Introduction to Machine Learning
NPFL 054

http://ufal.mff.cuni.cz/course/npfl054

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Lecture 3

Outline

- **Basic data analysis**
  - data for the Movie recommendation task
  - data for the Verb Pattern Recognition task
- **Clustering**
  - `USArrest` data set

Movie recommendation task (MOV)

Predict the user's rating for a given movie

	Toy Story (1995)	Star Wars (1977)	Some Like It Hot (1959)
Peter	?	5	4
Paul	2	5	?
Mary	2	4	?

E.g., predict Mary's rating for the *Some Like it Hot* movie

MOV – Available data

- **About users**

	age	**gender**	**occupation**	**zip code**
Peter	19	M	student	58644
Mary	50	F	healthcare	60657

- **About movies**

title	**action**	...	**IMDb rating**	**director**
Toy Story	0	...	8.3	John Lasseter
Some Like It Hot	0	...	8.3	Billy Wilder
Star Wars	1	...	8.7	George Lucas

MOV – Getting examples

- Create a database of movies to be rated by users
- Set up a rating scale allowing users to rate movies
- Record users' ratings
- Typically, the dataset of ratings is sparse.
  So do some pruning, like require a minimum of twenty ratings per user

MOV – Data

Basic statistics

number of ratings	100,000
number of movies	1,682
number of users	943

- Data comes from the MovieLens datasets
  – for more details, go to the course web page

MOV – Data representation

	1	**2**	**3**	**4**	**5-8**	**9-33**
vote id	MOVIE	USER	RATING	TIMESTAMP	user features	movie features
1	1	1	5	1997-09-23 00:02:38	24 M technician 85711	Toy Story (1995) ...
...	...	...	...	...	...	...
100,000	1682	916	3	...	...	...

See the feature description mov.pdf at
https://ufal.mff.cuni.cz/course/npfl054/materials

Data analysis

Machine learning process

1. Formulating the task (e.g., predict user's rating for a given movie)
2. Getting data (e.g., MOV data)
    - **Data analysis**
3. Building predictor
4. Evaluation

Data analysis

Deeper understanding the task by statistical view on the data
We exploit the data in order to make prediction of the target value.

- Build intuition and understanding for both the task and the data
- Ask questions and search for answers in the data
  - **What values do we see?**
  - **What associations do we see?**
- Do plotting and summarizing

Data analysis

We focus on

- Recap of methods for basic data exploration
- Analyzing distributions of values
- Analyzing association between features
- Analyzing association between features and target value

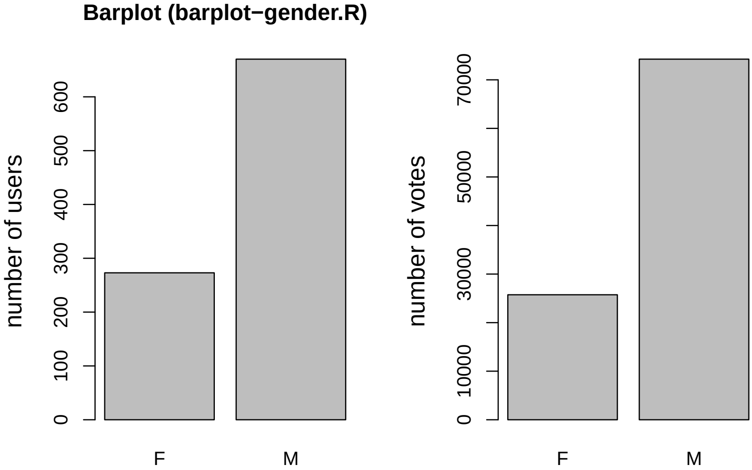
Methods for basic data exploration

Frequency tables display the frequency of categorical feature values.

```
# frequency of voting men and women
> table(examples$gender)
  F   M
25740 74260
```

Methods for basic data exploration

Bar plots visualize frequency tables



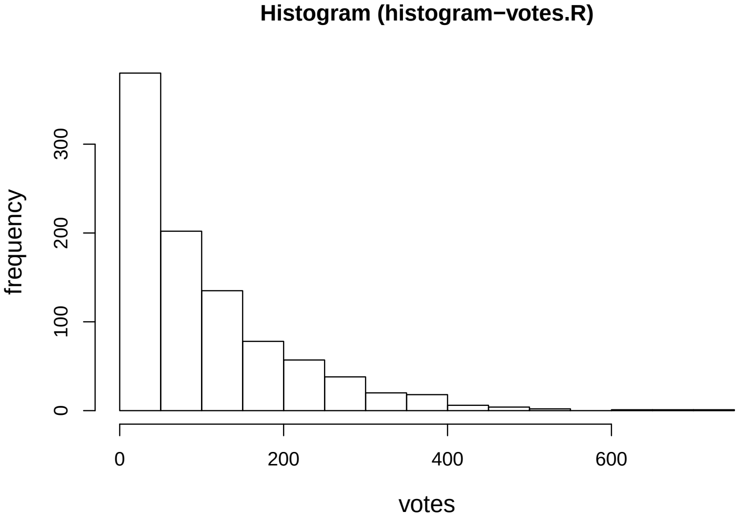
Methods for basic data exploration

Histograms visualize distribution of feature values.

Add a new feature VOTES for the number of votes of the users

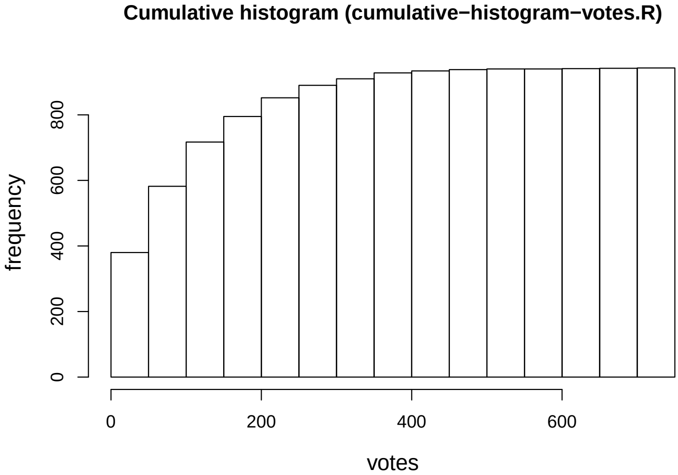
```
# get the number of votes for each user
> v <- as.data.frame(table(examples$user))
> users$votes <- v$Freq
> min(users$votes)
[1] 20
> max(users$votes)
[1] 737
```

Methods for basic data exploration



Methods for basic data exploration

Cumulative histograms visualize cumulative frequencies.



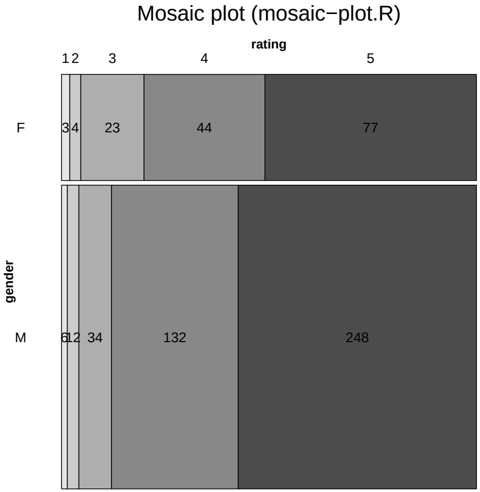
Methods for basic data exploration

Contingency tables display the frequency of values for combination of two categorical features.

```
> # Star Wars ratings
> movie <- subset(examples, movie == 50); nrow(movie) # 583
> # construct contingency table for gender and rating
> ct <- table(movie$gender, movie$rating)
> margin.table(ct)                # total sum
[1] 583
> addmargins(ct)                  # adds marginal sums by default
        1   2   3   4   5 Sum
  F     3   4  23  44  77 151
  M     6  12  34 132 248 432
  Sum   9  16  57 176 325 583
> round(prop.table(ct),3)         # prop.table generates proportions
        1     2     3     4     5
  F 0.005 0.007 0.039 0.075 0.132
  M 0.010 0.021 0.058 0.226 0.425
```

Methods for basic data exploration

Mosaic plots visualize contingency tables.



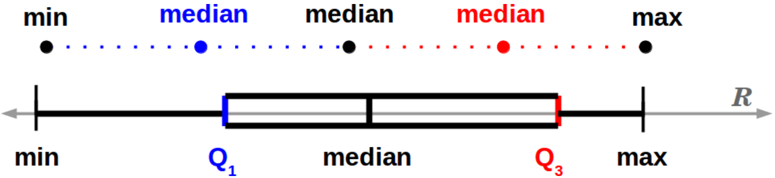
Methods for basic data exploration

Measures of center and variation

```
> min(users$votes);max(users$votes)
[1] 20
[1] 737
> mean(users$votes)
[1] 106.4
> median(users$votes)
[1] 65
> summary(users$votes) # five-number summary
   Min. 1st Qu.  Median    Mean 3rd Qu.    Max.
     20      33      65     106     148     737

> sd(users$votes) # standard deviation
[1] 100.93
```

Methods for basic data exploration

Box-and-whiskers plots visualize five-number summaries.



- Q_3 - Q_1 = interquartile range

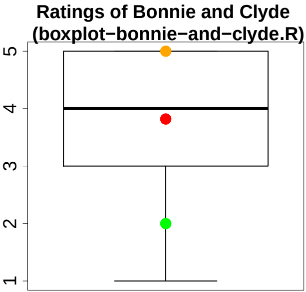
Methods for basic data exploration

Box-and-whiskers plots as indicators of

- centrality
- spread
- symmetry
- tail length

Methods for basic data exploration

Box-and-whiskers plots



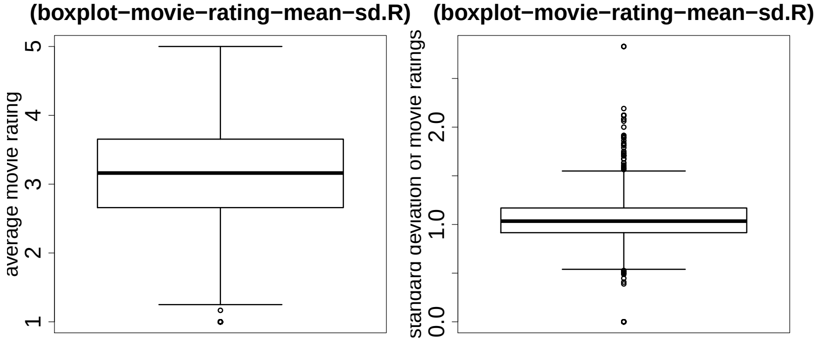
- the sample of 122 ratings

1	2	3	4	5
2	7	35	45	33

- $\mathrm{median}(\mathbf{x}) = 4$
- $\bar{\mathbf{x}} = 3.82$
- $sd(\mathbf{x}) = 0.95$
- the bottom whisker is much longer than the top whisker
- the sample is skewed to the left
- Peter's rating is in green and Mary's rating in orange

Methods for basic data exploration

- **Boxplots are of a great importance** to detect outliers and extreme values
- **Outlier** (**Extreme value**) is an observation that is distant from other observations, typically if it falls more than **1.5** (**3**)$*(Q_3 - Q_1)$ above Q_3 or below Q_1.



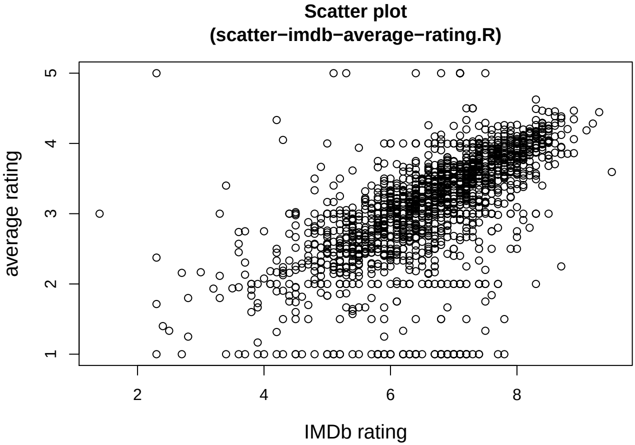
Methods for basic data exploration

Boxplots are of a great importance to detect outliers and extreme values

```
> boxplot <- boxplot(tapply(votes$rating, votes$movie, sd))
# analyze outliers
> boxplot$out[1:2]
     247      314
1.788854 0.000000
>
> subset(votes, movie == 247) # Turbo: A Power Rangers Movie
      user movie rating           timestamp
38147   38   247      5 1998-04-13 03:04:20
38148    1   247      1 1997-09-26 04:40:19
38149  374   247      1 1997-12-01 01:35:22
38150  222   247      1 1997-11-05 08:29:58
38151  782   247      1 1998-04-02 08:48:20

> movies[movies$movie == 247,]
247 Turbo: A Power Rangers Movie (1997)  28-Mar-1997 ...
```

Methods for basic data exploration

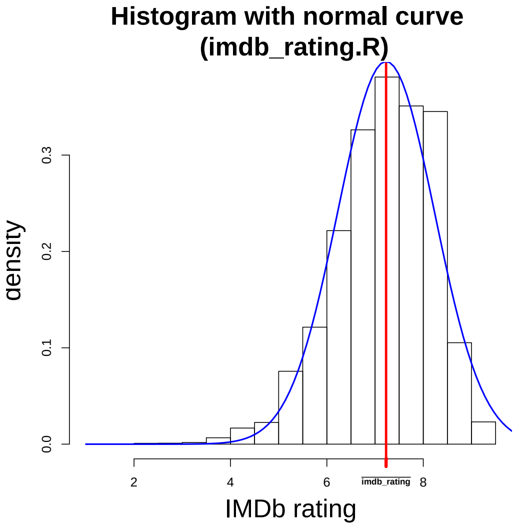
Scatter plots display values of two numerical features.



Analyzing distributions of values

Analyzing imdb_rating

- **What kind of probability distribution characterizes the IMDb ratings?**



Analyzing distributions of values

Analyzing imdb_rating

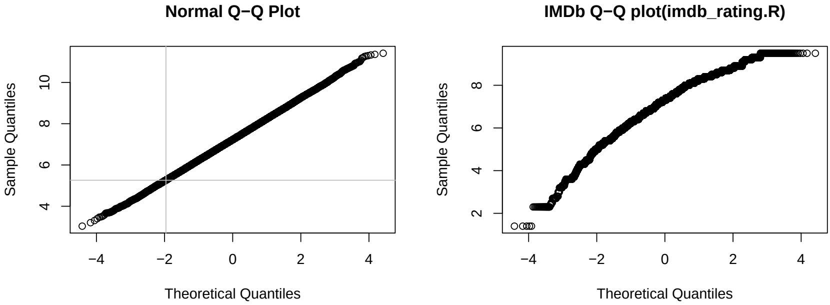
Does `imdb_rating` follow a normal distribution?

- Visualize the distribution using a quantile-quantile plot
- Use a distribution test

Analyzing distributions of values

Analyzing imdb_rating

Visualize the distribution using a quantile-quantile plot



- **Draw a conclusion**: `imdb_rating` does not follow a normal distribution.

Association between feature and target value
Numerical features

Pearson correlation coefficient is a measure of the linear relationship between two variables

- **For a population**

$$-1 \leq \rho_{X,Y} = \frac{\mathrm{cov}(X,Y)}{\sigma_X \sigma_Y} \leq +1$$

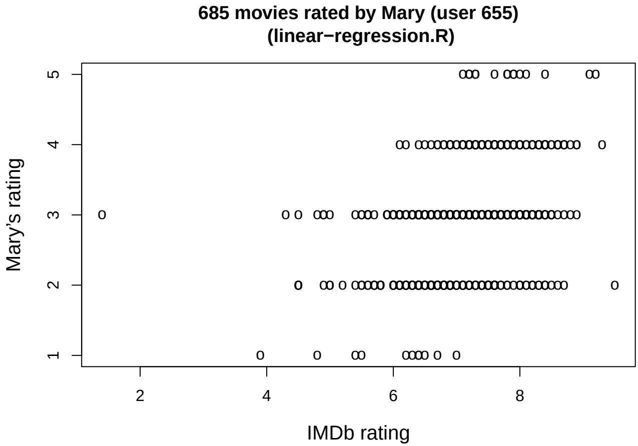
  - perfect negative correlation if $\rho = -1$
  - perfect positive correlation if $\rho = +1$
  - not linear relationship if $\rho = 0$

- **For a sample**

$$-1 \leq r_{X,Y} = \frac{\frac{1}{n-1}\sum_{i=1}^{n}(x_i - \bar{x})(y_i - \bar{y})}{s_X s_Y} \leq +1$$

Association between feature and target value
Numerical features

Association between Mary's ratings and the IMDb ratings



Association between feature and target value
Numerical features

$r(\mathrm{Peter's\ rating}, \mathrm{imdb\_rating})$	0,51
$r(\mathrm{Paul's\ rating}, \mathrm{imdb\_rating})$	0,44
$r(\mathrm{Mary's\ rating}, \mathrm{imdb\_rating})$	0,37

Association between features
Numerical features

$r(\text{Peter's rating}, \text{Mary's rating})$	0,29
$r(\text{Peter's rating}, \text{Paul's rating})$	0,29
$r(\text{Paul's rating}, \text{Mary's rating})$	0,24

Association between feature and target value
Categorical features

Pearson's χ^2 test
This test compares observed frequencies O_{ij} with theoretical frequencies E_{ij} that we would expect in case of statistical independence of X and Y. Test statistic $\chi^2 = \sum_{i=1}^{r} \sum_{j=1}^{s} \frac{(O_{ij} - E_{ij})^2}{E_{ij}}$ follows a χ^2 distribution with $(r-1)(s-1)$ degrees of freedom when the null hypothesis is true (r/s is the number of rows/columns in the contingency table).

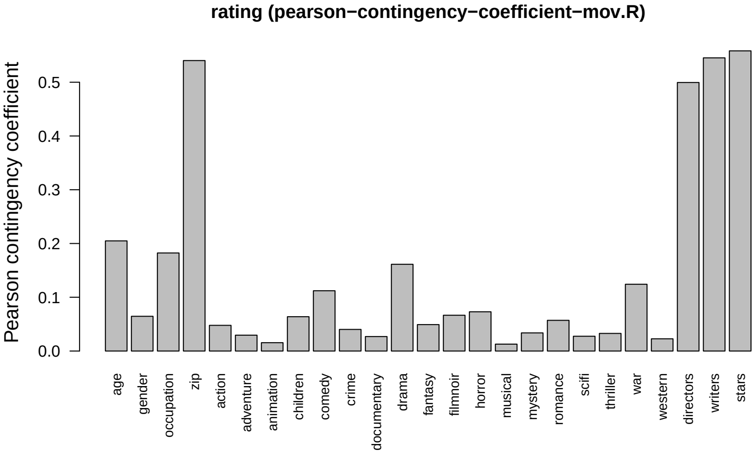
Pearson contingency coefficient

$$0 < \sqrt{\frac{\chi^2}{n + \chi^2}} < 1$$

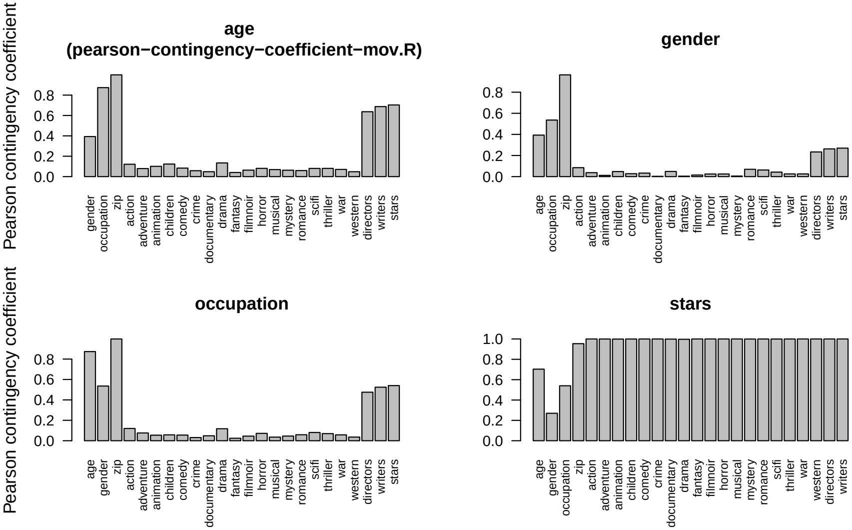
- perfect correlation if $\rightarrow 1$
- no correlation if $\rightarrow 0$

Note: Correction such that the coefficient can take values between 0 and 1 (which is not true if $r \neq s$): $\sqrt{\frac{\chi^2}{n+\chi^2}} \,/\, \sqrt{\frac{min(r;s)-1}{min(r;s)}}$

Association between feature and target value
Categorical features



Association between features
Categorical features



Analyzing values
Feature frequency

- **Feature frequency**

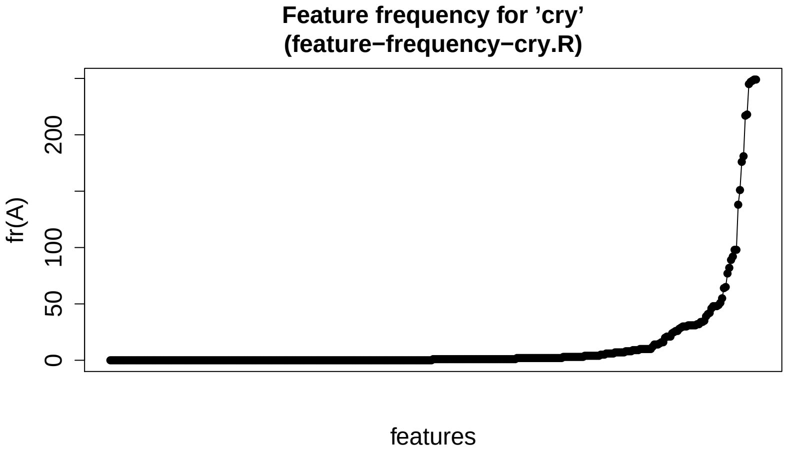
$$\mathrm{fr}(A_j) = \#\{\mathbf{x}_i \mid x_i^j > 0\}$$

where A_j is the j-th feature (binary), $\mathbf{x}_i$ is the feature vector of the i-th instance, and x_i^j is the value of A_j in $\mathbf{x}_i$.

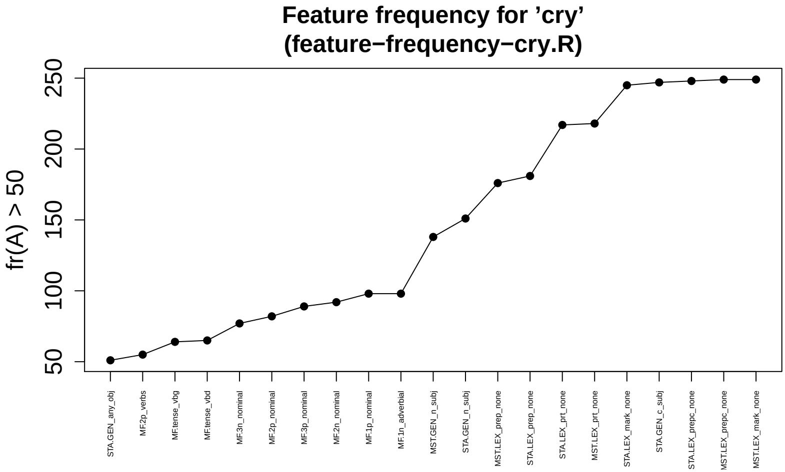
Analyzing values
Feature frequency – VPR data (cry)

```
> examples <- read.csv("cry.development.csv", sep="\t")
> c <- examples[,-c(1,ncol(examples))]
> nrow(examples)
[1] 250
> length(names(c)) # get the number of features
[1] 363
# compute feature frequency using the fr function (see feature-frequency-cry.R)
> ff <- apply(c, 2, fr) # apply fr to columns ('2') of c
> table(sort(ff))
  0   1   2   3   4   5   6   7   8   9  10  12  14  15  16  20
181  47  26  12   9   3   5   6   4   4   7   1   3   1   2   1

21 24 25 26 28  29  30  31  32  34  35  39  41  42  46  48  49
 3  1  1  2  1   1   3   5   2   2   1   1   1   1   1   3   1

51  55  64  65  77  82  89  92  98 138 151 176 181 217 218 245
 1   1   1   1   1   1   1   1   2   1   1   1   1   1   1   1

247 248 249
  1   1   2
```

Analyzing values
Feature frequency – VPR data (cry)



Analyzing values
Feature frequency – VPR data (cry)



Analyzing values
Feature frequency – VPR data (cry)

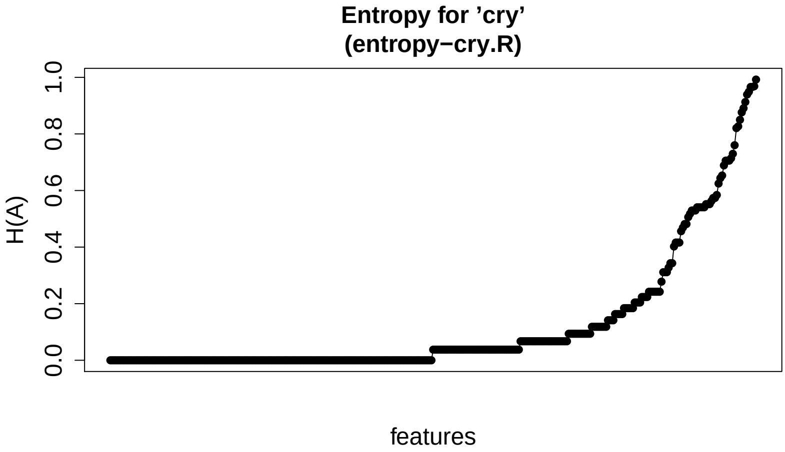
Filter out uneffective features from the CRY data

```
> examples <- read.csv("cry.development.csv", sep="\t")
> n <- nrow(examples)
> ## remove id and target class tp
> c <- examples[,-c(1,ncol(examples))]

> ## remove features with 0s only
> c.1 <- c[, !lapply(c,fr) == 0  ]
> ## remove features with 1s only
> c.2 <- c.1[, !lapply(c.1,fr) == n  ]
> ## remove column duplicates
> # unique removes duplicate rows
> c.effective <- data.frame(t(unique(t(as.matrix(c.2)))))

> ncol(c)             # get the number of input features
[1] 363
> ncol(c.effective)   # get the number of effective features
[1] 168
```

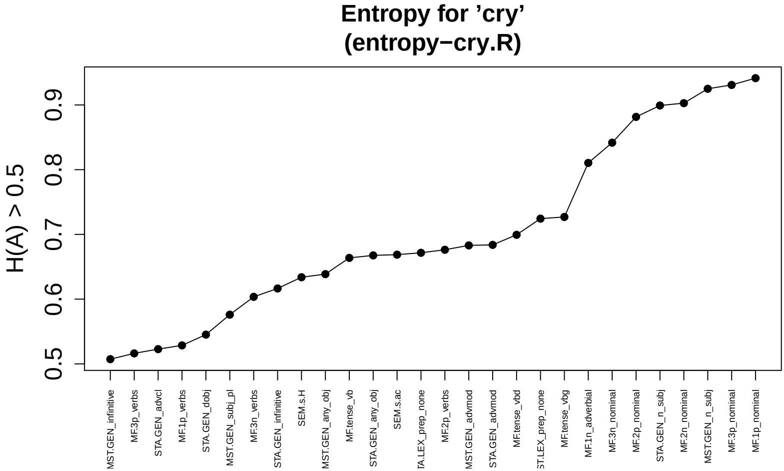
Analyzing values
Entropy – VPR data (cry)

```
# compute entropy using the entropy function (see entropy-cry.R)
> e <- apply(c, 2, entropy)
> table(sort(round(e,2)))
   0 0.04 0.07 0.09 0.12 0.14 0.16 0.18  0.2 0.22 0.24 0.28 0.31 0.33
 181   49   27   13    9    4    5    6    4    4    7    1    3    1

 0.34  0.4 0.42 0.46 0.47 0.48 0.51 0.52 0.53 0.54 0.55 0.56 0.57 0.58
    2    1    3    1    1    2    1    1    3    5    3    1    2    1

 0.62 0.64 0.65 0.69 0.71 0.73 0.76 0.82 0.83 0.85 0.88 0.89 0.91 0.94
    1    1    1    1    4    1    1    1    1    1    1    1    1    1

 0.95 0.97 0.99
    1    3    1
```

Analyzing values
Entropy – VPR data (cry)



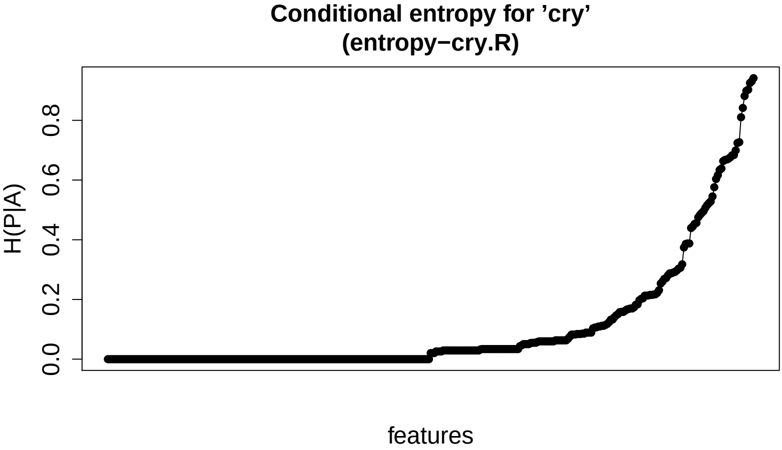
Analyzing values
Entropy – VPR data (cry)



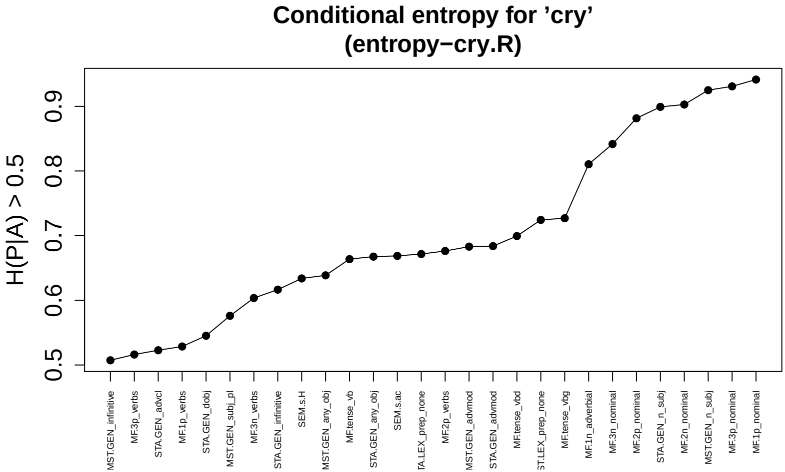
Association between feature and target value
Conditional entropy – VPR data (cry)

```
# compute conditional entropy using entropy.cond (see entropy-cry.R)
ce <- apply(c, 2, entropy.cond, y=examples$tp)
table(sort(round(ce,2)))
  0 0.02 0.03 0.04 0.05 0.06 0.07 0.08 0.09  0.1 0.11 0.12 0.13 0.14 0.15 0.16
 181    3   47    1    7   19    1    7    6    1    7    2    2    1    2    4
0.17 0.18  0.2 0.21 0.22 0.23 0.25 0.26 0.27 0.28 0.29  0.3 0.31 0.32 0.37 0.39
   5    2    3    3    5    1    1    1    2    1    4    2    1    1    1    3
0.44 0.45 0.46 0.48 0.49  0.5 0.51 0.52 0.53 0.55 0.58  0.6 0.62 0.63 0.64 0.66
   1    2    1    2    1    1    1    2    1    1    1    1    1    1    1    1
0.67 0.68  0.7 0.72 0.73 0.81 0.84 0.88  0.9 0.92 0.93 0.94
   3    3    1    1    1    1    1    1    2    1    1    1
```

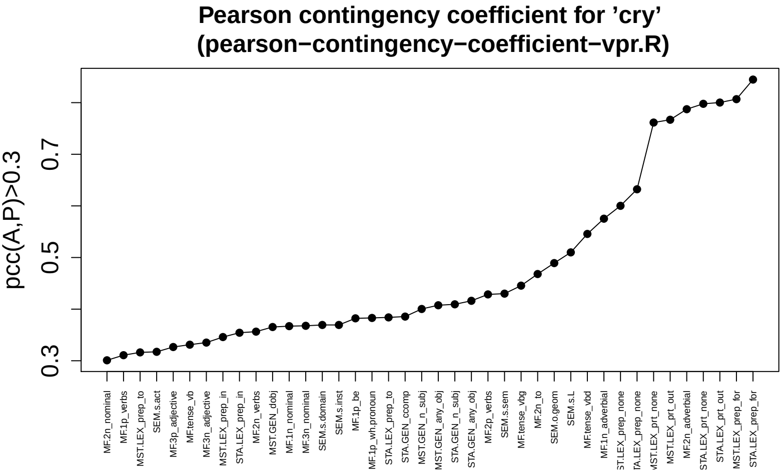
Association between feature and target value Conditional entropy – VPR data (cry)



Association between feature and target value
Conditional entropy – VPR data (cry)



Association between feature and target value
Pearson contingency coefficient – VPR data (cry)

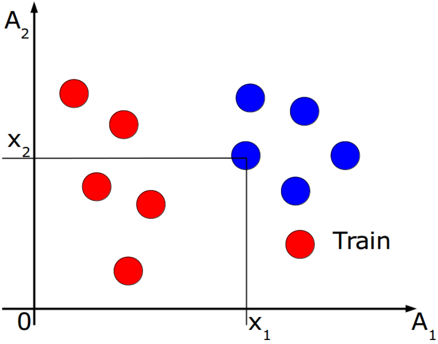


Pearson contingency coefficient for 'cry'
(pearson−contingency−coefficient−vpr.R)

Clustering
Supervised vs. Unsupervised learning

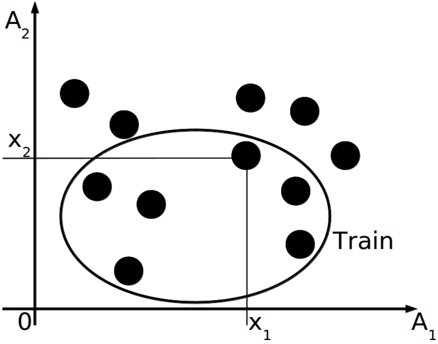
Supervised learning

$Data = \{\langle \mathbf{x}, y \rangle : \mathbf{x} \in X, y \in Y\}$



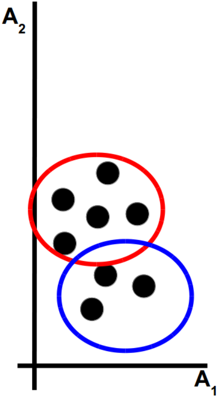
Unsupervised learning

$Data = \{\mathbf{x} : \mathbf{x} \in X\}$



Clustering

Clustering finds homogenous subgroups among the instances in the unlabeled data.



Clustering

Discovering structure

The most common criteria

- **Homogeneity**
  Objects within a same cluster should be similar each other
- **Separation**
  Objects in different clusters should be dissimilar from each other

Clustering
Similarity

The most common one:

- **Cosine similarity**

$$\mathrm{sim}(\mathbf{u},\mathbf{v}) = \mathbf{u}\cdot\mathbf{v}/\sqrt{\mathbf{u}\cdot\mathbf{u} * \mathbf{v}\cdot\mathbf{v}}$$

Clustering
Dissimilarity

Dissimilarity can be thought of as distance. The most common ones:

- **Euclidean distance** – continuous features

$$\mathrm{d}(\mathbf{u}, \mathbf{v}) = \sqrt{\sum_{i=1}^{m} (u_i - v_i)^2}$$

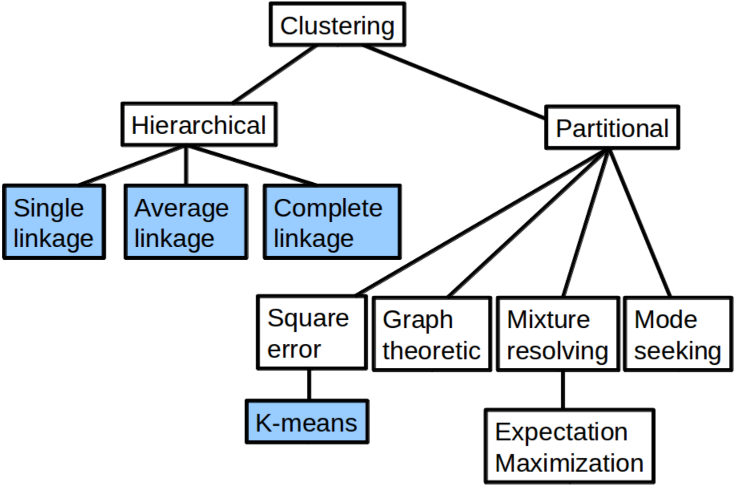
- **Manhattan distance** – continuous features

$$\mathrm{d}(\mathbf{u}, \mathbf{v}) = \sum_{i=1}^{m} |u_i - v_i|$$

- **Hamming distance** – categorical features

$$\mathrm{d}(\mathbf{u}, \mathbf{v}) = \sum_{i=1}^{m} (u_i \neq v_i)$$

Clustering algorithms



Credits: (Kononenko, Kukar, 2007)

Clustering algorithms

- $Data = \{\mathbf{x}_1, \mathbf{x}_2, \ldots, \mathbf{x}_n\}$
- A set of k clusters $C = \{C_1, C_2, \ldots, C_k\}$ containing the indeces of the instances
- $C_1 \cup \cdots \cup C_k = \{1, 2, \ldots, n\}$
- $C_j \cap C_i = \emptyset, \forall i \neq j$
- i-th cluster centroid $\mu(C_i) = \frac{1}{|C_i|} \sum_{\mathbf{x} \in C_i} \mathbf{x}$

Clustering algorithms
Loss functions

$d(\mathbf{x}_l, \mathbf{x}_j)$ – Euclidean distance

- **Within-cluster variation** $L(C_i)$

$$L(C_i) = \frac{1}{|C_i|} \sum_{\mathbf{x}_l, \mathbf{x}_j \in C_i} d(\mathbf{x}_l, \mathbf{x}_j)^2$$

- **Total within-cluster variation** $L(C_1, \dots, C_k)$

$$L(C_1, \dots, C_K) = \sum_{i=1}^{K} L(C_i)$$

K-means algorithm

K-means optimization problem

$$\mathrm{argmin}_{C_1,\ldots,C_K} L(C_1,\ldots,C_K) = \mathrm{argmin}_{C_1,\ldots,C_K} \sum_{i=1}^{K} L(C_i) \tag{1}$$

The number of all possible assignments of n instances into K clusters is

$$\frac{1}{K!}\sum_{k=1}^{K}(-1)^{K-k}\binom{K}{k}k^n$$

Computationally expensive :-(But ...

- Prove

$$\frac{1}{C_k}\sum_{\mathbf{x}_i,\mathbf{x}_j\in C_k} d(\mathbf{x}_i,\mathbf{x}_j)^2 = 2\sum_{\mathbf{x}\in C_k} d(\mathbf{x},\mu(C_k))^2$$

K-means algorithm

```
1. Create clusters $C_1^0, \ldots, C_K^0$:
    • randomly assign a number, from 1 to $K$, to each of the instance
2. while *total within-cluster variation does change* do
    a) for all clusters $C_i^t$, $i = 1, \ldots, K$ do
        $\mu(C_i^t) = \frac{1}{|C_i^t|} \sum_{\mathbf{x} \in C_i^t} \mathbf{x}$
    b) for all clusters $C_i^t$, $i = 1, \ldots, K$ do
        $C_i^{t+1} = \{\mathbf{x}; d(\mathbf{x}, \mu(C_i^t))^2 \leq d(\mathbf{x}, \mu(C_l^t))^2, \forall l \neq i\}$
```

This algorithm finds a local rather than a global optimum.

Dataset `USArrests` from the base R distribution

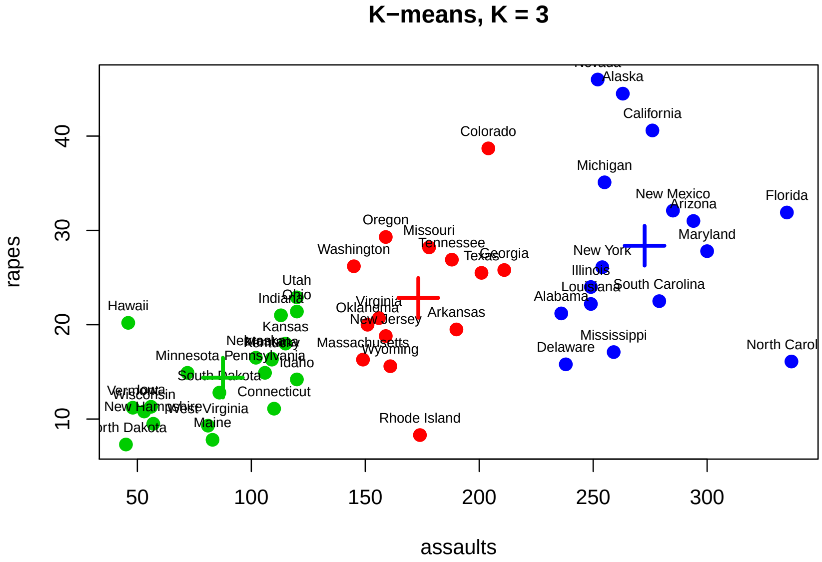
– statistics in arrests per 100,000 residents in each of the 50 US states in 1973

```
> attributes(USArrests)
$names
[1] "Murder"   "Assault"  "UrbanPop" "Rape"
#UrbanPop is the percent of the population living in urban areas
$class
[1] "data.frame"
$row.names
 [1] "Alabama"        "Alaska"         "Arizona"        "Arkansas"
 [5] "California"     "Colorado"       "Connecticut"    "Delaware"
 [9] "Florida"        "Georgia"        "Hawaii"         "Idaho"
[13] "Illinois"       "Indiana"        "Iowa"           "Kansas"
[17] "Kentucky"       "Louisiana"      "Maine"          "Maryland"
[21] "Massachusetts"  "Michigan"       "Minnesota"      "Mississippi"
[25] "Missouri"       "Montana"        "Nebraska"       "Nevada"
[29] "New Hampshire"  "New Jersey"     "New Mexico"     "New York"
[33] "North Carolina" "North Dakota"   "Ohio"           "Oklahoma"
[37] "Oregon"         "Pennsylvania"   "Rhode Island"   "South Carolina'
[41] "South Dakota"   "Tennessee"      "Texas"          "Utah"
[45] "Vermont"        "Virginia"       "Washington"     "West Virginia"
[49] "Wisconsin"      "Wyoming"
```

K-means algorithm with the `USArrests` data

```
> str(USArrests)
’data.frame’: 50 obs. of  4 variables:
 $ Murder  : num  13.2 10 8.1 8.8 9 7.9 3.3 5.9 15.4 17.4 ...
 $ Assault : int  236 263 294 190 276 204 110 238 335 211 ...
 $ UrbanPop: int  58 48 80 50 91 78 77 72 80 60 ...
 $ Rape    : num  21.2 44.5 31 19.5 40.6 38.7 11.1 15.8  ...

> d <- USArrests
> examples <- d[,c(2,4)]
> km.3 <- kmeans(examples, 3, nstart=20)
> km.3$tot.withinss
[1] 38435.53
> km.3$withinss
[1] 15847.167  7109.191 15479.168
```

K-means algorithm with the `USArrests` data



K-means algorithm with the `USArrests` data

Multiple initial cluster assignments (`nstart`)

```
> km.1 <- kmeans(examples,6,nstart=1)
> km.1$tot.withinss
[1] 13711.87
>
> km.20 <- kmeans(examples,6,nstart=20)
> km.20$tot.withinss
[1] 10282.92
```

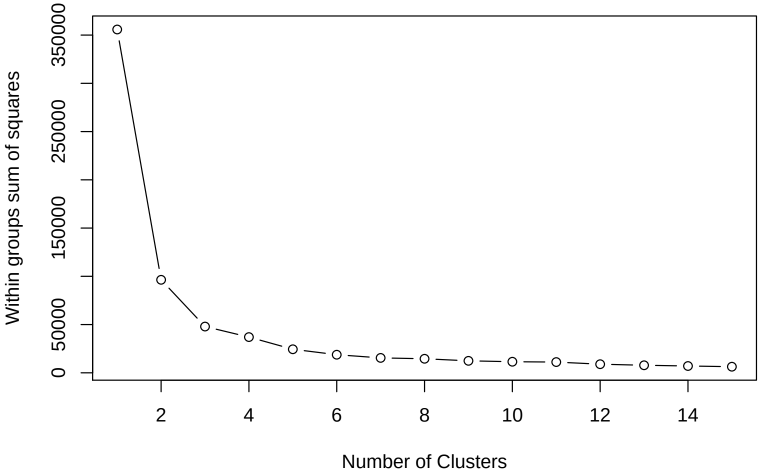
K-means algorithm with the `USArrests` data

Which K to choose?

```
> km.3 <- kmeans(d, 3, nstart=20)
> km.3$tot.withinss
[1] 47964.27
> km.3$withinss
[1]  9136.643 19263.760 19563.863
>
> wssplot(d) # to be presented in the lab
```

K-means algorithm with the `USArrests` data

Which K to choose?



K-means algorithm

Remarks

- The results depend on the initial clusters. The standard solution is to try a number of different starting points (see `nstart` in R).
  This is an annoyance that must be handled in an implementation.
- The results depend on the metric used to measure similarity.
- The results depend on the value of K.

Hierarchical clustering methods

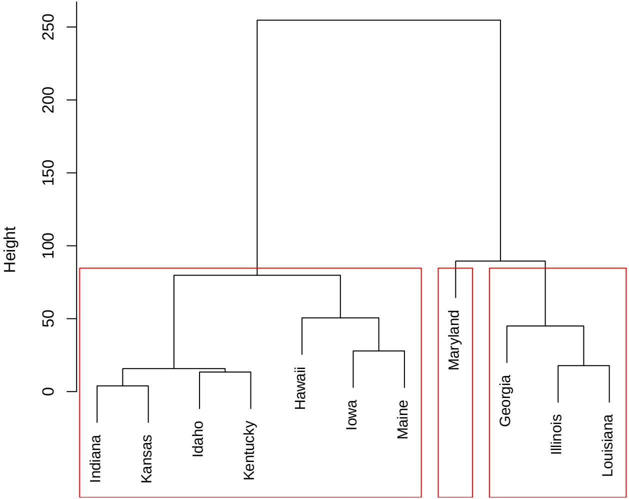
- do not require specification of the number of clusters.
- do produce tree-based representation of the instances, called **dendrogram**

Dendrogram

is a rooted binary tree where

- the root node represents an input data set $Data, |Data| = n$
- the internal nodes represent the groups of instances
- each non-terminal node has two daughter nodes
- each terminal node represents one of the input instances (n terminal nodes)

Dendrogram


Height
0
50
100
150
200
250
Indiana
Kansas
Idaho
Kentucky
Hawaii
Iowa
Maine
Maryland
Georgia
Illinois
Louisiana

How to read a dendrogram

- location of instances on the horizontal axis says nothing about the similarity
- location on the vertical axis: dissimilarity between the clusters when they were merged
- cutting the dendrogram $\sim$ getting clusters

Hierarchical clustering methods

Agglomerative (bottom-up) clustering

1. Start with each instance in its own singleton cluster
2. At each step, greedily merge 2 most similar clusters
3. Stop when there is a single cluster of all examples, else go to 2

Divisive (top-down) clustering

1. Start with all instances in the same cluster
2. At each step, remove the “outsiders” from the least cohesive cluster
3. Stop when each example is in its own singleton cluster, else go to 2

Agglomerative (bottom-up) hierarchical methods

```
1 for i := 1 to $n$ do $C_i := \{\mathbf{x}_i\}$ end
2 $C := \{C_1, C_2, \ldots, C_n\}$
3 $j := n + 1$
4 while $|C| > 1$
    1 $(C_{n_1}, C_{n_2}) := \mathrm{argmax}_{C_u, C_v \in C \times C} \mathrm{sim}(C_u, C_v)$
    2 $C_j = C_{n_1} \cup C_{n_2}$
    3 $C := C \setminus \{C_{n_1}, C_{n_2}\} \cup C_j$
    4 $j := j + 1$
```

Agglomerative hierarchical methods

Work with distance (dissimilarity) measures

- **dissimilarity between instances** $d(\mathbf{x}_i, \mathbf{x}_j)$
- **dissimilarity between clusters** $d(C_u, C_v)$
  - then 4.1. in the algorithm is

    $(C_{n_1}, C_{n_2}) := \mathrm{argmin}_{C_u, C_v \in C \times C}\, d(C_u, C_v)$

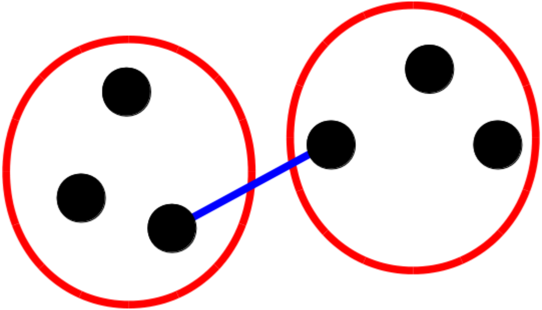
    where $d(C_u, C_v)$ is a **linkage function**

The choice of linkage function determines how we measure dissimilarity between clusters.

Dissimilarity between clusters
Single linkage clustering

The minimum dissimilarity between instances of each cluster

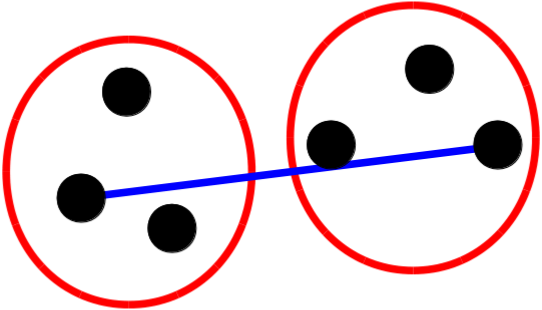
$$d(C_u, C_v) = \min_{\mathbf{x}_i \in C_u, \mathbf{x}_j \in C_v} d(\mathbf{x}_i, \mathbf{x}_j)$$



Dissimilarity between clusters
Complete linkage clustering

The maximum dissimilarity between instances of each cluster

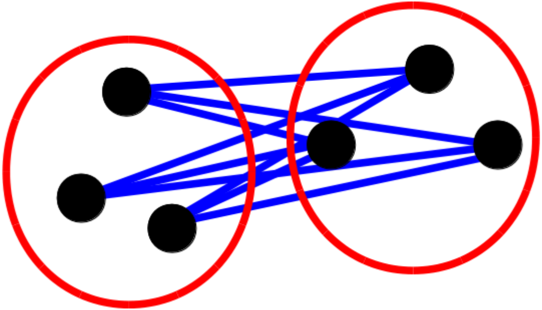
$$d(C_u, C_v) = \max_{\mathbf{x}_i \in C_u, \mathbf{x}_j \in C_v} d(\mathbf{x}_i, \mathbf{x}_j)$$



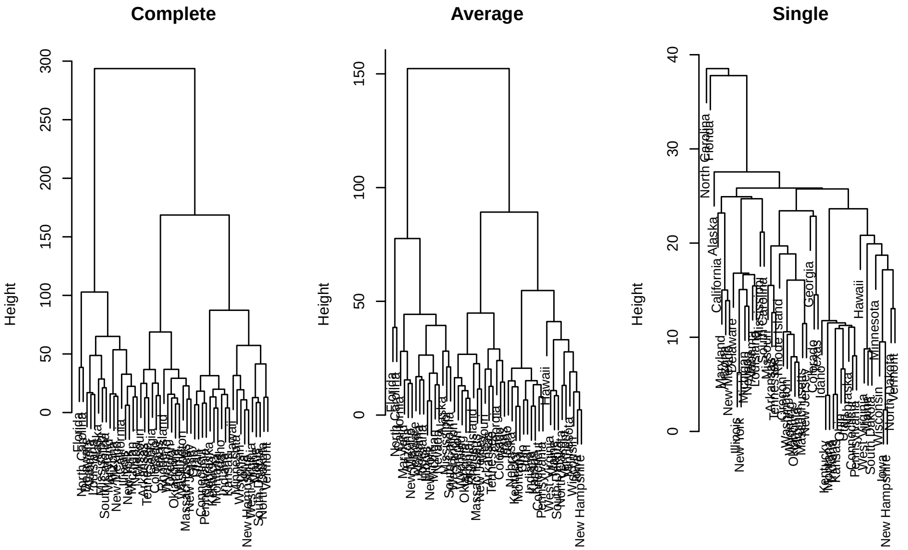
Dissimilarity between clusters
Average linkage clustering

The mean dissimilarity between instances of each cluster

$$d(C_u, C_v) = \frac{1}{|C_u||C_v|} \sum_{\mathbf{x}_i \in C_u} \sum_{\mathbf{x}_j \in C_v} d(\mathbf{x}_i, \mathbf{x}_j)$$



`USArrest` and the linkage methods



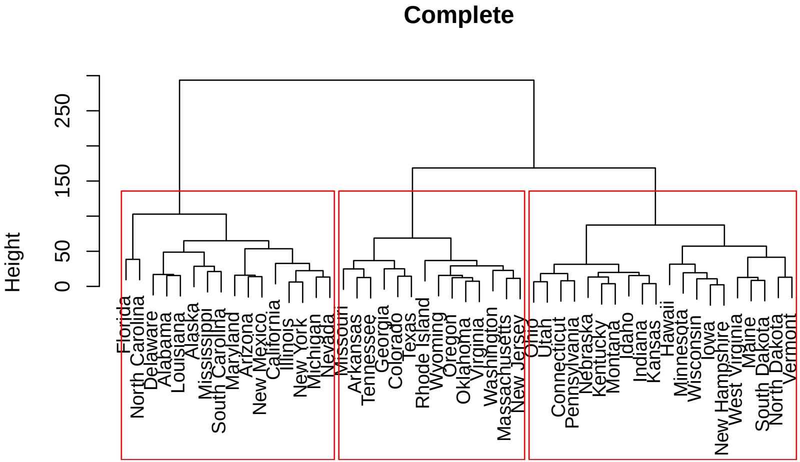
Complete

Average

Single

Cutting the dendrogram

```
> hc.complete <- hclust(dist(d), method = "complete")
# draw dendogram with red borders around the 3 clusters
> rect.hclust(hc.complete, k=3, border="red")
```



Cutting the dendrogram

Cut the dendrogram at height h. The interpretation of h is

- complete linkage: for each instance $\mathbf{x}_i$, EVERY other instance $\mathbf{x}_j$ in its cluster satisfies $d(\mathbf{x}_i, \mathbf{x}_j) \leq h$
- single linkage: for each instance $\mathbf{x}_i$, there is ANOTHER instance $\mathbf{x}_j$ in its cluster satisfies $d(\mathbf{x}_i, \mathbf{x}_j) \leq h$
- average linkage: no interpretation

Agglomerative hierarchical methods

Stopping criteria

- **Distance criterion**
  When the clusters are too far apart to be merged
- **Number criterion**
  When there is sufficiently small number of clusters

Key takeaways

- Examine the data before diving into the buiding predictor.
- Spot issues with data range, units, data type, and missing or invalid values.
- Visualization gives a sense of data distribution and relationships among variables.
- Visualization helps answer questions about the data.
- The goal of clustering is to discover or draw out similarities among subsets of your data.
- Different units cause different distances and potentially different clusterings.
- Different clustering algorithms will give different results. Consider different approaches, with different numbers of clusters.
- Consider the results from different heuristics for estimating the best number of clusters and explore various numbers of clusters.

Summary of Examination Requirements

- Methods for basic data exploration – plotting and summarizing
- Association between features
- Clustering algorithms: K-means, hierarchical agglomerative