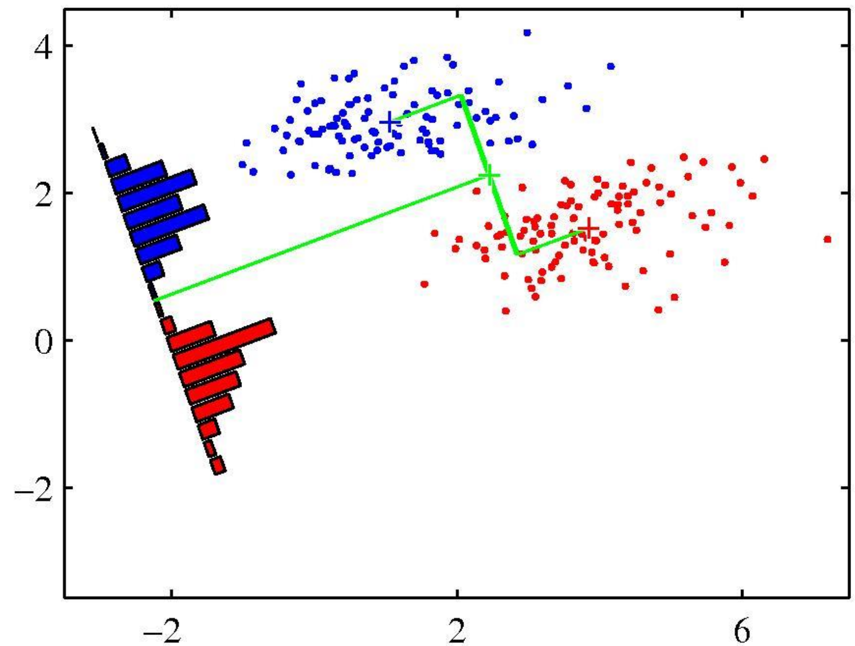
$$\mathbf{S}_{\mathrm{B}} = (\mathbf{m}_2 - \mathbf{m}_1)(\mathbf{m}_2 - \mathbf{m}_1)^{\mathrm{T}}$$

$$\mathbf{S}_{\mathrm{W}} = \sum_{n\in\mathcal{C}_1} (\mathbf{x}_n - \mathbf{m}_1)(\mathbf{x}_n - \mathbf{m}_1)^{\mathrm{T}} + \sum_{n\in\mathcal{C}_2} (\mathbf{x}_n - \mathbf{m}_2)(\mathbf{x}_n - \mathbf{m}_2)^{\mathrm{T}}$$

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

Fisher’s linear discriminant





The perceptron algorithm

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

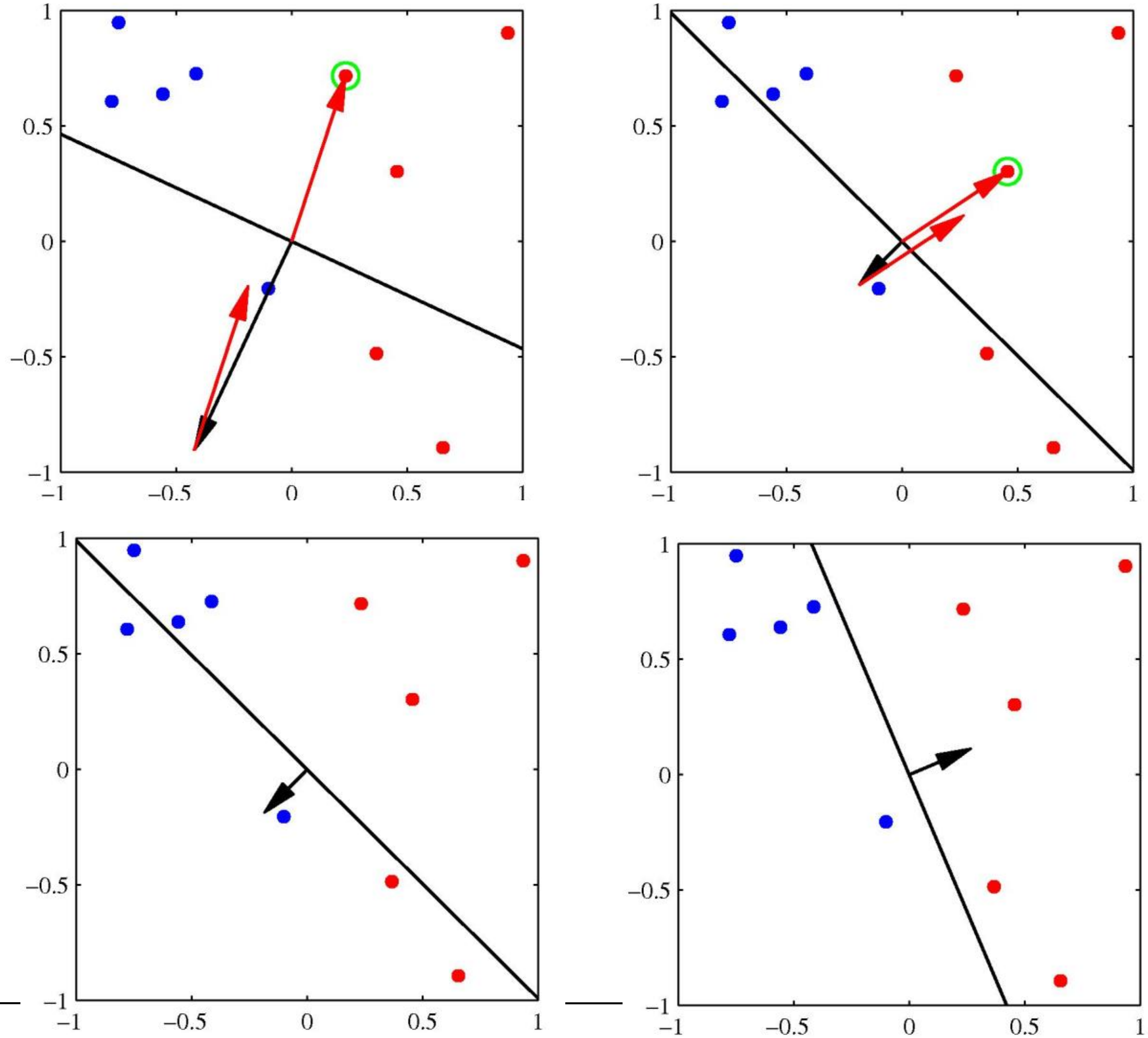
$$f(a) = \begin{cases} +1, & a \geqslant 0 \\ -1, & a < 0 \end{cases}$$

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

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

The perceptron convergence theorem states that if there exists an exact solution (in other words, if the training data set is linearly separable), then the perceptron learning algorithm is guaranteed to find an exact solution in a finite number of steps.

The perceptron algorithm



Probabilistic Generative Models

$$
\begin{aligned}
p(\mathcal{C}_1|\mathbf{x}) &= \frac{p(\mathbf{x}|\mathcal{C}_1)p(\mathcal{C}_1)}{p(\mathbf{x}|\mathcal{C}_1)p(\mathcal{C}_1) + p(\mathbf{x}|\mathcal{C}_2)p(\mathcal{C}_2)} \\
&= \frac{1}{1+\exp(-a)} = \sigma(a)
\end{aligned}
$$

σ(a) is the logistic sigmoid function

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

$$\sigma(-a) = 1 - \sigma(a)$$

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

a is the logit function

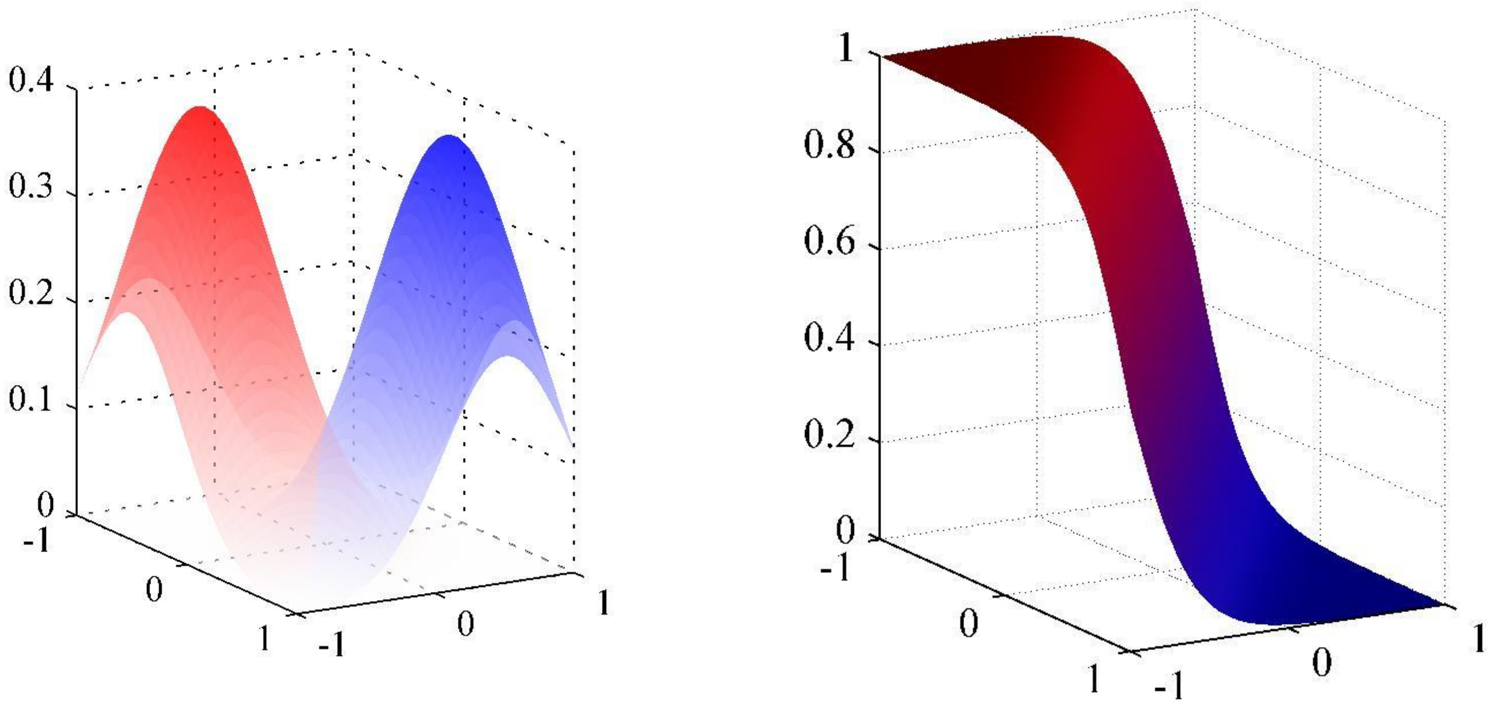
Probabilistic Generative Models

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

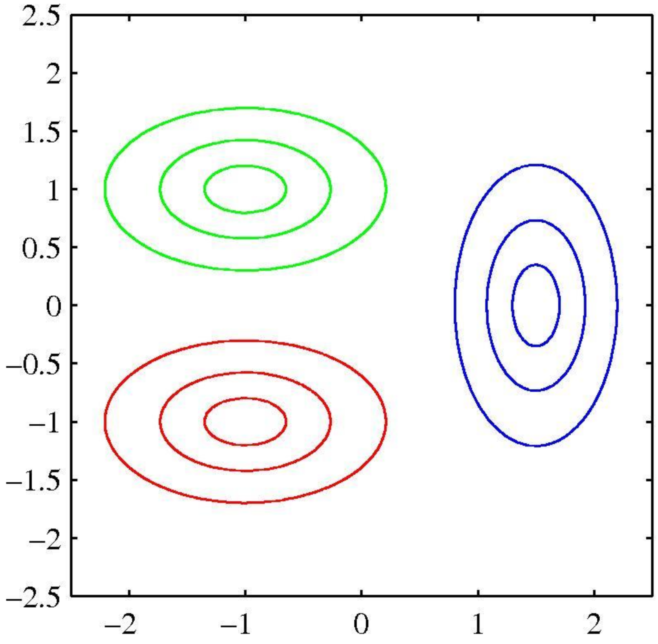
$$p(\mathcal{C}_1|\mathbf{x}) = \sigma(\mathbf{w}^{\mathrm{T}}\mathbf{x} + w_0)$$

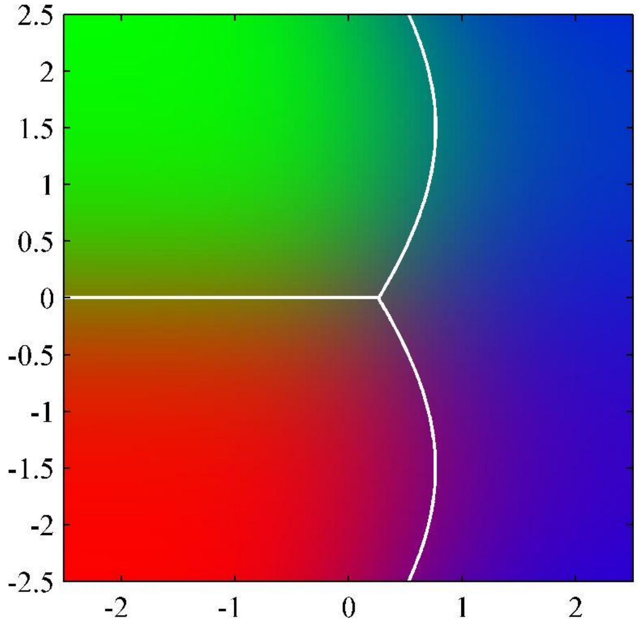
$$\begin{aligned} \mathbf{w} &= \mathbf{\Sigma}^{-1}(\boldsymbol{\mu}_1 - \boldsymbol{\mu}_2) \\ w_0 &= -\frac{1}{2}\boldsymbol{\mu}_1^{\mathrm{T}}\mathbf{\Sigma}^{-1}\boldsymbol{\mu}_1 + \frac{1}{2}\boldsymbol{\mu}_2^{\mathrm{T}}\mathbf{\Sigma}^{-1}\boldsymbol{\mu}_2 + \ln\frac{p(\mathcal{C}_1)}{p(\mathcal{C}_2)}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

Probabilistic Generative Models

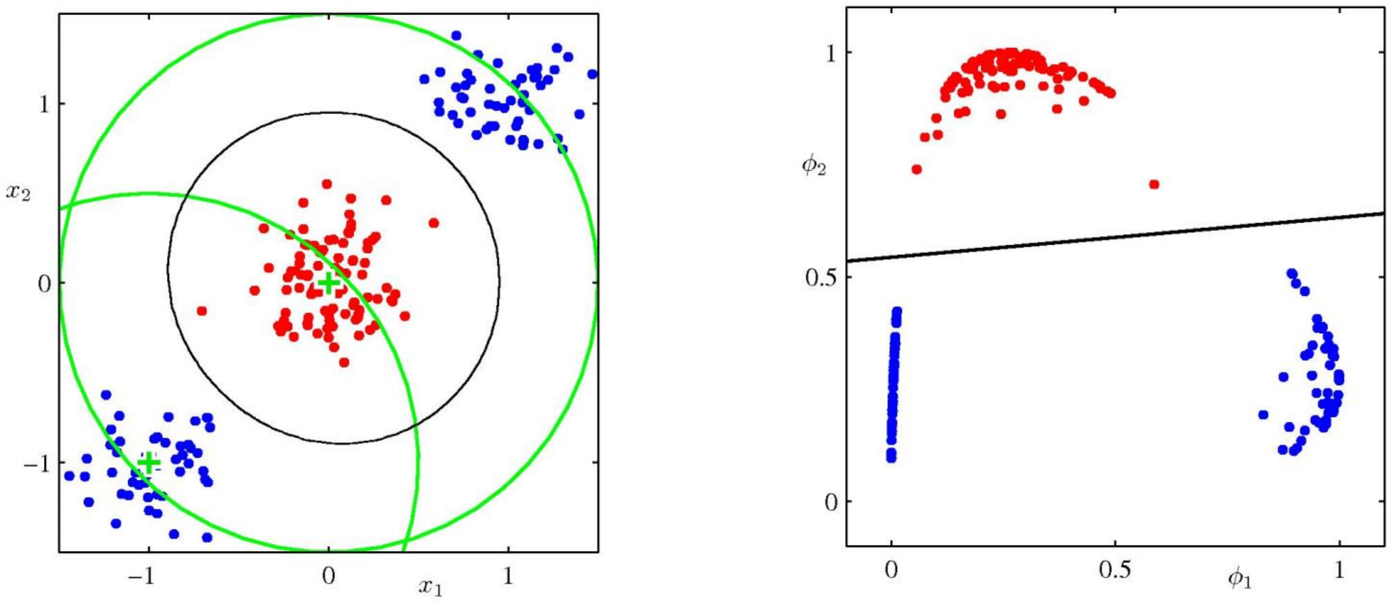


Probabilistic Generative Models





Probabilistic Discriminative Models



Probabilistic Discriminative Models

$$p(\mathcal{C}_1|\phi) = y(\phi) = \sigma\left(\mathbf{w}^{\mathrm{T}}\phi\right)$$

logistic regression

$$p(\mathcal{C}_2|\phi) = 1 - p(\mathcal{C}_1|\phi)$$

We use maximum likelihood to determine the parameters of the logistic regression model

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

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

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

Probabilistic Discriminative Models

For logistic regression, there is no longer a closed-form solution, due to the nonlinearity of the logistic sigmoid function

The error function can be minimized by an efficient iterative technique based on the Newton-Raphson iterative optimization scheme, which uses a local quadratic approximation to the log likelihood function.

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

$$\begin{aligned}\nabla E(\mathbf{w}) &= \sum_{n=1}^{N}(\mathbf{w}^{\mathrm{T}}\boldsymbol{\phi}_n - t_n)\boldsymbol{\phi}_n = \boldsymbol{\Phi}^{\mathrm{T}}\boldsymbol{\Phi}\mathbf{w} - \boldsymbol{\Phi}^{\mathrm{T}}\mathbf{t} \\ \mathbf{H} = \nabla\nabla E(\mathbf{w}) &= \sum_{n=1}^{N}\boldsymbol{\phi}_n\boldsymbol{\phi}_n^{\mathrm{T}} = \boldsymbol{\Phi}^{\mathrm{T}}\boldsymbol{\Phi}\end{aligned}$$

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

$$R_{nn} = y_n(1-y_n)$$

$$\mathbf{z} = \boldsymbol{\Phi}\mathbf{w}^{(\text{old})} - \mathbf{R}^{-1}(\mathbf{y}-\mathbf{t})$$

Probabilistic Discriminative Models

Not all choices of class-conditional density give rise to such a simple form for the posterior probabilities (for instance, if the class-conditional densities are modelled using Gaussian mixtures). This suggests that it might be worth exploring other types of discriminative probabilistic model.

$$a = \mathbf{w}^{\mathrm{T}}\boldsymbol{\phi}$$

$$p(t=1|a) = f(a)$$

f(·) is the activation function

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

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

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

$$\mathrm{erf}(a) = \frac{2}{\sqrt{\pi}}\int_{0}^{a} \exp(-\theta^2/2)\,\mathrm{d}\theta$$

$$\boldsymbol{\Phi}(a) = \frac{1}{2}\left\{1 + \frac{1}{\sqrt{2}}\mathrm{erf}(a)\right\}$$

probit regression

The Laplace Approximation

In many cases, we cannot integrate exactly over the parameter vector w since the posterior distribution is no longer Gaussian. It is therefore necessary to introduce some form of approximation.

$$p(z) = \frac{1}{Z} f(z) \qquad Z = \int f(z)\,\mathrm{d}z$$

$$\left.\frac{df(z)}{dz}\right|_{z=z_0} = 0 \qquad \ln f(z) \simeq \ln f(z_0) - \frac{1}{2}A(z-z_0)^2 \qquad A = -\left.\frac{d^2}{dz^2}\ln f(z)\right|_{z=z_0}$$

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

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

$$\ln f(\mathbf{z}) \simeq \ln f(\mathbf{z}_0) - \frac{1}{2}(\mathbf{z}-\mathbf{z}_0)^{\mathrm{T}}\mathbf{A}(\mathbf{z}-\mathbf{z}_0) \qquad \mathbf{A} = -\left.\nabla\nabla\ln f(\mathbf{z})\right|_{\mathbf{z}=\mathbf{z}_0}$$

$$f(\mathbf{z}) \simeq f(\mathbf{z}_0)\exp\left\{-\frac{1}{2}(\mathbf{z}-\mathbf{z}_0)^{\mathrm{T}}\mathbf{A}(\mathbf{z}-\mathbf{z}_0)\right\}$$

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

The Laplace Approximation

$$\begin{aligned} Z &= \int f(\mathbf{z})\,\mathrm{d}\mathbf{z} \\ &\simeq f(\mathbf{z}_0) \int \exp\left\{-\frac{1}{2}(\mathbf{z}-\mathbf{z}_0)^{\mathrm{T}}\mathbf{A}(\mathbf{z}-\mathbf{z}_0)\right\} \mathrm{d}\mathbf{z} \\ &= f(\mathbf{z}_0)\frac{(2\pi)^{M/2}}{|\mathbf{A}|^{1/2}} \end{aligned}$$

Consider a data set D and a set of models {Mi} having parameters {θi}.

$$p(\mathcal{D}) = \int p(\mathcal{D}|\boldsymbol{\theta})p(\boldsymbol{\theta})\,\mathrm{d}\boldsymbol{\theta}$$

$$f(\boldsymbol{\theta}) = p(\mathcal{D}|\boldsymbol{\theta})p(\boldsymbol{\theta})$$

$$Z = p(\mathcal{D})$$

$$\ln p(\mathcal{D}) \simeq \ln p(\mathcal{D}|\boldsymbol{\theta}_{\mathrm{MAP}}) + \underbrace{\ln p(\boldsymbol{\theta}_{\mathrm{MAP}}) + \frac{M}{2}\ln(2\pi) - \frac{1}{2}\ln|\mathbf{A}|}_{\text{Occam factor}}$$

where θ_{MAP} is the value of θ at the mode of the posterior distribution, and A is the Hessian matrix of second derivatives of the negative log posterior

$$\mathbf{A} = -\nabla\nabla \ln p(\mathcal{D}|\boldsymbol{\theta}_{\mathrm{MAP}})p(\boldsymbol{\theta}_{\mathrm{MAP}}) = -\nabla\nabla \ln p(\boldsymbol{\theta}_{\mathrm{MAP}}|\mathcal{D})$$

If we assume that the Gaussian prior distribution over parameters is broad, and that the Hessian has full rank

$$\ln p(\mathcal{D}) \simeq \ln p(\mathcal{D}|\boldsymbol{\theta}_{\mathrm{MAP}}) - \frac{1}{2}M\ln N$$

Bayesian Information Criterion (BIC)

Bayesian Logistic Regression

Exact Bayesian inference for logistic regression is intractable.

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

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

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

$$y_n = \sigma(\mathbf{w}^{\mathrm{T}}\phi_n)$$

To obtain a Gaussian approximation to the posterior distribution, we first maximize the posterior distribution to give the MAP (maximum posterior) solution w_{MAP}, which defines the mean of the Gaussian. The covariance is then given by the inverse of the matrix of second derivatives of the negative log likelihood, which takes the form

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

The Gaussian approximation to the posterior distribution therefore takes the form

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

Bayesian Logistic Regression

The predictive distribution for class C_1, given a new feature vector φ(x), is obtained by marginalizing with respect to the posterior distribution p(w|t), which is itself approximated by a Gaussian distribution q(w)

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

The corresponding probability for class C_2 given by

$$p(\mathcal{C}_2|\phi, \mathbf{t}) = 1 - p(\mathcal{C}_1|\phi, \mathbf{t})$$

Thus our variational approximation to the predictive distribution becomes

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

$$a = \mathbf{w}^{\mathrm{T}}\phi$$