

Introduction to Data Mining

- People have been seeking patterns in data since human life began: hunters seek patterns in animal migration behavior, farmers seek patterns in crop growth, politicians seek patterns in voter opinion and lovers seek patterns in their partners' responses...
- But we are overwhelmed with data. The amount of data in our lives seems to increase dramatically. As the volume of data increases, inexorably, the proportion of it that people understand decreases.
- Lying hidden in all this data is **information**, potentially useful information that is rarely made explicit or taken advantage of.

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- A scientist's job is to make sense of data, to discover the patterns that govern how the physical world works and encapsulate them in theories that can be used for predicting what will happen in new situations.
- **A tentative definition of Data Mining:** *Advanced methods for exploring and modeling relationships in large amounts of data.*
- There are other similar definitions. However, the term *exploring and modeling relationships in data* has a much longer history than the term *data mining*.
- Data mining analysis has been limited by the computing power. For example, the computer **IBM 7090** was a *transistorized* machine introduced in 1959. It had a processor speed of approximately 0.5 MHz and roughly 0.2 MB of RAM using *ferrite magnetic* cores.

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- Data sets were stored on cards and then transferred to magnetic tapes using a separate equipment.
- For instance, a data set with 600 rows and 4 columns would have used approximately 3000 cards. Tape storage was limited by the size of the room. The room pictured below contains the tape drives and controllers for the IBM 7090. The computer itself would need a **larger** room!!



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- In data mining, data are stored electronically and searchings are automated by computers.
- Computer performance has been doubling every 24 months. This has led to technological advances in storage structures and a corresponding increase in MB of storage space per dollar.
- **The Parkinson's law of data:** *Data expands to fill the space available for storage.*
- The amount of data in the world has been doubling every 18 to 24 months. Multi-gigabyte commercial databases are now commonplace.
- Economists, statisticians, forecasters, and communication engineers have long worked with the idea that patterns in data can be sought automatically, identified, validated, and used for prediction...

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- Historically, most data were generated or collected for **research purposes**. But, today, big companies have massive amounts of operational data which were not generated for **data analysis** in mind. It is aptly characterized as *opportunistic*. This is in contrast to experimental data where factors are controlled and varied in order to answer specific questions.
- The owners of the data and sponsors of the analyses are typically *not researchers*. The objectives are usually to support **business decisions**.
- **Database marketing** makes use of customer and transaction databases to improve product introduction, cross-sell, trade-up, and customer loyalty promotions.
- One of the facets of customer relationship management is concerned with identifying and profiling customers who are likely to switch brands or cancel services (*churn*). These customers can then be targeted for loyalty promotions.

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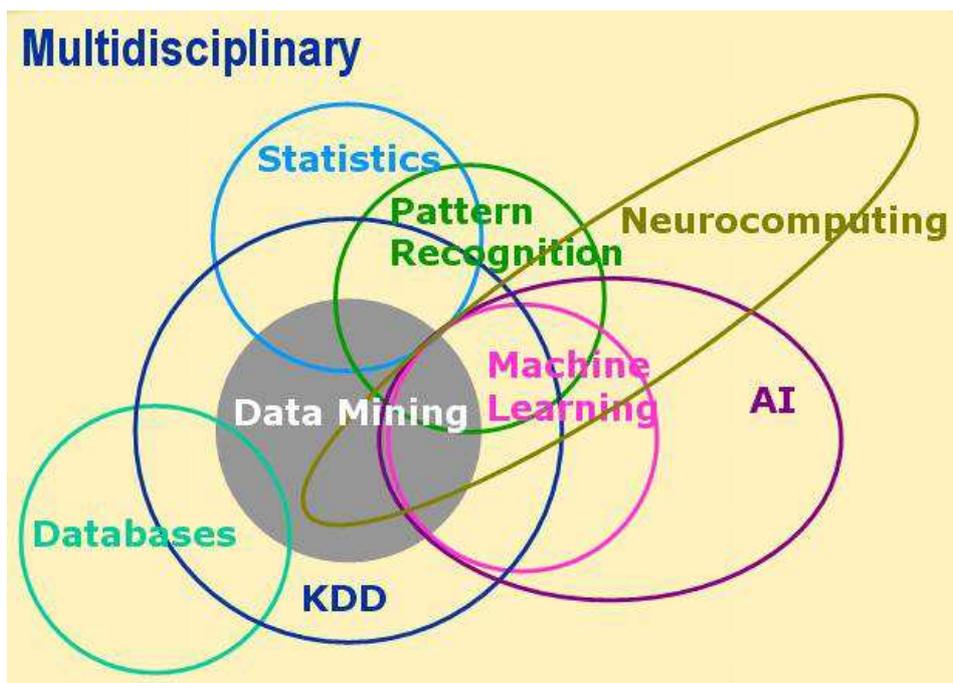
- **EXAMPLE: Credit scoring** is chiefly concerned with whether to extend credit to an applicant. The aim is to anticipate and reduce defaults and serious delinquencies. Other credit risk management concerns are the maintenance of existing credit lines (*should the credit limit be raised?*) and determining the best action to be taken on delinquent accounts.
- The aim of fraud detection is to uncover the patterns that characterize deliberate deception. These patterns are used by banks to prevent fraudulent credit card transactions and bad checks, by telecommunication companies to prevent fraudulent calling card transactions, and by insurance companies to identify fictitious or abusive claims.
- **EXAMPLE: Healthcare informatics** is concerned with decision-support systems that relate clinical information to patient outcomes. Practitioners and healthcare administrators use the information to improve the quality and cost effectiveness of different therapies and practices.

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DEFINITIONS I

- The analytical tools used in data mining were developed mainly by statisticians, artificial intelligence (AI) researchers, and database system researchers.
- One consequence of the multidisciplinary flavor of data mining methods is a **confusing terminology**. The same terms are often used in different senses and contexts and *synonyms* abound.
- **KDD** (*knowledge discovery in databases*) is a multidisciplinary research area concerned with the extraction of *patterns* from large databases. It is sometimes used synonymously with **data mining**.
- **Machine learning** is concerned with creating and understanding semiautomatic learning methods.
- **Pattern recognition** has its roots in engineering and is typically concerned with image classification.
- **Neurocomputing** is, itself, a multidisciplinary field concerned with *neural networks*.

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- Many people think data mining means magically discovering *hidden nuggets* of information without having to formulate the problem and without regard to the structure or content of the data. But, this is an *unfortunate misconception*.
- The database community has a tendency to view data mining methods as *only* more complicated types of *database queries*.
- For example, standard query tools can answer questions such as *how many surgeries, resulted in hospital, stays longer than 10 days?*
But data mining is needed for more complicated queries such as *which are the most important predictors of an excessive length of stay?*
- The problem translation step involves determining what analytical methods are relevant to the objectives.

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DEFINITIONS II

- **Predictive modeling** or *supervised prediction* or *supervised learning* is the **fundamental** data mining task. The training data set consists of **cases** or observations, examples, instances or records.
- Associated with each case is a vector of **input variables** (or predictors, features, explanatory variables, independent variables) and a **target variable** (or response, outcome, dependent variable). The **training data** is used to construct a model (rule) that can predict the values of the target from the inputs.
- The task is referred to as **supervised** because the prediction model is constructed from data where the target is known. It allows you to predict **new cases** when the target is unknown. Typically, the target is unknown because it refers to a future event.
- The **inputs** may be **numeric variables** such as *income*. They may be **nominal variables** such as *occupation*. They are often **binary variables** such as *home ownership*.

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EXAMPLE: The weather problem

Consider a simulated problem about **weather**, with 14 *examples* in the training set and four *attributes*: *outlook*, *temperature*, *humidity*, and *windy*. The *outcome* is whether to *play* or *not play* tennis.

In this problem there are 36 possible combinations ($3 \times 3 \times 2 \times 2 = 36$).

Outlook	Temperature	Humidity	Windy	Play
sunny	hot	high	false	no
sunny	hot	high	true	no
overcast	hot	high	false	yes
rainy	mild	high	false	yes
rainy	cool	normal	false	yes
rainy	cool	normal	true	no
overcast	cool	normal	true	yes
sunny	mild	high	false	no
sunny	cool	normal	false	yes
rainy	mild	normal	false	yes
sunny	mild	normal	true	yes
overcast	mild	high	true	yes
overcast	hot	normal	false	yes
rainy	mild	high	true	no

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A set of **rules**, learned from this information, might look as follows:

If outlook=sunny and humidity=high then play=no

If outlook=rainy and windy=true then play=no

If outlook=overcast then play=yes

If humidity=normal then play=yes

If none of the above then play=yes

- But these rules have to be interpreted in **order**.
- A set of rules that are intended to be interpreted in sequence is called a *decision list*.
- The rules, interpreted as a decision list, classify **correctly** all of the examples in the table whereas taken individually (*out of context*), may be **incorrect**.

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- The previous rules are **classification rules**: they predict the classification of the example in terms of whether to play or not.
- It is also possible to just look for any rules that *strongly associate* different attribute values. These are called **association rules**.
- Many association rules can be derived from the *weather data*. Some good ones are as follows:

If temperature=cool then humidity=normal

If humidity=normal and windy=false then play=yes

If outlook=sunny and play=no then humidity=high

If windy=false and play=no then outlook=sunny and humidity=high

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- There are many more rules that are less than 100% correct because, unlike classification rules, association rules can *predict any* of the **attributes**, not just a specified class, and can even predict more than one thing.
- For example, the fourth rule predicts both that **outlook** will be sunny and that **humidity** will be high.
- The search space, although finite, is extremely big, and it is generally quite impractical to enumerate all possible descriptions and then see which ones fit.
- In the weather problem there are $3 \times 3 \times 2 \times 2 = 36$ possibilities for each rule.

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- If we restrict the rule set to contain no more than 14 rules (because there are 14 examples in the training set), there are around 36^{14} possible different rule sets!!!
- Another way of looking at optimization in terms of searching, is to imagine it as a kind of *hill-climbing* in the *description space*. We try to find the description that best matches the set of examples, according to a pre-specified *matching criterion*.
- This is the way that most practical *machine learning methods* work. However, except in the most trivial cases, it is impractical to search the whole space exhaustively. Most practical algorithms involve *heuristic search* and they cannot guarantee to find the optimal description.

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Application with RWeka

```
library(RWeka)
x <- read.arff(system.file("arff", "weather.nominal.arff", package="RWeka"))
Apriori(x)
```

Best rules found:

1. outlook=overcast ==> play=yes
2. temperature=cool ==> humidity=normal
3. humidity=normal windy=FALSE ==> play=yes
4. outlook=sunny play=no ==> humidity=high
5. outlook=sunny humidity=high ==> play=no
6. outlook=rainy play=yes ==> windy=FALSE
7. outlook=rainy windy=FALSE ==> play=yes
8. temperature=cool play=yes ==> humidity=normal
9. outlook=sunny temperature=hot ==> humidity=high
10. temperature=hot play=no ==> outlook=sunny

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EXAMPLE: *Iris*

The *Iris dataset* (defined in 1935) is arguably one of the most famous dataset used in data mining. It contains 50 examples each of three types of plant: *Iris setosa*, *Iris versicolor*, and *Iris virginica*. There are four attributes: **sepal length**, **sepal width**, **petal length**, and **petal width** (all measured in *centimeters*).



Iris virginica



Iris versicolor



Iris setosa

	Sepal length	Sepal width	Petal length	Petal width	Type
1	5.1	3.5	1.4	0.2	<i>Iris setosa</i>
2	4.9	3.0	1.4	0.2	<i>Iris setosa</i>
3	4.7	3.2	1.3	0.2	<i>Iris setosa</i>
4	4.6	3.1	1.5	0.2	<i>Iris setosa</i>
...					
51	7.0	3.2	4.7	1.4	<i>Iris versicolor</i>
52	6.4	3.2	4.5	1.5	<i>Iris versicolor</i>
53	6.9	3.1	4.9	1.5	<i>Iris versicolor</i>
54	5.5	2.3	4.0	1.3	<i>Iris versicolor</i>
...					
102	5.8	2.7	5.1	1.9	<i>Iris virginica</i>
103	7.1	3.0	5.9	2.1	<i>Iris virginica</i>
104	6.3	2.9	5.6	1.8	<i>Iris virginica</i>
105	6.5	3.0	5.8	2.2	<i>Iris virginica</i>

All attributes have values that are **numeric**. The following set of rules might be learned from this dataset:

If petal length < 2.45 then Iris setosa

If sepal width < 2.10 then Iris versicolor

If sepal width < 2.45 and petal length < 4.55 then Iris versicolor

If sepal width < 2.95 and petal width < 1.35 then Iris versicolor

If petal length \geq 2.45 and petal length < 4.45 then Iris versicolor

If sepal length \geq 5.85 and petal length < 4.75 then Iris versicolor

If sepal width < 2.55 and petal length < 4.95 and

petal width < 1.55 then Iris versicolor

If petal length \geq 2.45 and petal length < 4.95 and

petal width < 1.55 then Iris versicolor

....

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DEFINITIONS: Concepts, Instances, and Attributes

- The input values take the form of *instances*, *attributes* and *concepts*.
- In general, *Information* takes the form of a set of *instances*. In the previous examples, each *instance* was an object or an individual.
- Each *instance* is characterized by the values of attributes that measure different aspects of the instance.
- There are many different types of *attributes*, although typical data mining methods deal only with **numeric** and **nominal** (categorical) ones.

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- In **classification learning**, the learning scheme is presented with a set of classified examples from which it is expected to learn a way of classifying *unseen* examples.
- In **association learning**, any association among features is sought, not just ones that predict a particular class value.
- In **clustering**, groups of examples that belong together are sought.
- In **numeric prediction**, the outcome to be predicted is not a discrete class but a numeric quantity.
- Regardless of the type of learning involved, it is defined what must be learned as the *concept*, and the output produced by a learning scheme is defined as the *concept description*.
- **Example:** the *weather example* is a classification problem. It presents a set of days together with a decision for each as to whether to play the game or not.

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- **Classification learning** is sometimes called *supervised* because the method operates under **supervision**. It is provided the *actual outcome* for each of the training examples.
- The outcome is called the *class* of the example.
- The success of classification learning can be determined by trying out the concept description that is learned, on an independent set of *test data* for which the true classifications are known.
- The *success rate* on test data gives an objective measure of how well the concept has been learned.
- In **association learning** there is no a specified class. The problem is to discover any structure in the data that is *interesting*.
- **Association rules** differ from **classification rules** in two ways: they can *predict any attribute*, not just the class, and they can predict **more than one** attribute's value at a time.

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- **Association rules** usually involve only *non-numeric* attributes. Thus, for example, you would not normally look for association rules in the *Iris dataset*.
- When there is no specified class, **clustering** is used to group items that *seem* to fall naturally together.
- Imagine a version of the *Iris* data in which the type of *Iris* is omitted. Then it is likely that the 150 instances fall into natural clusters corresponding to the three *Iris* types.
- The challenge is to find these clusters and assign the instances to them, and to be able to assign new instances to the clusters as well.
- It may be that one or more of the *Iris* types splits naturally into subtypes, in which case the data will exhibit more than three natural clusters.

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- Clustering may be followed by a **second step** of classification learning, in which rules that are learned give an intelligible description about how new instances should be placed into the clusters.
- **Numeric prediction** is a variant of classification learning in which the outcome is a numeric value rather than a category.
- With numeric prediction problems, the predicted value for new instances is often of less interest than the structure of the description that is learned. This structure is expressed in terms of which are the important attributes and how they relate to the numeric outcome.

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Association rules

- **Small example from the supermarket domain:** Consider a set of products (*items*) $I = \{milk, bread, butter, beer\}$ and a small database of possible purchases (*transactions*) containing the items with **1** codes for presence, and **0** for absence of an item.
- **Notations:** Let $I = \{i_1, i_2, \dots, i_n\}$ be a set of n binary attributes called **items** and $D = \{t_1, t_2, \dots, t_m\}$ be a set of transactions called the **database**.
- Each transaction in D has a unique transaction identification ID and contains a subset of the items in I .
- A **rule** is defined as an implication of the form $X \Rightarrow Y$ where $X, Y \subset I$ and $X \cap Y = \emptyset$.
- The sets of items (for short **itemsets**) X and Y are called antecedent (left-hand-side or *LHS*) and consequent (right-hand-side or *RHS*) of the rule respectively.

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Consider an the example of a database with 4 **items** and 5 **transactions**:

transaction ID	milk	bread	butter	beer
1	1	1	0	0
2	0	1	1	0
3	0	0	0	1
4	1	1	1	0
5	0	1	0	0

An example rule for the supermarket could be $\{milk, bread\} \Rightarrow \{butter\}$ meaning that if *milk* and *bread* is bought, customers also buy *butter*.

Note: This is a *naïf* example: datasets often contain thousands or millions of transactions...

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DEFINITIONS AND CONCEPTS IN ASSOCIATION RULE LEARNING

- The **SUPPORT** $\text{supp}(X)$ of an itemset X is defined as the **proportion** of transactions in the dataset which contain the itemset. It is equivalent to $P(X)$.
- In the example, the itemset $\{\textit{milk}, \textit{bread}, \textit{butter}\}$ has a support of $1/5 = 0.2$ since it occurs in 20% of all transactions (1 out of 5 transactions).
- The **CONFIDENCE** of a rule is defined as

$$\text{conf}(X \Rightarrow Y) = \frac{\text{supp}(X \cup Y)}{\text{supp}(X)} \equiv P(Y|X)$$

- For example, the rule $\{\textit{milk}, \textit{bread}\} \Rightarrow \{\textit{butter}\}$ has a confidence of $0.2/0.4 = 0.5$ in the database, which means that for 50% of the transactions containing *milk* and *bread* the rule are **correct**.
- **Confidence** can be interpreted as an estimate of the probability of finding Y (the right hand side (**RHS**) of the rule) in transactions which also contain X (the left hand side (**LHS**) of the rule).

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- The **LIFT** of a rule is defined as

$$\text{lift}(X \Rightarrow Y) = \frac{\text{supp}(X \cup Y)}{\text{supp}(X) \times \text{supp}(Y)} \equiv P(X \text{ and } Y)/P(X) \cdot P(Y)$$

It is the the ratio of the observed support to what expected if X and Y were independent.

The rule $\{\textit{milk}, \textit{bread}\} \Rightarrow \{\textit{butter}\}$ has a lift of $\frac{0.2}{0.4 \times 0.4} = 1.25$

- The **CONVICTION** of a rule is defined as

$$\text{conv}(X \Rightarrow Y) = \frac{1 - \text{supp}(Y)}{1 - \text{conf}(X \Rightarrow Y)} \equiv P(X)P(\text{not } Y)/P(X \text{ and not } Y)$$

Conviction is the ratio of the probability of X occurs without Y if they were independent, with respect to the probability of incorrect predictions.

- The rule $\{\textit{milk}, \textit{bread}\} \Rightarrow \{\textit{butter}\}$ has a **conviction** of $\frac{1-0.4}{1-0.5} = 1.2$. Then, if the association between X and Y were purely at random, the rule would be incorrect 20% more often.

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Example with `arules`

- We use the *Adult data set* from the UCI machine learning repository (Asuncion and Newman, 2007) provided by the package `arules`. The data originates from the U.S. census bureau database and contains 48842 observations with 14 attributes like age, work class, education, etc.
- In the original applications of the data, the attributes were used to predict the income level of individuals. Here it is added the attribute `income` with levels `small` and `large`, representing an income of $\leq 50,000\$$ and $> 50,000\$$, respectively.

```
library(arules)
data(AdultUCI)
dim(AdultUCI)
head(AdultUCI)
```

- `AdultUCI` has categorical and quantitative attributes and needs some preparations before it is suitable for association mining with `arules`.

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```
AdultUCI[["fnlwgt"]] <- NULL
AdultUCI[["education-num"]] <- NULL

AdultUCI[["age"]] <- ordered(cut(AdultUCI[["age"]], c(15,25,45,65,100)),
labels = c("Young", "Middle-aged", "Senior", "Old"))

AdultUCI[["hours-per-week"]] <- ordered(cut(AdultUCI[["hours-per-week"]],
c(0,25,40,60,168)), labels = c("Part-time", "Full-time", "Over-time", "Workaholic"))

AdultUCI[["capital-gain"]] <- ordered(cut(AdultUCI[["capital-gain"]],
c(-Inf, 0, median(AdultUCI[["capital-gain"]][AdultUCI[["capital-gain"]] >
0]), Inf)), labels = c("None", "Low", "High"))

AdultUCI[["capital-loss"]] <- ordered(cut(AdultUCI[["capital-loss"]],
c(-Inf, 0, median(AdultUCI[["capital-loss"]][AdultUCI[["capital-loss"]] >
0]), Inf)), labels = c("none", "low", "high"))
```

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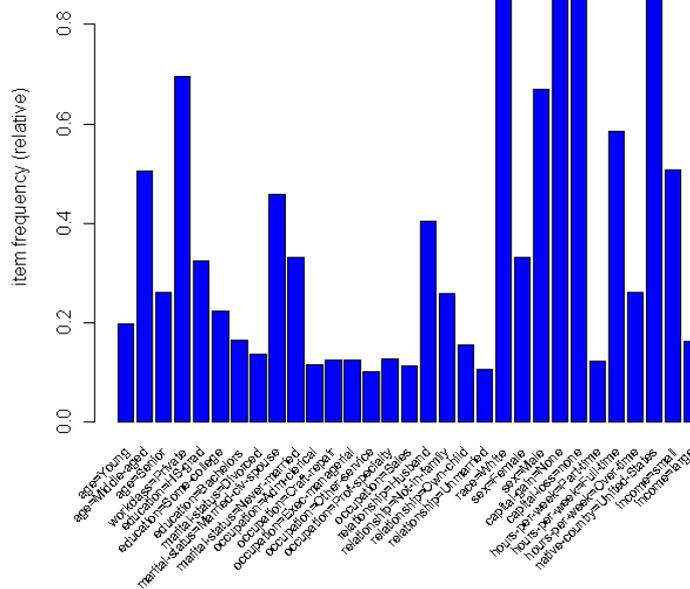
- The new data frame is called **Adult**:

```
Adult <- as(AdultUCI, "transactions")
Adult
summary(Adult)
```

- The summary of the transaction data set gives a rough overview showing the most frequent items, the length distribution of the transactions and the extended item information which shows which variable and value were used to create each binary item.
- To see which items are important in the data set we can only plot the item frequency for items with a support greater than 10%.

```
itemFrequencyPlot(Adult, support=0.1, cex.names=0.65, col="pink")
```

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- Next, we call the function `apriori` to find all rules with a minimum support of 1% and a confidence of 0.6.

```
rules <- apriori(Adult, parameter=list(support=0.01, confidence=0.6))
rules
```

- First, the function prints the used parameters. The parameter `maxlen` (maximum size of the mined frequent `itemsets`) is by default restricted to 5. Longer association rules are only mined if `maxlen` is set to a higher value.
- The result of the mining algorithm is a set of 276443 rules. For an overview of the mined rules `summary` can be used. It shows the number of rules, the most frequent items contained in the left-hand-side (*LHS*) and the right-hand-side (*RHS*) and their respective length distributions and summary statistics for the quality measures returned by the mining algorithm.

```
summary(rules)
```

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- As typical for association rule mining, the number of rules found is huge. It is useful to produce separate subsets of rules with the command `subset`. Consider variable `income` in the right-hand-side (*RHS*) of the rule, and a `lift` value greater than 1.2.

```
rulesIncomeSmall <- subset(rules, subset=rhs %in% "income=small" & lift>1.2)
rulesIncomeLarge <- subset(rules, subset=rhs %in% "income=large" & lift>1.2)
```

- We now have a set with rules for persons with a **small income** and a set for persons with a **large income**. For comparison, we inspect for both sets the three rules with the highest confidence, using `sort()`.

```
inspect(head(sort(rulesIncomeSmall, by="confidence"), n=3))
inspect(head(sort(rulesIncomeLarge, by="confidence"), n=3))
```

- From the rules we see that workers in the **private sector working part-time**, or in the service industry, tend to have a **small income**. While persons with **high capital** gain who are born in the US tend to have a **large income**.

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Graphing rules with arulesViz

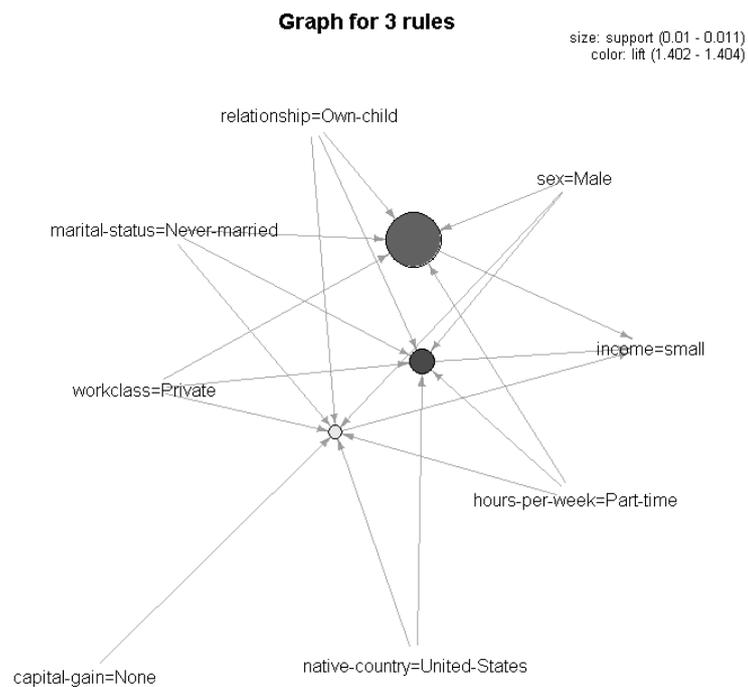
It is possible also to plot the obtained rules by using *schemes*:

```
library(arulesViz)

plot(head(sort(rulesIncomeSmall, by="confidence"), n=3),
method="graph", control=list(type="items"))

plot(head(sort(rulesIncomeLarge, by="confidence"), n=3),
method="graph", control=list(type="items"))
```

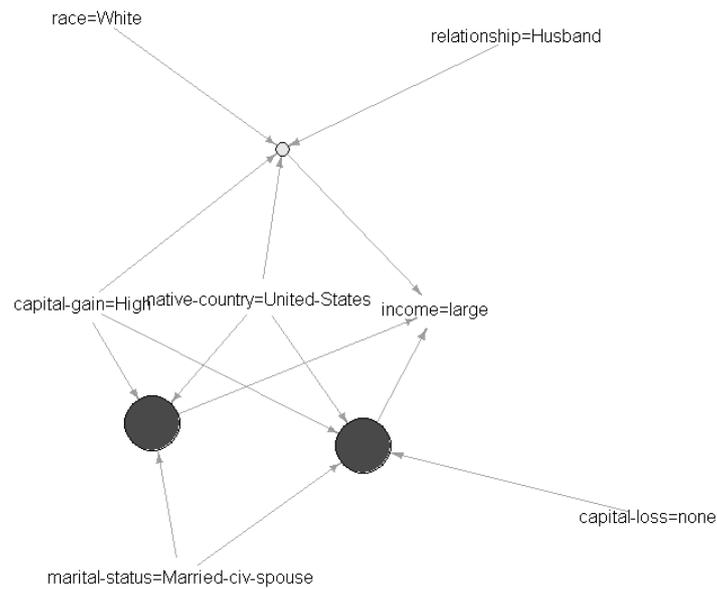
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Graph for 3 rules

size: support (0.013 - 0.016)
color: lift (4.264 - 4.266)



Sampling with arules

- Taking samples from large databases is useful if the original database does not fit into memory. Moreover, sampling can speed-up the process with little degradation of accuracy.
- **Example:** We choose a minimum support of 5%, an error rate for support equal to 10% and a confidence level of 90%. The sample size is computed as $n = \frac{-2 \ln(c)}{\tau \epsilon^2}$, for support $\tau = \text{supp}(X) = 0.05$ and error rate of support $\epsilon = 0.2$, at a given confidence level $1 - c = 0.9$.

```
data(Adult)
supp <- 0.05
epsilon <- 0.1
c <- 0.1
n <- -2*log(c) / (supp*(epsilon^2))
n
```

- With `sample` we produce a sample of size n *with replacement* from the database.

```
# n=9210.34
AdultSample <- sample(Adult, n, replace=TRUE)
```

- The sample can be compared with the original database (the *population*), by using an item frequency plot. The item frequencies in the sample are displayed as bars, and the item frequencies in the original database are represented by a line.

```
itemFrequencyPlot(AdultSample, population=Adult, support=supp, cex.names=0.7)
```

- It is obtained in this example, that mining the sample instead of the whole data base results in a speed-up factor of roughly 5.

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- To evaluate the accuracy for the itemsets mined from the sample, we analyze the difference between the two sets.

```
itemsets <- eclat(Adult, parameter=list(support=supp), control=list(verbose=FALSE))
itemsetsSample <- eclat(AdultSample, parameter=list(support=supp),
control=list(verbose=FALSE))
itemsets
itemsetsSample
```

- The two sets have roughly the same size. To check if the sets contain similar itemsets, we match the sets and see what fraction of frequent itemsets found in the database were also found in the sample.

```
matching <- match(itemsets, itemsetsSample, nomatch=0)
sum(matching > 0)/length(itemsets)
```

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- Almost all frequent itemsets were found using the sample. Only itemsets with support very close to the minimum support, were missed or not found.

```
summary(quality(itemsets[which(!matching)]))$support)
summary(quality(itemsetsSample[-matching]))$support)
```

- For the frequent itemsets which were found in the database and in the sample, we can calculate the accuracy level showing the error rate.

```
supportItemsets <- quality(itemsets[which(matching > 0)])$support
supportSample <- quality(itemsetsSample[matching])$support
accuracy <- 1 - abs(supportSample - supportItemsets)/supportItemsets
summary(accuracy)
```

- The summary shows that sampling resulted in finding the support of itemsets with high accuracy.