CS 1675 Intro to Machine Learning
Lecture 8

- **Logistic regression**
- **Generative classification model**

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Classification

- **Data:** $D = \{d_1, d_2, .., d_n\}$
  $d_i = < \mathbf{x}_i, y_i >$
  - y_i **represents a discrete class value**
- **Goal: learn** $f : X \rightarrow Y$

- **Binary classification**
  - **A special case when** $Y \in \{0,1\}$

- **First step:**
  - we need to devise a model of the function f

Discriminant functions

- A common way to represent a **classifier is by using**
  - **Discriminant functions**
- **Works for both the binary and multi-way classification**
- **Idea:**
  - For every class $i = 0,1, \ldots k$ define a function $g_i(\mathbf{x})$ mapping $X \rightarrow \Re$
  - When the decision on input **x** should be made choose the class with the highest value of $g_i(\mathbf{x})$

$$y^* = \arg\max_i \; g_i(\mathbf{x})$$

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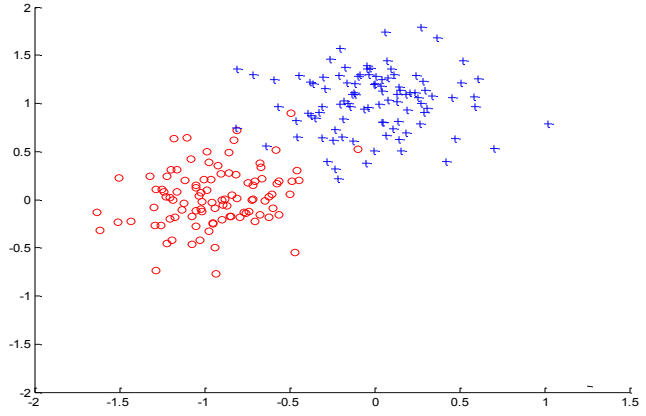
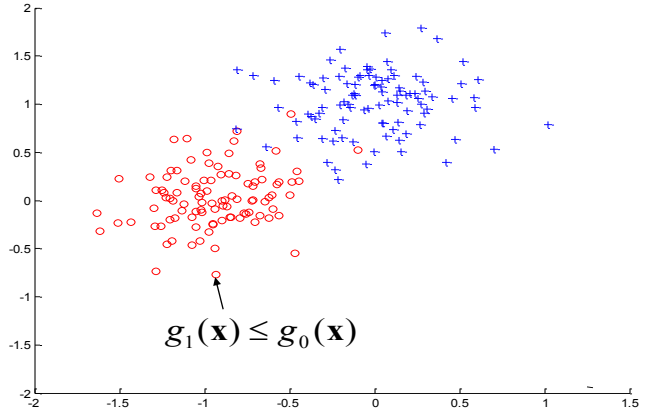
- So what happens with the input space? Assume a binary case.

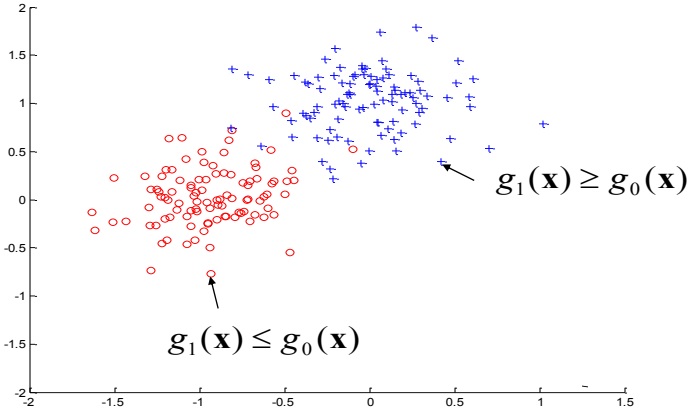
Discriminant functions



Discriminant functions

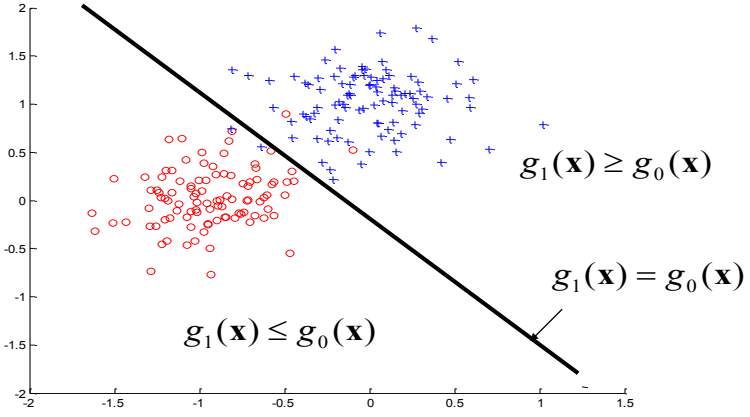


Discriminant functions

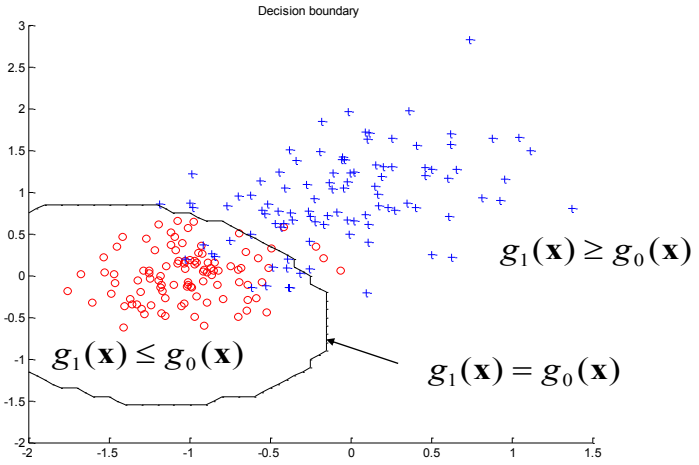


Discriminant functions

- **Decision boundary:** discriminant functions are equal



Quadratic decision boundary



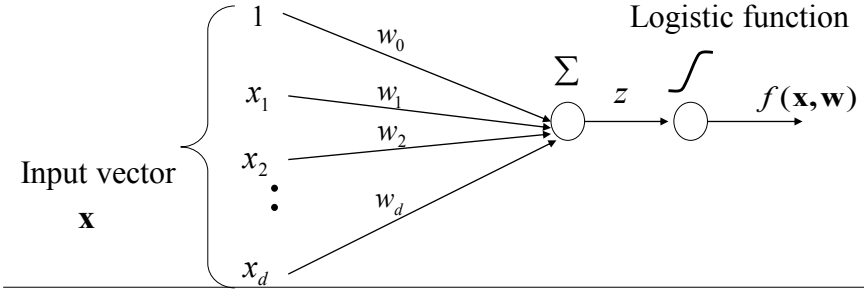
Logistic regression model

- **Defines a linear decision boundary**
- **Discriminant functions:**

$$g_1(\mathbf{x}) = g(\mathbf{w}^T\mathbf{x}) \qquad g_0(\mathbf{x}) = 1 - g(\mathbf{w}^T\mathbf{x})$$

- **where** $g(z) = 1/(1+e^{-z})$ - is a logistic function

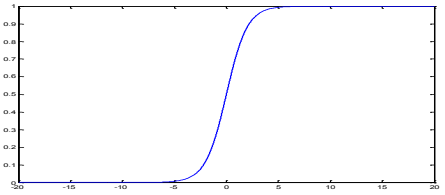
$$f(\mathbf{x},\mathbf{w}) = g_1(\mathbf{w}^T\mathbf{x}) = g(\mathbf{w}^T\mathbf{x})$$



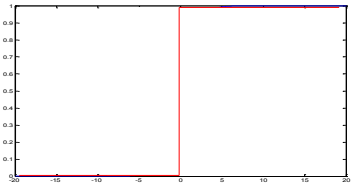
Logistic function

Function: $$g(z) = \frac{1}{(1+e^{-z})}$$

- Is also referred to as a **sigmoid function**
- takes a real number and outputs the number in the interval [0,1]
- Models a smooth switching function; replaces hard threshold function



Logistic (smooth) switching



Threshold (hard) switching

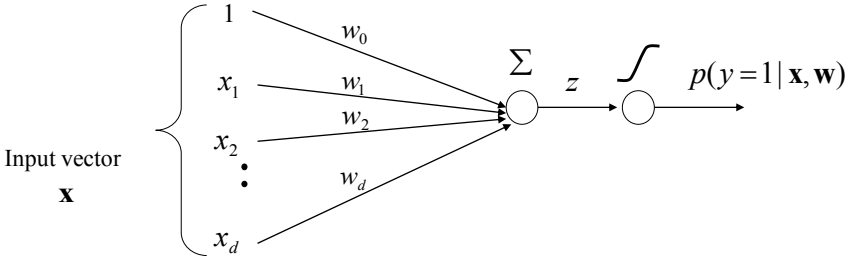
Logistic regression model

- **Discriminant functions:**

$$g_1(\mathbf{x}) = g(\mathbf{w}^T\mathbf{x}) \qquad g_0(\mathbf{x}) = 1 - g(\mathbf{w}^T\mathbf{x})$$

- **Values of discriminant functions vary in interval [0,1]**
  - **Probabilistic interpretation**

$$f(\mathbf{x},\mathbf{w}) = p(y=1 \mid \mathbf{w},\mathbf{x}) = g_1(\mathbf{x}) = g(\mathbf{w}^T\mathbf{x})$$



Logistic regression

- We learn **a probabilistic function**

$$f : X \rightarrow [0,1]$$

  - where f describes the probability of class 1 given $\mathbf{x}$

$$f(\mathbf{x},\mathbf{w}) = g_1(\mathbf{w}^T\mathbf{x}) = p(y=1 \mid \mathbf{x},\mathbf{w})$$

Note that: $p(y=0 \mid \mathbf{x},\mathbf{w}) = 1 - p(y=1 \mid \mathbf{x},\mathbf{w})$

- Making decisions with the logistic regression model:

?

Logistic regression

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- Making decisions with the logistic regression model:

If $p(y=1 \mid \mathbf{x}) \geq 1/2$ then choose **1**
Else choose **0**

Linear decision boundary

- Logistic regression model defines a **linear decision boundary**
- **Why?**
- **Answer:** Compare two **discriminant functions**.
- **Decision boundary:** $g_1(\mathbf{x}) = g_0(\mathbf{x})$
- For the boundary it must hold:

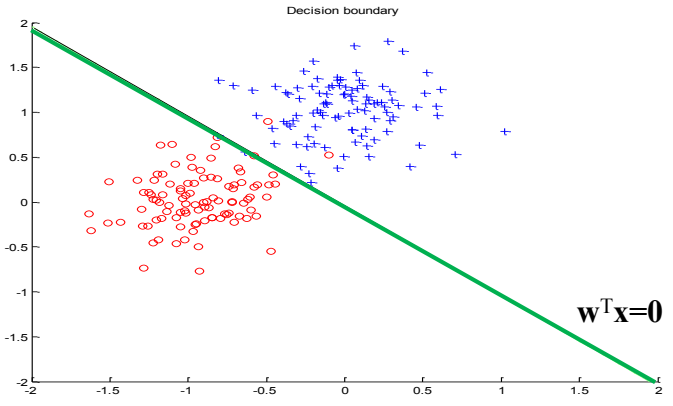
$$\log \frac{g_o(\mathbf{x})}{g_1(\mathbf{x})} = \log \frac{1 - g(\mathbf{w}^T\mathbf{x})}{g(\mathbf{w}^T\mathbf{x})} = 0$$

$$\log \frac{g_o(\mathbf{x})}{g_1(\mathbf{x})} = \log \frac{\frac{\exp -(\mathbf{w}^T\mathbf{x})}{1+\exp -(\mathbf{w}^T\mathbf{x})}}{\frac{1}{1+\exp -(\mathbf{w}^T\mathbf{x})}} = \log \exp -(\mathbf{w}^T\mathbf{x}) = \mathbf{w}^T\mathbf{x} = 0$$

Logistic regression model. Decision boundary

- **LR defines a linear decision boundary**

  Example: 2 classes (blue and red points)



Logistic regression: parameter learning

Likelihood of outputs

- **Let**

$$D_i =< \mathbf{x}_i, y_i > \quad \mu_i = p(y_i = 1 \mid \mathbf{x}_i, \mathbf{w}) = g(z_i) = g(\mathbf{w}^T \mathbf{x})$$

- **Then**

$$L(D, \mathbf{w}) = \prod_{i=1}^{n} P(y = y_i \mid \mathbf{x}_i, \mathbf{w}) = \prod_{i=1}^{n} \mu_i^{\,y_i} (1 - \mu_i)^{1 - y_i}$$

- **Find weights w that maximize the likelihood of outputs**
  - Apply the log-likelihood trick. The optimal weights are the same for both the likelihood and the log-likelihood

$$l(D, \mathbf{w}) = \log \prod_{i=1}^{n} \mu_i^{\,y_i} (1 - \mu_i)^{1 - y_i} = \sum_{i=1}^{n} \log \mu_i^{\,y_i} (1 - \mu_i)^{1 - y_i} =$$

$$= \sum_{i=1}^{n} y_i \log \mu_i + (1 - y_i) \log(1 - \mu_i)$$

Logistic regression: parameter learning

- **Notation:** $\mu_i = p(y_i = 1 \mid \mathbf{x}_i, \mathbf{w}) = g(z_i) = g(\mathbf{w}^T \mathbf{x})$
- **Log likelihood**

$$l(D, \mathbf{w}) = \sum_{i=1}^{n} y_i \log \mu_i + (1 - y_i) \log(1 - \mu_i)$$

- **Derivatives of the loglikelihood**

$$\frac{\partial}{\partial w_j} l(D, \mathbf{w}) = \sum_{i=1}^{n} x_{i,j} (y_i - g(z_i))$$

Nonlinear in weights !!

$$\nabla_{\mathbf{w}} l(D, \mathbf{w}) = \sum_{i=1}^{n} \mathbf{x}_i (y_i - g(\mathbf{w}^T \mathbf{x}_i)) = \sum_{i=1}^{n} \mathbf{x}_i (y_i - f(\mathbf{w}, \mathbf{x}_i))$$

- **Gradient descent:**

$$\mathbf{w}^{(k)} \leftarrow \mathbf{w}^{(k-1)} - \alpha(k) \nabla_{\mathbf{w}} [-l(D, \mathbf{w})] \mid_{\mathbf{w}^{(k-1)}}$$

$$\mathbf{w}^{(k)} \leftarrow \mathbf{w}^{(k-1)} + \alpha(k) \sum_{i=1}^{n} [y_i - f(\mathbf{w}^{(k-1)}, \mathbf{x}_i)] \mathbf{x}_i$$

Derivation of the gradient

- **Log likelihood** $l(D,\mathbf{w}) = \sum_{i=1}^{n} y_i \log \mu_i + (1-y_i)\log(1-\mu_i)$
- **Derivatives of the loglikelihood**

$$\frac{\partial}{\partial w_j} l(D,\mathbf{w}) = \sum_{i=1}^{n} \frac{\partial}{\partial z_i}\left[y_i \log g(z_i) + (1-y_i)\log(1-g(z_i))\right]\frac{\partial z_i}{\partial w_j}$$

$$\frac{\partial z_i}{\partial w_j} = x_{i,j}$$

Derivative of a logistic function

$$\frac{\partial g(z_i)}{\partial z_i} = g(z_i)(1-g(z_i))$$

$$\frac{\partial}{\partial z_i}\left[y_i \log g(z_i) + (1-y_i)\log(1-g(z_i))\right] = y_i \frac{1}{g(z_i)}\frac{\partial g(z_i)}{\partial z_i} + (1-y_i)\frac{-1}{1-g(z_i)}\frac{\partial g(z_i)}{\partial z_i}$$

$$= y_i(1-g(z_i)) + (1-y_i)(-g(z_i)) = y_i - g(z_i)$$

$$\nabla_{\mathbf{w}} l(D,\mathbf{w}) = \sum_{i=1}^{n} -\mathbf{x}_i(y_i - g(\mathbf{w}^T\mathbf{x}_i)) = \sum_{i=1}^{n} -\mathbf{x}_i(y_i - f(\mathbf{w},\mathbf{x}_i))$$

Logistic regression. Online gradient descent

- **On-line component of the loglikelihood**

$$J_{\text{online}}(D_i,\mathbf{w}) = -\left[y_i \log \mu_i + (1-y_i)\log(1-\mu_i)\right]$$

- **On-line learning update for weight w** $J_{online}(D_k,\mathbf{w})$

$$\mathbf{w}^{(k)} \leftarrow \mathbf{w}^{(k-1)} - \alpha(k)\nabla_{\mathbf{w}}[J_{online}(D_k,\mathbf{w})]\,|_{\mathbf{w}^{(k-1)}}$$

- **ith update for the logistic regression** and $D_k = <\mathbf{x}_k, y_k>$

$$\mathbf{w}^{(k)} \leftarrow \mathbf{w}^{(k-1)} + \alpha(k)[y_i - f(\mathbf{w}^{(k-1)},\mathbf{x}_k)]\mathbf{x}_k$$

Online logistic regression algorithm

Online-logistic-regression (*stopping_criterion*)

initialize weights $\mathbf{w} = (w_0, w_1, w_2 \ldots w_d)$

while *stopping_criterion = FALSE*

do **select** next data point $D_i =< \mathbf{x}_i, y_i >$

set $\alpha(i)$

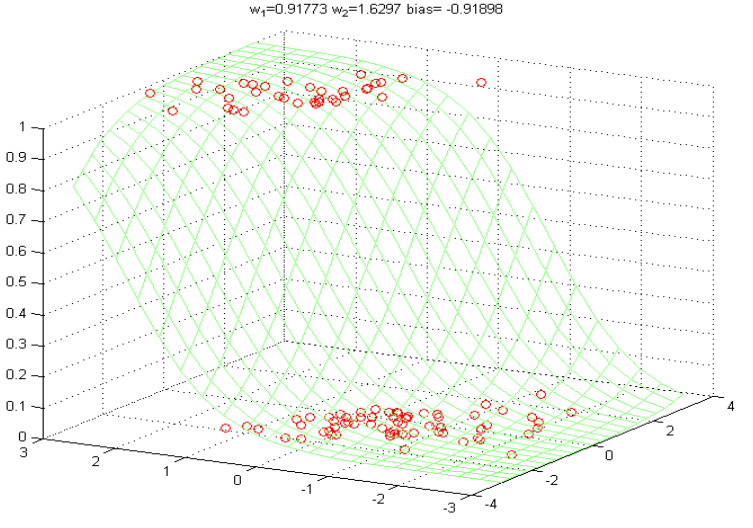
update weights (in parallel)

$$\mathbf{w} \leftarrow \mathbf{w} + \alpha(i)[y_i - f(\mathbf{w}, \mathbf{x}_i)]\mathbf{x}_i$$

end

return weights $\mathbf{w}$

Online algorithm. Example.



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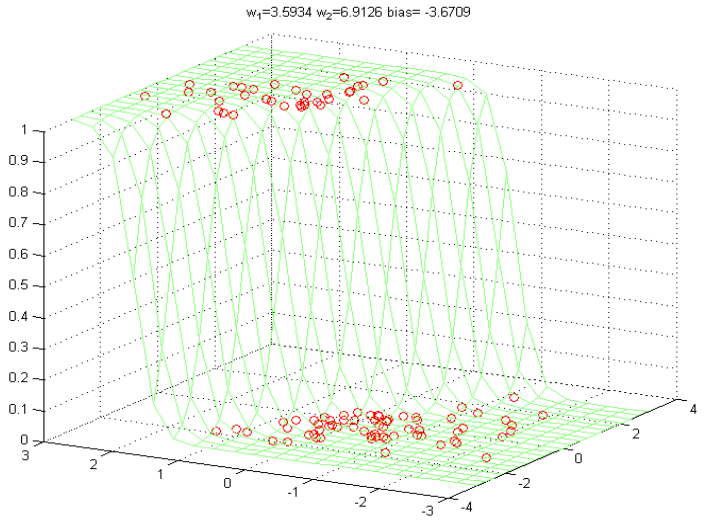
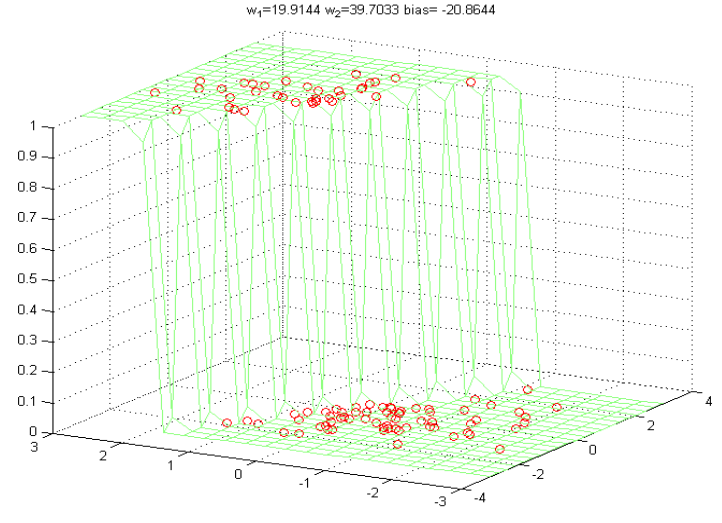


Online algorithm. Example.



Generative approach to classification

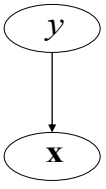
Logistic regression: **learns a model of** $p(y \mid \mathbf{x})$

Generative approach:

1. **Represents and learns the joint distribution** $p(\mathbf{x}, y)$
2. **Uses it to define probabilistic discriminant functions**

E.g. $g_o(\mathbf{x}) = p(y=0 \mid \mathbf{x})$ $g_1(\mathbf{x}) = p(y=1 \mid \mathbf{x})$

Typical joint model $p(\mathbf{x}, y) = p(\mathbf{x} \mid y)p(y)$



- $p(\mathbf{x} \mid y)$ = **Class-conditional distributions (densities)**

  binary classification: two class-conditional distributions

  $p(\mathbf{x} \mid y=0)$ $p(\mathbf{x} \mid y=1)$

- $p(y)$ = **Priors on classes** - probability of class y

  binary classification: Bernoulli distribution

  $p(y=0) + p(y=1) = 1$

Generative approach to classification

Typical joint model $p(\mathbf{x}, y) = p(\mathbf{x} \mid y)p(y)$

- $p(\mathbf{x} \mid y)$ = **Class-conditional distributions (densities)**

  binary classification: two class-conditional distributions

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- $p(y)$ = **Priors on classes**
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  - for binary classification: Bernoulli distribution

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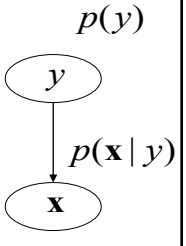
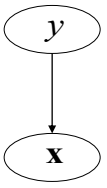


Quadratic discriminant analysis (QDA)

Model:

- **Class-conditional distributions**
  - **multivariate normal distributions**

$$\mathbf{x} \sim N(\boldsymbol{\mu}_0, \boldsymbol{\Sigma}_0) \quad \text{for} \quad y = 0$$
$$\mathbf{x} \sim N(\boldsymbol{\mu}_1, \boldsymbol{\Sigma}_1) \quad \text{for} \quad y = 1$$



Multivariate normal $\mathbf{x} \sim N(\boldsymbol{\mu}, \boldsymbol{\Sigma})$

$$p(\mathbf{x} \mid \boldsymbol{\mu}, \boldsymbol{\Sigma}) = \frac{1}{(2\pi)^{d/2}|\boldsymbol{\Sigma}|^{1/2}} \exp\left[-\frac{1}{2}(\mathbf{x}-\boldsymbol{\mu})^T \boldsymbol{\Sigma}^{-1}(\mathbf{x}-\boldsymbol{\mu})\right]$$

- **Priors on classes (class 0,1)** $y \sim Bernoulli$
  - **Bernoulli distribution**

$$p(y, \theta) = \theta^y (1-\theta)^{1-y} \qquad y \in \{0,1\}$$

Learning of parameters of the QDA model

Density estimation in statistics

- We see examples – we do not know the parameters of Gaussians (class-conditional densities)

$$p(\mathbf{x} \mid \boldsymbol{\mu}, \boldsymbol{\Sigma}) = \frac{1}{(2\pi)^{d/2}|\boldsymbol{\Sigma}|^{1/2}} \exp\left[-\frac{1}{2}(\mathbf{x}-\boldsymbol{\mu})^T \boldsymbol{\Sigma}^{-1}(\mathbf{x}-\boldsymbol{\mu})\right]$$

- **ML estimate of parameters** of a multivariate normal $N(\boldsymbol{\mu}, \boldsymbol{\Sigma})$ for a set of n examples of $\mathbf{x}$

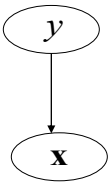
  Optimize log-likelihood: $l(D, \boldsymbol{\mu}, \boldsymbol{\Sigma}) = \log \prod_{i=1}^{n} p(\mathbf{x}_i \mid \boldsymbol{\mu}, \boldsymbol{\Sigma})$

$$\hat{\boldsymbol{\mu}} = \frac{1}{n}\sum_{i=1}^{n} \mathbf{x}_i \qquad \hat{\boldsymbol{\Sigma}} = \frac{1}{n}\sum_{i=1}^{n} (\mathbf{x}_i - \hat{\boldsymbol{\mu}})(\mathbf{x}_i - \hat{\boldsymbol{\mu}})^T$$

- How about **class priors**?

Learning Quadratic discriminant analysis (QDA)

- **Learning Class-conditional distributions**
  - **Learn parameters of 2 multivariate normal distributions**



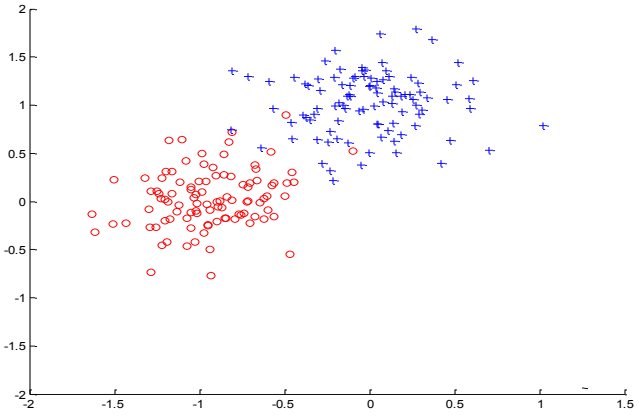
$$\mathbf{x} \sim N(\boldsymbol{\mu}_0, \boldsymbol{\Sigma}_0) \quad \text{for} \quad y = 0$$
$$\mathbf{x} \sim N(\boldsymbol{\mu}_1, \boldsymbol{\Sigma}_1) \quad \text{for} \quad y = 1$$

  - **Use the density estimation methods**

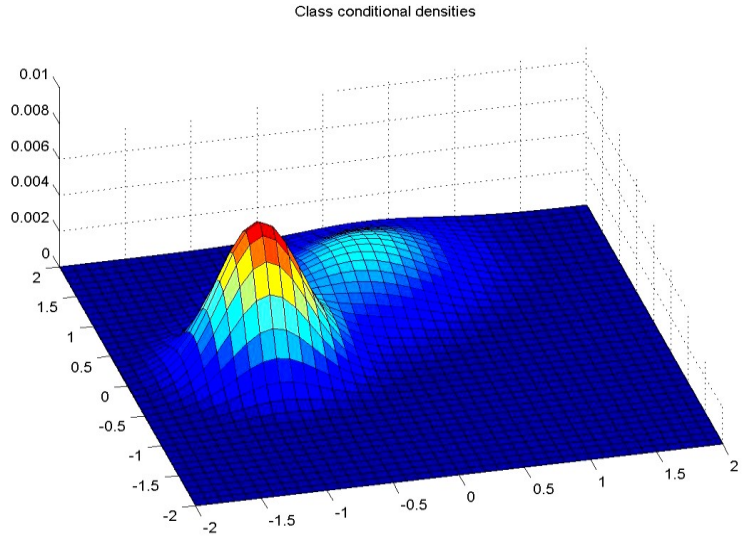
- **Learning Priors on classes (class 0,1)** $y \sim Bernoulli$
  - **Learn the parameter of the Bernoulli distribution**
  - **Again use the density estimation methods**

$$p(y, \theta) = \theta^{y}(1-\theta)^{1-y} \qquad y \in \{0,1\}$$

QDA



2 Gaussian class-conditional densities



QDA: Making class decision

Basically we need to design discriminant functions

- **Posterior of a class** – choose the class with better posterior probability

$$\underbrace{p(y=1\,|\,\mathbf{x})}_{g_1(\mathbf{x})} > \underbrace{p(y=0\,|\,\mathbf{x})}_{g_0(\mathbf{x})} \quad \Rightarrow \quad \begin{array}{l}\text{then } y=1 \\ \text{else } y=0\end{array}$$

$$p(y=1\,|\,\mathbf{x}) = \frac{p(\mathbf{x}\,|\,\mu_1,\Sigma_1)p(y=1)}{p(\mathbf{x}\,|\,\mu_0,\Sigma_0)p(y=0)+p(\mathbf{x}\,|\,\mu_1,\Sigma_1)p(y=1)}$$

- **It is sufficient to compare:**

$$p(\mathbf{x}\,|\,\mu_1,\Sigma_1)p(y=1) > p(\mathbf{x}\,|\,\mu_0,\Sigma_0)p(y=0)$$

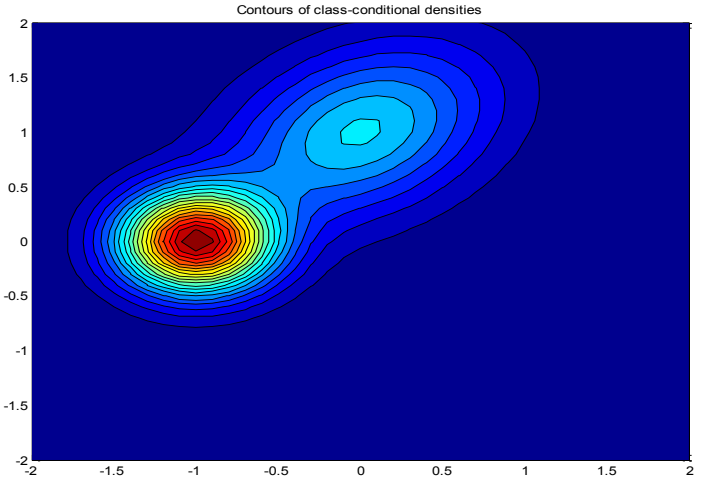
QDA: Making class decision

Alternative discriminant functions:

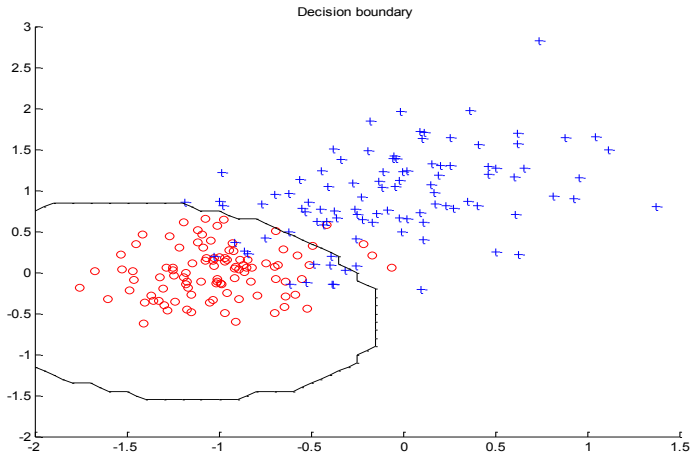
- **Ignore the prior on the classes**
- **Use likelihood of data**:
  - chooses the class (Gaussian) that explains the input data (**x**) better (likelihood of the data)

$$\underbrace{p(\mathbf{x} \mid \mu_1, \Sigma_1)}_{g_1(\mathbf{x})} > \underbrace{p(\mathbf{x} \mid \mu_0, \Sigma_0)}_{g_0(\mathbf{x})} \quad \Rightarrow \quad \begin{array}{l} \text{then } y=1 \\ \text{else } y=0 \end{array}$$

QDA: Quadratic decision boundary

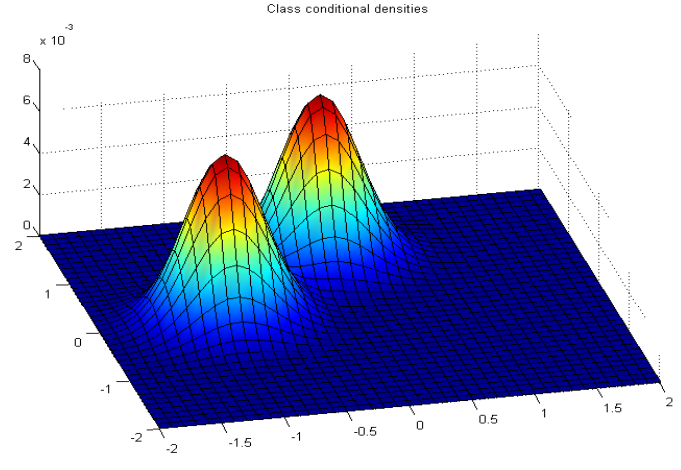


QDA: Quadratic decision boundary

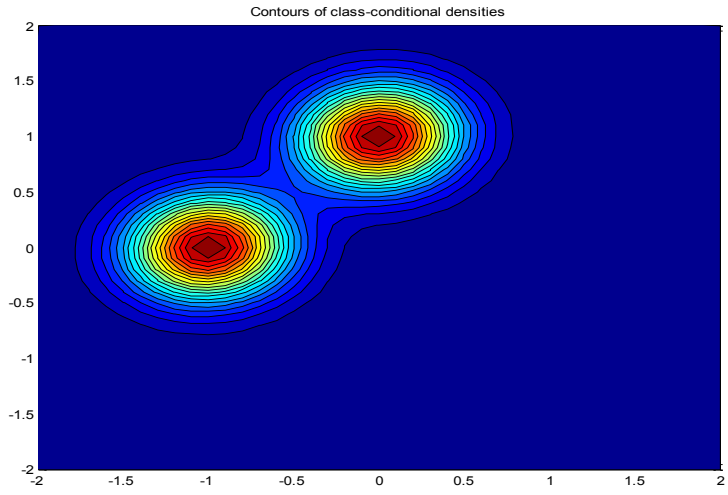


Linear discriminant analysis (LDA)

- **Assume covariances** are the same $\mathbf{x} \sim N(\boldsymbol{\mu}_0, \boldsymbol{\Sigma}),\ y = 0$
  $\mathbf{x} \sim N(\boldsymbol{\mu}_1, \boldsymbol{\Sigma}),\ y = 1$



LDA: Linear decision boundary



LDA: linear decision boundary