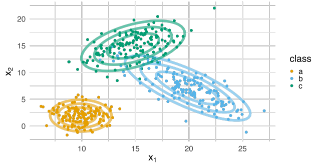
Introduction to Machine Learning

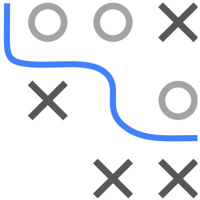
Classification
Discriminant Analysis



Learning goals

- LDA and QDA construction principle based on generative approach
- How are their parameters estimated
- Linear and quadratic decision boundaries

LINEAR DISCRIMINANT ANALYSIS



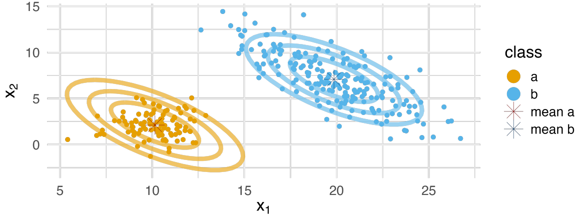
Generative approach, following Bayes' theorem:

$$\pi_k(\mathbf{x}) \approx \mathbb{P}(y = k \mid \mathbf{x}) = \frac{\mathbb{P}(\mathbf{x}|y = k)\mathbb{P}(y = k)}{\mathbb{P}(\mathbf{x})} = \frac{p(\mathbf{x}|y = k)\pi_k}{\sum\limits_{j=1}^{g} p(\mathbf{x}|y = j)\pi_j}$$

Assume that distribution $p(\mathbf{x}|y = k)$ per class is **multivariate Gaussian**:

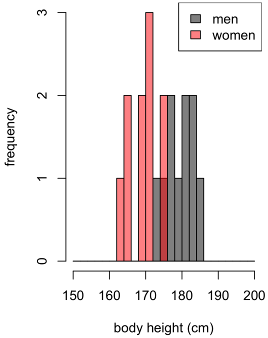
$$p(\mathbf{x}|y = k) = \frac{1}{(2\pi)^{\frac{p}{2}}|\Sigma|^{\frac{1}{2}}} \exp\left(-\frac{1}{2}(\mathbf{x} - \boldsymbol{\mu_k})^T \Sigma^{-1} (\mathbf{x} - \boldsymbol{\mu_k})\right)$$

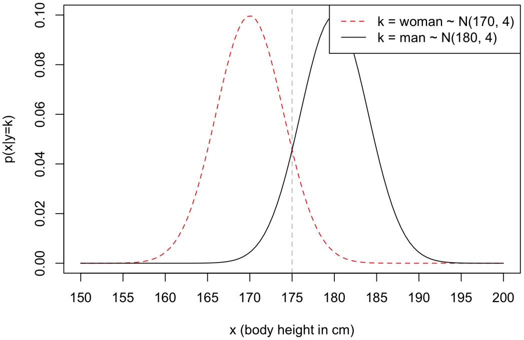
with **equal covariance structure**, so $\Sigma_k = \Sigma \quad \forall k$



UNIVARIATE EXAMPLE

- Classify a new person as male or female based on their height (naive toy example, unrealistic in many ways)
- We will compute in the true DGP, so we assume we know all distributions and their params; we use the LDA setup

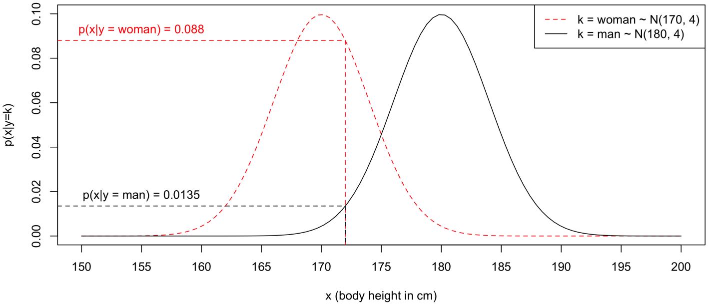




Optimal separation is located at the intersection (= decision boundary)!

UNIVARIATE EXAMPLE: EQUAL CLASS SIZES

Let's compute posterior probability that a 172 cm tall person is male

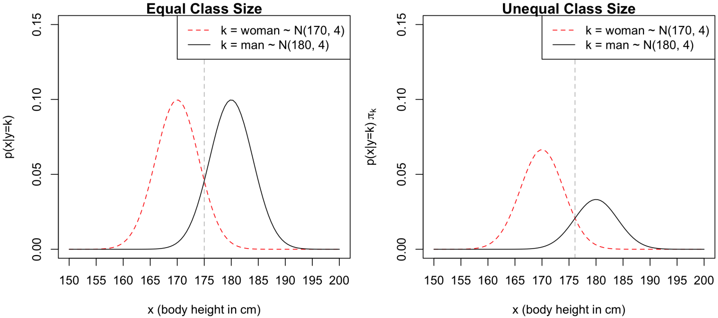


Assuming equal class sizes, prior probs π_k cancel out (since $\pi_{man} = \pi_{woman}$):

$$\mathbb{P}(y = \text{man} \mid \mathbf{x}) = \frac{p(\mathbf{x} \mid y = \text{man})}{p(\mathbf{x} \mid y = \text{man}) + p(\mathbf{x} \mid y = \text{woman})} = \frac{0.0135}{0.0135 + 0.088} = 0.133$$

UNIVARIATE EXAMPLE: UNEQUAL CLASS SIZES

For unequal class sizes (e.g., $\pi_{woman} = 2\pi_{man}$), the prior probs matter and cause a shift of the decision boundary towards the smaller class

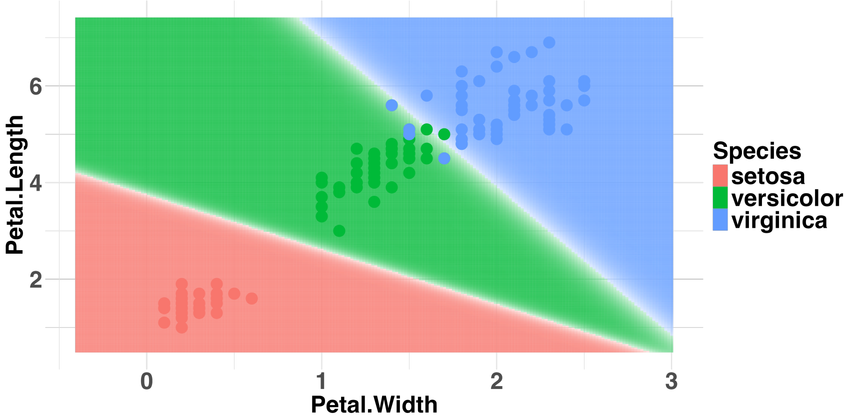


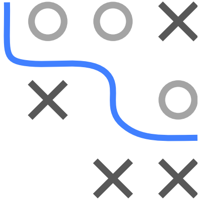
$$\mathbb{P}(y = \text{man} \mid \mathbf{x}) = \frac{p(\mathbf{x} \mid y = \text{man})\pi_{man}}{p(\mathbf{x} \mid y = \text{man})\pi_{man} + p(\mathbf{x} \mid y = \text{woman})\pi_{woman}}$$

$$= \frac{0.0135 \cdot \frac{1}{3}}{0.0135 \cdot \frac{1}{3} + 0.088 \cdot \frac{2}{3}} = 0.0712$$

LDA AS LINEAR CLASSIFIER

Because of the equal covariance structure of all class-specific Gaussians, the decision boundaries of LDA are always linear





LDA AS LINEAR CLASSIFIER

Can easily prove this by showing that posteriors can be written as affine-linear functions - up to rank-preserving transformation:

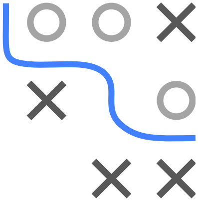
$$\pi_k(\mathbf{x}) = \frac{\pi_k \cdot p(\mathbf{x}|y=k)}{p(\mathbf{x})} = \frac{\pi_k \cdot p(\mathbf{x}|y=k)}{\sum\limits_{j=1}^{g} \pi_j \cdot p(\mathbf{x}|y=j)}$$

As the denominator is the same for all classes we only need to consider

$$\pi_k \cdot p(\mathbf{x}|y=k)$$

and show that this can be written as a linear function of **x**.

LDA AS LINEAR CLASSIFIER



$$
\begin{aligned}
& \pi_k \cdot p(\mathbf{x}|y=k) \\
\propto \quad & \pi_k \exp\left(-\tfrac{1}{2}\mathbf{x}^T\Sigma^{-1}\mathbf{x} - \tfrac{1}{2}\boldsymbol{\mu}_k^T\Sigma^{-1}\boldsymbol{\mu}_k + \mathbf{x}^T\Sigma^{-1}\boldsymbol{\mu}_k\right) \\
= \quad & \exp\left(\log \pi_k - \tfrac{1}{2}\boldsymbol{\mu}_k^T\Sigma^{-1}\boldsymbol{\mu}_k + \mathbf{x}^T\Sigma^{-1}\boldsymbol{\mu}_k\right)\exp\left(-\tfrac{1}{2}\mathbf{x}^T\Sigma^{-1}\mathbf{x}\right) \\
= \quad & \exp\left(w_{0k} + \mathbf{x}^T\boldsymbol{w}_k\right)\exp\left(-\tfrac{1}{2}\mathbf{x}^T\Sigma^{-1}\mathbf{x}\right) \\
\propto \quad & \exp\left(w_{0k} + \mathbf{x}^T\boldsymbol{w}_k\right)
\end{aligned}
$$

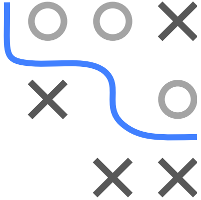
by defining $w_{0k} := \log \pi_k - \frac{1}{2}\boldsymbol{\mu}_k^T\Sigma^{-1}\boldsymbol{\mu}_k$ and $\boldsymbol{w}_k := \Sigma^{-1}\boldsymbol{\mu}_k$.

By finally taking the log, we can write our transformed scores as linear:

$$f_k(\mathbf{x}) = w_{0k} + \mathbf{x}^T\boldsymbol{w}_k$$

- The above is a little bit “lax” so lets carefully check
- We left out several (pos) multiplicative constants
- $\exp\left(-\frac{1}{2}\mathbf{x}^T\Sigma^{-1}\mathbf{x}\right)$ contains $\mathbf{x}$ but is the same for all classes
- $\log(at+b)$ is still isotonic for $a > 0$

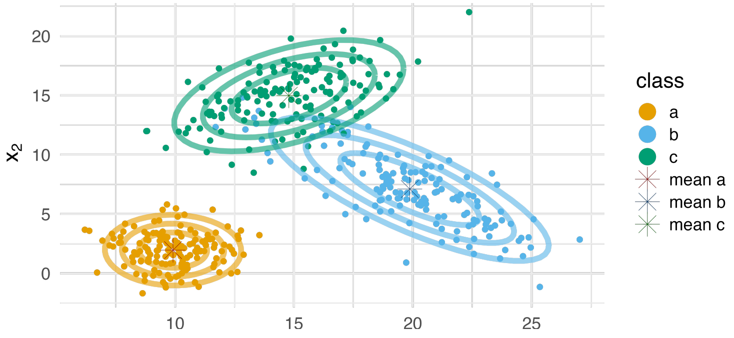
QUADRATIC DISCRIMINANT ANALYSIS



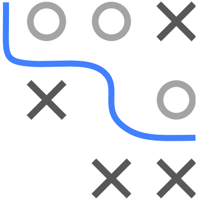
Doesn't assume equal covariances Σ_k per class, so generalizes LDA:

$$p(\mathbf{x}|y=k) = \frac{1}{(2\pi)^{\frac{p}{2}}|\Sigma_k|^{\frac{1}{2}}} \exp\left(-\frac{1}{2}(\mathbf{x}-\boldsymbol{\mu_k})^T\Sigma_k^{-1}(\mathbf{x}-\boldsymbol{\mu_k})\right)$$

$\Rightarrow$ Better data fit but **requires estimation of more parameters** (Σ_k)!

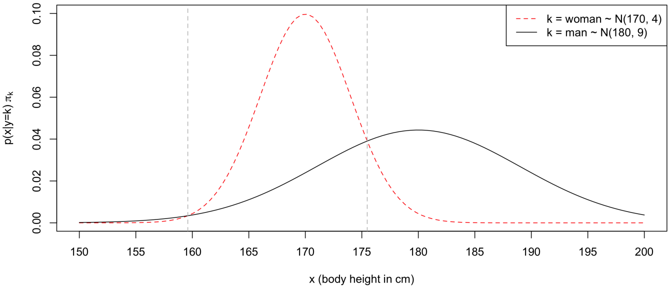


UNIVARIATE EXAMPLE WITH QDA



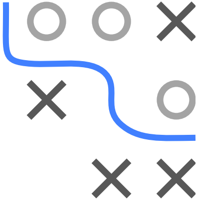
Different covariance matrices lead to multiple classification rules:

- $x < 159.6$ is being assigned to class *man*.
- $159.6 < x < 175.5$ is being assigned to class *woman*.
- $x > 175.5$ is being assigned to class *man*.



$\Rightarrow$ The separation function is quadratic, we learn a curved decision boundary (in 1D a little bit weird, as we learn an interval)

QDA DECISION BOUNDARIES

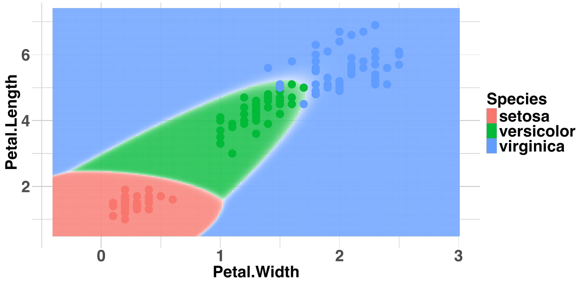


$$
\begin{aligned}
\pi_k(\mathbf{x}) &\propto \pi_k \cdot p(\mathbf{x}|y=k) \\
&\propto \pi_k |\Sigma_k|^{-\frac{1}{2}} \exp\left(-\frac{1}{2}\mathbf{x}^T\Sigma_k^{-1}\mathbf{x} - \frac{1}{2}\boldsymbol{\mu}_{\boldsymbol{k}}^T\Sigma_k^{-1}\boldsymbol{\mu}_{\boldsymbol{k}} + \mathbf{x}^T\Sigma_k^{-1}\boldsymbol{\mu}_{\boldsymbol{k}}\right)
\end{aligned}
$$

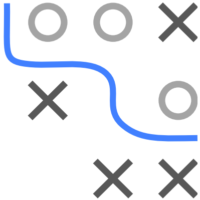
Taking log, we get a quadratic discriminant function in x:

$$
\log \pi_k - \frac{1}{2}\log|\Sigma_k| - \frac{1}{2}\boldsymbol{\mu}_{\boldsymbol{k}}^T\Sigma_k^{-1}\boldsymbol{\mu}_{\boldsymbol{k}} + \mathbf{x}^T\Sigma_k^{-1}\boldsymbol{\mu}_{\boldsymbol{k}} - \frac{1}{2}\mathbf{x}^T\Sigma_k^{-1}\mathbf{x}
$$

Allowing for curved decision boundaries:



PARAMETER ESTIMATION



Parameters $\boldsymbol{\theta}$ are estimated in a straightforward manner by:

$$\hat{\pi}_k = \frac{n_k}{n}, \text{ where } n_k \text{ is the number of class-}k\text{ observations}$$

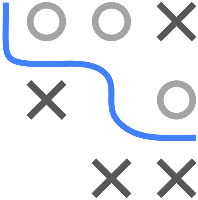
$$\hat{\boldsymbol{\mu}}_{\boldsymbol{k}} = \frac{1}{n_k} \sum_{i:y^{(i)}=k} \mathbf{x}^{(i)}$$

$$\hat{\Sigma}_k = \frac{1}{n_k - 1} \sum_{i:y^{(i)}=k} (\mathbf{x}^{(i)} - \hat{\boldsymbol{\mu}}_{\boldsymbol{k}})(\mathbf{x}^{(i)} - \hat{\boldsymbol{\mu}}_{\boldsymbol{k}})^T \qquad \text{(QDA)}$$

$$\hat{\Sigma} = \frac{1}{n - g} \sum_{k=1}^{g} \sum_{i:y^{(i)}=k} (\mathbf{x}^{(i)} - \hat{\boldsymbol{\mu}}_{\boldsymbol{k}})(\mathbf{x}^{(i)} - \hat{\boldsymbol{\mu}}_{\boldsymbol{k}})^T \quad \text{(LDA)}$$

As $\hat{\Sigma}_k, \hat{\Sigma}$ are $p \times p$ matrices (for p features), estimating all $\hat{\Sigma}_k$ involves $\frac{p(p+1)}{2} \cdot g$ parameters across g classes (vs. just $\frac{p(p+1)}{2}$ for LDA's $\hat{\Sigma}$) (in addition to estimating priors and class means)

QDA PARAMETER ESTIMATION EXAMPLE



E.g., for a simple two-class, 2-dimensional dataset:

Class 1: $\mathbf{x}_1 = \begin{pmatrix} 1 \\ 2 \end{pmatrix}, \mathbf{x}_2 = \begin{pmatrix} 2 \\ 3 \end{pmatrix}$, Class 2: $\mathbf{x}_3 = \begin{pmatrix} 6 \\ 8 \end{pmatrix}, \mathbf{x}_4 = \begin{pmatrix} 7 \\ 9 \end{pmatrix}, \mathbf{x}_5 = \begin{pmatrix} 8 \\ 10 \end{pmatrix}$

Class priors: $\hat{\pi}_1 = \frac{n_1}{n} = \frac{2}{5} = 0.4, \quad \hat{\pi}_2 = \frac{n_2}{n} = \frac{3}{5} = 0.6$

Class means: $\hat{\boldsymbol{\mu}}_\mathbf{1} = \frac{1}{2}(\mathbf{x}_1 + \mathbf{x}_2) = \begin{pmatrix} 1.5 \\ 2.5 \end{pmatrix}, \quad \hat{\boldsymbol{\mu}}_\mathbf{2} = \frac{1}{3}(\mathbf{x}_3 + \mathbf{x}_4 + \mathbf{x}_5) = \begin{pmatrix} 7 \\ 9 \end{pmatrix}$

Class covariances:

$$(\mathbf{x}_1 - \hat{\boldsymbol{\mu}}_\mathbf{1})(\mathbf{x}_1 - \hat{\boldsymbol{\mu}}_\mathbf{1})^\top = \begin{pmatrix} 0.25 & 0.25 \\ 0.25 & 0.25 \end{pmatrix} = (\mathbf{x}_2 - \hat{\boldsymbol{\mu}}_\mathbf{1})(\mathbf{x}_2 - \hat{\boldsymbol{\mu}}_\mathbf{1})^\top$$

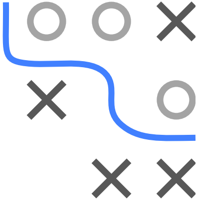
$$\Rightarrow \hat{\Sigma}_1 = \frac{1}{1}\left(\begin{pmatrix} 0.25 & 0.25 \\ 0.25 & 0.25 \end{pmatrix} + \begin{pmatrix} 0.25 & 0.25 \\ 0.25 & 0.25 \end{pmatrix}\right) = \begin{pmatrix} 0.5 & 0.5 \\ 0.5 & 0.5 \end{pmatrix}$$

$$(\mathbf{x}_3 - \hat{\boldsymbol{\mu}}_\mathbf{2})(\mathbf{x}_3 - \hat{\boldsymbol{\mu}}_\mathbf{2})^\top = \begin{pmatrix} 1 & 1 \\ 1 & 1 \end{pmatrix} = (\mathbf{x}_5 - \hat{\boldsymbol{\mu}}_\mathbf{2})(\mathbf{x}_5 - \hat{\boldsymbol{\mu}}_\mathbf{2})^\top,$$

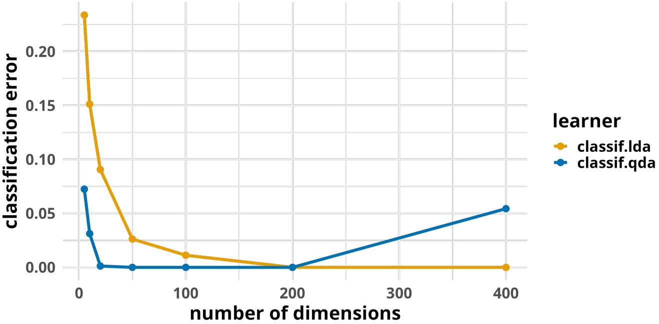
$$(\mathbf{x}_4 - \hat{\boldsymbol{\mu}}_\mathbf{2})(\mathbf{x}_4 - \hat{\boldsymbol{\mu}}_\mathbf{2})^\top = \begin{pmatrix} 0 & 0 \\ 0 & 0 \end{pmatrix}$$

$$\Rightarrow \hat{\Sigma}_2 = \frac{1}{2}\left(\begin{pmatrix} 1 & 1 \\ 1 & 1 \end{pmatrix} + \begin{pmatrix} 0 & 0 \\ 0 & 0 \end{pmatrix} + \begin{pmatrix} 1 & 1 \\ 1 & 1 \end{pmatrix}\right) = \begin{pmatrix} 1 & 1 \\ 1 & 1 \end{pmatrix}$$

DISCRIMINANT ANALYSIS COMPARISON



- We benchmark on simple toy data set(s)
- Normally distributed data per class, but unequal cov matrices
- And then increase dimensionality
- We might assume that QDA always wins here ...



$\Rightarrow$ LDA might be preferable over QDA in higher dimensions!