Lecture 5

Classification II

ISLR 4, ESL 4

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Classification Discriminative vs. Generative

	Discriminative	Generative
Output for an input x	estimate $\hat{g}(x)$ of class $g(x)$	probability distribution $\{p_g(x) \mid g \in G\}$, $p_g(x)$ is the probability that x belongs to class g
Main idea	the classifier returns an estimate of the output, which discriminates between different classes	the classifier generates the output with some probability
Performance measure	loss function that measures the deviation between estimate and output, e.g. 0-1 loss	(log-)likelihood of the estimator generating the output $\sum_{i=1}^{n} \log p_{g_i}(x)$
Optimization problem	Minimize the loss function	Maximize the likelihood

Bayesian Classification

Bayesian Methods

- Bayes' formula

Probability of the input, given the output, i.e. class density

Posterior (probability of the output given the input) → $$\Pr(Y \mid X) = \frac{\Pr(X \mid Y)\Pr(Y)}{\Pr(X)}$$ ← Prior probability of the output; ← Prior probability of the input

- $\Pr(X)$ is a normalizing constant that only depends on the input data and often need not be computed

Bayesian classification for K classes

- use Bayes' formula to determine posterior density per class $\Pr(Y = k \mid X = x)$

$$p_k(x) = \Pr(Y = k \mid X = x) = \frac{\pi_k f_k(x)}{\sum_{\ell=1}^{K} \pi_\ell f_\ell(x)}$$

class density

- we compute $p_k(x)$ by estimating the class prior probabilities π_k and the class densities $f_k(X)$
- we estimate the prior class probabilities from data, $\pi_k = \frac{1}{n}\sum_{i=1}^{n} I(y_i = k)$
- we **somehow** determine the probability density for point x for a class k
- we then classify each point to its most probable class

Linear Discriminant Analysis

Model assumptions

- every class is Gaussian-distributed

$$f_k(x) = \frac{1}{\sqrt{2\pi}\sigma_k} \exp\left(-\frac{1}{2\sigma_k^2}(x-\mu_k)^2\right)$$

- all classes have the same variance

$$\sigma_1^2 = \sigma_2^2 = \cdots = \sigma_K^2 = \sigma^2$$

The Bayesian classifier now becomes

$$p_k(x) = \frac{\pi_k f_k(x)}{\sum_{\ell=1}^{K} \pi_\ell f_\ell(x)} = \frac{\pi_k \frac{1}{\sqrt{2\pi}\sigma_k} \exp\left(-\frac{1}{2\sigma_k^2}(x-\mu_k)^2\right)}{\sum_{l=1}^{K} \pi_l \frac{1}{\sqrt{2\pi\sigma^2}} \exp\left(-\frac{1}{2\sigma^2}(x-\mu_l)^2\right)}$$

- the logarithm of the numerator

$$-\frac{x^2}{2\sigma^2} + x \cdot \frac{\mu_k}{\sigma^2} - \frac{\mu_k^2}{2\sigma^2} + \log \pi_k - \log\left(\sqrt{2\pi}\sigma\right)$$

Linear Discriminant Analysis

The Bayes-optimal choice is to classify $\boldsymbol{x}$ to the class with the largest discriminant

- the discriminant of a class $\boldsymbol{k}$ is the log-probability that cancels in the log odds

$$\log\left(\frac{p_k(x)}{p_l(x)}\right) = \delta_k(x) - \delta_l(x)$$

- where

$$\delta_k(x) = x \cdot \frac{\mu_k}{\sigma^2} - \frac{\mu_k^2}{2\sigma^2} + \log \pi_k$$

  is the log-numerator from previous slide with the class-independent terms removed

Example Linear Discriminant Analysis

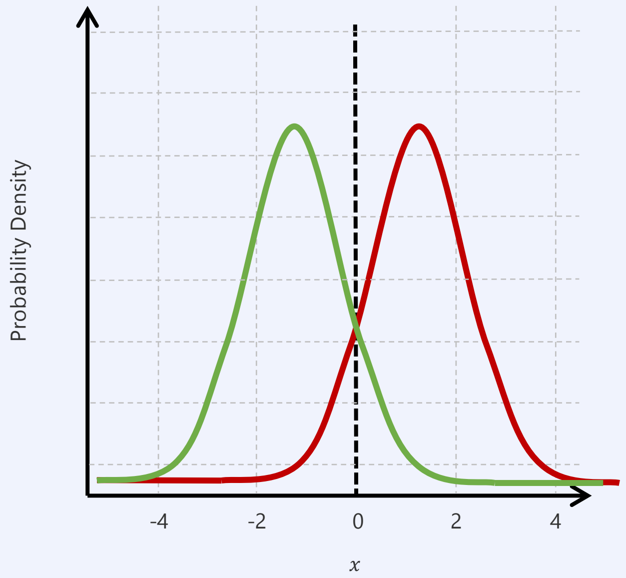
If $\pi_1 = \pi_2$ we classify an observation x to class 1 if

$$2x(\mu_1 - \mu_2) > \mu_1^2 - \mu_2^2$$

- the Bayes decision boundary is the set of points for which both discriminants are equal, i.e.

$$x = \frac{\mu_1^2 - \mu_2^2}{2(\mu_1 - \mu_2)} = \frac{\mu_1 + \mu_2}{2}$$

- the figure shows two 1D normal density functions.
- the dashed line represents the Bayes decision boundary, at which an observation is equally likely to belong to either class



$\mu_1 = -1.25$
$\mu_2 = 1.25$
$\sigma_1 = \sigma_2 = 1$

Fitting Univariate LDA Models

In general, we do not know the underlying class densities

- we estimate these using the finite training sample

$$\hat{\mu}_k = \frac{1}{n_k} \sum_{i:y_i=k} x_i$$

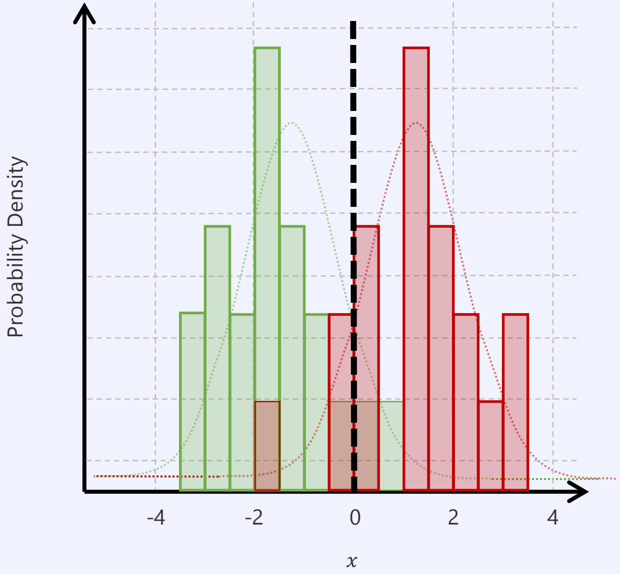
$$\hat{\sigma}^2 = \frac{1}{n-K} \sum_{k=1}^{K} \sum_{i:y_i=k} (x_i - \hat{\mu}_k)^2$$

$$\pi = n_k/n$$

- we assign x to the class with the largest fitted discriminant

$$\hat{\delta}_k(x) = x \cdot \frac{\hat{\mu}_k}{\hat{\sigma}^2} - \frac{\hat{\mu}_k^2}{2\hat{\sigma}^2} + \log \hat{\pi}_k$$

- note that the discriminants are linear (!)



LDA fit over 20 samples per class, fitted decision boundary in dashed black. Bayes error 10.6%, LDA test error 11.1%

Multivariate LDA

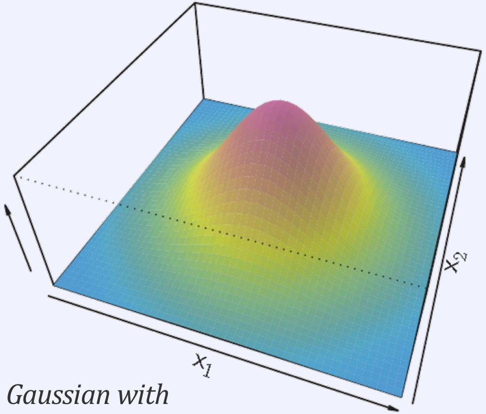
Model assumptions

- each class is a multivariate Gaussian
- the covariance matrix is the same for all classes

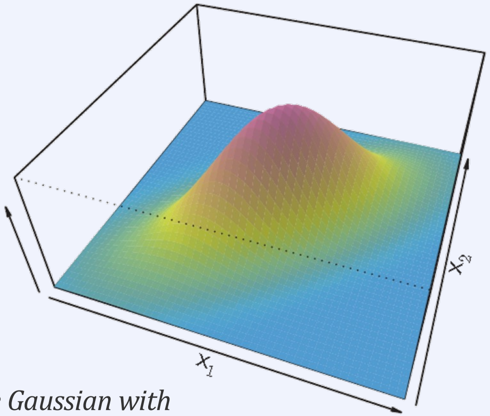
$$f_{k(x)} = \frac{1}{(2\pi)^{\frac{p}{2}}|\boldsymbol{\Sigma}|^{\frac{1}{2}}} \exp\left(-\frac{1}{2}(x-\mu_k)^T\boldsymbol{\Sigma}^{-1}(x-\mu_k)\right)$$

$$\delta_k(x) = x^T\boldsymbol{\Sigma}^{-1}\mu_k - \frac{1}{2}\mu_k^T\boldsymbol{\Sigma}^{-1}\mu_k + \log\pi_k$$

- $\boldsymbol{\Sigma}$ is the $p{\times}p$ covariance matrix of the inputs $\boldsymbol{\Sigma} = \mathrm{Cov}(x)$



Multivariate Gaussian with two uncorrelated predictors



Multivariate Gaussian with two correlated predictors (0.7)

Multivariate LDA

Model assumptions

- each class is a multivariate Gaussian
- the covariance matrix is the same for all classes

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

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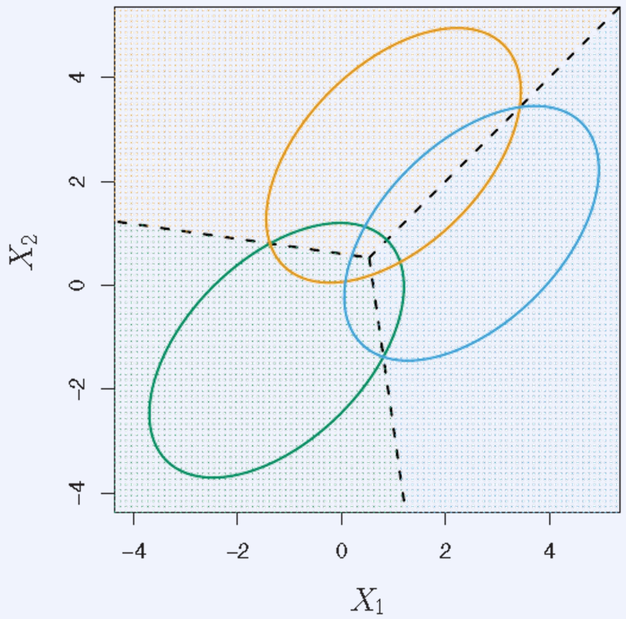


2D synthetic data example with three classes. Ellipses contain 95% of the class probability mass, the Bayes decision boundaries are dashed

Multivariate LDA

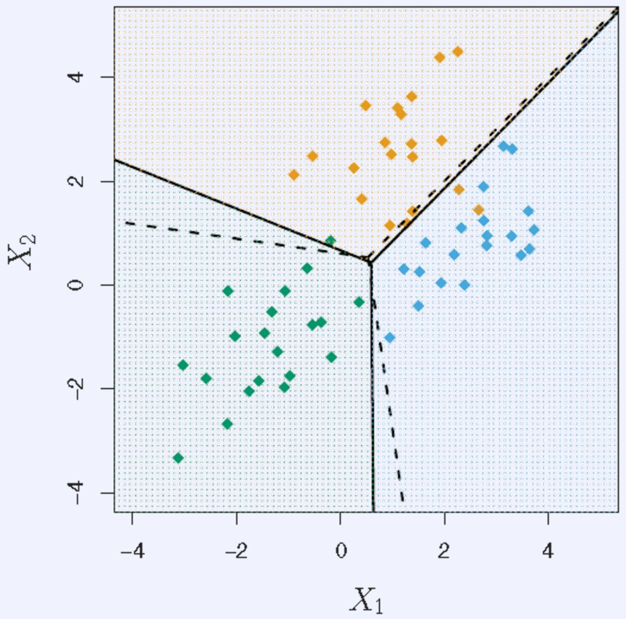
Model assumptions

- each class is a multivariate Gaussian
- the covariance matrix is the same for all classes

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

$$\delta_k(x) = x^T\mathbf{\Sigma}^{-1}\mu_k - \frac{1}{2}\mu_k^T\mathbf{\Sigma}^{-1}\mu_k + \log\pi_k$$

- $\mathbf{\Sigma}$ is the $p \times p$ covariance matrix of the inputs $\mathbf{\Sigma} = \mathrm{Cov}(x)$
- model is fitted using sample estimates similar to the 1D case
- μ easy, but $\mathbf{\Sigma}$ is the hardest to estimate



LDA fit of data set comprising 20 samples from each class, decision boundary in black

Multivariate LDA

Example **default** with **balance** and **student** as inputs

- training error for LDA is 2.75%
- data is highly unbalanced, we have only 3,33% positives
- the No-only classifier has an error of already only 3,33%

Sensitivity $\text{Sens} = TP/(TP+FN) = TP/P^*$

- fraction of correctly predicted positives

Specificity $\text{Spec} = TN/(TN+FP) = TN/N^*$

- fraction of correctly predicted negatives

- No $\text{Sens} = \frac{0}{333} = 0\%$, $\text{Spec} = \frac{9{,}667}{9{,}667} = 100\%$
- LDA $\text{Sens} = \frac{81}{333} = 24.3\%$, $\text{Spec} = \frac{9{,}644}{9{,}667} = 99.8\%$
- LDA approximates the Bayes classifier, it minimizes error on all observations

LDA Model Results

Prediction	True Default Status No (−)	Yes (+)	Total
No (−)	9,644	252	9,896
Yes (+)	23	81	104
Total	**9,667**	**333**	**10,000**

Prediction	True Default Status No (−)	Yes (+)	Total
No (−)	TN	FN	N
Yes (+)	FP	TP	P
Total	N^*	P^*	n

Confusion matrix

Type-1 error
False positive

Type-2 error
False negative

Types of Errors – a handy guide

Type I error
(false positive)

Type II error
(false negative)

Multivariate LDA

Biasing the classifier trades sensitivity for specificity

$$\log((p_k(x))/(p_l(x))) = \delta_k(x) - \delta_l(x)$$

- move the decision threshold between class **no** or **yes** from
  $$\Pr(\textbf{default} = \text{yes} \mid X = x) = 0.5$$
- we can increase sensitivity by choosing
  $\Pr(\textbf{default} = \text{yes} \mid X = x) < 0.5$
  as this assigns more points to class **yes**
- for $\Pr(\textbf{default} = \text{yes} \mid X = x) < 0.2$
  - Sens = 195/333 = 58.6%
  - Spec = 9,432/9,667 = 97.6%
  - Error = 373/10,000 = 3.73%

For a threshold of 0.5 we get
Sens = 24.3%, Spec = 99.8%, Error=2.75%

Prediction	True Default Status No (−)	Yes (+)	Total
No (−)	9,644	252	9,896
Yes (+)	23	81	104
Total	**9,667**	**333**	**10,000**

Prediction	True Default Status No (−)	Yes (+)	Total
No (−)	9,432	138	9,570
Yes (+)	235	195	430
Total	**9,667**	**333**	**10,000**

While for a threshold of 0.2 we have
Sens = 58.6%, Spec = 97.6%, Error=3.73%

Multivariate LDA

Biasing the classifier trades sensitivity for specificity

$$\log((p_k(x))/(p_l(x))) = \delta_k(x) - \delta_l(x)$$

- move the decision threshold between class **no** or **yes** from
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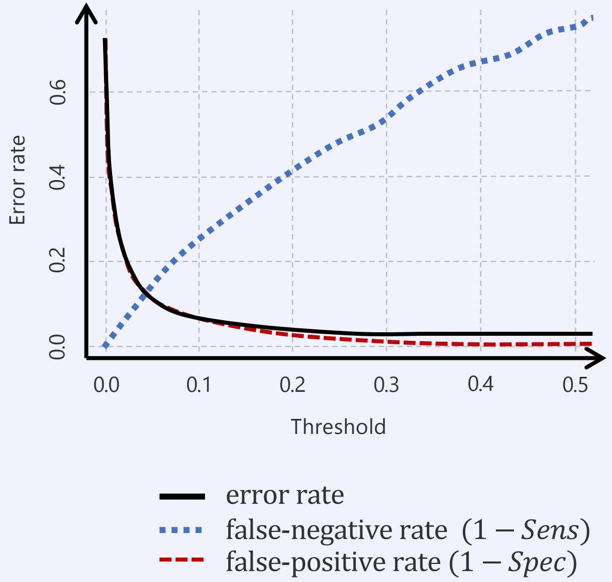
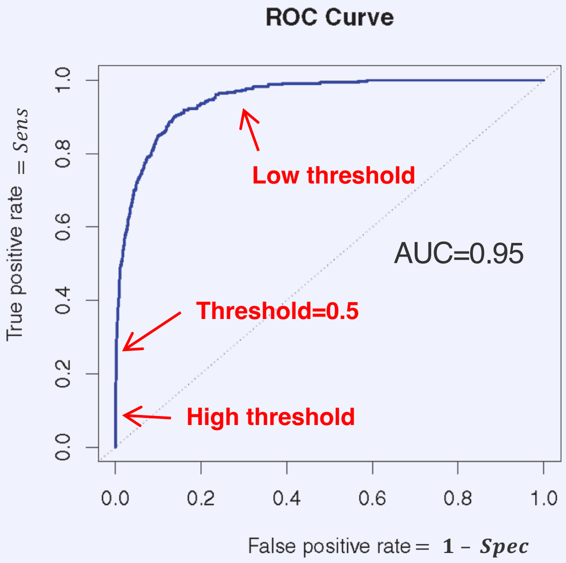
- for $\Pr(\textbf{default} = \text{yes} \mid X = x) < 0.2$
  - Sens = $195/333 = 58.6\%$
  - Spec = $9{,}432/9{,}667 = 97.6\%$
  - Error = $373/10{,}000 = 3.73\%$
- error rates change smoothly when we move the threshold



ROC Curves

Receiver-Operating Characteristic (ROC) curves plot $Sens$ against $1 - Spec$ for all thresholds

- Area Under the ROC-Curve (AUC) measures the quality of a classifier independent of the choice of that threshold
- optimally $Spec = Sens = 1$ for any threshold ($AUC = 1$)
- random classifier performs on the diagonal ($AUC = 0.5$)
- if the ROC curve goes below the diagonal, we can improve accuracy by inverting the classifier



ROC curves are not influenced by imbalance of the data

- balance only affects locations of a threshold along the curve

Quadratic Discriminant Analysis (QDA)

We give up the assumption that the covariances of all classes are all the same

For QDA we have

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

$$\delta_k(x) = -\frac{1}{2}x^T\mathbf{\Sigma}_k^{-1}x + x^T\mathbf{\Sigma}_k^{-1}\mu_k - \frac{1}{2}\mu_k^T\mathbf{\Sigma}_k^{-1}\mu_k + \log\pi_k$$

For LDA we had

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

$$\delta_k(x) = x^T\mathbf{\Sigma}^{-1}\mu_k - \frac{1}{2}\mu_k^T\mathbf{\Sigma}^{-1}\mu_k + \log\pi_k$$

Quadratic Discriminant Analysis (QDA)

We give up the assumption that the covariances of all classes are all the same

For QDA we have

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

$$\delta_k(x) = -\frac{1}{2}x^T \mathbf{\Sigma}_k^{-1} x + x^T \mathbf{\Sigma}_k^{-1}\mu_k - \frac{1}{2}\mu_k^T \mathbf{\Sigma}_k^{-1}\mu_k + \log \pi_k$$

For LDA we had

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

$$\delta_k(x) = x^T \mathbf{\Sigma}^{-1}\mu_k - \frac{1}{2}\mu_k^T \mathbf{\Sigma}^{-1}\mu_k + \log \pi_k$$

Quadratic Discriminant Analysis (QDA)

In QDA every class has its own covariance matrix

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

$$\delta_k(x) = -\frac{1}{2}x^T\boldsymbol{\Sigma}_k^{-1}x + x^T\boldsymbol{\Sigma}_k^{-1}\mu_k - \frac{1}{2}\mu_k^T\boldsymbol{\Sigma}_k^{-1}\mu_k + \log\pi_k$$

- class boundaries are now quadratic curves
- we fit a different covariance matrix estimate per class
- LDA has $(2K+p+1)p/2$ parameters,
- QDA has $Kp(p+3)/2$ parameters

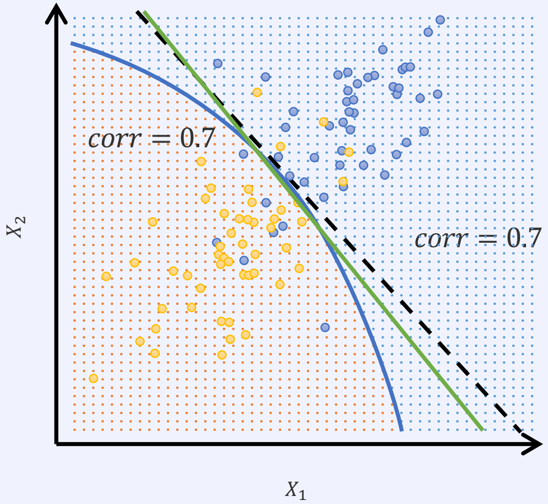
Example

- for $p = 4, K = 2$, LDA has 18 parameters, QDA has 28 parameters
- for $p = 8, K = 2$, LDA has 52 parameters, QDA has 88 parameters

Example LDA vs. QDA

Two-class problem with $\Sigma_1 = \Sigma_2$

QDA overtrains



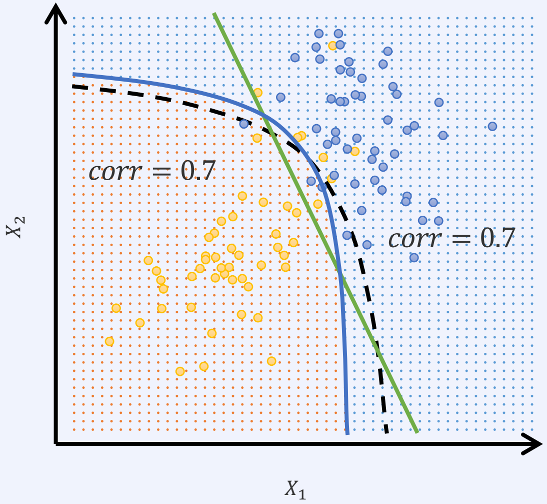
Bayes decision boundary

LDA decision boundary

QDA decision boundary

Two-class problem with $\Sigma_1 \neq \Sigma_2$

LDA overtrains



Bayes decision boundary

LDA decision boundary

QDA decision boundary

Fitting LDA and QDA Models

Again, we use sample estimates

- $\hat{\mu}_k = \frac{1}{n_k}\sum_{i:y_i=k} x_i$
- $\widehat{\boldsymbol{\Sigma}} = \frac{1}{n-K}\sum_{k=1}^{K}\sum_{i:y_i=k}(x_i - \hat{\mu}_k)(x_i - \hat{\mu}_k)^T$
- $\widehat{\boldsymbol{\Sigma}}_k = \frac{1}{n_k-K}\sum_{i:y_i=k}(x_i - \hat{\mu}_k)(x_i - \hat{\mu}_k)^T$
- $\pi_k = n_k/n$

To simplify calculation we use the eigenvalue decomposition of the covariance matrices

$$\widehat{\boldsymbol{\Sigma}}_k = \boldsymbol{U}_k \boldsymbol{D}_k \boldsymbol{U}_k^T$$

- $\boldsymbol{U}_k$ is a $p \times p$ orthonormal matrix
- $\boldsymbol{D}_k$ is a diagonal matrix of decreasing positive eigenvalues $\boldsymbol{d}_{kl}$

The main terms in the discriminants,

$$\delta_k(x) = -\frac{1}{2}\log\left|\widehat{\boldsymbol{\Sigma}}_k\right| - \frac{1}{2}(x-\mu_k)^T\widehat{\boldsymbol{\Sigma}}_k^{-1}(x-\mu_k) + \log \pi_k$$

then turn into

$$\log\left|\widehat{\boldsymbol{\Sigma}}_k\right| = \sum_l \log d_{kl}$$

$$(x-\hat{\mu}_k)^T\hat{\Sigma}_k^{-1}(x-\hat{\mu}_k) = \left[\boldsymbol{U}_k^T(x-\hat{\mu}_k)\right]^T D_k^{-1}\left[U_k^T(x-\hat{\mu}_k)\right]$$

The LDA estimator

- Step 1: Normalize $\boldsymbol{X}$ to spherical covariance

$$X^* \leftarrow \boldsymbol{D}^{-1/2}\boldsymbol{U}^T X$$

- Step 2: Classify to the closest class centroid in the transformed space, where distance is weighted by the class prior probabilities $\boldsymbol{\pi}_k$

Comparing Different Classifiers

Comparison of the Classification Methods

We now know four classifiers: k-NN, LDA, QDA and logistic regression

- when should we use which?

Logistic regression and LDA are surprisingly closely related

- univariate binary setting $p_2(x) = 1 - p_1(x)$
- log-odds for LDA are $\log \frac{p_1(x)}{1-p_1(x)} = c_0 + c_1 x$

  (difference of two linear discriminants)
- while for logistic regression $\log \frac{p_1(x)}{1-p_1(x)} = \beta_0 + \beta_1 x$

Similar, but different

- β_0 and β_1 are maximum likelihood estimates
- c_0 and c_1 are estimated from sample mean and variance of Gaussian distribution
- relationship extends to multivariate data: LR and LDA often give similar results – but not always!
- LDA makes stronger assumptions

Comparison of the Classification Methods

We now know four classifiers: k-NN, LDA, QDA and logistic regression

- when should we use which?

k-NN is nonparametric and tends to work better for strongly nonlinear settings

- it does not allow for inference, i.e. we do not get a model that we can learn from

QDA is a compromise between LDA and k-NN

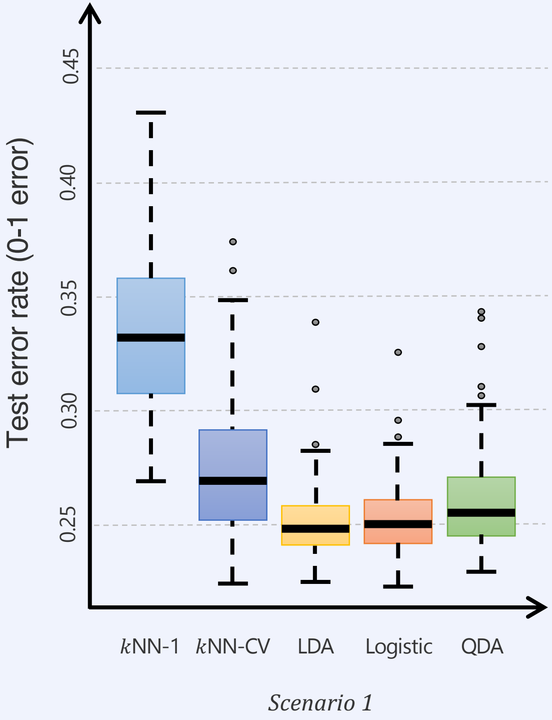
Comparing the Classification Methods

Scenario 1

- 100 random training data sets, $p = 2$ predictors, $K = 2$ classes
- 20 observations per class
- observations in different classes uncorrelated normal variables with different means and the same variance (spherical Gaussian)
- this matches the LDA assumptions of LDA

Observations

- LDA works very well
- logistic regression assumes a linear decision boundary, performs only slightly worse than LDA
- k-NN overtrains, as does QDA



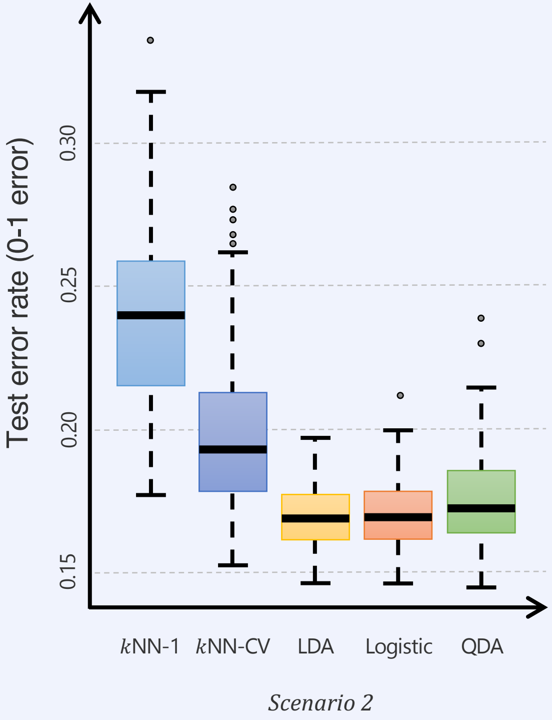
Comparing the Classification Methods

Scenario 2

- 100 random training data sets, $p = 2$ predictors, $K = 2$ classes
- like scenario 1, but predictors in each class now have a correlation of -0.5 (elliptical multivariate Gaussian)

Observations

- relative performances are similar to scenario 1



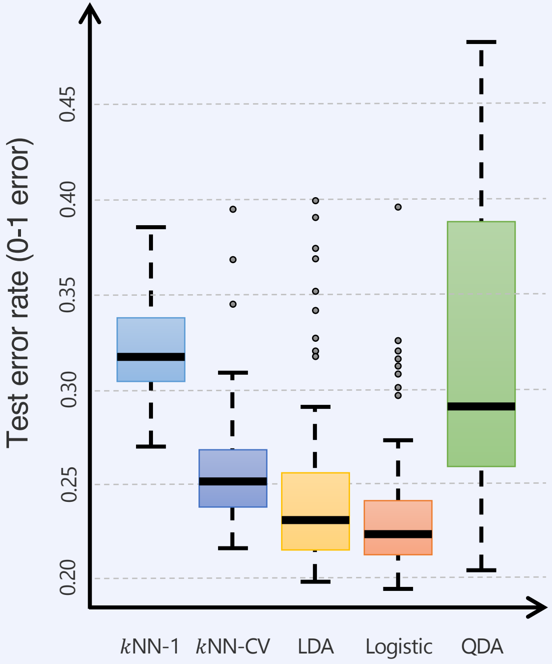
Comparing the Classification Methods

Scenario 3

- 100 random training data sets, $p = 2$ predictors, $K = 2$ classes
- X_1 and X_2 are generated using a $\boldsymbol{t}$-distribution
- more extreme points than with a Gaussian
- decision boundary is linear, but, setup violates LDA assumption

Observations

- logistic regression performs best
- QDA deteriorates because of non-normality of the data



Scenario 3

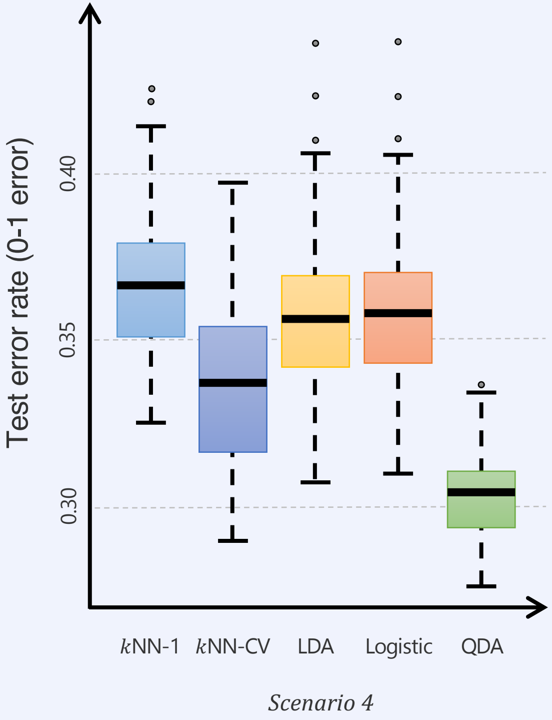
Comparing the Classification Methods

Scenario 4

- 100 random training data sets, $p = 2$ predictors, $K = 2$ classes
- class 1: normal distribution with correlation 0.5 to predictors
- class 2: normal distribution with correlation -0.5 to predictors
- assumptions of QDA are met (but not LDA!)

Observations

- QDA outperforms all other methods



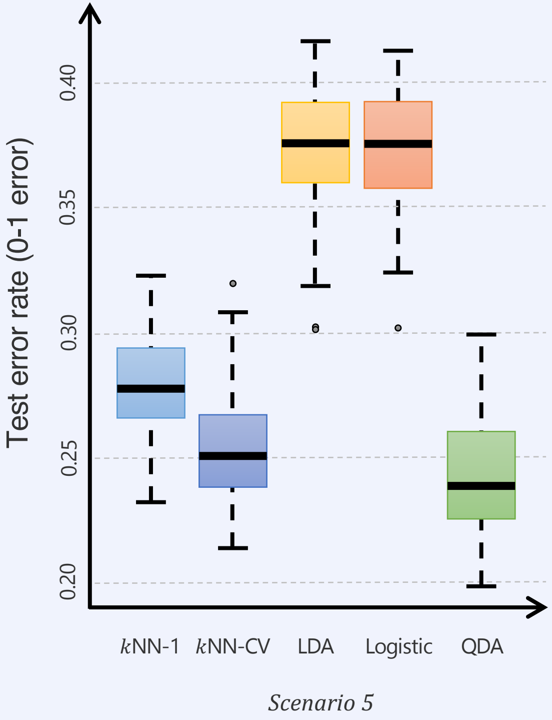
Comparing the Classification Methods

Scenario 5

- 100 random training data sets, $p = 2$ predictors, $K = 2$ classes
- two normal distributions with uncorrelated predictors
- inputs X_1^2, X_2^2 and $X_1 X_2$, not X_1 and X_2
- the decision boundary is quadratic

Observations

- QDA performs best
- kNN (CV) follows closely
- the linear methods all perform poorly



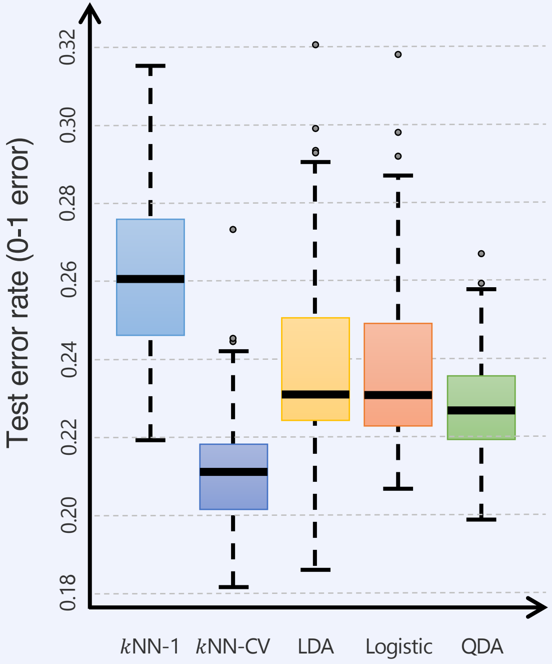
Comparing the Classification Methods

Scenario 6

- 100 random training data sets, $p = 2$ predictors, $K = 2$ classes
- like 5, but responses sampled from a complicated linear function

Observations

- even QDA cannot model data well
- k-NN-1 overtrains
- k-NN (CV) outperforms all parametric approaches
- smoothness must be chosen carefully



Scenario 6