Inteligencia Artificial

UTN – FRVM

5º Año Ing. en Sistemas de Información

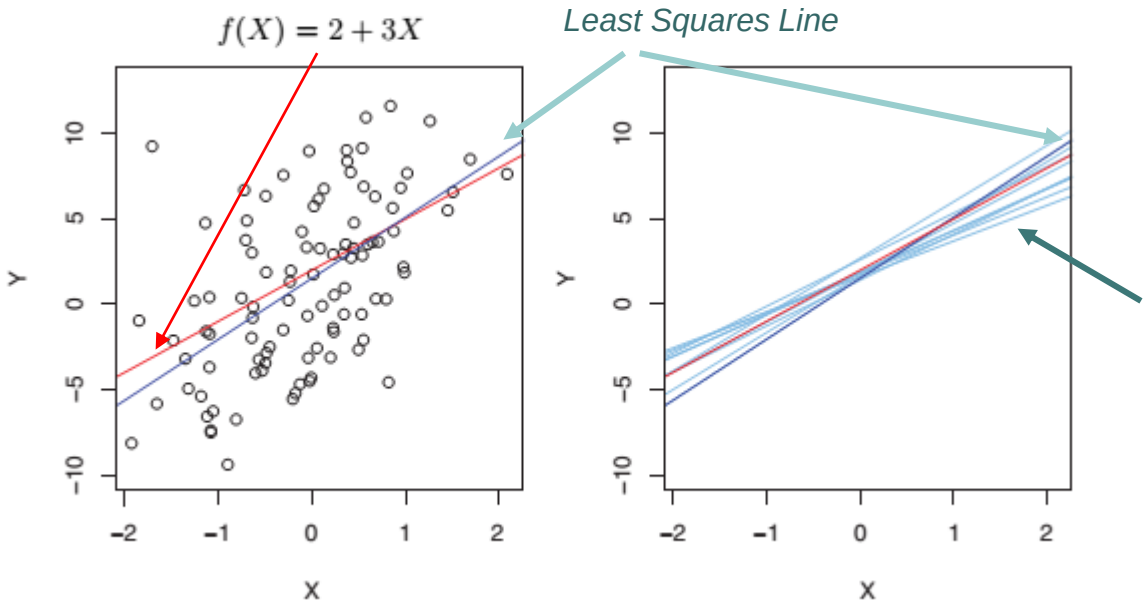
Agenda

- *Accuracy of the Coefficient Estimates*.
- K-Nearest Neighbours.
- Resampling Methods.
- Classification

Accuracy of the Coefficient Estimates

$$Y = \beta_0 + \beta_1 X + \epsilon.$$

- Here β_0 is the intercept term—that is, the expected value of *Y* when *X* = 0, and β_1 is the slope—the average increase in *Y* associated with a one-unit increase in *X*.
- We typically assume that the error term is independent of *X*.



Separate random set of observations. Each least squares line is different, but on average, the least squares lines are quite close to the population regression line.

Standard Error

- The average of $\hat{\mu}$'s over many data sets will be very close to μ.
- How far off will that single estimate of $\hat{\mu}$ be?

$$\mathrm{Var}(\hat{\mu}) = \mathrm{SE}(\hat{\mu})^2 = \frac{\sigma^2}{n}$$

Standard deviation of each realization of y_i of Y

the standard error tells us the average amount that this estimate $\hat{\mu}$ differs from the actual value of μ

$$\mathrm{SE}(\hat{\beta}_0)^2 = \sigma^2 \left[\frac{1}{n} + \frac{\bar{x}^2}{\sum_{i=1}^{n}(x_i - \bar{x})^2}\right], \quad \mathrm{SE}(\hat{\beta}_1)^2 = \frac{\sigma^2}{\sum_{i=1}^{n}(x_i - \bar{x})^2}$$

$$\sigma^2 = \mathrm{Var}(\epsilon)$$

Standard Error

- In general, σ^2 is not known, but can be estimated from the data.
- The estimate of σ is known as the *residual standard error (RSE)*

Residual sum of squares

$$\mathrm{RSE} = \sqrt{\mathrm{RSS}/(n-2)}.$$

$$\mathrm{RSS} = (y_1 - \hat{\beta}_0 - \hat{\beta}_1 x_1)^2 + (y_2 - \hat{\beta}_0 - \hat{\beta}_1 x_2)^2 + \ldots + (y_n - \hat{\beta}_0 - \hat{\beta}_1 x_n)^2$$

Standard errors can be used to compute *confidence intervals*. A 95 % confidence interval is defined as a range of values such that with 95 % interval probability, the range will contain the true unknown value of the parameter.

$$\hat{\beta}_1 \pm 2 \cdot \mathrm{SE}(\hat{\beta}_1)$$

Hypothesis tests

- H_0:There is no relationship between X and Y *(Null Hypothesis)* $\beta_1 = 0 \quad Y = \beta_0 + \epsilon$
- H_a:There is some relationship between X and Y *(Alternative Hypothesis)*

$$t = \frac{\hat{\beta}_1 - 0}{\mathrm{SE}(\hat{\beta}_1)}$$

	Coefficient	Std. error	t-statistic
Intercept	7.0325	0.4578	15.36
TV	0.0475	0.0027	17.67

Assessing the Accuracy of the Model

- The quality of a linear regression fit is typically assessed using two related quantities: the *residual standard error* (RSE) and the R^2 statistic.
- **RSE**: it is the average amount that the response will deviate from the true regression line. Problem? Units of Y (Which is a good RSE?)

$$\mathrm{RSE} = \sqrt{\frac{1}{n-2}\mathrm{RSS}} = \sqrt{\frac{1}{n-2}\sum_{i=1}^{n}(y_i - \hat{y}_i)^2}$$

- R2: takes the form of a *proportion —the proportion of variance explained*— and so it always takes on a value between 0 and 1, and is independent of the scale of *Y*

$$R^2 = \frac{\mathrm{TSS} - \mathrm{RSS}}{\mathrm{TSS}} = 1 - \frac{\mathrm{RSS}}{\mathrm{TSS}}$$

the amount of variability that is left unexplained after performing the regression

the amount of variability inherent in the response before the regression is performed

$$\mathrm{TSS} = \sum(y_i - \bar{y})^2$$

the amount of variability in the response that is removed by performing the regression.

K-Nearest Neighbours

- Many approaches attempt to estimate the *conditional distribution* of *Y* given *X*, and then classify a given observation to the class with highest *estimated* probability.

- Given a positive integer *K* and a test observation x_0, the *KNN* classifier first identifies the neighbors *K* points in the training data that are closest to x_0, represented by N_0

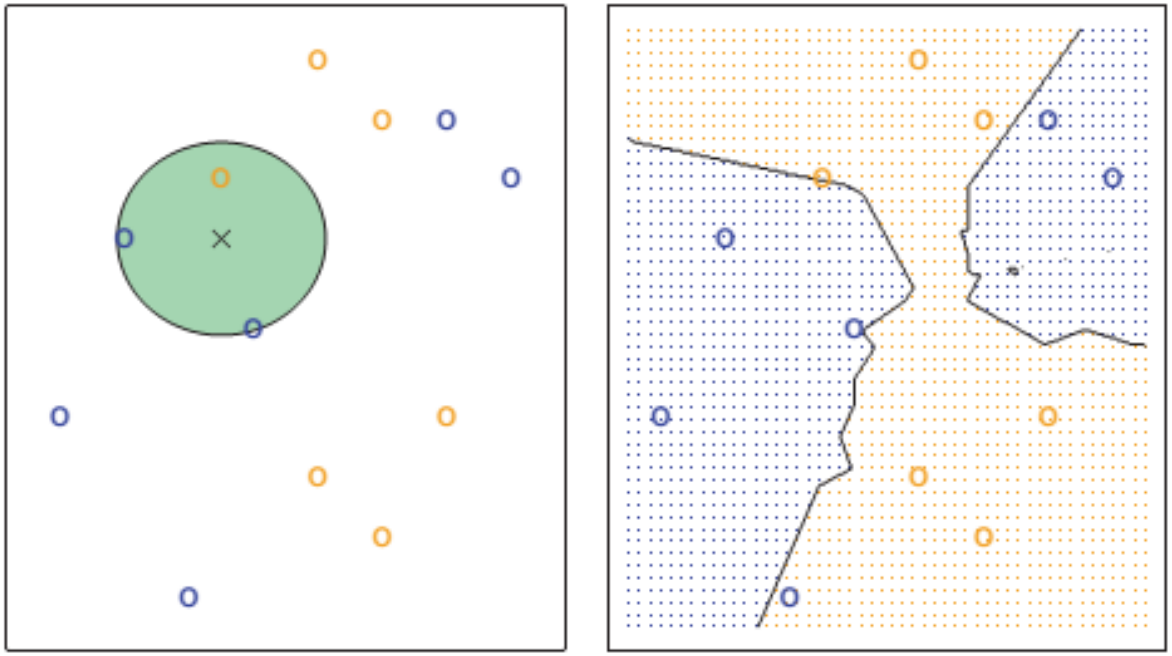
- The conditional probability for class *j* as the fraction of points in N_0 whose response values equal *j:*

$$\Pr(Y = j|X = x_0) = \frac{1}{K} \sum_{i \in \mathcal{N}_0} I(y_i = j)$$

$$d(x_i, x_j) = \sqrt{\sum_{r=1}^{p} (x_{ri} - x_{rj})^2}$$

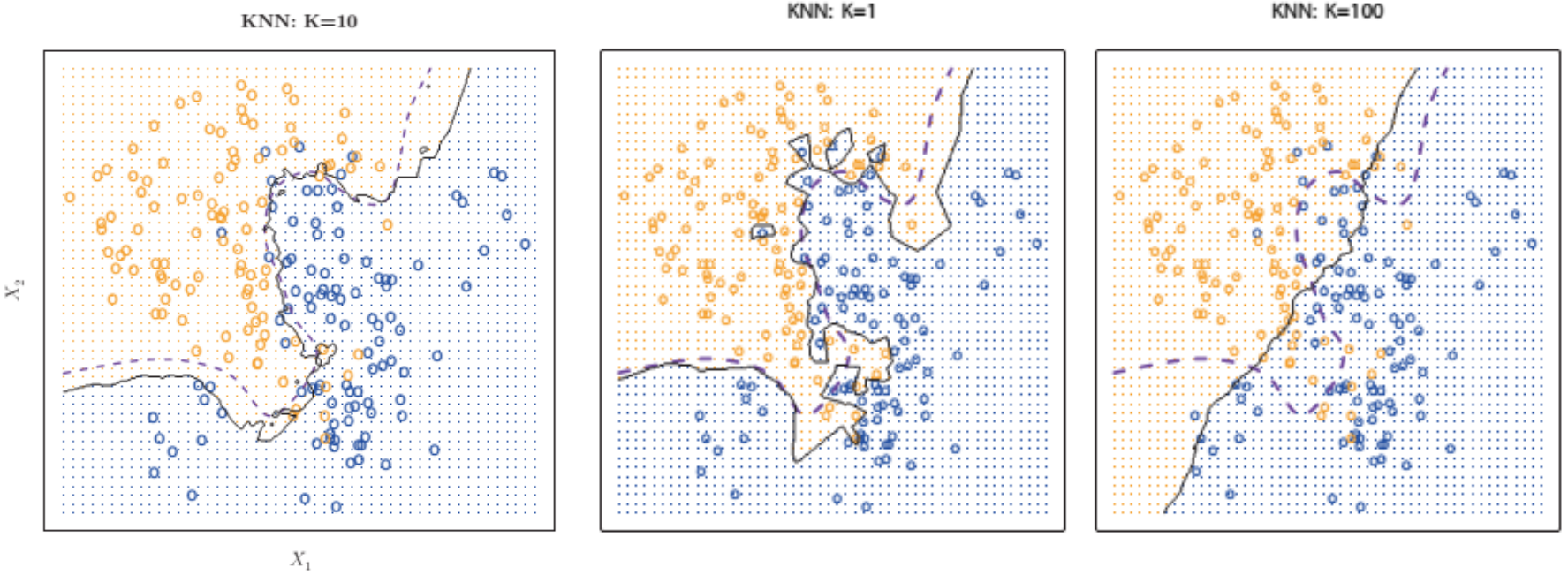
$$d = |\mathbf{x} - \mathbf{y}| = \sqrt{\sum_{i=1}^{n} |x_i - y_i|^2} \ .$$

KNN



- *The **KNN** approach, using K = 3, is illustrated in a simple situation with six blue observations and six orange observations.*
- ***Left**: a test observation at which a predicted class label is desired is shown as a black cross. The three closest points to the test observation are identified, and it is predicted that the test observation belongs to the most commonly-occurring class, in this case blue.*
- ***Right**: The KNN decision boundary for this example is shown in black. The blue grid indicates the region in which a test observation will be assigned to the blue class, and the orange grid indicates the region in which it will be assigned to the orange class.*

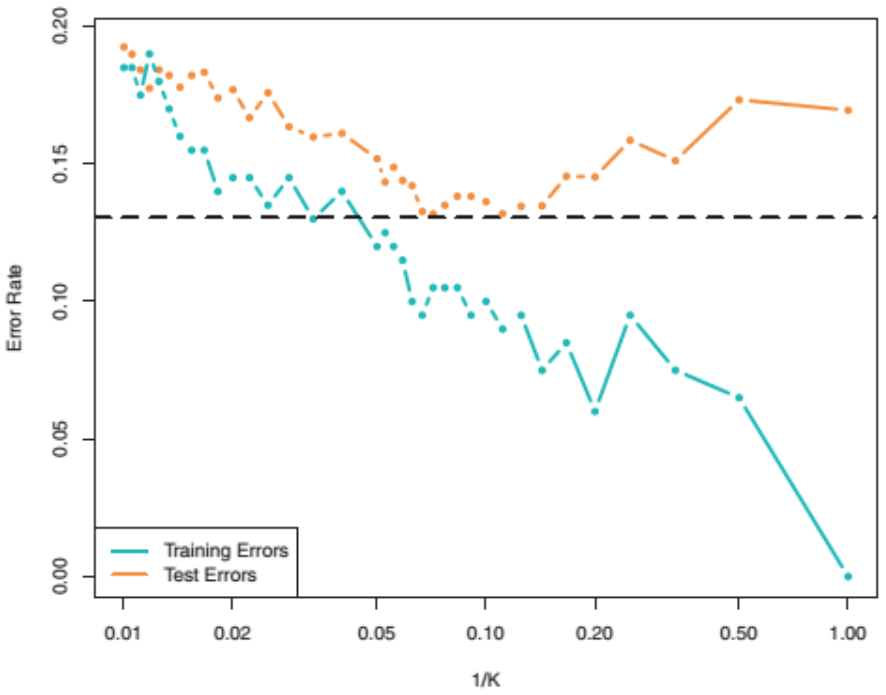
KNN



Test Errors 0.1363 0.1695 0.1925

- *The black curve indicates the KNN decision boundary using K* = 10, 1, 100*. The Bayes decision boundary is shown as a purple dashed line.*

KNN Training-Test Errors



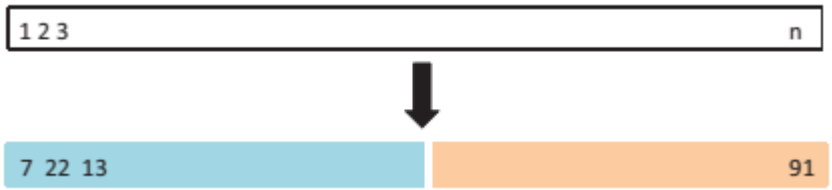
- *The **KNN** training error rate (blue, 200 observations) and test error rate (orange, 5,000 observations), as the level of flexibility (assessed using 1/K) increases, or equivalently as the number of neighbors K decreases. The black dashed line indicates the Bayes error rate. The jumpiness of the curves is due to the small size of the training data set.*

Resampling Methods

- ***Resampling methods*** involve repeatedly drawing samples from a training set and refitting a model of interest on each sample in order to obtain additional information about the fitted model.
- In order to estimate the variability of a linear regression fit, we can repeatedly draw different samples from the training data, fit a linear regression to each new sample, and then examine the extent to which the resulting fits differ.
- Such an approach may allow us to obtain information that would not be available from fitting the model only once using the original training sample.
- Resampling approaches can be computationally expensive, because they involve fitting the same statistical method multiple times using different subsets of the training data.
- ***Cross-validation*** and the ***bootstrap***.
- ***Cross-validation*** can be used to estimate the test error associated with a given statistical learning method in order to evaluate its performance, or to select the appropriate level of flexibility.
- The process of evaluating a model's performance is known as *model assessment*, whereas the process of selecting the proper level of flexibility for a model is known as *model selection*.
- The ***bootstrap*** is used in several contexts, most commonly to provide a measure of accuracy of a parameter estimate or of a given selection statistical learning method.

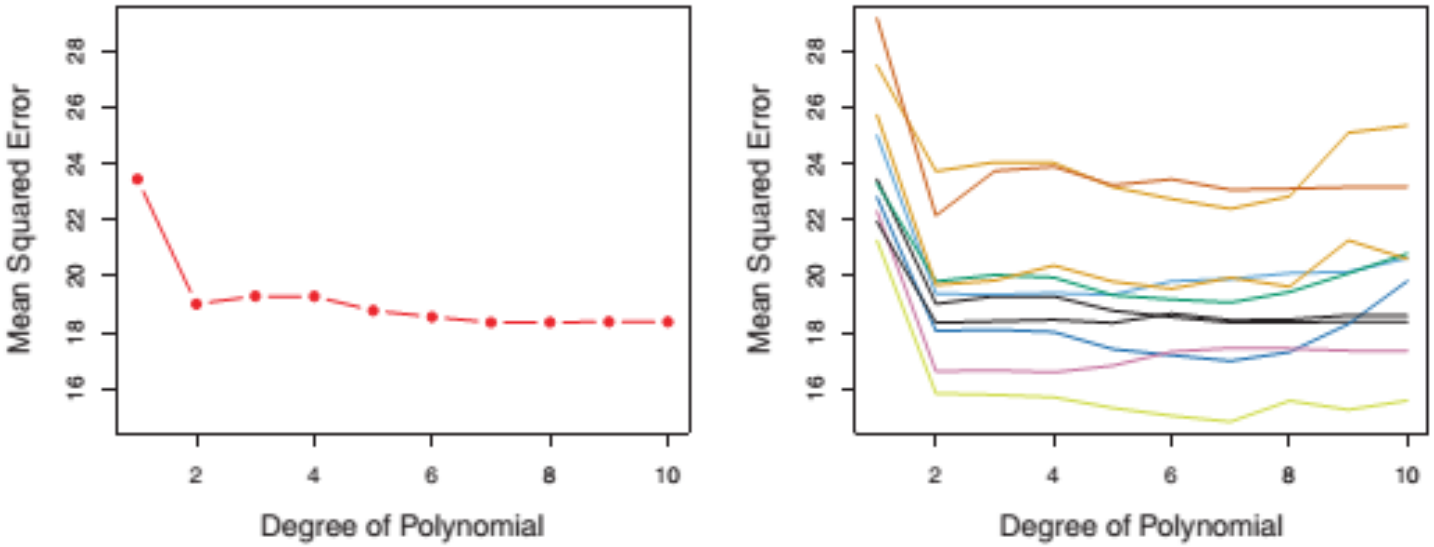
Cross-Validation

- In the absence of a very large designated test set that can be used to directly estimate the test error rate, a number of techniques can be used to estimate this quantity using the available training data.
- *The Validation Set Approach*



- *A schematic display of the validation set approach. A set of **n** observations are randomly split into a training set (shown in blue, containing observations 7, 22, and 13, among others) and a validation set (shown in beige, and containing observation 91, among others). The statistical learning method is fit on the training set, and its performance is evaluated on the validation set.*

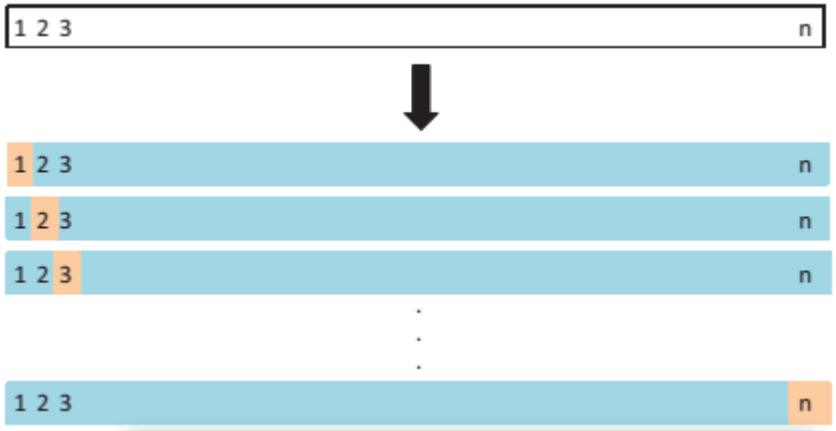
Validation set approach

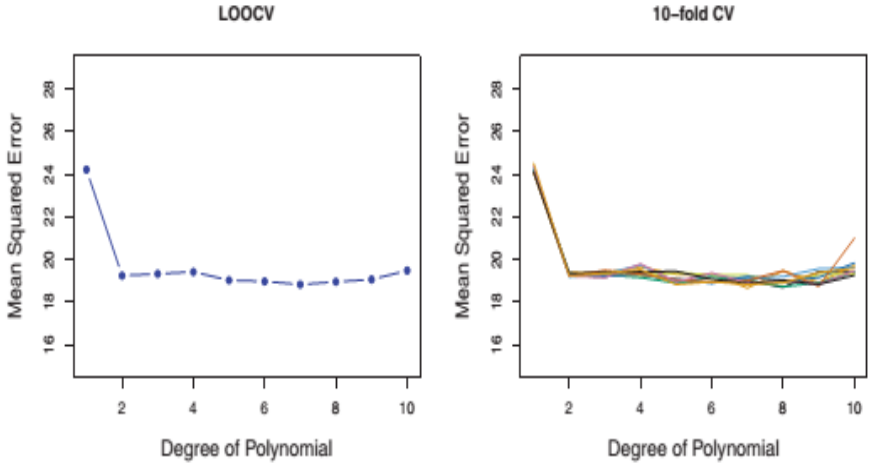


- *The validation set approach was used on the* Auto *data set in order to estimate the test error that results from predicting* mpg *using polynomial functions of* horsepower*.*
- Left: *Validation error estimates for a single split into training and validation data sets.*
- Right: *The validation method was repeated ten times, each time using a different random split of the observations into a training set and a validation set. This illustrates the variability in the estimated test MSE that results from this approach.*

Leave - One - Out Cross - Validation

- Involves splitting the set of observations into two parts.
- However, instead of creating two subsets of comparable size, a single observation (x_1,y_1) is used for the validation set, and the remaining observations $\{(x_2,y_2), \ldots, (x_n,y_n)\}$ make up the training set.





$$\mathrm{CV}_{(n)} = \frac{1}{n}\sum_{i=1}^{n}\mathrm{MSE}_i.$$

k-Fold Cross-Validation

- This approach involves randomly dividing the set of observations into *k* groups, or *folds*, of approximately equal size.
- The first fold is treated as a validation set, and the method is fit on the remaining $k - 1$ folds.
- The mean squared error, MSE_1, is then computed on the observations in the held-out fold. This procedure is repeated *k* times

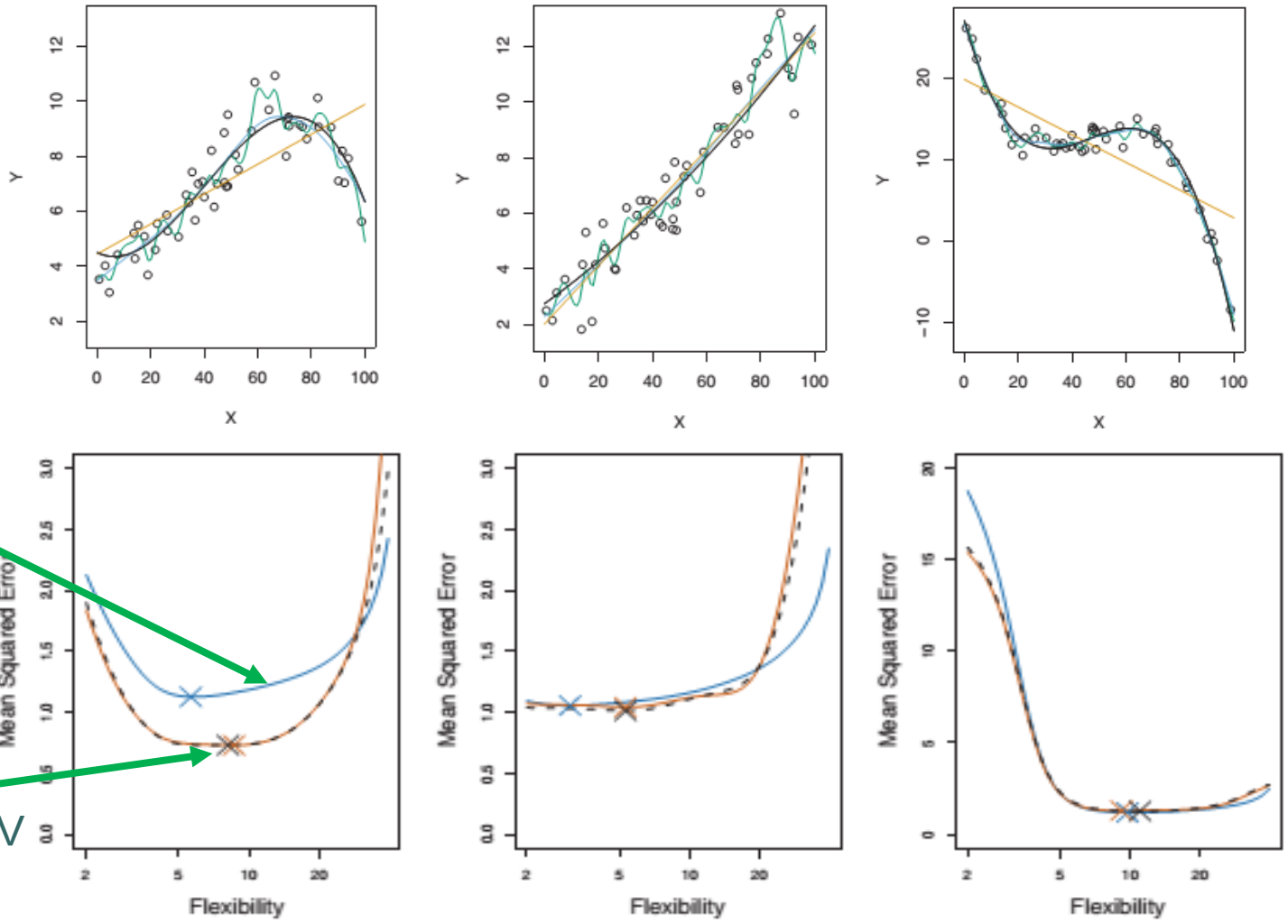
k-Fold Cross-Validation

- This process results in *k* estimates of the test error, MSE_1, MSE_2,..., MSE_k. The *k*-fold CV estimate is computed by averaging these values.

$$\text{CV}_{(k)} = \frac{1}{k} \sum_{i=1}^{k} \text{MSE}_i.$$

- Cross-validation is a very general approach that can be applied to almost any statistical learning method.

k-Fold Cross-Validation



An overview of Classification

- Classification problems occur often, perhaps even more so than regression problems. Some examples include:

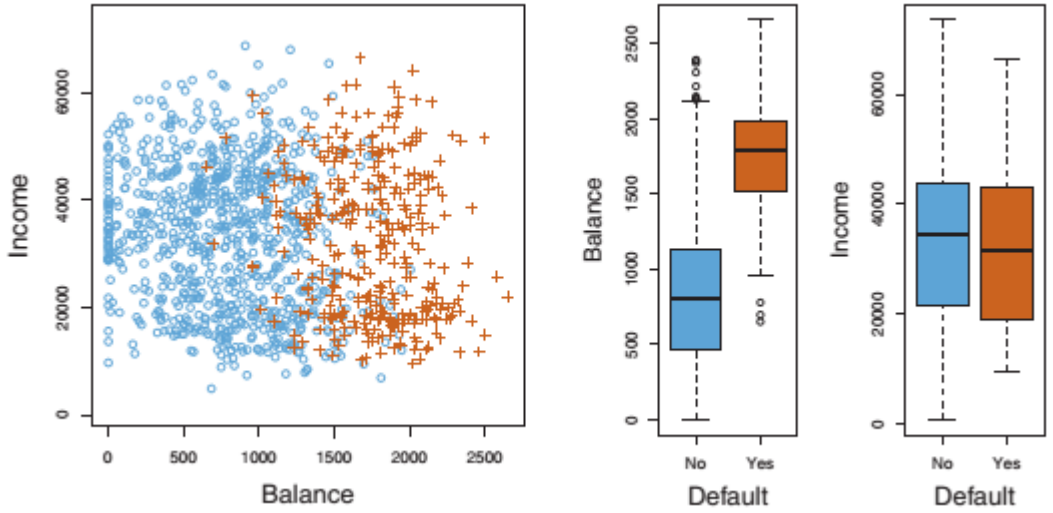
- A person arrives at the emergency room with a set of symptoms that could possibly be attributed to one of three medical conditions. Which of the three conditions does the individual have?

- An online banking service must be able to determine whether or not a transaction being performed on the site is fraudulent, on the basis of the user's IP address, past transaction history, and so forth.

- On the basis of DNA sequence data for a number of patients with and without a given disease, a biologist would like to figure out which DNA mutations are deleterious (disease-causing) and which are not.

Default Dataset

- We are interested in predicting whether an individual will default on his or her credit card payment, on the basis of annual income and monthly credit card balance.

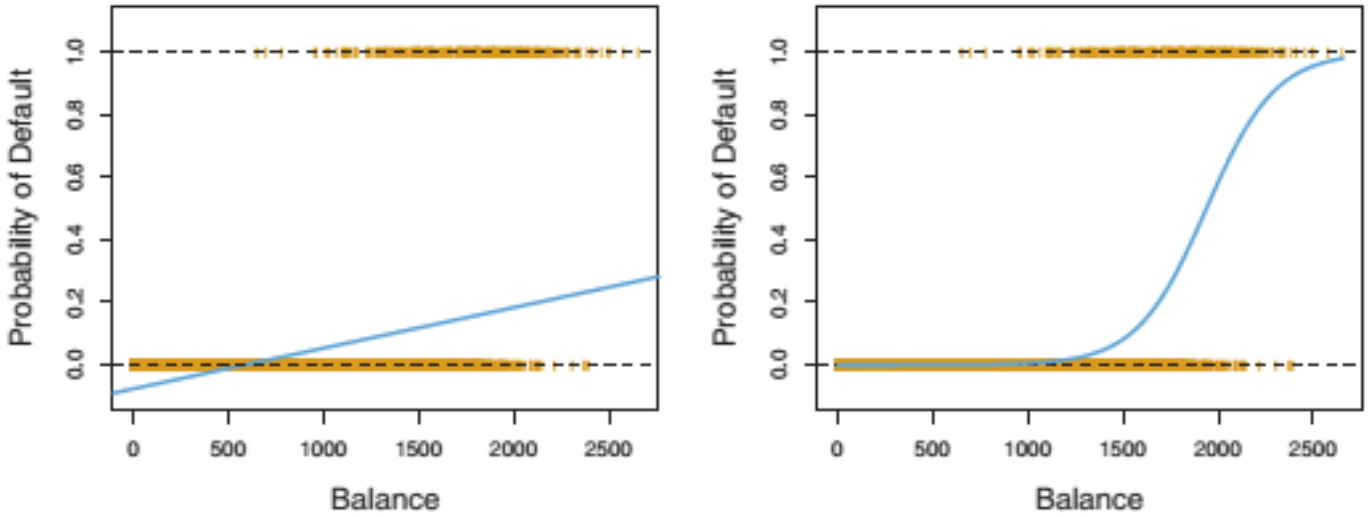


- *The* Default *data set.* Left: *The annual incomes and monthly credit card balances of a number of individuals. The individuals who defaulted on their credit card payments are shown in orange, and those who did not are shown in blue.* Center: *Boxplots of* balance *as a function of* default *status.* Right: *Boxplots of* income *as a function of* default *status.*

Logistic Regression

- Consider again the Default data set, where the response default falls into one of two categories, Yes or No.
- Rather than modeling this response *Y* directly, logistic regression models the *probability* that *Y* belongs to a particular category.

Logistic Regression



- *Classification using the* Default *data.*
- ***Left***: *Estimated probability of* default *using linear regression. The orange ticks indicate the 0/1 values coded for* default(No *or* Yes*).*
- ***Right***: *Predicted probabilities of* default *using logistic regression. All probabilities lie between* 0 *and* 1*.*

Logistic Regression

- For the Default data, logistic regression models the probability of default.
- For example, the probability of default given balance can be written as *Pr(default = Yes|balance), abbreviated as* ***p(balance)***
- For example, one might predict default = Yes for any individual for whom ***p(balance)*** > 0.5
- Alternatively, if a company wishes to be conservative in predicting individuals who are at risk for default, then they may choose to use a lower threshold, such as ***p(balance) > 0.1***

The Logistic Model

- How should we model the relationship between $p(X) = \Pr(Y = 1|X)$ and X? (For convenience we are using the generic 0/1 coding for the response).

$$p(X) = \beta_0 + \beta_1 X.$$

- For balances close to zero we predict a negative probability of default; if we were to predict for very large balances, we would get values bigger than 1.

- These predictions are not sensible, since of course the true probability of default, regardless of credit card balance, must fall between 0 and 1.

Logistic Regression

- Any time a straight line is fit to a binary response that is coded as 0 o r 1 , in principle we can always predict $p(X) < 0$ for some values of X and $p(X) > 1$ for others (unless the range of X is limited).
- To avoid this problem, we must model $p(X)$ using a function that gives outputs between 0 and 1 for all values of X.
- In logistic regression, we use the *logistic function*

$$p(X) = \frac{e^{\beta_0+\beta_1 X}}{1 + e^{\beta_0+\beta_1 X}}.$$

$$\ell(\beta_0, \beta_1) = \prod_{i:y_i=1} p(x_i) \prod_{i':y_{i'}=0} (1 - p(x_{i'})).$$

- We seek estimates for β_0 and β_1 such that the predicted probability $\hat{p}(x_i)$ of default for each individual, corresponds as closely as possible to the individual's observed default status.
- We try to find $\hat{\beta}_0$ and $\hat{\beta}_1$ such that plugging these estimates into the model for $p(X)$, yields a number close to one for all individuals who defaulted, and a number close to zero for all individuals who did not.

Making Predictions

- Once the coefficients have been estimated, it is a simple matter to compute the probability of default for any given credit card balance.
- For example, using the coefficient estimates, we predict that the default probability for an individual with a balance of \$1, 000 is

$$\hat{p}(X) = \frac{e^{\hat{\beta}_0+\hat{\beta}_1 X}}{1+e^{\hat{\beta}_0+\hat{\beta}_1 X}} = \frac{e^{-10.6513+0.0055\times 1{,}000}}{1+e^{-10.6513+0.0055\times 1{,}000}} = 0.00576$$

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

→ Multiple predictors