Lecture 6: Classification

Reading: Sections 4.3, 4.4

GU4241/GR5241 Statistical Machine Learning

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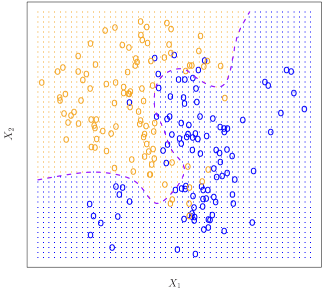
Classification problems

Supervised learning with a **qualitative or categorical** response.

Just as common, if not more common than regression:

- *Medical diagnosis:* Given the symptoms a patient shows, predict which of 3 conditions they are attributed to.
- *Online banking:* Determine whether a transaction is fraudulent or not, on the basis of the IP address, client's history, etc.
- *Web searching:* Based on a user's history, location, and the string of a web search, predict which link a person is likely to click.
- *Online advertising:* Predict whether a user will click on an ad or not.

Classification problem



ISL Figure 2.13

Recall:

- $X = (X_1, X_2)$ are inputs.
- Color $Y \in \{\text{Yellow}\ , \text{Blue}\}$ is the output.
- (X, Y) have a joint distribution.
- Purple line is *Bayes boundary* — the best we could do if we knew the joint distribution of (X, Y)

Review: Bayes classifier

Suppose $P(Y \mid X)$ is known. Then, given an input x_0, we predict the response

$$\hat{y}_0 = \mathsf{argmax}_{\,y}\; P(Y = y \mid X = x_0).$$

The Bayes classifier minimizes the expected 0-1 loss:

$$E\left[\frac{1}{m}\sum_{i=1}^{m}\mathbf{1}(\hat{y}_i \neq y_i)\right]$$

This minimum 0-1 loss (the best we can hope for) is the **Bayes error rate**.

Example: Spam Filtering

Representing emails

- $\mathbf{Y} = \{$ spam, email $\}$
- $\mathbf{X} = \mathbb{R}^d$
- Each axis is labelled by one possible word.
- d = number of distinct words in vocabulary
- x_j = number of occurences of word j in email represented by $\mathbf{x}$

For example, if axis j represents the term "the", $x_j = 3$ means that "the" occurs three times in the email $\mathbf{x}$. This representation is called a **vector space model of text**.

Example dimensions

	george	you	your	hp	free	hpl	!	our	re	edu
spam	0.00	2.26	1.38	0.02	0.52	0.01	0.51	0.51	0.13	0.01
email	1.27	1.27	0.44	0.90	0.07	0.43	0.11	0.18	0.42	0.29

With Bayes equation

$$f(\mathbf{x}) = \underset{y \in \{\text{spam},\text{email}\}}{\text{argmax}} P(y|\mathbf{x}) = \underset{y \in \{\text{spam},\text{email}\}}{\text{argmax}} p(\mathbf{x}|y)P(y)$$

Naive Bayes

Simplifying assumption

The classifier is called a **naive Bayes** classifier if it assumes

$$p(\mathbf{x}|y) = \prod_{j=1}^{d} p_j(x_i|y) \ ,$$

i.e. if it treats the individual dimensions of $\mathbf{x}$ as conditionally independent given y.

In spam example

- Corresponds to the assumption that the number of occurrences of a word carries information about y.
- Co-occurrences (how often do given combinations of words occur?) is neglected.

Estimation

Class prior

The distribution $P(y)$ is easy to estimate from training data:

$$P(y) = \frac{\#\text{observations in class } y}{\#\text{observations}}$$

Class-conditional distributions

The class conditionals $p(x|y)$ usually require a modeling assumption. Under a given model:

- Separate the training data into classes.
- Estimate $p(x|y)$ on class y by maximum likelihood.

Strategy: estimate $P(Y \mid X)$

If we have a good estimate for the conditional probability $\hat{P}(Y \mid X)$, we can use the classifier:

$$\hat{y}_0 = \text{argmax}_y \, \hat{P}(Y = y \mid X = x_0).$$

Suppose Y is a binary variable. Could we use a linear model?

$$P(Y = 1|X) = \beta_0 + \beta_1 X_1 + \cdots + \beta_1 X_p$$

Problems:

- This would allow probabilities $<$0 and $>$1.
- Difficult to extend to more than 2 categories.

Logistic regression

We model the joint probability as:

$$P(Y = 1 \mid X) = \frac{e^{\beta_0 + \beta_1 X_1 + \cdots + \beta_p X_p}}{1 + e^{\beta_0 + \beta_1 X_1 + \cdots + \beta_p X_p}},$$

$$P(Y = 0 \mid X) = \frac{1}{1 + e^{\beta_0 + \beta_1 X_1 + \cdots + \beta_p X_p}}.$$

This is the same as using a linear model for the log odds:

$$\log \left[\frac{P(Y = 1 \mid X)}{P(Y = 0 \mid X)} \right] = \beta_0 + \beta_1 X_1 + \cdots + \beta_p X_p.$$

Fitting logistic regression

The training data is a list of pairs $(y_1, x_1), (y_2, x_2), \ldots, (y_n, x_n)$. In the linear model

$$\log\left[\frac{P(Y = 1 \mid X)}{P(Y = 0 \mid X)}\right] = \beta_0 + \beta_1 X_1 + \cdots + \beta_p X_p,$$

we don't observe the left hand side.

We cannot use a least squares fit.

Fitting logistic regression

Solution:

The likelihood is the probability of the training data, for a fixed set of coefficients $\beta_0, \ldots, \beta_p$:

$$\prod_{i=1}^{n} P(Y = y_i \mid X = x_i)$$

$$= \underbrace{\prod_{i;y_i=1} \frac{e^{\beta_0+\beta_1 x_{i1}+\cdots+\beta_p x_{ip}}}{1+e^{\beta_0+\beta_1 x_{i1}+\cdots+\beta_p x_{ip}}}}_{\text{Probability of responses} = 1} \underbrace{\prod_{j;y_j=0} \frac{1}{1+e^{\beta_0+\beta_1 x_{j1}+\cdots+\beta_p x_{jp}}}}_{\text{Probability of responses} = 0}$$

- Choose estimates $\hat{\beta}_0, \ldots, \hat{\beta}_p$ which maximize the likelihood.
- Solved with numerical methods (e.g. Newton's algorithm).

Logistic regression in R

```
> glm.fit=glm(Direction~Lag1+Lag2+Lag3+Lag4+Lag5+Volume,
    data=Smarket,family=binomial)
> summary(glm.fit)

Call:
glm(formula = Direction ~ Lag1 + Lag2 + Lag3 + Lag4 + Lag5
    + Volume, family = binomial, data = Smarket)

Deviance Residuals:
   Min      1Q  Median      3Q     Max
 -1.45   -1.20    1.07    1.15    1.33

Coefficients:
            Estimate Std. Error z value Pr(>|z|)
(Intercept) -0.12600    0.24074   -0.52     0.60
Lag1        -0.07307    0.05017   -1.46     0.15
Lag2        -0.04230    0.05009   -0.84     0.40
Lag3         0.01109    0.04994    0.22     0.82
Lag4         0.00936    0.04997    0.19     0.85
Lag5         0.01031    0.04951    0.21     0.83
Volume       0.13544    0.15836    0.86     0.39
```

Logistic regression in R

- We can estimate the Standard Error of each coefficient.
- The z-statistic is the equivalent of the t-statistic in linear regression:

$$z = \frac{\hat{\beta}_j}{\mathsf{SE}(\hat{\beta}_j)}.$$

- The p-values are test of the null hypothesis $\beta_j = 0$ (Wald's test).
- Other possible hypothesis tests: likelihood ratio test (chi-square distribution).

Example: Predicting credit card `default`

Predictors:

- `student`: 1 if student, 0 otherwise.
- `balance`: credit card balance.
- `income`: person's income.

In this dataset, there is *confounding*, but little collinearity.

- Students tend to have higher balances. So, `balance` is explained by `student`, but not very well.
- People with a high `balance` are more likely to default.
- Among people with a given `balance`, students are less likely to default.

Example: Predicting credit card `default`

Predictors:

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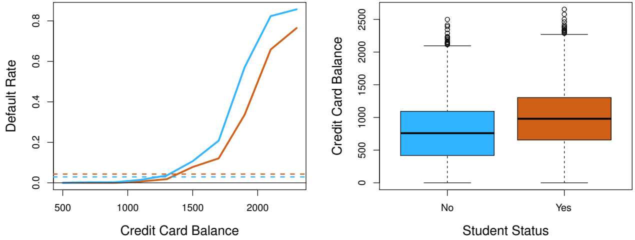
- `income`: person's income.



Example: Predicting credit card `default`

Logistic regression using only `balance`:

	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

Logistic regression using only `student`:

	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

Logistic regression using all 3 predictors:

	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

Extending logistic regression to more than 2 categories

Multinomial logistic regression:

Suppose Y takes values in $\{1, 2, \ldots, K\}$, then we use a linear model for the log odds against a baseline category (e.g. 1):

$$\log\left[\frac{P(Y = 2 \mid X)}{P(Y = 1 \mid X)}\right] = \beta_{0,2} + \beta_{1,2}X_1 + \cdots + \beta_{p,2}X_p,$$

$$\cdots$$

$$\log\left[\frac{P(Y = K \mid X)}{P(Y = 1 \mid X)}\right] = \beta_{0,K} + \beta_{1,K}X_1 + \cdots + \beta_{p,K}X_p.$$

Some issues with logistic regression

- The coefficients become unstable when there is collinearity. Furthermore, this affects the convergence of the fitting algorithm.
- When the classes are well separated, the coefficients become unstable. This is always the case when $p \geq n - 1$.

Main strategy in Chapter 4

Find an estimate $\hat{P}(Y \mid X)$. Then, given an input x_0, we predict the response as in a Bayes classifier:

$$\hat{y}_0 = \text{argmax}_{\,y}\ \hat{P}(Y = y \mid X = x_0).$$

Linear Discriminant Analysis (LDA)

Strategy: Instead of estimating $P(Y \mid X)$, we will estimate:

1. $\hat{P}(X \mid Y)$: Given the response, what is the distribution of the inputs.
2. $\hat{P}(Y)$: How likely are each of the categories.

Then, we use *Bayes rule* to obtain the estimate:

$$\hat{P}(Y = k \mid X = x) = \frac{\hat{P}(X = x \mid Y = k)\hat{P}(Y = k)}{\hat{P}(X = x)}$$

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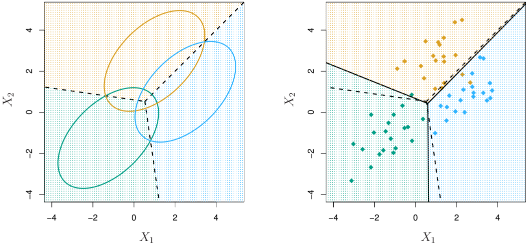
$$\hat{P}(Y = k \mid X = x) = \frac{\hat{P}(X = x \mid Y = k)\hat{P}(Y = k)}{\sum_j \hat{P}(X = x \mid Y = j)\hat{P}(Y = j)}$$

Linear Discriminant Analysis (LDA)

Strategy: Instead of estimating $P(Y \mid X)$, we will estimate:

1. We model $\hat{P}(X = x \mid Y = k) = \hat{f}_k(x)$ as a *Multivariate Normal Distribution*:



2. $\hat{P}(Y = k) = \hat{\pi}_k$ is estimated by the fraction of training samples of class k.

LDA has linear decision boundaries

Suppose that:

- We know $P(Y = k) = \pi_k$ exactly.
- $P(X = x|Y = k)$ is Mutivariate Normal with density:

$$f_k(x) = \frac{1}{(2\pi)^{p/2}|\mathbf{\Sigma}|^{1/2}} e^{-\frac{1}{2}(x-\mu_k)^T \mathbf{\Sigma}^{-1}(x-\mu_k)}$$

μ_k : Mean of the inputs for category k.
$\mathbf{\Sigma}$: Covariance matrix (common to all categories).

Then, what is the Bayes classifier?

LDA has linear decision boundaries

By Bayes rule, the probability of category k, given the input x is:

$$P(Y = k \mid X = x) = \frac{f_k(x)\pi_k}{P(X = x)}$$

The denominator does not depend on the response k, so we can write it as a constant:

$$P(Y = k \mid X = x) = C \times f_k(x)\pi_k$$

Now, expanding $f_k(x)$:

$$P(Y = k \mid X = x) = \frac{C\pi_k}{(2\pi)^{p/2}|\mathbf{\Sigma}|^{1/2}} e^{-\frac{1}{2}(x-\mu_k)^T \mathbf{\Sigma}^{-1}(x-\mu_k)}$$

LDA has linear decision boundaries

$$P(Y = k \mid X = x) = \frac{C\pi_k}{(2\pi)^{p/2}|\mathbf{\Sigma}|^{1/2}} e^{-\frac{1}{2}(x-\mu_k)^T \mathbf{\Sigma}^{-1}(x-\mu_k)}$$

Now, let us absorb everything that does not depend on k into a constant C':

$$P(Y = k \mid X = x) = C'\pi_k e^{-\frac{1}{2}(x-\mu_k)^T \mathbf{\Sigma}^{-1}(x-\mu_k)}$$

and take the logarithm of both sides:

$$\log P(Y = k \mid X = x) = \log C' + \log \pi_k - \frac{1}{2}(x-\mu_k)^T \mathbf{\Sigma}^{-1}(x-\mu_k).$$

This is the same for every category, k.

LDA has linear decision boundaries

$$P(Y = k \mid X = x) = \frac{C\pi_k}{(2\pi)^{p/2}|\mathbf{\Sigma}|^{1/2}} e^{-\frac{1}{2}(x-\mu_k)^T \mathbf{\Sigma}^{-1}(x-\mu_k)}$$

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This is the same for every category, k.
So we want to find the maximum of this over k.

LDA has linear decision boundaries

Goal, maximize the following over k:

$$\begin{aligned}
&\log \pi_k - \frac{1}{2}(x-\mu_k)^T \mathbf{\Sigma}^{-1}(x-\mu_k). \\
=&\log \pi_k - \frac{1}{2}\left[x^T \mathbf{\Sigma}^{-1} x + \mu_k^T \mathbf{\Sigma}^{-1}\mu_k\right] + x^T \mathbf{\Sigma}^{-1}\mu_k \\
=&C'' + \log \pi_k - \frac{1}{2}\mu_k^T \mathbf{\Sigma}^{-1}\mu_k + x^T \mathbf{\Sigma}^{-1}\mu_k
\end{aligned}$$

We define the objective:

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

At an input x, we predict the response with the highest $\delta_k(x)$.

LDA has linear decision boundaries

What is the decision boundary? It is the set of points in which 2 classes do just as well:

$$\delta_k(x) = \delta_\ell(x)$$

$$\log \pi_k - \frac{1}{2}\mu_k^T \mathbf{\Sigma}^{-1}\mu_k + x^T \mathbf{\Sigma}^{-1}\mu_k = \log \pi_\ell - \frac{1}{2}\mu_\ell^T \mathbf{\Sigma}^{-1}\mu_\ell + x^T \mathbf{\Sigma}^{-1}\mu_\ell$$

LDA has linear decision boundaries

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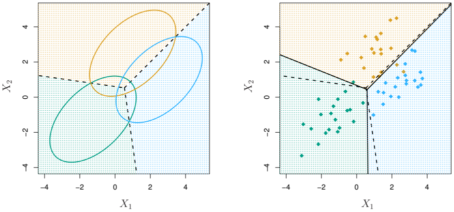
This is a linear equation in x.



Estimating π_k

$$\hat{\pi}_k = \frac{\#\{i\ ;\ y_i = k\}}{n}$$

In English, the fraction of training samples of class k.

Estimating the parameters of $f_k(x)$

Estimate the center of each class μ_k:

$$\hat{\mu}_k = \frac{1}{\#\{i\ ;\ y_i = k\}} \sum_{i\ ;\ y_i = k} x_i$$

Estimate the common covariance matrix $\mathbf{\Sigma}$:

- One predictor ($p = 1$):

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

- Many predictors ($p > 1$): Compute the vectors of deviations $(x_1 - \hat{\mu}_{y_1}), (x_2 - \hat{\mu}_{y_2}), \ldots, (x_n - \hat{\mu}_{y_n})$ and use an unbiased estimate of its covariance matrix, $\mathbf{\Sigma}$.

LDA prediction

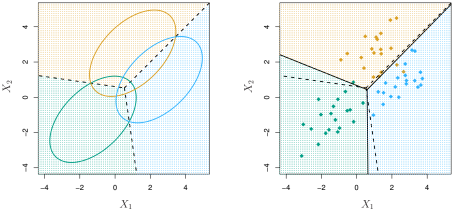
For an input x, predict the class with the largest:

$$\hat{\delta}_k(x) = \log \hat{\pi}_k - \frac{1}{2}\hat{\mu}_k^T \hat{\mathbf{\Sigma}}^{-1}\hat{\mu}_k + x^T \hat{\mathbf{\Sigma}}^{-1}\hat{\mu}_k$$

The decision boundaries are defined by:

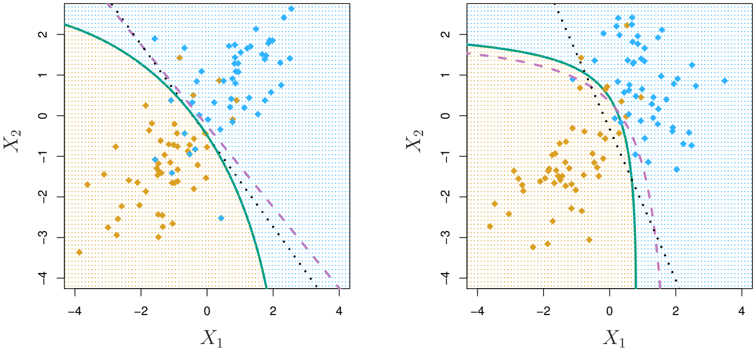
$$\log \hat{\pi}_k - \frac{1}{2}\hat{\mu}_k^T \hat{\mathbf{\Sigma}}^{-1}\hat{\mu}_k + x^T \hat{\mathbf{\Sigma}}^{-1}\hat{\mu}_k = \log \hat{\pi}_\ell - \frac{1}{2}\hat{\mu}_\ell^T \hat{\mathbf{\Sigma}}^{-1}\hat{\mu}_\ell + x^T \hat{\mathbf{\Sigma}}^{-1}\hat{\mu}_\ell$$

Solid lines in:



Quadratic discriminant analysis (QDA)

The assumption that the inputs of every class have the same covariance $\mathbf{\Sigma}$ can be quite restrictive:



Quadratic discriminant analysis (QDA)

In **quadratic discriminant analysis** we estimate a mean $\hat{\mu}_k$ and a covariance matrix $\hat{\mathbf{\Sigma}}_k$ for each class separately.

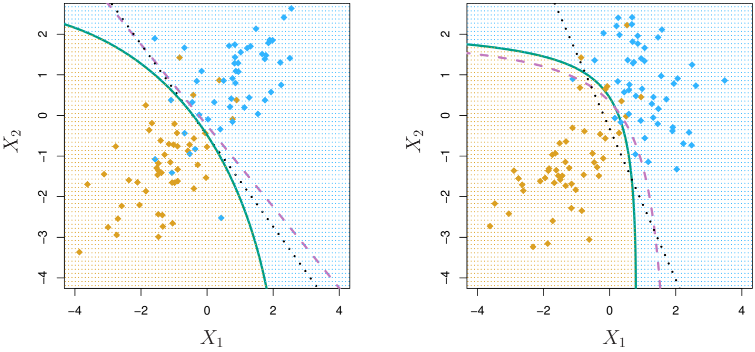
Given an input, it is easy to derive an objective function:

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

This objective is now quadratic in x and so are the decision boundaries.

Quadratic discriminant analysis (QDA)

- Bayes boundary (– – –)
- LDA (· · · · · ·)
- QDA (——).



Evaluating a classification method

We have talked about the 0-1 loss:

$$\frac{1}{m}\sum_{i=1}^{m}\mathbf{1}(y_i \neq \hat{y}_i).$$

It is possible to make the wrong prediction for some classes more often than others. The 0-1 loss doesn't tell you anything about this.

A much more informative summary of the error is a **confusion matrix**:

		Predicted class		
		− or Null	+ or Non-null	Total
True class	− or Null	True Neg. (TN)	False Pos. (FP)	N
	+ or Non-null	False Neg. (FN)	True Pos. (TP)	P
	Total	N*	P*	

Example. Predicting `default`

Used LDA to predict credit card default in a dataset of 10K people.

Predicted "yes" if $P(\texttt{default} = \text{yes}|X) > 0.5$.

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

- The error rate among people who do **not** default (false positive rate) is very low.
- However, the rate of false negatives is 76%.
- It is possible that false negatives are a bigger source of concern!
- One possible solution: Change the threshold.

Example. Predicting `default`

Changing the threshold to 0.2 makes it easier to classify to "yes".

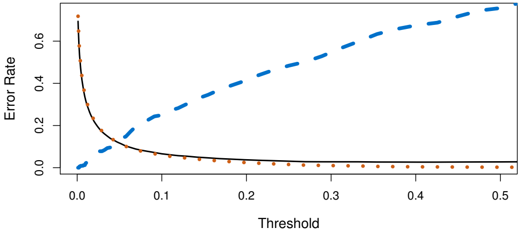
Predicted "yes" if $P(\texttt{default} = \text{yes}|X) > 0.2$.

		True default status		
		No	Yes	Total
Predicted	No	9,432	138	9,570
default status	Yes	235	195	430
	Total	9,667	333	10,000

Note that the rate of false positives became higher! That is the price to pay for fewer false negatives.

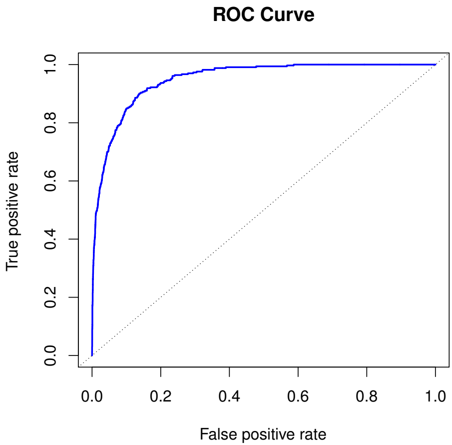
Example. Predicting `default`

Let's visualize the dependence of the error on the threshold:



- – – – False negative rate (error for defaulting customers)
- · · · · · False positive rate (error for non-defaulting customers)
- —— 0-1 loss or total error rate.

Example. The ROC curve



- Displays the performance of the method for any choice of threshold.
- The area under the curve (AUC) measures the quality of the classifier:
  - 0.5 is the AUC for a random classifier
  - The closer AUC is to 1, the better.

Thinking about the loss function is important

Most of the **regression** methods we've studied aim to minimize the RSS, while **classification** methods aim to minimize the 0-1 loss.

In classification, we often care about certain kinds of error more than others; i.e. the natural loss function is not the 0-1 loss.

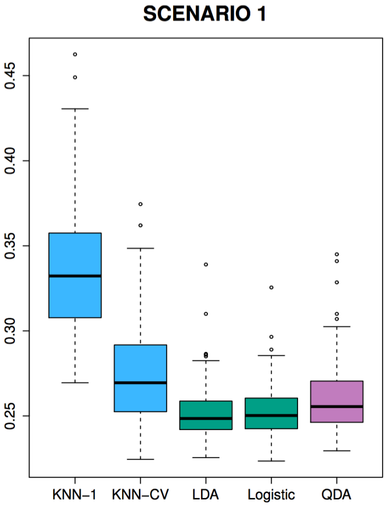
Even if we use a method which minimizes a certain kind of training error, we can *tune* it to optimize our true loss function.

- e.g. Find the threshold that brings the False negative rate below an acceptable level.

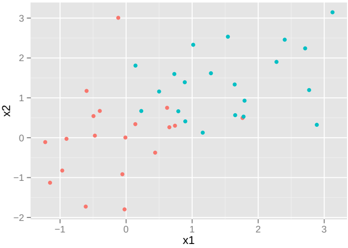
Comparing classification methods through simulation

1. Simulate data from several different known distributions with 2 predictors and a binary response variable.
2. Compare the test error (0-1 loss) for the following methods:
   - KNN-1
   - KNN-CV ("optimal" KNN)
   - Logistic regression
   - Linear discriminant analysis (LDA)
   - Quadratic discriminant analysis (QDA)

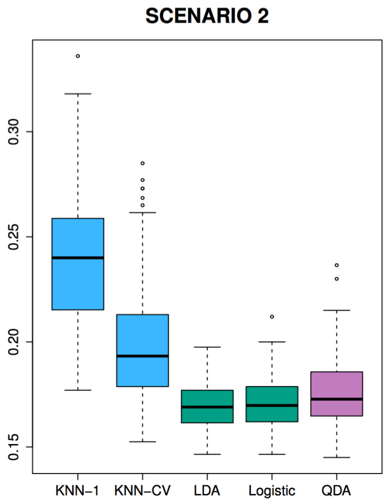
Scenario 1



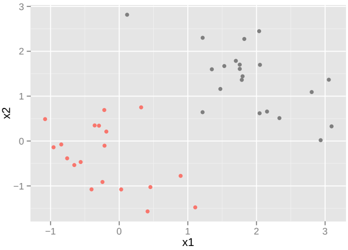
- X_1, X_2 standard normal.
- No correlation in either class.



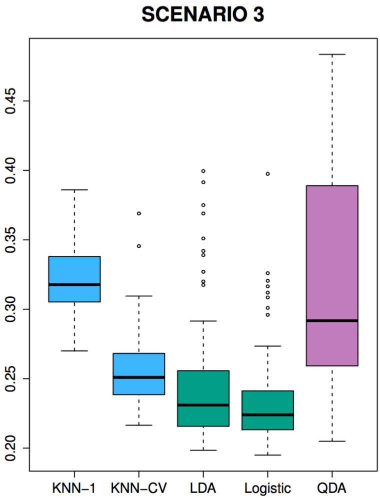
Scenario 2



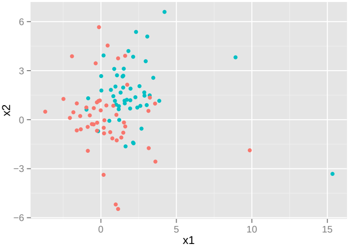
- X_1, X_2 standard normal.
- Correlation is -0.5 in both classes.



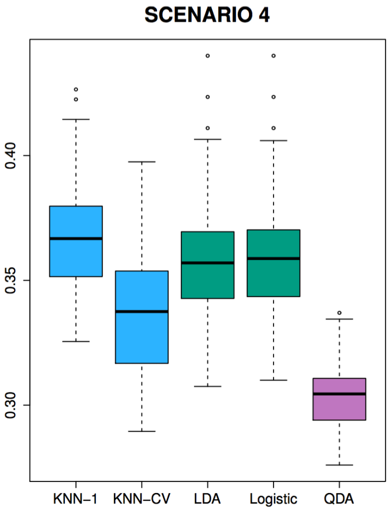
Scenario 3



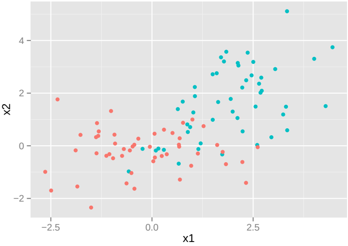
- X_1, X_2 Student t random variables.
- No correlation in either class.



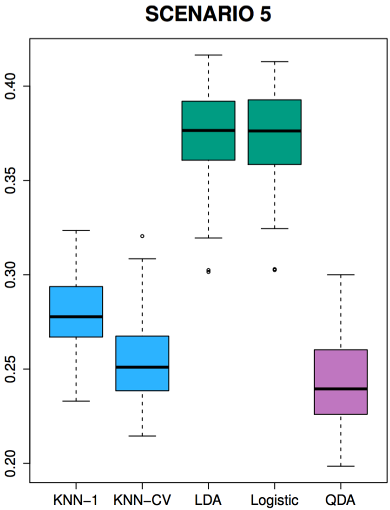
Scenario 4



- X_1, X_2 standard normal.
- First class has correlation 0.5, second class has correlation -0.5.



Scenario 5

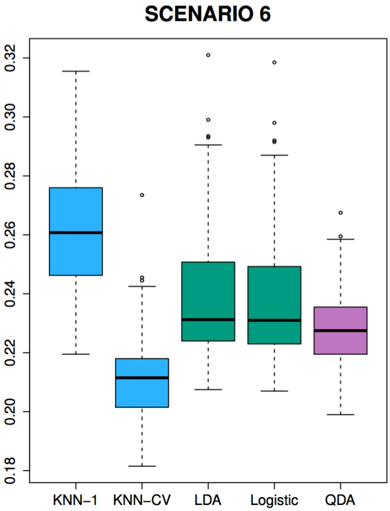


- X_1, X_2 uncorrelated, standard normal.
- Response Y was sampled from:

$$P(Y=1|X) = \frac{e^{\beta_0+\beta_1(X_1^2)+\beta_2(X_2^2)+\beta_3(X_1X_2)}}{1+e^{\beta_0+\beta_1(X_1^2)+\beta_2(X_2^2)+\beta_3(X_1X_2)}}.$$

- The true decision boundary is quadratic.

Scenario 6



- X_1, X_2 uncorrelated, standard normal.
- Response Y was sampled from:

$$P(Y=1|X) = \frac{e^{f_{\text{nonlinear}}(X_1,X_2)}}{1+e^{f_{\text{nonlinear}}(X_1,X_2)}}.$$

- The true decision boundary is very rough.