COM 525000 – Statistical Learning

Lecture 4 – Classification

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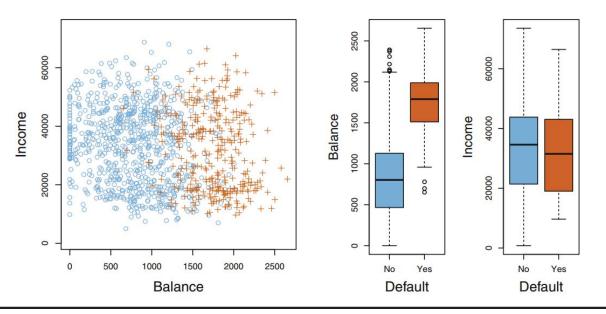
Classification

- Classification refers to the prediction of qualitative or categorical responses based on the observation.
 - → Often done by predicting the probability of each of the categories (similar to *regression*).
- Three widely-used classifiers:
 - Logistic regression;
 - Linear discriminant analysis;
 - k nearest neighbors.
- Other methods, such as generalized additive models (Chapter 7), trees, random forests, boosting (Chapter 8), and support vector machines (Chapter 9).

Motivating Example

Example: (Simulated Default Data Set)

Annual income versus credit card balance of 10,000 individuals, and their default status.



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Estimating Quantitative Values

 Question: Why not assign quantitative values to different categories and predict these values?

E.g., for stroke, drug overdose, epileptic seizure, let

$$Y = \begin{cases} 1, & \text{if stroke} \\ 2, & \text{if drug overdose} \\ 3, & \text{if epileptic seizure} \end{cases}$$

and estimate the value of Y. (\rightarrow implies ordering.)

This is "ok" in the binary case, e.g.,

$$Y = \begin{cases} 1, & \text{if default} \\ 0, & \text{if no default.} \end{cases}$$

→ Large and small predicted values represents two different directions (instead of an ordering).

Estimating Probabilities

 By using linear regression to predict Y, the predicted response can be given by

$$\hat{Y} = \begin{cases} 1, & \hat{f}(X) = X^T \beta \ge 0.5 \\ 0, & \hat{f}(X) = X^T \beta < 0.5. \end{cases}$$

• In estimation theory, the estimator that minimizes the squared loss function $L(Y,f(X))=(Y-f(X))^2$ is

$$f^*(x) = \arg\min_{c} E_{Y|X} \left[(Y - c)^2 | X = x \right]$$
$$= E[Y|X = x]$$
$$= \Pr(Y = 1 | X = x) \left(\triangleq p(x) \right)$$

The linear least squares solution $\hat{f}(X) = X^T \beta$ can be viewed as a linear approximation of this function.

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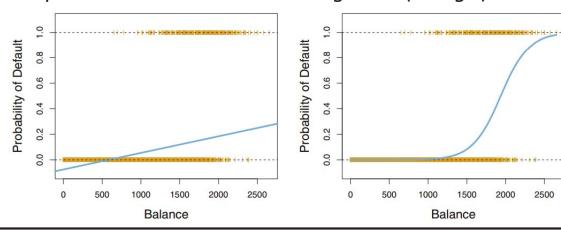
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Linear vs Logistic Model (p = 1)

- Linear model: $p(X) = \beta_0 + \beta_1 X$ (may go beyond [0,1])
- Logistic model:

$$\log\left(\frac{p(X)}{1-p(X)}\right) = \beta_0 + \beta_1 X \Rightarrow p(X) = \frac{e^{\beta_0 + \beta_1 X}}{1 + e^{\beta_0 + \beta_1 X}}$$

→Imposes a linear model on the log-odds (or logit).



Estimating β_0 and β_1 (p=1)

• Maximum likelihood method: Choose β_0 and β_1 to maximize the likelihood that y_1, \ldots, y_n are the responses given that the inputs are x_1, \ldots, x_n , i.e.,

$$\ell(\beta_0, \beta_1) = \prod_{i=1} \Pr(Y = y_i | X = x_i; \beta_0, \beta_1)$$
$$= \prod_{i:y_i=1} p(x_i; \beta_0, \beta_1) \prod_{i:y_i=0} (1 - p(x_i; \beta_0, \beta_1)).$$



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Logistic Regression on the Default Data Set

0.5	Coefficient	Std. error	Z-statistic	P-value
Intercept	-10.6513	0.3612	-29.5	< 0.0001
balance	0.0055	0.0002	24.9	< 0.0001

 E.g., the estimated probability of default for an individual with balance \$1000 is

$$\hat{p}(X) = \frac{e^{\hat{\beta}_0 + \hat{\beta}_1 X}}{1 + e^{\hat{\beta}_0 + \hat{\beta}_1 X}} =$$

- → For balance \$2000, this estimated prob. is 0.586.
- For qualitative variable, such as "student", we can define dummy variable

$$X = \begin{cases} 1, & \text{if student,} \\ 0, & \text{if not student.} \end{cases}$$

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Multiple Logistic Regression (1/2)

• For the case with multiple predictors X_1, X_2, \dots, X_p ,

$$\log\left(\frac{p(X)}{1-p(X)}\right) = \beta_0 + \beta_1 X_1 + \dots + \beta_p X_p \Big(= X^T \beta\Big).$$

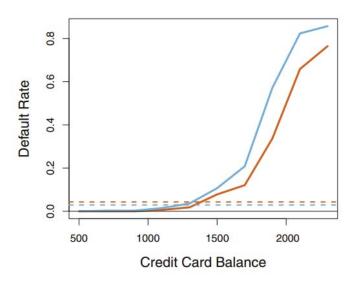
Example:

	Coefficient	Std. error	Z-statistic	P-value
Intercept	-10.8690	0.4923	-22.08	< 0.0001
balance	0.0057	0.0002	24.74	< 0.0001
income	0.0030	0.0082	0.37	0.7115
student[Yes]	-0.6468	0.2362	-2.74	0.0062

	Coefficient	Std. error	Z-statistic	P-value
Intercept	-3.5041	0.0707	-49.55	< 0.0001
student[Yes]	0.4049	0.1150	3.52	0.0004

→ Student less likely to default for *fixed* balance and income, but more likely to default on the average.

Multiple Logistic Regression (2/2)



- students
- non-students

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Estimating the Coefficients

• By adopting the maximum likelihood method, the coefficients $\beta = (\beta_0, \beta_1, \dots, \beta_p)^T$ are chosen to maximize

$$\log \ell(\beta) = \sum_{i=1}^{n} \left[y_i \log p(x_i; \beta) + (1 - y_i) \log(1 - p(x_i; \beta)) \right]$$

$$= \sum_{i=1}^{n} \left[y_i \beta^T x_i - \log(1 + e^{\beta^T x_i}) \right]$$

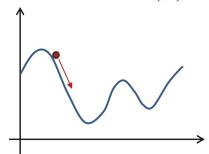
$$= -\sum_{i=1}^{n} \log \left(1 + e^{-(2y_i - 1)\beta^T x_i} \right)$$

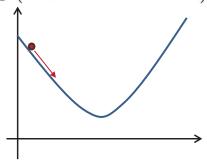
- → concave and, thus, has a unique global maximum.
- Numerical methods, e.g., gradient descent, iteratively reweighted least squares (IRLS).

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Gradient Descent (1/3)

• Gradient descent is like having a ball roll down a hilly surface, e.g., $J(\beta) = \sum_{i=1}^n \log \left(1 + e^{-(2y_i - 1)\beta^T x_i}\right)$.





- 1. Start at random point $\beta(0)$.
- 2. In iteration k+1, take a step along the steepest slope

$$\beta(k+1) = \beta(k) - \eta \nabla J(\beta(k))$$

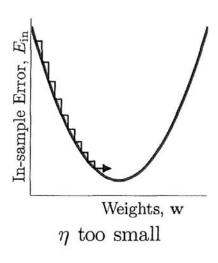
where
$$\nabla J(\beta(k)) = -\sum_{i=1}^{n} \frac{(2y_i - 1)x_i}{1 + e^{-(2y_i - 1)\beta(k)^T x_i}}$$
.

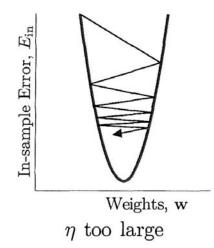
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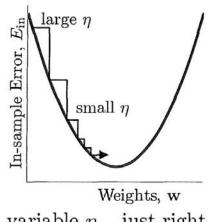
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Gradient Descent (2/3)

Gradient Descent (3/3)







variable η just right

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Iteratively Reweighted Least Squares (1/2)

Newton-Raphson algorithm uses update method

$$\beta(k+1) = \beta(k) - \left(\frac{\partial^2 \log \ell(\beta)}{\partial \beta \partial \beta^T}\right)^{-1} \frac{\partial \log \ell(\beta)}{\partial \beta} \Big|_{\beta = \beta(k)}$$

The first derivative is given by

$$\frac{\partial \log \ell(\beta)}{\partial \beta} = \sum_{i=1}^{n} x_i (y_i - p(x_i; \beta)) = \mathbf{X}^T (\mathbf{y} - \mathbf{p}(\beta))$$

where $\mathbf{p}(\beta) = [p(x_1; \beta), \dots, p(x_n; \beta)]^T$ and the second derivative or Hessian matrix is

$$\frac{\partial^2 \log \ell(\beta)}{\partial \beta \partial \beta^T} = -\sum_{i=1}^n x_i x_i^T p(x_i; \beta) (1 - p(x_i; \beta)) = -\mathbf{X}^T \mathbf{W}(\beta) \mathbf{X}$$

where $\mathbf{W}(\beta) = \operatorname{diag}(\mathbf{p}(\beta))(\mathbf{I} - \operatorname{diag}(\mathbf{p}(\beta))).$

Iteratively Reweighted Least Squares (2/2)

That is, we have

• The update in each iteration is the solution to the weighted least squares problem:

$$\beta(k+1) \leftarrow \arg\min_{\beta} (\mathbf{z}(k) - \mathbf{X}\beta)^T \mathbf{W}(\beta(k)) (\mathbf{z}(k) - \mathbf{X}\beta)$$

→ Iteratively reweighted least squares (IRLS)

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Multinomial Logistic Regression (1/2)

- Suppose that there are K > 2 classes (represented by the response variable $Y \in \{1, ..., K\}$).
- Goal: Model the log-posterior probabilities

$$\log p_k(x) = \log \Pr(Y = k | X = x), \ k = 1, \dots, K,$$
 as linear functions while satisfying $\sum_{k=1}^K p_k(x) = 1.$

The model is given by

$$\log\left(\frac{p_1(x)}{p_K(x)}\right) = \beta_1^T x$$

$$\log\left(\frac{p_2(x)}{p_K(x)}\right) = \beta_2^T x$$

$$\vdots$$

$$\log\left(\frac{p_{K-1}(x)}{p_K(x)}\right) = \beta_{K-1}^T x$$



$$p_k(x) = \frac{e^{\beta_k^T x}}{1 + \sum_{\ell=1}^{K-1} e^{\beta_\ell^T x}}$$
 for $k = 1, \dots, K-1$
$$p_K(x) = \frac{1}{1 + \sum_{\ell=1}^{K-1} e^{\beta_\ell^T x}}$$

Multinomial Logistic Regression (2/2)

The coefficients are chosen to maximize

$$\log \ell(\beta) = \sum_{k=1}^{K} \sum_{i:y_i=k} \log p_k(x_i; \beta_k)$$

• Given coefficient estimates $\hat{\beta}_1, \dots, \hat{\beta}_K$, where, $\hat{\beta}_K = 0$, the predicted output for new input x_0 is given by

$$\hat{Y}(x_0) = \arg\max_{k \in \{1, \dots, K\}} \frac{e^{\hat{\beta}_k^T x_0}}{1 + \sum_{\ell=1}^{K-1} e^{\hat{\beta}_\ell^T x_0}}$$

$$\left(= \arg\max_{k \in \{1, \dots, K\}} \Pr(Y = k | X = x_0) \right)$$

→ The (estimated) maximum a posterior probability (MAP) detector.

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Bayes Theory for Classification (1/3)

- Suppose that there are K classes and, thus, the response variable $Y \in \{1, 2, ..., K\}$.
- Let $\pi_k = \Pr(Y = k)$ be the prior probability that Y = k, and let $f_k(x) \triangleq \Pr(X = x | Y = k)$ be the conditional density function of X given Y = k.
- A classifier can be described as

$$\hat{Y}(x) = \begin{cases} 1, & x \in \mathcal{R}_1 \\ 2, & x \in \mathcal{R}_2 \end{cases}$$
$$\vdots & \vdots \\ K, & x \in \mathcal{R}_K \end{cases}$$

where \mathcal{R}_k is the decision region for class k. Here, $\mathcal{R}_k \cup \mathcal{R}_\ell = \emptyset$ and $\cup_{k=1}^K \mathcal{R}_k = \mathcal{X}$.

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Bayes Theory for Classification (2/3)

• The probability of prediction error is $Pr(\hat{Y}(X) \neq Y) =$

→ To minimize the error probability, we should let $x \in \mathcal{R}_k$ whenever $\Pr(Y = k | X = x) > \Pr(Y = \ell | X = x), \ \forall \ell \neq k$.

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Bayes Theory for Classification (3/3)

 The prediction that minimizes the probability of classification error is given by

$$\hat{Y}(x) = \arg \max_{k \in \{1, ..., K\}} \Pr(Y = k | X = x)$$

$$= \arg \max_{k \in \{1, ..., K\}} \frac{\pi_k f_k(x)}{\sum_{l=1}^K \pi_l f_l(x)} \Big(\triangleq p_k(x) \Big).$$

- → Logistic regression aims to estimate the log of the posterior probability using a linear model.
- \rightarrow Why not estimate π_k and $f_k(x)$ directly?

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Gaussian with Equal Variance Assumption

- Estimating π_k is relatively easy, but estimating $f_k(x)$ can be more difficult unless assuming a simple form.
- Suppose that $f_k(x)$ is assumed to be **Gaussian**, i.e.,

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

with equal variance $\sigma_1^2 = \cdots = \sigma_K^2 = \sigma^2$.

(Recall that μ_k and σ_k^2 are the mean and variance parameters for the kth class.)

In this case, we have

$$p_k(x) = \frac{\pi_k \frac{1}{\sqrt{2\pi}\sigma} \exp\left(-\frac{1}{2\sigma^2} (x - \mu_k)^2\right)}{\sum_{\ell=1}^K \pi_\ell \frac{1}{\sqrt{2\pi}\sigma} \exp\left(-\frac{1}{2\sigma^2} (x - \mu_\ell)^2\right)}.$$

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Bayes Classifier in the Gaussian Case (1/2)

 Under the Gaussian and equal variance assumption, the Bayes classifier yields

$$\hat{Y}(x) = \arg \max_{k \in \{1,...,K\}} p_k(x) =$$

$$\rightarrow \delta_k(x) \triangleq x \frac{\mu_k}{\sigma^2} - \frac{\mu_k^2}{2\sigma^2} + \log \pi_k$$
 is the classification criterion.

Bayes Classifier in the Gaussian Case (2/2)

• For K=2 and $\pi_1=\pi_2$, the Bayes classifier decides on class 1 if

$$\delta_1(x) > \delta_2(x) \Rightarrow$$

and decides on class 2, otherwise.

• The Bayes decision boundary is given by x such that $\delta_1(x) = \delta_2(x)$. That is,

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Linear Discriminant Analysis for p=1

• Linear discriminant analysis (LDA) assumes that $f_k(x)$ is Gaussian with equal variance and applies the Bayes classifier with estimates

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

where n_k is the number of observations in class k.

• This yields the approximated classification criterion

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

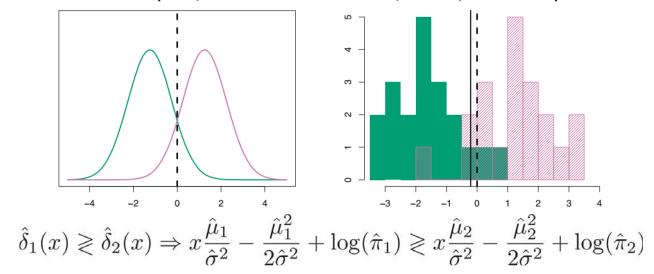
In LDA, the classification is performed by taking

$$\hat{Y} = \arg \max_{k \in \{1, \dots, K} \hat{\delta}_k(x).$$

Example

Left: the Gaussian density functions for two classes.

• Right: histogram of 20 random observations from each class (i.e., $n_1 = n_2 = 20$ and, thus, $\hat{\pi}_1 = \hat{\pi}_2$).



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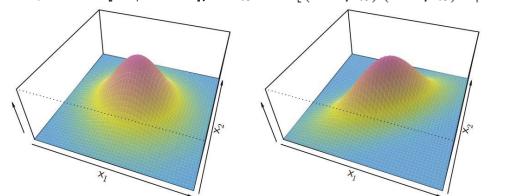
Multivariate Gaussian

• Consider the case with p predictors $X = (X_1, X_2, \dots, X_p)^T$.

• The density function under class k is assumed to be multivariate Gaussian, i.e.,

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

where $\mu_k = E[X|Y = k]$, $\Sigma_k = E[(x - \mu_k)(x - \mu_k)^T|Y = k]$.



Linear Discriminant Analysis for p>1

• For $\Sigma_1 = \cdots = \Sigma_K = \Sigma$, the Bayes classifier is

$$\hat{Y}(x) = \arg\max_{k \in \{1,...,K\}} p_k(x) = \arg\max_{k \in \{1,...,K\}} \delta_k(x)$$

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

• LDA approximates the Bayes classifier by replacing the parameters μ_k, Σ, π_k with their estimates

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

and $\hat{\pi}_k = \frac{n_k}{n}$. That is, the classification is given by

$$\hat{Y}(x) = \arg \max_{k \in \{1, \dots, K\}} \hat{\delta}_k(x)$$

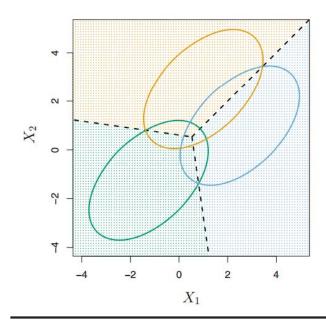
$$= \arg\max_{k \in \{1, \dots, K\}} x^T \hat{\boldsymbol{\Sigma}}^{-1} \hat{\mu}_k - \frac{1}{2} \hat{\mu}_k^T \hat{\boldsymbol{\Sigma}}^{-1} \hat{\mu}_k + \log \hat{\pi}_k.$$

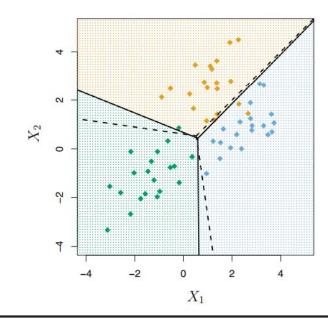
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Example

• The boundary between classes k and ℓ is given by the line $\delta_k(x) = \delta_\ell(x)$ for the Bayes classifier, and by the line $\hat{\delta}_k(x) = \hat{\delta}_\ell(x)$ for the LDA classifier.





Confusion Matrix (1/2)

 For the Default data set, fitting the LDA model to the 10,000 training data yields training error rate 2.75%.
 (Here, the predictors are balance & student status.)

	-	True default status		
		No	Yes	Total
Predicted	No	9,644	252	9,896
$default\ status$	Yes	23	81	104
	Total	9,667	333	10,000

- → Training errors are usually less than test errors.
- →Only 3.33% of individuals in the data set default (i.e., a *null* classifier has only 3.33% error rate).

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Confusion Matrix (2/2)

Sensitivity (specificity) is the percentage of true (non-)
defaulters that are correctly identified.

		True default status		
		No	Yes	Total
$\overline{Predicted}$	No	9,644	252	9,896
$default\ status$	Yes	23	81	104
	Total	9,667	333	10,000

- Only $\frac{81}{333}=24.3\%$ of defaulters were correctly identified.
 - → sensitivity=24.3% (i.e., error rate in "default"=75.7%)
- $-\frac{9644}{9667}$ = 99.8% of non-defaulters were correctly identified. → specificity=99.8% (i.e., error rate in "non-default"=0.2%)

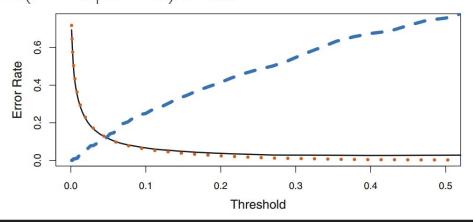
Remark: Bayes classifier minimizes the average error rate, not the individual error rates in different classes.

Average vs Conditional Error Rate

Recall that, in the Default data set, we have

$$Y = \begin{cases} 1, & \text{if default} \\ 0, & \text{if no default.} \end{cases}$$

• The Bayes classifier yields $\hat{Y}=1$ for input X=x if $\Pr(Y=1|X=x)>\Pr(Y=0|X=x)=1-\Pr(Y=1|X=x)$ $\Rightarrow \Pr(Y=1|X=x)>0.5$

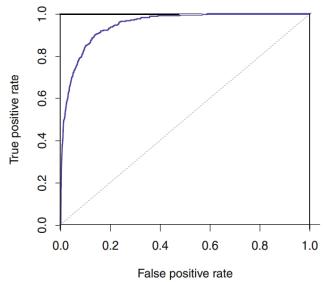


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Receiver Operating Characteristics (ROC)

 The receiver operating characteristics (ROC) curve displays the true positive rate vs false positive rates.



→ The overall performance of a classifier can be measured by the area under the (ROC) curve (AUC).

Quadratic Discriminant Analysis

- Quadratic discriminant analysis (QDA) is similar to LDA, but assuming a different variance for each class.
- That is, for class k, $X \sim \mathcal{N}(\mu_k, \Sigma_k)$.
- Under this assumption, the Bayes classifier is

$$\hat{Y}(x) = \arg \max_{k \in \{1, \dots, K\}} \delta_k(x)$$

where

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

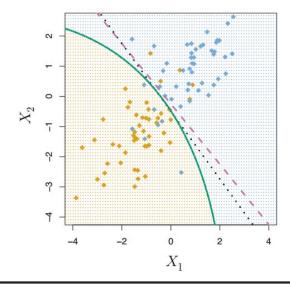
- \rightarrow quadratic in terms of variable x.
- QDA is more flexible but has much more parameters to estimate. → problematic with small training data

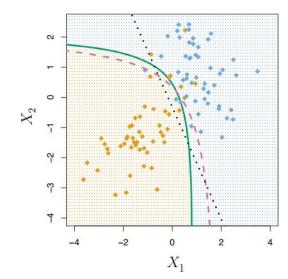
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Example: LDA vs QDA

- Left: Two Gaussian classes have a common correlation of 0.7 among the predictors.
- Right: Orange class has correlation 0.7 and blue class has correlation -0.7.





Comparison of Classification Methods (1/3)

- Two-class case with $p_1(x)$ and $p_2(x)=1-p_1(x)$ being the prob. that X=x belongs to classes 1 and 2.
- In logistic regression, we let

$$\log\left(\frac{p_1(x)}{1 - p_1(x)}\right) = \beta_0 + \beta_1 x$$

In LDA, we assume that

$$p_k(x) = \frac{\pi_k \frac{1}{\sqrt{2\pi}\sigma} \exp\left(-\frac{1}{2\sigma^2} (x - \mu_k)^2\right)}{\sum_{l=1}^2 \pi_l \frac{1}{\sqrt{2\pi}\sigma} \exp\left(-\frac{1}{2\sigma^2} (x - \mu_l)^2\right)}, \ k = 1, 2$$

and, thus,

$$\log\left(\frac{p_1(x)}{1-p_1(x)}\right) = \log\frac{\pi_1}{\pi_2} - \frac{\mu_1^2 - \mu_2^2}{2\sigma^2} + \frac{\mu_1 - \mu_2}{\sigma^2}x = c_0 + c_1x.$$

→ LR and LDA apply different fitting procedures.

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Comparison of Classification Methods (2/3)

In QDA, we assume that

$$p_k(x) = \frac{\pi_k \frac{1}{\sqrt{2\pi}\sigma_k} \exp\left(-\frac{1}{2\sigma_k^2} (x - \mu_k)^2\right)}{\sum_{l=1}^2 \pi_l \frac{1}{\sqrt{2\pi}\sigma_l} \exp\left(-\frac{1}{2\sigma^2} (x - \mu_l)^2\right)}, \ k = 1, 2$$

and thus

$$\log\left(\frac{p_1(x)}{1-p_1(x)}\right) = \log\frac{\pi_1/\sigma_1}{\pi_2/\sigma_2} - \frac{1}{2\sigma_1^2}(x-\mu_1)^2 + \frac{1}{2\sigma_2^2}(x-\mu_2)^2$$
$$= c_0 + c_1x + c_2x^2.$$

→ Related to 2nd order polynomial logistic regression.

Comparison of Classification Methods (3/3)

kNN classification is done by taking

$$\hat{Y}(x) = \arg\max_{k' \in \{1, ..., K\}} \frac{1}{k} \sum_{i: x_i \in \mathcal{N}_k(x)} \mathbf{1}_{\{y_i = k'\}} \Big(\approx \Pr(Y = k' | X = x) \Big).$$

- → non-parametric
- Flexibility: kNN>QDA>LDA

Example: In the following, we simulate 100 random training sets from several different known distributions with 2 predictors and a binary response variable.

Compare between (1) kNN-1, (2) kNN-CV, (3) Logistic Regression, (4) LDA, (5) QDA.

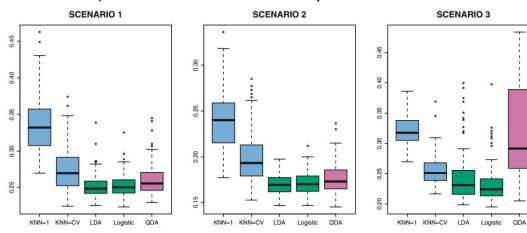
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Example (1/2)

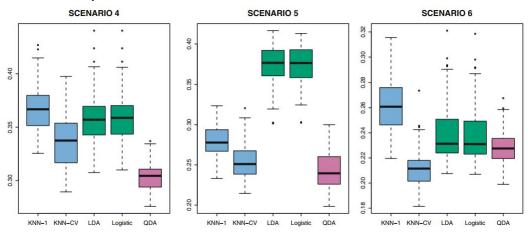
- **Scenario 1:** 20 training observations in each class, uncorrelated normal with different means.
- Scenario 2: Same as Scenario 1 but with correlation of -0.5 among the two predictors.
- **Scenario 3:** The two predictors generated from the student t-distribution, with 50 observations per class.



ass,

Example (2/2)

- **Scenario 4:** Normal with correlation of 0.5 in class 1 and -0.5 in class 2. Means differ between classes.
- Scenario 5: Normal with uncorrelated predictors. Responses were sampled $\Pr(Y=1|X=x)=\frac{e^{\beta_0+\beta_1X_1^2+\beta_2X_2^2+\beta_3X_1X_2}}{1+e^{\beta_0+\beta_1X_1^2+\beta_2X_2^2+\beta_3X_1X_2}}.$
- **Scenario 6:** Same as Scenario 5, but responses sampled from a more complicated non-linear function.



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