DISCRIMINANT ANALYSIS

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Machine Learning

Outline

1. Introduction
2. LDA. Equal spherical covariance matrices
3. LDA. Equal covariance matrices
4. QDA. Arbitrary covariance matrices
5. Conclusions

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Assumptions

- Assume the class-conditional density function $f(\mathbf{x}|c_r)$ follows a multivariate Gaussian $\mathbf{X}|c_r \sim \mathcal{N}(\mathbf{x}|\boldsymbol{\mu}_r, \boldsymbol{\Sigma}_r)$, i.e.

$$f(\mathbf{x}|c_r, \boldsymbol{\mu}_r, \boldsymbol{\Sigma}_r) = \frac{1}{(2\pi)^{n/2}|\boldsymbol{\Sigma}_r|^{1/2}} \exp\left\{-\frac{1}{2}(\mathbf{x}-\boldsymbol{\mu}_r)^T\boldsymbol{\Sigma}_r^{-1}(\mathbf{x}-\boldsymbol{\mu}_r)\right\},$$

  where $\boldsymbol{\mu}_r$ is the n-dimensional mean vector, $\boldsymbol{\Sigma}_r$ is the $n \times n$ covariance matrix and $|\boldsymbol{\Sigma}_r|$ its determinant, $r = 1, ..., R$

- Search for $c^* = \arg\text{máx}_r\, p(C = c_r|\mathbf{x})$, or equivalently maximize the discriminant function:

$$\begin{aligned} g_r(\mathbf{x}) &= \ln f(\mathbf{x}|c_r) + \ln p(C = c_r) \\ &= -\frac{1}{2}(\mathbf{x}-\boldsymbol{\mu}_r)^T\boldsymbol{\Sigma}_r^{-1}(\mathbf{x}-\boldsymbol{\mu}_r) - \frac{n}{2}\ln 2\pi - \frac{1}{2}\ln|\boldsymbol{\Sigma}_r| + \ln p(C = c_r) \end{aligned}$$

- Applying $g_r(\mathbf{x})$, the feature space is divided into R **decision regions**, $\mathcal{R}_1, ..., \mathcal{R}_R$: $\mathbf{x}$ is in $\mathcal{R}_r$ if $g_r(\mathbf{x}) = c_r$

Estimation of parameters

- Parameters estimated from data with their maximum likelihood estimates:

$$
\begin{aligned}
\hat{\boldsymbol{\mu}}_r &= \frac{1}{N_r} \sum_{i:c^i=c_r} \mathbf{x}^i \quad \textit{(sample mean)} \\
\hat{\boldsymbol{\Sigma}}_r &= \frac{1}{N_r} \sum_{i:c^i=c_r} (\mathbf{x}^i - \hat{\boldsymbol{\mu}}_r)(\mathbf{x}^i - \hat{\boldsymbol{\mu}}_r)^T \quad \textit{(sample covariance)} \\
\hat{p}(C = c_r) &= \frac{N_r}{N} \quad \textit{(relative frequency of class-}c_r\textit{ observations)}
\end{aligned}
$$

- Applying a multivariate Gaussian goodness-of-fit test will be necessary

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LDA. Equal spherical covariance matrices

Linear discriminant analysis

- $\mathbf{X}|c_r$ has zero covariances and the same variance σ^2 in $\mathbf{\Sigma}_r$ (for all c_r), i.e. X_i are conditionally independent
  - $\mathbf{\Sigma}_r = \sigma^2\mathbf{I} \Rightarrow |\mathbf{\Sigma}_r| = \sigma^{2n}$ and $\mathbf{\Sigma}_r^{-1} = (1/\sigma^2)\mathbf{I}$
- 2nd and 3rd addends in $g_r(\mathbf{x})$ can be ignored (do not depend on r) and

$$g_r(\mathbf{x}) = -\frac{1}{2\sigma^2}(\mathbf{x} - \boldsymbol{\mu}_r)^T(\mathbf{x} - \boldsymbol{\mu}_r) + \ln p(C = c_r)$$

or equivalently ($\mathbf{x}^T\mathbf{x}$ does not depend on r) we obtain the linear function

$$g_r(\mathbf{x}) = \mathbf{w}_r^T\mathbf{x} + w_{r0}$$

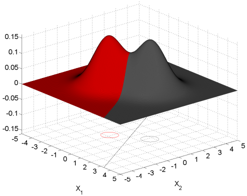
where

$$\begin{aligned} \mathbf{w}_r &= \frac{1}{\sigma^2}\boldsymbol{\mu}_r \\ w_{r0} &= -\frac{1}{2\sigma^2}\boldsymbol{\mu}_r^T\boldsymbol{\mu}_r + \ln p(C = c_r) \end{aligned}$$

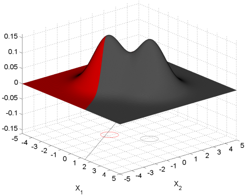
LDA. Equal spherical covariance matrices

- Decision boundary, defined by $g_r(\mathbf{x}) = g_k(\mathbf{x})$, is $\mathbf{w}^T(\mathbf{x} - \mathbf{x}_0) = 0$

$$\begin{aligned} \mathbf{w} &= \boldsymbol{\mu}_r - \boldsymbol{\mu}_k \\ \mathbf{x}_0 &= \frac{1}{2}(\boldsymbol{\mu}_r + \boldsymbol{\mu}_k) - \frac{\sigma^2}{(\boldsymbol{\mu}_r - \boldsymbol{\mu}_k)^T(\boldsymbol{\mu}_r - \boldsymbol{\mu}_k)} \ln \frac{p(c_r)}{p(c_k)}(\boldsymbol{\mu}_r - \boldsymbol{\mu}_k) \end{aligned}$$



$p(c_1) = p(c_2) = .5$



$p(c_1) = .99, p(c_2) = .01$

The decision boundary is a hyperplane orthogonal to $\mathbf{w}$ (line linking the means) and passes through point $\mathbf{x}_0$.

- In (a), the hyperplane passes through the halfway point between the means: if $p(c_1) = p(c_2) \rightarrow \mathbf{x}_0 = \frac{1}{2}(\boldsymbol{\mu}_1 + \boldsymbol{\mu}_2)$
- In (b), the decision is biased in favor of c_1

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LDA. Equal covariance matrices

Linear discriminant analysis

- Assume **homoscedasticity** $\boldsymbol{\Sigma}_r = \boldsymbol{\Sigma}$, i.e., all equal although arbitrary
- The shared $\boldsymbol{\Sigma}$ is estimated using the whole data set as the pooled sample covariance matrix

$$\hat{\boldsymbol{\Sigma}} = \frac{1}{N-R} \sum_{r=1}^{R} \sum_{i:c^i=c_r} (\mathbf{x}_i - \hat{\boldsymbol{\mu}}_r)(\mathbf{x}_i - \hat{\boldsymbol{\mu}}_r)^T$$

- The discriminant function is

$$g_r(\mathbf{x}) = -\frac{1}{2}(\mathbf{x} - \boldsymbol{\mu}_r)^T \boldsymbol{\Sigma}^{-1} (\mathbf{x} - \boldsymbol{\mu}_r) + \ln p(C = c_r)$$

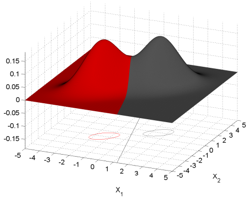
and since $\mathbf{x}^T \boldsymbol{\Sigma}^{-1} \mathbf{x}$ does not depend on r either, $g_r(\mathbf{x}) = \mathbf{w}_r^T \mathbf{x} + w_{r0}$, where

$$\begin{aligned} \mathbf{w}_r &= \boldsymbol{\Sigma}^{-1} \boldsymbol{\mu}_r \\ w_{r0} &= -\frac{1}{2} \boldsymbol{\mu}_r^T \boldsymbol{\Sigma}^{-1} \boldsymbol{\mu}_r + \ln p(C = c_r) \end{aligned}$$

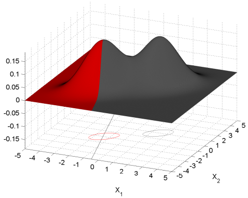
LDA. Equal covariance matrices

- Decision boundary is again a hyperplane $\mathbf{w}^T(\mathbf{x} - \mathbf{x}_0) = 0$, where

$$\begin{aligned} \mathbf{w} &= \boldsymbol{\Sigma}^{-1}(\boldsymbol{\mu}_r - \boldsymbol{\mu}_k) \\ \mathbf{x}_0 &= \frac{1}{2}(\boldsymbol{\mu}_r + \boldsymbol{\mu}_k) - \frac{1}{(\boldsymbol{\mu}_r - \boldsymbol{\mu}_k)^T \boldsymbol{\Sigma}^{-1} (\boldsymbol{\mu}_r - \boldsymbol{\mu}_k)} \ln \frac{p(c_r)}{p(c_k)} (\boldsymbol{\mu}_r - \boldsymbol{\mu}_k) \end{aligned}$$



$p(c_1) = p(c_2) = .5$



$p(c_1) = .99, p(c_2) = .01$

The decision boundary is not necessarily orthogonal to the line linking the means

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QDA. Arbitrary covariance matrices

Quadratic discriminant analysis

- Assume different covariance matrices for each class label, $\mathbf{\Sigma}_r$
- Only 2nd addend in $g_r(\mathbf{x})$ can be ignored and g_r is now quadratic

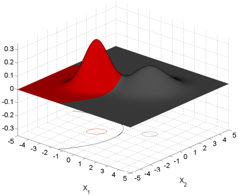
$$g_r(\mathbf{x}) = \mathbf{x}^T \mathbf{W}_r \mathbf{x} + \mathbf{w}_r^T \mathbf{x} + w_{r0}$$

where

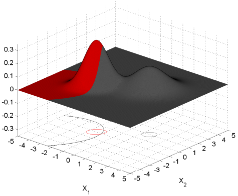
$$\begin{aligned}
\mathbf{W}_r &= -\frac{1}{2}\mathbf{\Sigma}_r^{-1} \\
\mathbf{w}_r &= \mathbf{\Sigma}_r^{-1}\boldsymbol{\mu}_r \\
w_{r0} &= -\frac{1}{2}\boldsymbol{\mu}_r^T \mathbf{\Sigma}_r^{-1} \boldsymbol{\mu}_r - \frac{1}{2}\ln|\mathbf{\Sigma}_r| + \ln p(C = c_r)
\end{aligned}$$

QDA. Arbitrary covariance matrices

- For C binary, the decision boundaries are hyperquadrics with any general form: hyperplanes, pairs of hyperplanes, hyperspheres, hyperellipsoids, hyperparaboloids, etc.
- For more than two classes, the extension is straightforward and may result in many different and complicated regions



$p(c_1) = p(c_2) = .5$



$p(c_1) = .99, p(c_2) = .01$

Regions separated by the hyperbola

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Conclusions

Summary

- Gaussian assumption for class-conditional density
- Linear and quadratic cases
- More assumptions than logistic regression
- Since $g_r(\mathbf{x}) = \ln p(C = c_r, \mathbf{X} = \mathbf{x})$, then
  $g_r(\mathbf{x}) - g_R(\mathbf{x}) = \ln \frac{f(C=r,\mathbf{X}=\mathbf{x})}{f(C=R,\mathbf{X}=\mathbf{x})} = \ln \frac{p(C=r|\mathbf{x})}{p(C=R|\mathbf{x})}$, that in LDA is a linear combination
  $\beta'_{r0} + \beta'_{r1}x_1 + \cdots + \beta'_{rn}x_n$ *As in LOGREG*
  - $\Rightarrow$ logistic regression and LDA have the same form: the log-posterior odds for a pair of classes is a linear function of $\mathbf{x}$
  - $\Rightarrow$ However, parameters are estimated differently:
    - $f(\mathbf{x}, c) = f(\mathbf{x})p(c|\mathbf{x})$, with $p(c|\mathbf{x})$ in a logit-linear form *in both*
    - Logistic fits the parameters of $p(c|\mathbf{x})$ by maximizing the *conditional* log-likelihood. A **discriminative** classifier (and ignors $f(\mathbf{x})$)
    - LDA, by maximizing the *full* log-likelihood. A **generative** classifier based on the joint density $f(\mathbf{x}, c) = f(\mathbf{x}|c)p(c)$, where $f(\cdot|\cdot)$ is a Gaussian density (and $f(\mathbf{x})$ is a Gaussian mixture density, not ignored)

In Weka

LDA, QDA within *Functions* [install them from the Package Manager]

Bibliography

Texts

- Bielza, C., Larrañaga, P. (2021) *Data-Driven Computational Neuroscience. Machine Learning and Statistical Models*, Cambridge University Press [Chap. 8]
- R. Duda, P. Hart, D.G. Stork (2001) *Pattern Classification*, John Wiley & Sons, 2nd Ed. [Chap 2]

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