Lecture 5: Clustering, Linear Regression

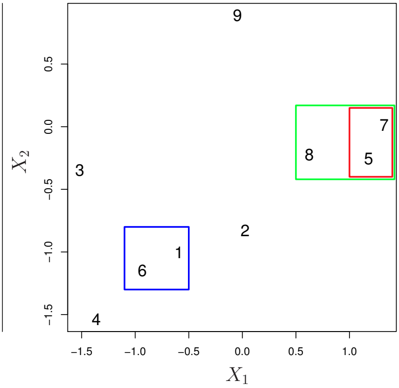
Reading: Chapter 10, Sections 3.1-3.2

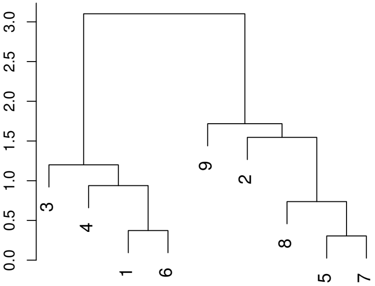
STATS 202: Data mining and analysis

October 2, 2019

Hierarchical clustering

Most algorithms for hierarchical clustering are *agglomerative*.



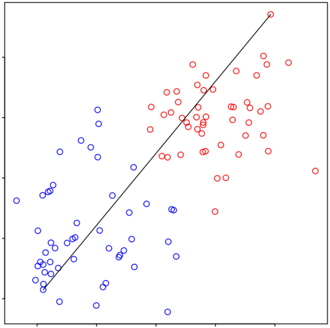


The output of the algorithm is a *dendogram*. We must be careful about how we interpret the dendogram.

Notion of distance between clusters

At each step, we link the 2 clusters that are "closest" to each other.

Hierarchical clustering algorithms are classified according to the notion of distance between clusters.



Complete linkage:
The distance between 2 clusters is the *maximum* distance between any pair of samples, one in each cluster.

Notion of distance between clusters

At each step, we link the 2 clusters that are "closest" to each other.

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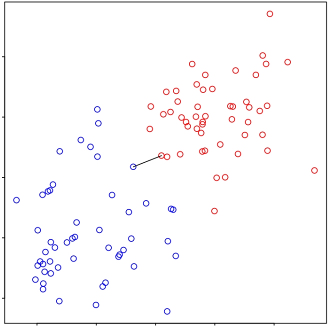
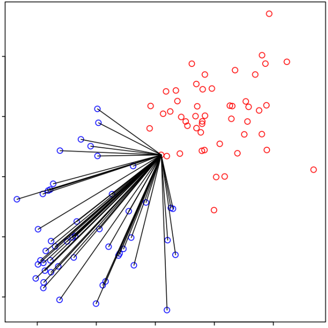


Single linkage:
The distance between 2 clusters is the *minimum* distance between any pair of samples, one in each cluster.

Notion of distance between clusters

At each step, we link the 2 clusters that are “closest” to each other.

Hierarchical clustering algorithms are classified according to the notion of distance between clusters.



Average linkage:
The distance between 2 clusters is the average of all pairwise distances.

Example

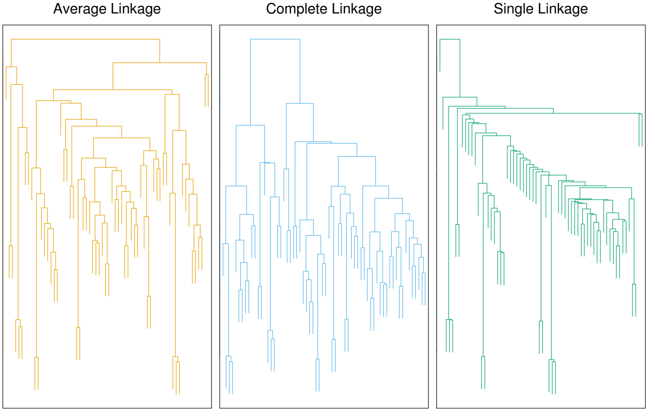


Figure 10.12

Clustering is riddled with questions and choices

- Is clustering appropriate? i.e. Could a sample belong to more than one cluster?
  - Mixture models, soft clustering, topic models.
- How many clusters are appropriate?
  - Choose subjectively — depends on the inference sought.
  - There are formal methods based on gap statistics, mixture models, etc.
- Are the clusters robust?
  - Run the clustering on different random subsets of the data. Is the structure preserved?
  - Try different clustering algorithms. Are the conclusions consistent?
  - Most important: temper your conclusions.

Clustering is riddled with questions and choices

- Should we scale the variables before doing the clustering?
  - Variables with larger variance have a larger effect on the Euclidean distance between two samples.

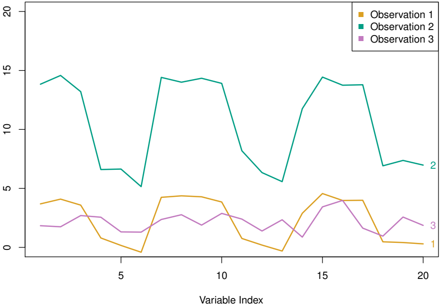
	(	Area in acres,	Price in US$,	Number of houses	)
Property 1	(	10,	450,000,	4	)
Property 2	(	5,	300,000,	1	)

- Does Euclidean distance capture dissimilarity between samples?

Correlation distance

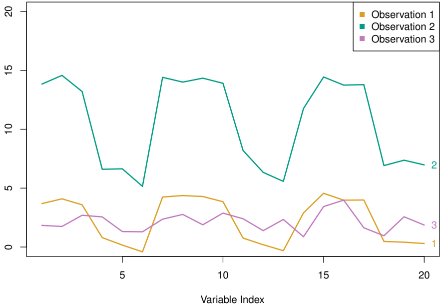
Example: Suppose that we want to cluster customers at a store for market segmentation.

- Samples are customers
- Each variable corresponds to a specific product and measures the number of items bought by the customer during a year.



Correlation distance

- Euclidean distance would cluster all customers who purchase few things (orange and purple).
- Perhaps we want to cluster customers who purchase *similar* things (orange and teal).
- Then, the **correlation distance** may be a more appropriate measure of dissimilarity between samples.



Simple linear regression

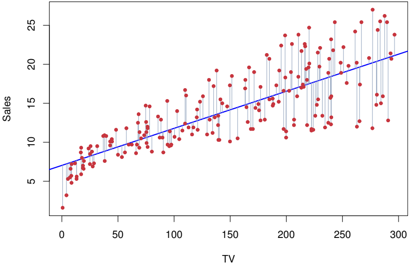


Figure 3.1

$$y_i = \beta_0 + \beta_1 x_i + \varepsilon_i$$

$$\varepsilon_i \sim \mathcal{N}(0, \sigma) \quad \text{i.i.d.}$$

The estimates $\hat{\beta}_0$ and $\hat{\beta}_1$ are chosen to minimize the residual sum of squares (RSS):

$$\begin{aligned} \text{RSS} &= \sum_{i=1}^{n} (y_i - \hat{y}_i)^2 \\ &= \sum_{i=1}^{n} (y_i - \hat{\beta}_0 - \hat{\beta}_1 x_i)^2. \end{aligned}$$

Estimates $\hat{\beta}_0$ and $\hat{\beta}_1$

A little calculus shows that the minimizers of the RSS are:

$$\hat{\beta}_1 = \frac{\sum_{i=1}^{n}(x_i - \overline{x})(y_i - \overline{y})}{\sum_{i=1}^{n}(x_i - \overline{x})^2},$$

$$\hat{\beta}_0 = \overline{y} - \hat{\beta}_1 \overline{x}.$$

Assesing the accuracy of $\hat{\beta}_0$ and $\hat{\beta}_1$

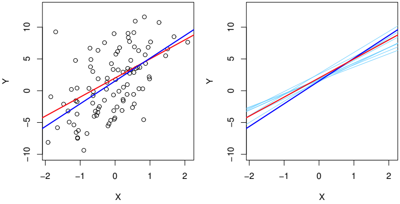


Figure 3.3

The Standard Errors for the parameters are:

$$\text{SE}(\hat{\beta}_0)^2 = \sigma^2 \left[\frac{1}{n} + \frac{\overline{x}^2}{\sum_{i=1}^n (x_i - \overline{x})^2} \right]$$

$$\text{SE}(\hat{\beta}_1)^2 = \frac{\sigma^2}{\sum_{i=1}^n (x_i - \overline{x})^2}.$$

The 95% confidence intervals:

$$\hat{\beta}_0 \pm 2 \cdot \text{SE}(\hat{\beta}_0)$$

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

Hypothesis test

H_0: There is no relationship between X and Y.

H_a: There is some relationship between X and Y.

$$H_0\colon\ \beta_1 = 0.$$

$$H_a\colon\ \beta_1 \neq 0.$$

Test statistic: $\quad t = \frac{\hat{\beta}_1 - 0}{\mathsf{SE}(\hat{\beta}_1)}.$

Under the null hypothesis, this has a t-distribution with $n-2$ degrees of freedom.

	Coefficient	Std. error	t-statistic	p-value
Intercept	7.0325	0.4578	15.36	< 0.0001
TV	0.0475	0.0027	17.67	< 0.0001

TABLE 3.1. *For the* Advertising *data, coefficients of the least squares model for the regression of number of units sold on TV advertising budget. An increase of $1,000 in the TV advertising budget is associated with an increase in sales by around 50 units (Recall that the* sales *variable is in thousands of units, and the* TV *variable is in thousands of dollars).*

Interpreting the hypothesis test

- If we reject the null hypothesis, can we conclude that there is significant evidence of a linear relationship?
  - No. A quadratic relationship may be a better fit, for example.
- If we don't reject the null hypothesis, can we assume there is no relationship between X and Y?
  - No. This test is only powerful against certain monotone alternatives. There could be more complex non-linear relationships.

Multiple linear regression

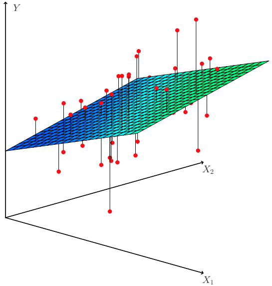


Figure 3.4

$$Y = \beta_0 + \beta_1 X_1 + \cdots + \beta_p X_p + \varepsilon$$

$$\varepsilon \sim \mathcal{N}(0, \sigma) \quad \text{i.i.d.}$$

or, in matrix notation:

$$E\mathbf{y} = \mathbf{X}\beta,$$

where $\mathbf{y} = (y_1, \ldots, y_n)^T$, $\beta = (\beta_0, \ldots, \beta_p)^T$ and $\mathbf{X}$ is our usual data matrix with an extra column of ones on the left to account for the intercept.

Multiple linear regression answers several questions

- Is at least one of the variables X_i useful for predicting the outcome Y?
- Which subset of the predictors is most important?
- How good is a linear model for these data?
- Given a set of predictor values, what is a likely value for Y, and how accurate is this prediction?

The estimates $\hat{\beta}$

Our goal again is to minimize the RSS:

$$\begin{aligned}
\text{RSS} &= \sum_{i=1}^{n} (y_i - \hat{y}_i)^2 \\
&= \sum_{i=1}^{n} (y_i - \hat{\beta}_0 - \hat{\beta}_1 x_{i,1} - \cdots - \hat{\beta}_p x_{i,p})^2.
\end{aligned}$$

One can show that this is minimized by the vector $\hat{\beta}$:

$$\hat{\beta} = (\mathbf{X}^T \mathbf{X})^{-1} \mathbf{X}^T \mathbf{y}.$$

Which variables are important?

Consider the hypothesis:

$H_0 : \beta_{p-q+1} = \beta_{p-q+2} = \cdots = \beta_p = 0.$

Let RSS_0 be the residual sum of squares for the model which excludes these variables. The F-statistic is defined by:

$$F = \frac{(\mathsf{RSS}_0 - \mathsf{RSS})/q}{\mathsf{RSS}/(n-p-1)}.$$

Under the null hypothesis, this has an F-distribution.

Example: If $q = p$, we test whether any of the variables is important.

$$\mathsf{RSS}_0 = \sum_{i=1}^{n} (y_i - \overline{y})^2$$

Which variables are important?

A multiple linear regression in R has the following output:

```
Residuals:
    Min      1Q  Median      3Q     Max
-15.594  -2.730  -0.518   1.777  26.199

Coefficients:
              Estimate Std. Error t value Pr(>|t|)
(Intercept)  3.646e+01  5.103e+00   7.144 3.28e-12 ***
crim        -1.080e-01  3.286e-02  -3.287 0.001087 **
zn           4.642e-02  1.373e-02   3.382 0.000778 ***
indus        2.056e-02  6.150e-02   0.334 0.738288
chas         2.687e+00  8.616e-01   3.118 0.001925 **
nox         -1.777e+01  3.820e+00  -4.651 4.25e-06 ***
rm           3.810e+00  4.179e-01   9.116  < 2e-16 ***
age          6.922e-04  1.321e-02   0.052 0.958229
dis         -1.476e+00  1.995e-01  -7.398 6.01e-13 ***
rad          3.060e-01  6.635e-02   4.613 5.07e-06 ***
tax         -1.233e-02  3.761e-03  -3.280 0.001112 **
ptratio     -9.527e-01  1.308e-01  -7.283 1.31e-12 ***
black        9.312e-03  2.686e-03   3.467 0.000573 ***
lstat       -5.248e-01  5.072e-02 -10.347  < 2e-16 ***
---
Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1

Residual standard error: 4.745 on 492 degrees of freedom
Multiple R-Squared: 0.7406,     Adjusted R-squared: 0.7338
F-statistic: 108.1 on 13 and 492 DF,  p-value: < 2.2e-16
```

Which variables are important?

The t-statistic associated to the ith predictor is the square root of the F-statistic for the null hypothesis which sets only $\beta_i = 0$.

A low p-value indicates that the predictor is important.

Warning: If there are many predictors, even under the null hypothesis, some of the t-tests will have low p-values just by chance.

How many variables are important?

When we select a subset of the predictors, we have 2^p choices.

A way to simplify the choice is to greedily add variables (or to remove them from a baseline model). This creates a sequence of models, from which we can select the best.

- **Forward selection:** Starting from a *null model* (the intercept), include variables one at a time, minimizing the RSS at each step.
- **Backward selection:** Starting from the *full model*, eliminate variables one at a time, choosing the one with the largest p-value at each step.
- **Mixed selection:** Starting from a *null model*, include variables one at a time, minimizing the RSS at each step. If the p-value for some variable goes beyond a threshold, eliminate that variable.

Choosing one model in the range produced is a form of *tuning*.

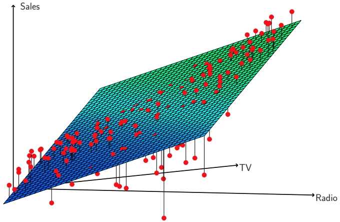
How good is the fit?

To assess the fit, we focus on the residuals.

- The RSS always decreases as we add more variables.
- The residual standard error (RSE) corrects this:

$$\text{RSE} = \sqrt{\frac{1}{n-p-1}\text{RSS}}.$$

- Visualizing the residuals can reveal phenomena that are not accounted for by the model; eg. synergies or interactions:



How good are the predictions?

The function `predict` in R outputs predictions from a linear model:

```
> predict(lm.fit,data.frame(lstat=(c(5,10,15))),
        interval="confidence")
    fit   lwr   upr
1 29.80 29.01 30.60
2 25.05 24.47 25.63
3 20.30 19.73 20.87
```

Confidence intervals reflect the uncertainty on $\hat{\beta}$.

```
> predict(lm.fit,data.frame(lstat=(c(5,10,15))),
        interval="prediction")
    fit    lwr   upr
1 29.80 17.566 42.04
2 25.05 12.828 37.28
3 20.30  8.078 32.53
```

Prediction intervals reflect uncertainty on $\hat{\beta}$ and the irreducible error ε as well.