Statistical Machine Learning
Hilary Term 2020

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Slide credits and other course material can be found at:
http://www.stats.ox.ac.uk/~palamara/SML20.html

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Plug-in Classification

- Consider the 0-1 loss and the risk:

$$\mathbb{E}\Big[L(Y, f(X))\Big|X = x\Big] = \sum_{k=1}^{K} L(k, f(x))\mathbb{P}(Y = k|X = x)$$

  The Bayes classifier provides a solution that minimizes the risk:

$$f_{\text{Bayes}}(x) \quad = \quad \arg\max_{k=1,\dots,K} \pi_k g_k(x).$$

- We know neither the conditional density g_k nor the class probability π_k!
- The **plug-in classifier** chooses the class

$$f(x) = \arg\max_{k=1,\dots,K} \widehat{\pi}_k \widehat{g}_k(x),$$

- where we plugged in
  - estimates $\widehat{\pi}_k$ of π_k and $k = 1, \dots, K$ and
  - estimates $\widehat{g}_k(x)$ of conditional densities,
- **Linear Discriminant Analysis** is an example of plug-in classification.

Summary: **Linear Discriminant Analysis**

- **LDA**: a plug-in classifier assuming multivariate normal conditional density $g_k(x) = g_k(x|\mu_k, \Sigma)$ for each class k sharing the **same covariance** Σ:

$$X|Y = k \sim \mathcal{N}(\mu_k, \Sigma),$$
$$g_k(x|\mu_k, \Sigma) = (2\pi)^{-p/2}|\Sigma|^{-1/2} \exp\left(-\frac{1}{2}(x-\mu_k)^\top \Sigma^{-1}(x-\mu_k)\right).$$

- LDA minimizes the squared **Mahalanobis distance** between x and $\widehat{\mu}_k$, offset by a term depending on the estimated class proportion $\widehat{\pi}_k$:

$$\begin{aligned}
f_{\text{LDA}}(x) &= \underset{k\in\{1,\dots,K\}}{\operatorname{argmax}} \log \widehat{\pi}_k g_k(x|\widehat{\mu}_k, \widehat{\Sigma}) \\
&= \underset{k\in\{1,\dots,K\}}{\operatorname{argmax}} \underbrace{\left(\log \widehat{\pi}_k - \frac{1}{2}\widehat{\mu}_k^\top \widehat{\Sigma}^{-1}\widehat{\mu}_k\right) + \left(\widehat{\Sigma}^{-1}\widehat{\mu}_k\right)^\top x}_{\text{terms depending on } k \text{ linear in } x} \\
&= \underset{k\in\{1,\dots,K\}}{\operatorname{argmin}} \frac{1}{2}\underbrace{(x-\widehat{\mu}_k)^\top \widehat{\Sigma}^{-1}(x-\widehat{\mu}_k)}_{\text{squared Mahalanobis distance}} - \log \widehat{\pi}_k.
\end{aligned}$$

LDA projections

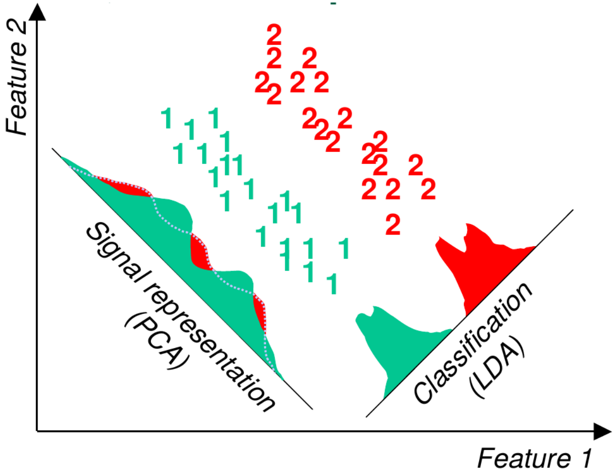
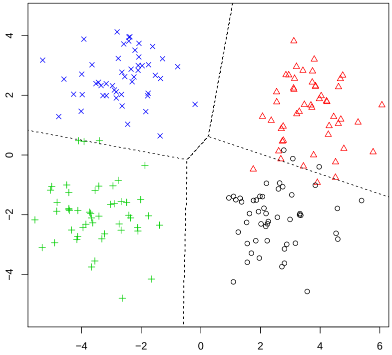
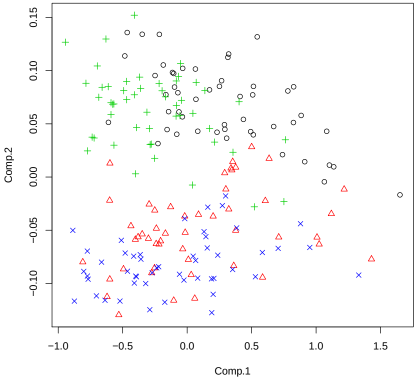


Figure by R. Gutierrez-Osuna

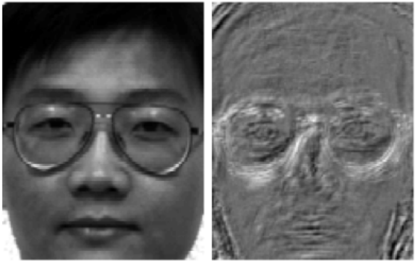
LDA vs PCA projections





LDA separates the groups better.

Fisherfaces



Eigenfaces vs. Fisherfaces, Belhumeur et al. 1997

http://ieeexplore.ieee.org/document/598228/

Conditional densities with different covariances

Given training data with K classes, assume a parametric form for conditional density $g_k(x)$, where for each class

$$X|Y = k \quad \sim \ \mathcal{N}(\mu_k, \Sigma_k),$$

i.e., instead of assuming that every class has a different mean μ_k with the **same** covariance matrix Σ (LDA), we now allow each class to have its own covariance matrix.
Considering $\log \pi_k g_k(x)$ as before,

$$\begin{aligned}
\log \pi_k g_k(x) &= \text{const} + \log(\pi_k) - \frac{1}{2}\left(\log|\Sigma_k| + (x-\mu_k)^T\Sigma_k^{-1}(x-\mu_k)\right) \\
&= \text{const} + \log(\pi_k) - \frac{1}{2}\left(\log|\Sigma_k| + \mu_k^T\Sigma_k^{-1}\mu_k\right) \\
&\qquad + \mu_k^T\Sigma_k^{-1}x - \frac{1}{2}x^T\Sigma_k^{-1}x \\
&= a_k + b_k^T x + x^T c_k x.
\end{aligned}$$

A **quadratic** discriminant function instead of linear.

Quadratic decision boundaries

Again, by considering that we choose class k over k',

$$
\begin{aligned}
a_k + b_k^T x + x^T c_k x - (a_{k'} + b_{k'}^T x + x^T c_{k'} x) \\
= a_\star + b_\star^T x + x^T c_\star x > 0
\end{aligned}
$$

we see that the decision boundaries of the Bayes Classifier are quadratic surfaces.

- The plug-in Bayes Classifer under these assumptions is known as the **Quadratic Discriminant Analysis** (QDA) Classifier.

QDA

LDA classifier:

$$\boxed{f_{\mathsf{LDA}}(x) = \underset{k \in \{1,\dots,K\}}{\arg\min} \left\{ (x - \widehat{\mu}_k)^T \widehat{\Sigma}^{-1} (x - \widehat{\mu}_k) - 2\log(\widehat{\pi}_k) \right\}}$$

QDA classifier:

$$\boxed{f_{\mathsf{QDA}}(x) = \underset{k \in \{1,\dots,K\}}{\arg\min} \left\{ (x - \widehat{\mu}_k)^T \widehat{\Sigma}_k^{-1} (x - \widehat{\mu}_k) - 2\log(\widehat{\pi}_k) + \log(|\widehat{\Sigma}_k|) \right\}}$$

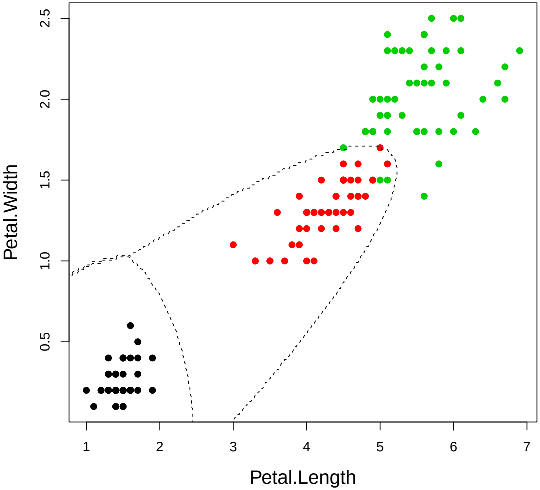
for each point $x \in \mathcal{X}$ where the plug-in estimate $\widehat{\mu}_k$ is as before and $\widehat{\Sigma}_k$ is (in contrast to LDA) estimated for each class $k = 1, \dots, K$ separately:

$$\widehat{\Sigma}_k = \frac{1}{n_k} \sum_{j : y_j = k} (x_j - \widehat{\mu}_k)(x_j - \widehat{\mu}_k)^T.$$

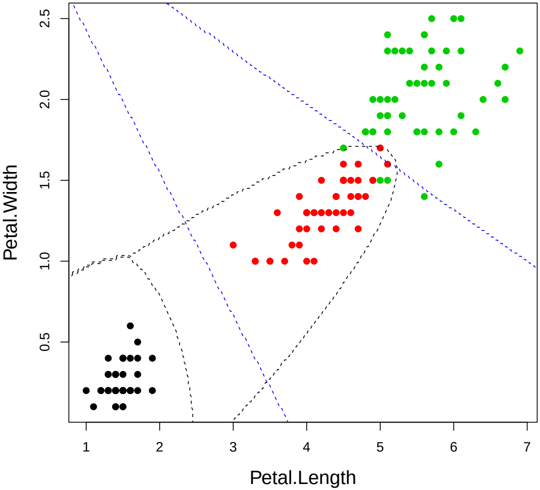
Computing and plotting the QDA boundaries.

```
##fit QDA
iris.qda <- qda(x=iris.data,grouping=ct)

##create a grid for our plotting surface
x <- seq(-6,6,0.02)
y <- seq(-4,4,0.02)
z <- as.matrix(expand.grid(x,y),0)
m <- length(x)
n <- length(y)


iris.qdp <- predict(iris.qda,z)$class
contour(x,y,matrix(iris.qdp,m,n),
        levels=c(1.5,2.5), add=TRUE, d=FALSE, lty=2)
```

Iris example: QDA boundaries



Iris example: QDA boundaries



LDA or QDA?

- Having seen both LDA and QDA in action, it is natural to ask which is the "better" classifier.
- If the covariances of different classes are very distinct, QDA will probably have an advantage over LDA.
- Parametric models are only ever approximations to the real world, allowing **more flexible decision boundaries** (QDA) may seem like a good idea. However, there is a price to pay in terms of increased variance and potential **overfitting**.

Regularized Discriminant Analysis

In the case where data is scarce, to fit

- LDA, need to estimate $K \times p + p \times p$ parameters
- QDA, need to estimate $K \times p + K \times p \times p$ parameters.

Using LDA allows us to better estimate the covariance matrix Σ. Though QDA allows more flexible decision boundaries, the estimates of the K covariance matrices Σ_k are more variable.
RDA combines the strengths of both classifiers by regularizing each covariance matrix Σ_k in QDA to the single one Σ in LDA

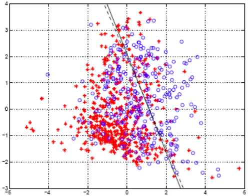
$$\Sigma_k(\alpha) = \alpha\Sigma_k + (1-\alpha)\Sigma \qquad \text{for some } \alpha \in [0, 1].$$

This introduces a new parameter α and allows for a continuum of models between LDA and QDA to be used. Can be selected by Cross-Validation for example.

Logistic regression

Review

- In LDA and QDA, we estimate $p(x|y)$, but for classification we are mainly interested in $p(y|x)$
- Why not estimate that directly? Logistic regression[1] is a popular way of doing this.



[1] Despite the name “regression”, we are using it for classification!

Logistic regression

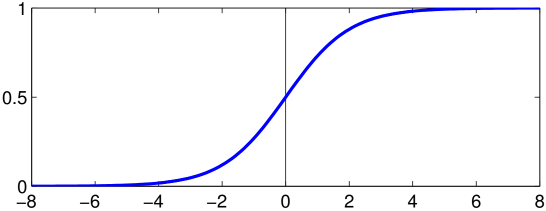
- One of the most popular methods for classification
- Linear model on the probabilities
- Dates back to work on population growth curves by Verhulst [1838, 1845, 1847]
- Statistical use for classification dates to Cox [1960s]
- Independently discovered as the perceptron in machine learning [Rosenblatt 1957]
- Main example of “discriminative” as opposed to “generative” learning
- Naïve approach to classification: we could do linear regression assigning specific values to each class. Logistic regression refines this idea and provides a more suitable model.

Logistic regression

- Statistical perspective: consider $\mathcal{Y} = \{0, 1\}$. Generalised linear model with Bernoulli likelihood and logit link:

$$Y|X = x, a, b \sim \text{Bernoulli}\left(s(a + b^\top x)\right)$$

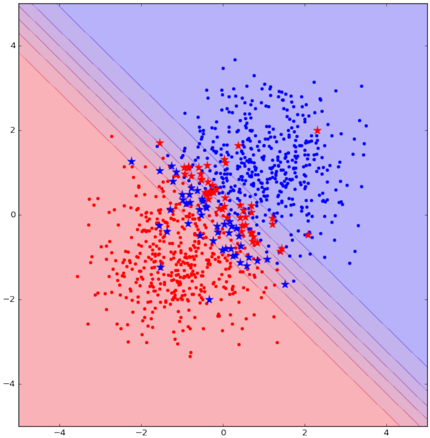
$$s(a + b^\top x) = \tfrac{1}{1+\exp(-(a+b^\top x))}.$$

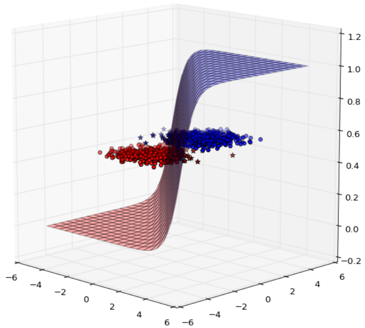


- ML perspective: a **discriminative classifier**. Consider binary classification with $\mathcal{Y} = \{+1, -1\}$. Logistic regression uses a parametric model on the conditional $Y|X$, not the joint distribution of (X, Y):

$$p(Y = y|X = x; a, b) = \frac{1}{1 + \exp(-y(a + b^\top x))}.$$

Prediction Using Logistic Regression





Hard vs Soft classification rules

- Consider using LDA for binary classification with $\mathcal{Y} = \{+1, -1\}$. Predictions are based on linear decision boundary:

$$\begin{aligned}\widehat{y}_{\text{LDA}}(x) &= \text{sign}\left\{\log \widehat{\pi}_{+1} g_{+1}(x|\widehat{\mu}_{+1}, \widehat{\Sigma}) - \log \widehat{\pi}_{-1} g_{-1}(x|\widehat{\mu}_{-1}, \widehat{\Sigma})\right\} \\ &= \text{sign}\left\{a + b^\top x\right\}\end{aligned}$$

  for a and b depending on fitted parameters $\widehat{\theta} = (\widehat{\pi}_{+1}, \widehat{\pi}_{-1}, \widehat{\mu}_{+1}, \widehat{\mu}_{-1}, \Sigma)$.
- Quantity $a + b^\top x$ can be viewed as a soft classification rule. Indeed, it is modelling the difference between the log-discriminant functions, or equivalently, the **log-odds ratio**:

$$a + b^\top x = \log \frac{p(Y = +1|X = x; \widehat{\theta})}{p(Y = -1|X = x; \widehat{\theta})}.$$

- $f(x) = a + b^\top x$ corresponds to the "confidence of predictions" and loss can be measured as a function of this confidence:
  - exponential loss: $L(y, f(x)) = e^{-yf(x)}$,
  - log-loss: $L(y, f(x)) = \log(1 + e^{-yf(x)})$,
  - hinge loss: $L(y, f(x)) = \max\{1 - yf(x), 0\}$.

Linearity of log-odds and logistic function

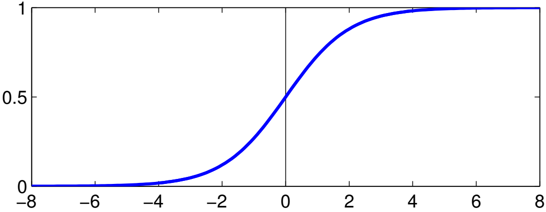
- $a + b^\top x$ models the **log-odds ratio**:

$$\log \frac{p(Y = +1|X = x; a, b)}{p(Y = -1|X = x; a, b)} = a + b^\top x.$$

- Solve explicitly for conditional class probabilities (using $p(Y = +1|X = x; a, b) + p(Y = -1|X = x; a, b) = 1$):

$$p(Y = +1|X = x; a, b) = \frac{1}{1 + \exp(-(a + b^\top x))} =: s(a + b^\top x)$$
$$p(Y = -1|X = x; a, b) = \frac{1}{1 + \exp(+(a + b^\top x))} = s(-a - b^\top x)$$

where $s(z) = 1/(1 + \exp(-z))$ is the **logistic function**.



Fitting the parameters of the hyperplane

How to learn a and b given a training data set $(x_i, y_i)_{i=1}^n$?

- Consider maximizing the **conditional log likelihood** for $\mathcal{Y} = \{+1, -1\}$:

$$p(Y = y_i | X = x_i; a, b) = p(y_i | x_i) = \begin{cases} s(a + b^\top x_i) & \text{if} \quad Y = +1 \\ 1 - s(a + b^\top x_i) & \text{if} \quad Y = -1 \end{cases}$$

- Noting that $1 - s(z) = s(-z)$, we can write the log-likelihood using the compact expression:

$$\log p(y_i | x_i) = \log s(y_i(a + b^\top x_i)).$$

- And the log-likelihood over the whole i.i.d. data set is:

$$\ell(a, b) = \sum_{i=1}^n \log p(y_i | x_i) = \sum_{i=1}^n \log s(y_i(a + b^\top x_i)).$$

Fitting the parameters of the hyperplane

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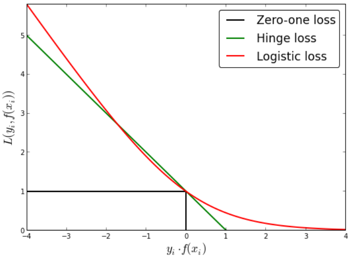
$$\ell(a,b) = \sum_{i=1}^n \log p(y_i|x_i) = \sum_{i=1}^n \log s(y_i(a + b^\top x_i)).$$

- Equivalent to minimizing the empirical risk associated with the **log loss**:

$$\widehat{R}_{\text{log}}(f_{a,b}) = \frac{1}{n}\sum_{i=1}^n -\log s(y_i(a+b^\top x_i)) = \frac{1}{n}\sum_{i=1}^n \log(1+\exp(-y_i(a+b^\top x_i)))$$



Could we use the 0-1 loss?

- With the 0-1 loss, the risk becomes:

$$\widehat{R}(f_{a,b}) = \frac{1}{n}\sum_{i=1}^{n} \text{step}(-y_i(a + b^\top x_i))$$

- But what is the gradient? ...