Probabilistic Generative Models

Machine Learning

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Probabilistic Generative Models

- Binary Classification

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

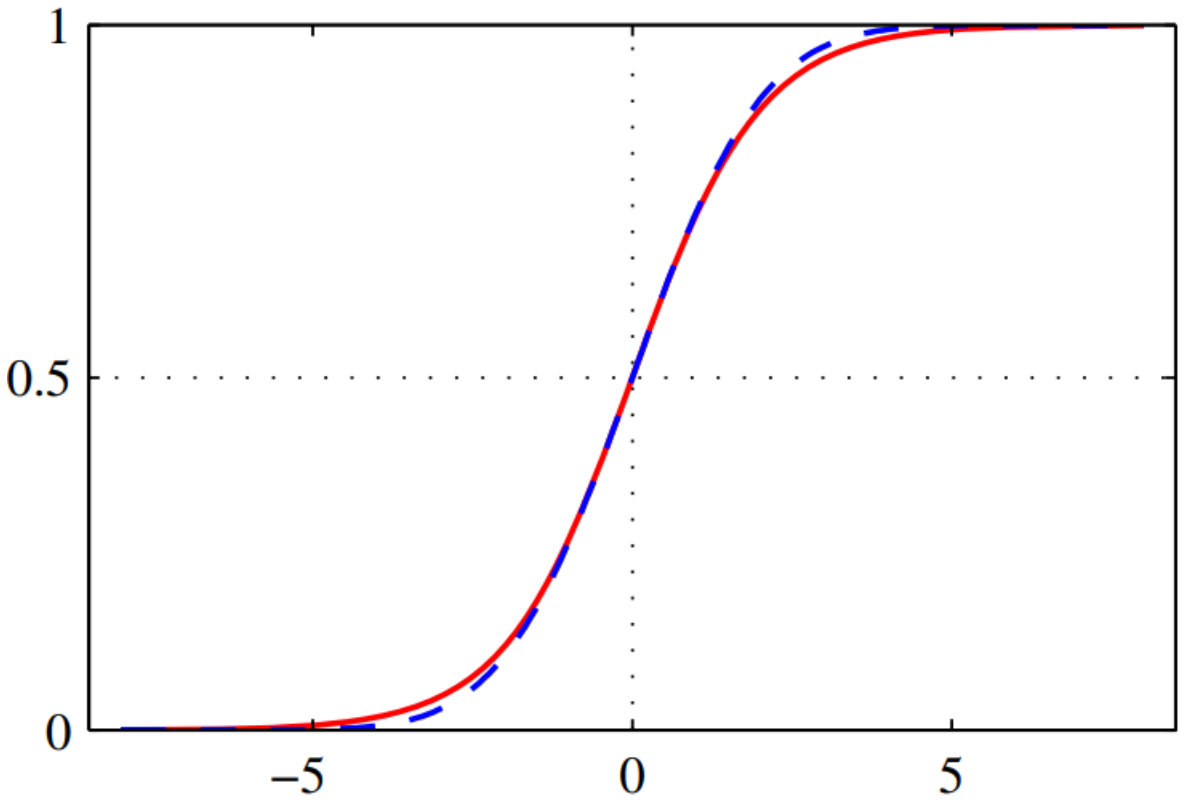
where we have defined

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

and $\sigma(a)$ is the *logistic sigmoid* function defined by

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

Logistic sigmoid function



Logistic sigmoid function

- Interesting properties

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

- The inverse of the logistic sigmoid is given by

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

and is known as the *logit* function.

Probabilistic Generative Models

For the case of $K > 2$ classes, we have

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

$$= \frac{\exp(a_k)}{\sum_j \exp(a_j)}$$

softmax function

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

Continuous inputs :
Class-conditional densities are Gaussian

Assume that all classes share the same covariance matrix

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

- For two classes

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

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

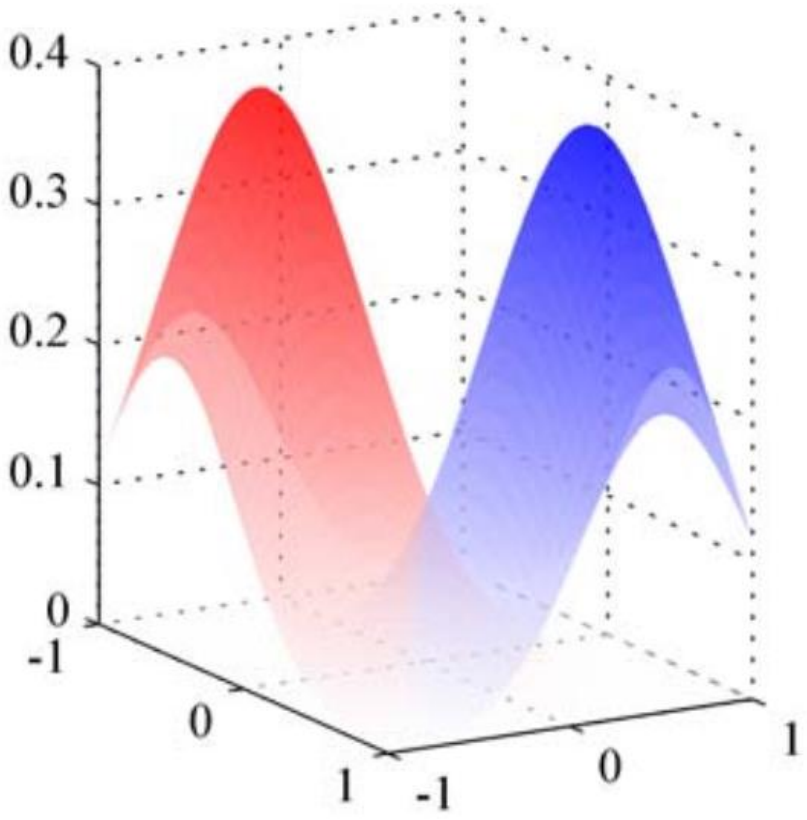
$$w_0 = -\frac{1}{2}\boldsymbol{\mu}_1^{\mathrm{T}}\mathbf{\Sigma}^{-1}\boldsymbol{\mu}_1 + \frac{1}{2}\boldsymbol{\mu}_2^{\mathrm{T}}\mathbf{\Sigma}^{-1}\boldsymbol{\mu}_2 + \ln\frac{p(\mathcal{C}_1)}{p(\mathcal{C}_2)}$$

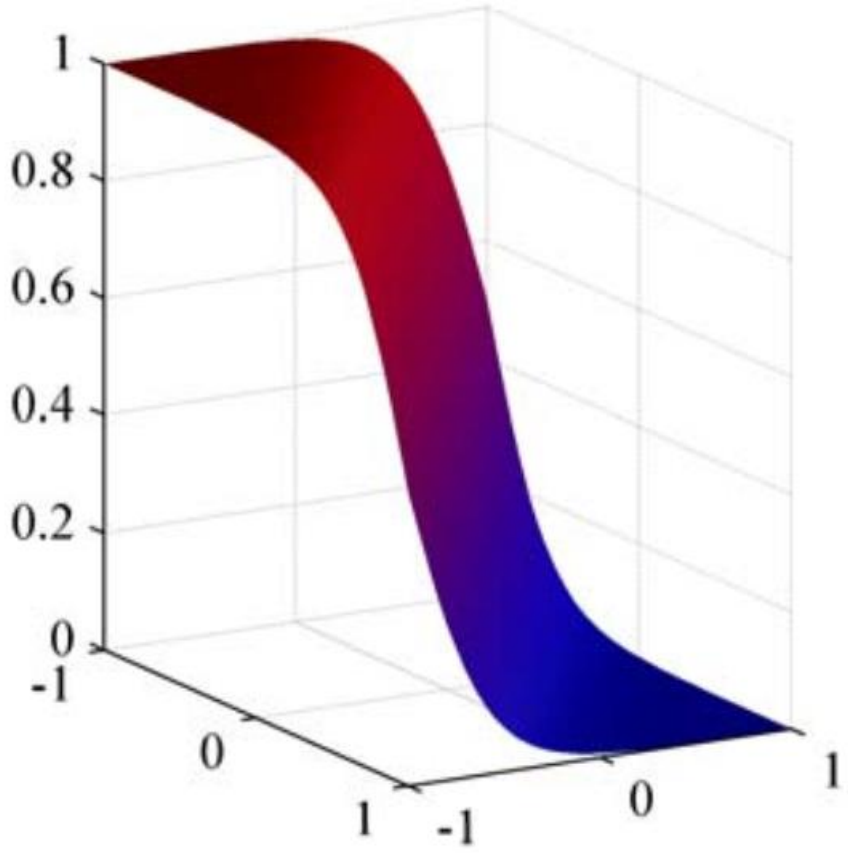
$$a = \ln\frac{p(\mathbf{x}|\mathcal{C}_1)p(\mathcal{C}_1)}{p(\mathbf{x}|\mathcal{C}_2)p(\mathcal{C}_2)}$$

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

Continuous inputs :

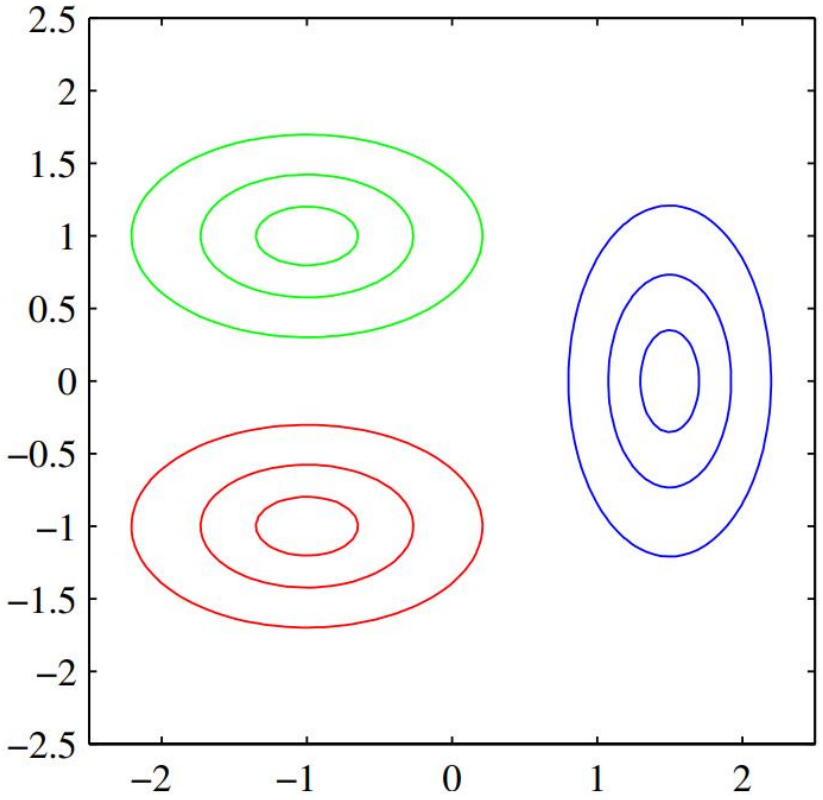
Class-conditional densities are Gaussian

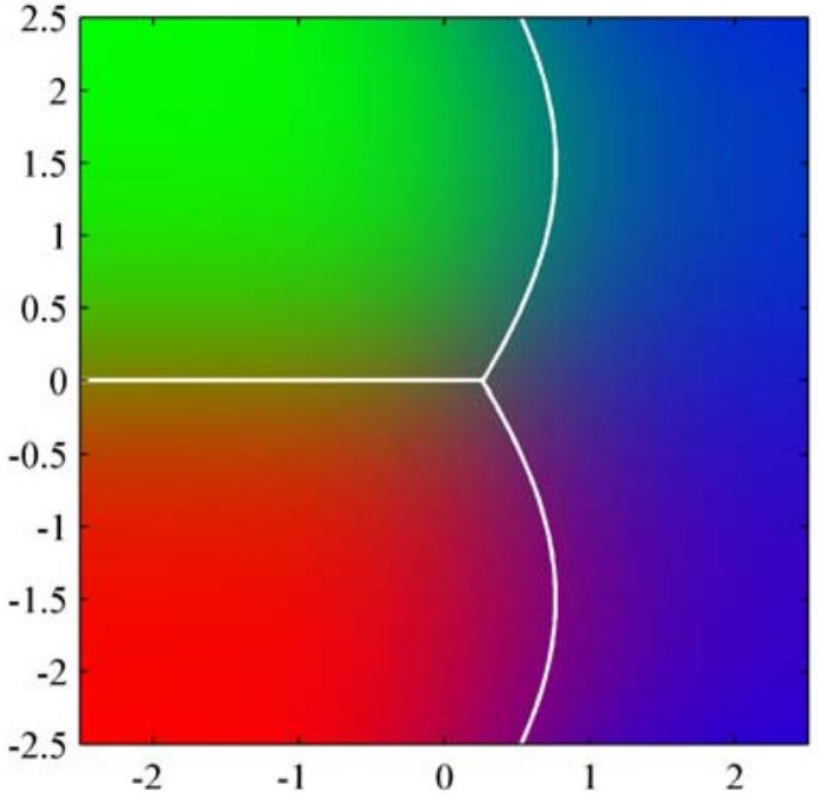




Continuous inputs :
Class-conditional densities are Gaussian

Assume that all classes have different covariance matrix
Quadratic Discriminant





Maximum likelihood solution:

Class-conditional densities; Gaussian, Shared Covariance

- For K=2

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

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

Thus the likelihood function is given by

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

Maximum likelihood solution:

Class-conditional densities; Gaussian, Shared Covariance

- Consider first the maximization with respect to π
- The terms in the log likelihood function that depend on π are

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

Setting the derivative with respect to π equal to zero and rearranging, we obtain

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

Maximum likelihood solution:

Class-conditional densities; Gaussian, Shared Covariance

- maximization with respect to $\boldsymbol{\mu}_1$

$$\sum_{n=1}^{N} t_n \ln \mathcal{N}(\mathbf{x}_n|\boldsymbol{\mu}_1, \boldsymbol{\Sigma}) = -\frac{1}{2}\sum_{n=1}^{N} t_n(\mathbf{x}_n - \boldsymbol{\mu}_1)^{\mathrm{T}}\boldsymbol{\Sigma}^{-1}(\mathbf{x}_n - \boldsymbol{\mu}_1) + \text{const}$$

Setting the derivative with respect to $\boldsymbol{\mu}$ to zero and rearranging, we obtain

$$\boldsymbol{\mu}_1 = \frac{1}{N_1}\sum_{n=1}^{N} t_n \mathbf{x}_n \qquad \boldsymbol{\mu}_2 = \frac{1}{N_2}\sum_{n=1}^{N} (1 - t_n)\mathbf{x}_n$$

Maximum likelihood solution:

Class-conditional densities; Gaussian, Shared Covariance

- the maximum likelihood solution for the shared covariance

$$-\frac{1}{2}\sum_{n=1}^{N} t_n \ln|\boldsymbol{\Sigma}| - \frac{1}{2}\sum_{n=1}^{N} t_n (\mathbf{x}_n - \boldsymbol{\mu}_1)^{\mathrm{T}} \boldsymbol{\Sigma}^{-1} (\mathbf{x}_n - \boldsymbol{\mu}_1)$$

$$-\frac{1}{2}\sum_{n=1}^{N} (1 - t_n) \ln|\boldsymbol{\Sigma}| - \frac{1}{2}\sum_{n=1}^{N} (1 - t_n) (\mathbf{x}_n - \boldsymbol{\mu}_2)^{\mathrm{T}} \boldsymbol{\Sigma}^{-1} (\mathbf{x}_n - \boldsymbol{\mu}_2)$$

$$= -\frac{N}{2}\ln|\boldsymbol{\Sigma}| - \frac{N}{2}\mathrm{Tr}\left\{\boldsymbol{\Sigma}^{-1}\mathbf{S}\right\}$$

Maximum likelihood solution:

Class-conditional densities; Gaussian, Shared Covariance

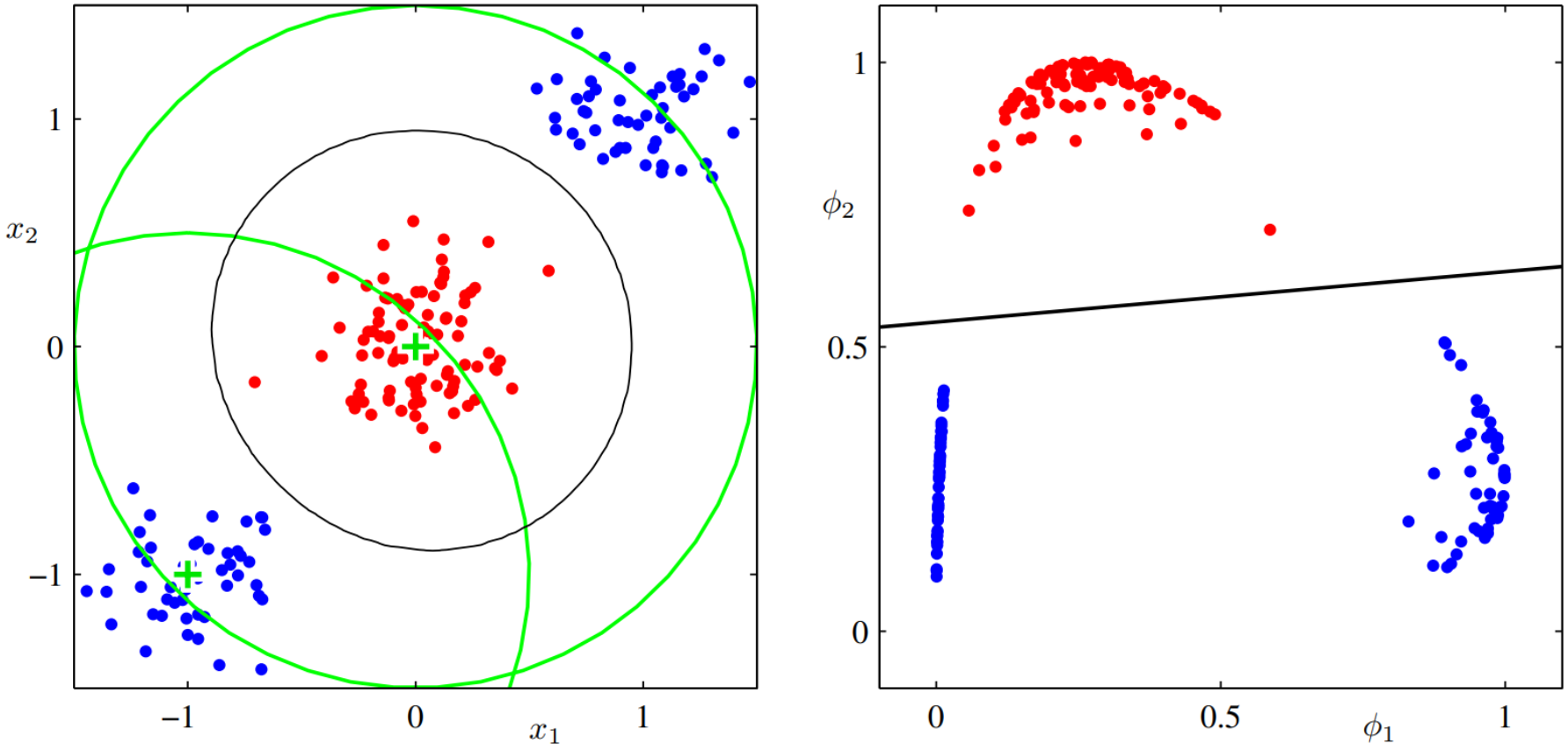
$$= -\frac{N}{2}\ln|\boldsymbol{\Sigma}| - \frac{N}{2}\mathrm{Tr}\left\{\boldsymbol{\Sigma}^{-1}\mathbf{S}\right\}$$

where we have defined

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

Probabilistic Discriminative Models

Fixed basis functions



Logistic Regression

- In our discussion of generative approaches, we saw that under rather general assumptions,

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

$\sigma(\cdot)$ is the *logistic sigmoid* function

M-dimensional feature space $\boldsymbol{\phi}$, this model has M adjustable parameters.

Maximum likelihood for logistic regression

For a data set $\{\boldsymbol{\phi}_n, t_n\}$, where $t_n \in \{0, 1\}$ and $\boldsymbol{\phi}_n = \boldsymbol{\phi}(\mathbf{x}_n)$, the likelihood function can be written

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

where $\mathbf{t} = (t_1, \ldots, t_N)^{\mathrm{T}}$ and $y_n = p(\mathcal{C}_1|\boldsymbol{\phi}_n)$.

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

where $y_n = \sigma(a_n)$ and $a_n = \mathbf{w}^{\mathrm{T}} \boldsymbol{\phi}_n$

Derivative of Error function w.r.t. **w**

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

$$\begin{aligned}
\frac{\partial E}{\partial y_n} &= \frac{1 - t_n}{1 - y_n} - \frac{t_n}{y_n} \\
&= \frac{y_n(1 - t_n) - t_n(1 - y_n)}{y_n(1 - y_n)} \\
&= \frac{y_n - y_n t_n - t_n + y_n t_n}{y_n(1 - y_n)} \\
&= \frac{y_n - t_n}{y_n(1 - y_n)}.
\end{aligned}$$

$$\frac{\partial y_n}{\partial a_n} = \frac{\partial \sigma(a_n)}{\partial a_n} = \sigma(a_n)\,(1 - \sigma(a_n)) = y_n(1 - y_n)$$

$$\nabla a_n = \phi_n$$

$$\begin{aligned}
\nabla E &= \sum_{n=1}^{N} \frac{\partial E}{\partial y_n} \frac{\partial y_n}{\partial a_n} \nabla a_n \\
&= \sum_{n=1}^{N} (y_n - t_n)\phi_n
\end{aligned}$$

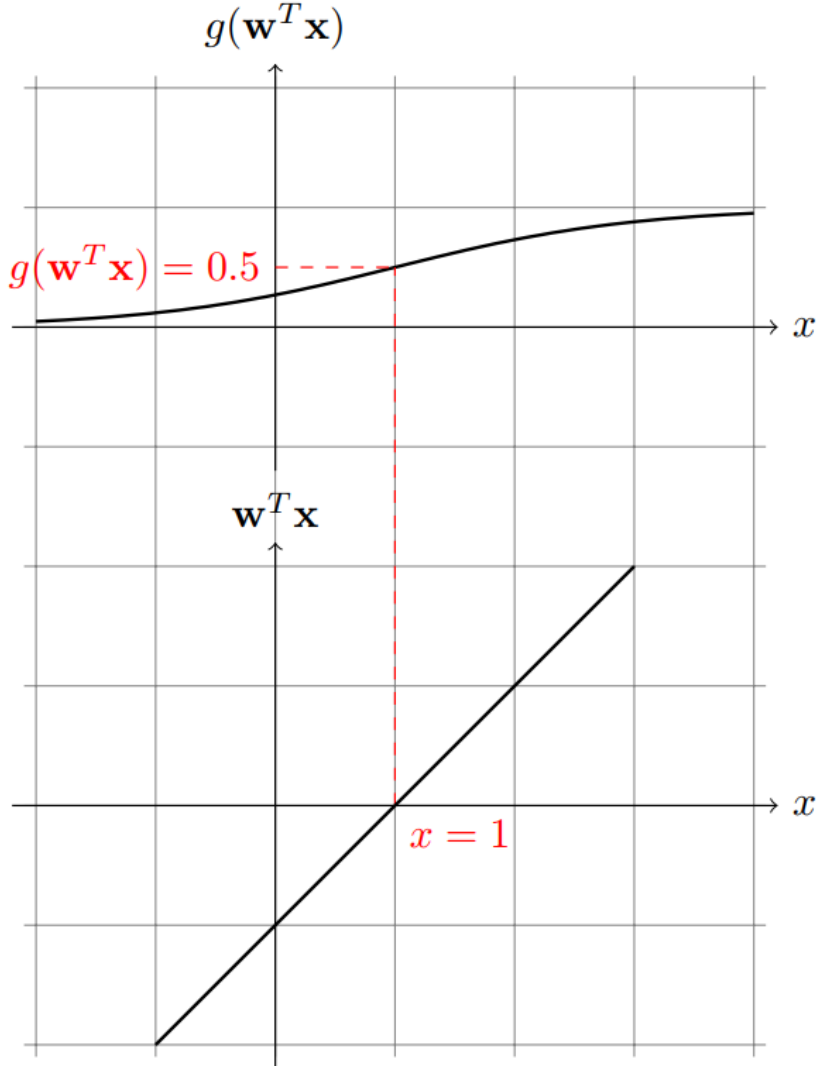
$$\mathbf{w}^{(\tau+1)} = \mathbf{w}^{(\tau)} - \eta \nabla E_n$$

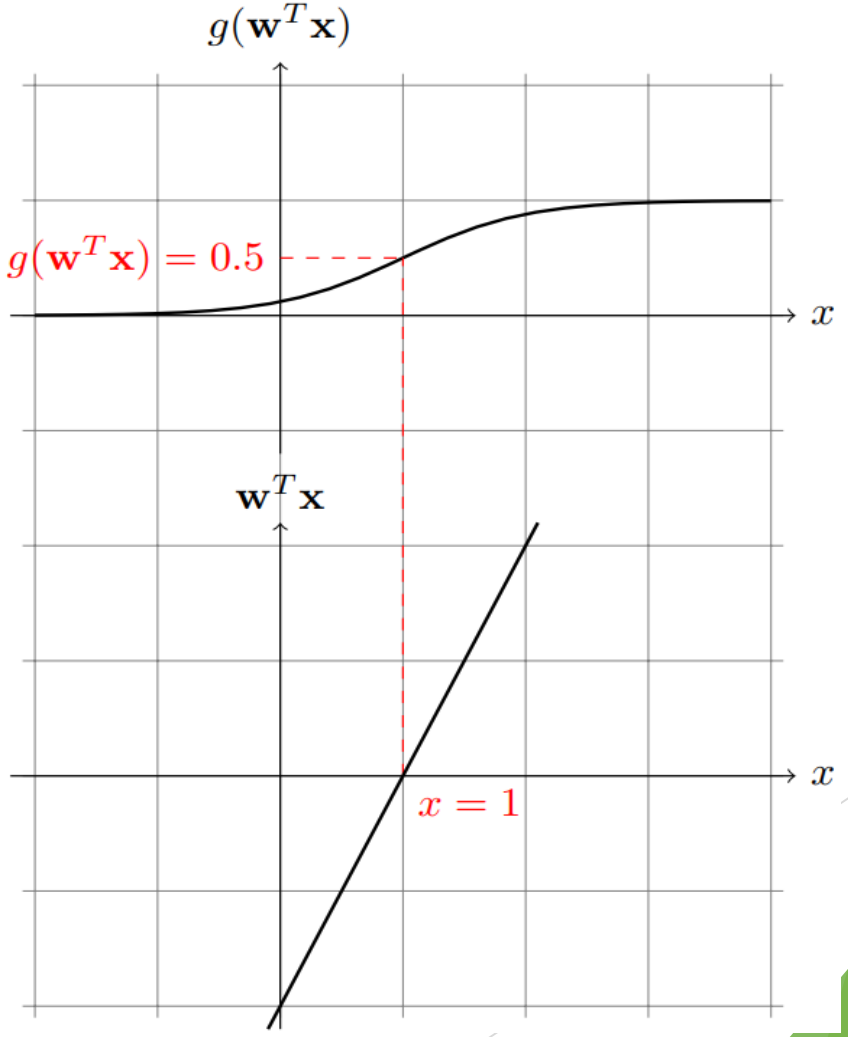
Overfitting ???

- When data is linearly separable.
- The decision boundary is comprised of all the **x** for which we say $p(y = 1|\mathbf{x},\mathbf{w}) = 0.5$
- This implies that $\mathbf{w}^T\mathbf{x} = 0$
- For example: $\mathbf{w}^T\mathbf{x} = w_0 + w_1 x$ $\mathbf{w} = \begin{bmatrix} w_0 \\ w_1 \end{bmatrix}, \mathbf{x} = \begin{bmatrix} 1 \\ x \end{bmatrix}$
- Boundary is simply the point where $x = -\frac{w_0}{w_1}$

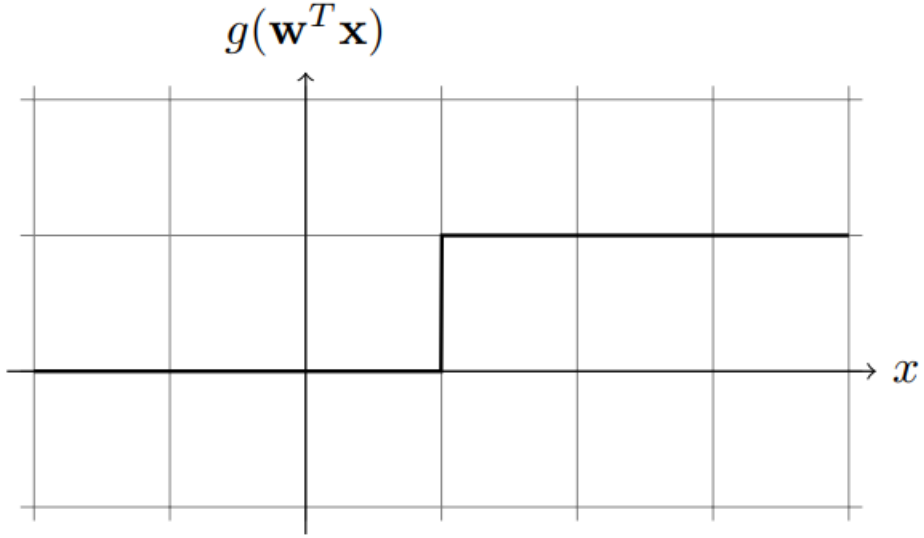
Overfitting ???

In this example, $w_0 = -1, w_1 = 1$





Overfitting ???



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