

Machine Learning

Lecture BigData Analytics

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Disclaimer: Big Data software is constantly updated, code samples may be outdated.

Outline

- 1 Introduction
- 2 Methodology
- 3 Classification
- 4 Regression
- 5 Clustering
- 6 Association Rule Mining
- 7 Meta-Learning
- 8 Summary

Data Mining (Knowledge Discovery) [1,35]

Definition

- **Data mining:** process of discovering patterns in large data sets
 - (Semi-)Automatic analysis of large data to identify interesting patterns
 - Using artificial intelligence, machine learning, statistics and databases

Tasks / Problems for data mining

- **Classification:** predict the category of samples
- **Regression:** find a function to model numeric data with the least error
- **Anomaly detection:** identify unusual data (relevant or error)
- **Association rule learning:** identify relationships between variables
- **Clustering:** discover and classify similar data into structures and groups
- **Summarization:** find a compact representation of the data

Terminology for Input Data [1, 40]

- **Sample:** instances (subset) of the unit of observation
- **Feature:** measurable property of a phenomenon (explanatory variable)
 - The set of features is usually written as vector (f_1, \dots, f_n)
- **Label/response:** outcome/property of interest for analysis/prediction
 - Dependent variable
 - Discrete in classification, continuous in regression

Forms of features/labels

- **Numeric:** a (potentially discrete) number characterizes the property
 - e.g., age of people
- **Categorical/nominal:** a set of classes
 - e.g., eye color
 - Dichotomous (binary) variable: contains only two classes (Male: Yes/No)
- **Ordinal:** an ordered set of classes
 - e.g., babies, teens, adults, elderly

Example Data

Imagine we have data about alumni from the university

Field of study	Gender	Age	Succ. exams	Fail. exams	Avg. grade*	Graduate	Dur. studies
CS	M	24	21	1	2.0	Yes	10
CS	M	22	5	2	1.7	Enrolled	2
Physics	F	23	20	1	1.3	Enrolled	6
Physics	M	25	8	10	3.0	No	10

- Categorical: field of study, gender, graduate, (favourite colour)
- Numeric: age, successful/failed exams, duration of studies
- Numeric: average grade; Ordinal: very good, good, average, failed

Our goal defines the machine learning problem

- Predict if a student will graduate \Rightarrow classification
 - Prescriptive analysis: we may want to support these students better
- Predict the duration (in semesters) for the study \Rightarrow regression
- Clustering to see if there are interesting classes of students
 - We could label these, e.g., the prodigies, the lazy, ...
 - Probably not too helpful for the listed features

Terminology for Learning [40]

- **Online learning:** update the model constantly while it is applied
- **Offline (batch) learning:** learn from data (training phase), then apply
- **Supervised learning:** feature and label are provided in the training
- **Unsupervised learning:** no labels provided, relevant structures must be identified by the algorithms, i.e., descriptive task of pattern discovery
- **Reinforcement learning:** algorithm tries to perform a goal while interacting with the environment
 - Humans use reinforcement, (semi)-supervised and unsupervised learning

Overview of Machine Learning Algorithms (Excerpt)

Classification

- k-Nearest neighbor
- Naive bayes
- Decision trees
- Classification rule learners

Regression/Numeric prediction

- Linear regression
- Regression trees
- Model trees

Regression & classification

- Neuronal networks
- Support vector machines

Pattern detection

- Association rules
- k-means clustering
- density-based clustering
- model-based clustering

Meta-learning algorithms

- Bagging
- Boosting
- Random forests

Machine Learning in Practice [1]

Process / Phases

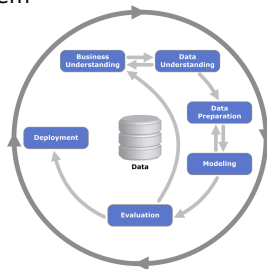
- 1 Data collection: combining data into a single source
- 2 Data exploration and preparation: inspection and data cleanup
- 3 Model training: depending on machine learning task choose algorithm
- 4 Model evaluation: check accuracy of the model
- 5 Model improvement: if necessary try to improve accuracy by utilizing advanced methods or providing additional input

Cross Industry Standard Process for Data Mining [39]

CRISP-DM is a commonly used methodology from data mining experts

Phases

- **Business understanding:** business objectives, requirements, constraints; converting the problem to a data mining problem
- **Data understanding:** collecting initial data, exploration, assessing data quality, identify interesting subsets
- **Data preparation:** creation of derived data from the raw data (data munging)
- **Modeling:** modeling techniques are selected and applied to create models, assess model quality/validation
- **Evaluation** (wrt business): check business requirements, review construction of the model(s), decide use
- **Deployment:** applying the model for knowledge extraction; creating a report, implementing repeatable data mining process



Source: Kenneth Jensen [38]

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Normalization of Data [1, p. 72]

- Several algorithms require that numeric variables are normalized
 - The numbers of the feature vector are treated identically
 - Example: in the features (age, income, is_male), income is >> age
- Treatment: scale features similar, e.g., all values between 0 and 1

Min-Max normalization

- $$X_{new} = \frac{X - \min(X)}{\max(X) - \min(X)}$$

Z-Score standardization

- $$X_{new} = \frac{X - \text{mean}(X)}{\text{StdDev}(X)}$$
- Especially useful for normal distributed data

Dummy Coding [1]

- Problem: distance is not defined for categorical data
 - Regression does not make sense for categorical data
- Dummy coding transforms N classes into N-1 dummy (proxy) variables
 - 0 indicates instance is of given class
 - 1 indicates use other class
 - The last class is the reference class
- Dummy coding works well for features
 - Independent prediction of several “feature” classes must be resolved, i.e., more than one class is predicted as 1

Example

- Color: Red, blue, green
- Dummy variables: color_red, color_blue, color_green
- Color green could be omitted and be the reference

Treating Missing Data [32, 33, 1, p.300]

- Problem: a feature is not available for an example

Alternatives

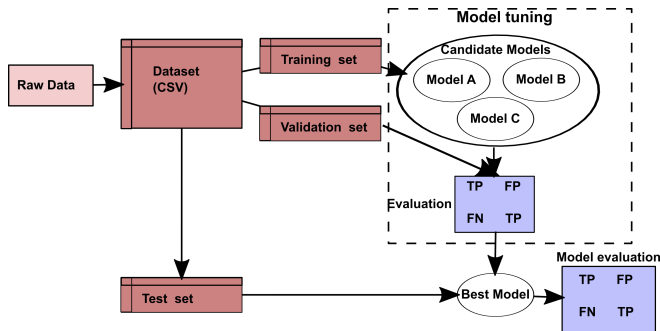
- Deletion: remove examples with missing (N/A) data
 - Problem: we may have many features of which many examples miss one
- Imputation: replace N/A with substitution values
 - Hot-deck imputation: replace value with a random value from similar entity
 - Last observation carried forward: simply use last observed value
 - Replace with median, mean (of similar entities)
 - Interpolation (or Kriging)
 - Apply a regression model
 - Statistic regression: replace with mean + random variance
- Replacing too many instances may complicate analysis/exploration

Strategy for Learning [40]

- Goal: Learn properties of the population from a sample
- Data quality is usually suboptimal
 - Erroneous samples (random noise, ambivalent data)
 - **Overfitting**: a model describes noise in the sample instead of population properties
 - **Underfitting**: a model ignores small but important patterns
 - **Robust** algorithms reduce the chance of fitting noise
- How accurate is a specific model on the **population**?
 - Should we train a model on our data and check its accuracy on the same?
 - As the model is trained on the data, it should be able to be accurate
 - A lookup table might reproduce the data perfectly but is not useful
 - Resubstitution error: training/testing with the same data
 - Shows how well the model can fit
 - A bad fit can be an indicator for ambivalent/erroneous data
 - A bad fit can also show that the method is not appropriate for the data
 - Personally, I always do check model quality first on the resubstitution error

Systematic Testing with the Holdout Method

- Split data into **training** (50%), **test** (25%) and **validation** (25%) set
 - Training set: build/train model from this data sample
 - Validation set: check model quality and refine the models
 - Test set: check final model accuracy on this set (expected accuracy)
- Once the best model is identified, train it on complete data set



Holdout method. The figure is based on [1, p.337].

Supplementary Strategies

Problems

- Sometimes we have not sufficient training samples
- Suboptimal selection of training samples may cause problems
 - Classification: some classes may have only a few training samples

k-fold cross validation

- Prevents cases in which we partition data suboptimally
- See next slide

Leave-one-out cross validation

- Builds model with all elements except one
- Compute model accuracy on the last (test) element
- Repeat the process for each element

k-fold cross validation

- 1 Split data into k sets
- 2 For all permutations: train from k-1 sets, validate with remaining set
- 3 Compute average error metrics

Example with the iris data set

```
1 library(cvTools)
2 set.seed(123) # initialize random seed generator
3
4 data(iris)
5 # create 10 folds
6 f = cvFolds(nrow(iris), K=10, R=1, type="random")
7
8 # retrieve all sets
9 for (set in 1:10){
10   validation = iris[ f$subsets[f$which == set] , ] # 135 elements
11   training = iris[ f$subsets[f$which != set], ] # 15 elements
12
13   # TODO Now build your model with training data and validate it
14   # TODO Build error metrics for this repeat
15 }
16
17 # Output aggregated error metrics for all repeats
18
19 # Some packages perform the k-cross validation for you
```

Creating only one training set

```
1 # create two classes, train and validation set
2 mask = sample(2, nrow(iris), repl=T, prob=c(0.9,0.1))
3 validation = iris[mask==1, ]
4 training = iris[mask==2, ]
```

Stratified sampling [11]

- Stratification: dividing the population into homogeneous subgroups before sampling
 - e.g., for clinical trials: people (not) having a disease and smokers, 4 groups
 - Draw the same number of random samples from each group
- If we have the data already:
 - Split the observed samples into classes and distribute these instances across training/test/validation set
 - Alternatively: Draw the same number of elements from each class

Example problem: class imbalance problem [1, p. 312]

- Consider we have test A for a disease
 - We know that 990 people are healthy and 10 people have the disease
 - Assume the test always reports “healthy”
 - Is this a good test? It is correct in 99% of cases!
- ⇒ A careful assessment of model performance is needed

Evaluating Model Performance

- Idea: compare true value with predicted “value” on the training data
- Algorithms return the predicted class/numeric value
 - Classification returns the class (e.g., color, healthy: yes/no)
 - Regression the numeric value
- Algorithms may return a probability of the prediction
 - Likelihood that the value was correct on the training/test set
 - Sometimes the choice is tight, i.e., 49% class A vs. 51% class B
 - We may skip such results and say we cannot determine the class!
- There are different metrics to assess the quality of the model
 - Metrics depend on the problem: classification vs. regression

Assessing Correctness of Classification Models

Confusion matrix

- Visualizes the performance of the classification
- Shows count in observation (row) and prediction class (column)

	Class A	Class B	Class C
Class A	AA	AB	AC
Class B	BA	BB	BC
Class C	CA	CB	CC

- Often one class is of interest (e.g., class A)
 - True positive (TP): observation is true, predicted as true (AA)
 - False positive (FP): observation is false, prediction is true (BA, CA)
 - True negative (TN): observation is false, predicted as false (BB, CC)
 - False negative (FN): observation is true, prediction is false (else)
- There are useful metrics defined on these values
 - Accuracy, error rate, sensitivity, specificity, precision, recall
 - Kappa statistic: correctness vs. random correctness
 - F-measure (F-score): weights precision and recall equally

Evaluating Model Performance for Numerical Data

- **Residual:** difference of observation¹ and estimated (predicted) value
 - Residual (error): $e = o - e$
 - In our test/validation set we have n samples for which we compute residuals
- **Mean absolute error:** $MAE = \frac{1}{n} \sum_{i=1}^n |e_i|$
- **Mean square error:** $MSE = \sqrt{\frac{1}{n} \sum_{i=1}^n (o_i - e_i)^2}$
- **Mean absolute percentage error:** $MAPE = \frac{100}{n} \sum_{i=1}^n \left| \frac{o_i - e_i}{o_i} \right|$
- We may compute correlation of observation and estimation

¹Also called actual value, but I prefer observation since we do not know if it is the true value.

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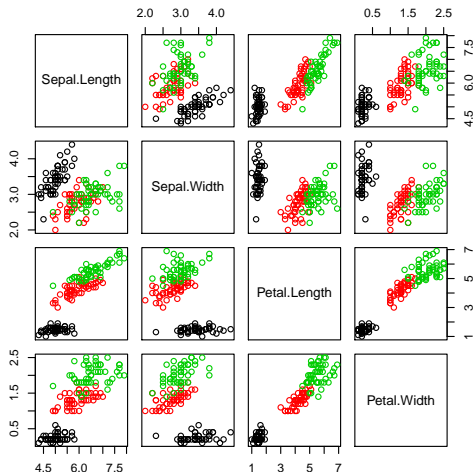
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Classification: Supervised Learning

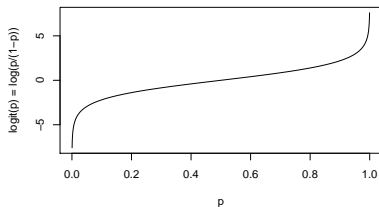
- Goal: Identify/predict the class of previously unknown instances



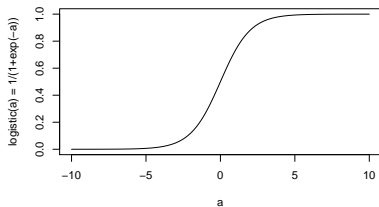
Each class (flower type) is visualized in its own color

Generalized Linear Model (GLM) [34]

- LM expects numeric data and normal distribution of error values
- GLM is a linear model that map the response via a link function
 - e.g., improve accuracy for binary result variable by computing a probability



Plot of $\text{logit}(p)$



$\text{logit}^{-1}(\alpha) = \text{logistic}(\alpha)$ (for binary)

Example in R

```
1 d$female = (d$gender == "female") # convert into dichotomous var
2 d$grade = factor(d$grade) # convert variable into a categorical var
3
4 m = glm(formula = graduate ~ female + age + grade + exams_succ + exams_fail,
        ↪ family=binominal(link="probit"), data=d)
```


k-Nearest Neighbor (k-NN) [1]

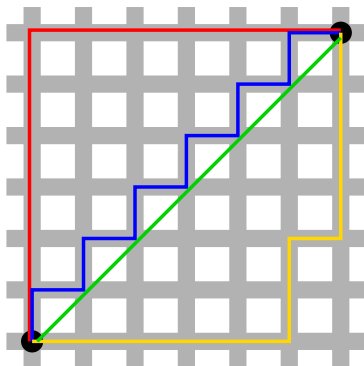
- Prediction: compute distance of new sample to k nearest samples
 - Majority of neighbors vote for new class
- Strengths:
 - Simple and effective supervised learning algorithm
 - No assumption about data distribution
 - Fast training
- Weaknesses:
 - Does not create a model
 - Parameter k needs to be set
 - Slow classification
 - Normalization (min/max) required, nominal features and missing data?

Example in R

```
1 library(kknn)
2 m = kknn(Species ~ Sepal.Width + Petal.Length + Petal.Width + Sepal.Length, train=training, test=validation, k=3)
3
4 # Create a confusion matrix
5 table(validation$Species, m$fit)
6 #           setosa versicolor virginica
7 # setosa      3           0           0
8 # versicolor  0           7           0
9 # virginica   0           1           4
```

Supporting Topic: Distance Metrics

- Consider two vectors $v = (v_1, \dots, v_n)$ and $w = (w_1, \dots, w_n)$
- Euclidean distance: $d(v, w) = \sqrt{(v_1 - w_1)^2 + \dots + (v_n - w_n)^2}$
- Manhattan distance: $d(v, w) = |(v_1 - w_1)| + \dots + |(v_n - w_n)|$



Red: Manhattan distance. Green: diagonal, euclidean distance. Blue, yellow: equivalent Manhattan distances [12]

Naive Bayes [1]

- Idea: predict class based on probabilities of occurrence in the training
 - e.g., email containing *medication*, *viagra*, *shop* is likely Spam
- Based on Bayesian methods
 - $P(A)$: Probability outcome A is observed = count A / count all observations
 - Assume independence: $P(A \cap B) = P(B|A) \cdot P(A) = P(A|B) \cdot P(B)$
 - $P(A|B) = \frac{P(A \cap B)}{P(B)} = \frac{P(B|A) \cdot P(A)}{P(B)}$ (Probability of A under condition B)
- Naive assumptions: independence and equal importance of features
- Classification: $P(C_L | F_1, \dots, F_n) = \frac{1}{Z} p(C_L) \prod_{i=1}^n p(F_i | C_L)$
- Strengths:
 - Simple, fast and effective
 - Works well with noisy and missing data
 - Small number of training samples required
 - Probability for a prediction can be obtained (confidence)
- Weaknesses:
 - Assumes that all features are equally important
 - Suboptimal for datasets with many numeric features
 - Probabilities are less reliable than predicted classes

Example: Spam Filter [1]

- Goal: Classify an email as Ham or Spam based on text
- $w_i = 1$, if a word occurs in message i , 0 otherwise
- Summarize w_i based on the labels and create tables

Probability table calculated from the training set for each word

Frequency	Medication		Total
	Yes	No	
Spam	4	16	20
Ham	1	79	80
Total	5	95	100

Frequency	Shop		Total
	Yes	No	
Spam	3	17	20
Ham	20	60	80
Total	23	77	100

Classification of new e-mails

- $P(\text{Spam}|\text{Medication}, \text{Shop}) = 4/20 \cdot 3/20 \cdot 20/100 = 0.006$
 - $P(\text{Ham}|\text{Medication}, \text{Shop}) = 1/80 \cdot 20/80 \cdot 80/100 = 0.0025$
- ⇒ $P(\text{Spam}) = 0.006 / (0.006 + 0.0025) = 70.6\%$

Data Pre-Processing [1]

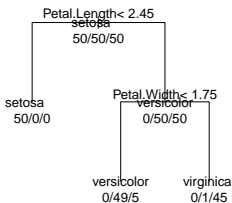
- Problem: predict 0 if a feature is missing in a class level while training
 - e.g., in our Spam classifier a word is never seen in a spam email
 - Observation in practice leads to multiplication with zero
 - Solution: missing data is treated with the Laplace estimator:
Add 1 to the count of each class-feature to ensure it occurs
 - Other values work too, but ensure that probability for class sum to 1
 - Alternative: Ignore attribute from calculation

Likelihood	Medication		Total
	Yes	No	
Spam	5/22	17/22	22
Ham	2/82	80/82	82
Total	7	97	104

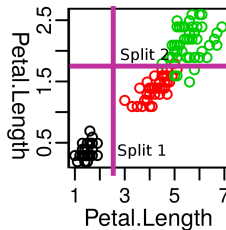
- Predicting numeric features with Naive Bayes
 - Create interval classes (bins) for numeric data
 - e.g., Class 1 are all instances between 0 and 10
 - Selection of cut points should be inspired by data distribution
 - Quantiles are (trivial but) potential cut points
 - Alternative: use a probability density function
 - Training: estimate parameters based on distribution of a class
 - Prediction for x : multiply by PDF(x) (instead of probability of a class)

Decision Trees

- Tree data structures, a node indicates an attribute and threshold
 - Follow left edge if value is below threshold otherwise right
 - Leafs are decisions
 - Can separate data horizontally and vertically
- Classification trees (for classes) and regression trees for continuous vars
- Various algorithms to construct a tree
 - CART: Pick the attribute to maximize information gain of the split
- Knowledge (decision rules) can be extracted from the tree
- Tree pruning: Recursively remove unlikely leafs (reduces overfitting)



(a) Tree for iris data



(b) Split of the values

Decision Trees with R

- Rpart package supports regression (method="anova")
- Classification (with two classes method="poisson" else "class")
- Control object defines requirements for splitting
(e.g., observations per leaf, cost complexity (cp) factor)

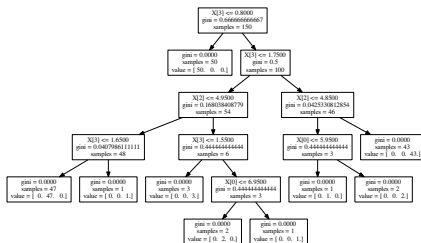
```
1 library(rpart)
2 data(iris) # The iris data (from the slide before)
3 # Create a classification tree based on all inputs
4 m = rpart(Species ~ Sepal.Width + Petal.Length + Petal.Width + Sepal.Length, data=iris, method="class",
5 control = rpart.control(minsplit=5, cp = 0.05)) # require a minimum number of 5 observations
6 summary(m) # print details of the tree
7
8 plot(m, compress=T, uniform=T, margin=0.7) # plot the tree
9 text(m, use.n=T, all=T) # add text to the tree, plot all nodes not only leafs
10 m = prune(m, cp=0.05) # prune the tree, won't change anything here
11
12 p = predict(m, iris[150,], type="class") # predict class of data in the data frame, here one instance virginica
13 p = predict(m, iris[150,], type="prob") # predict probabilities
14 # setosa versicolor virginica
15 # 150 0 0.02173913 0.9782609
16
17 # Confusion matrix, training and test data is identical to show ambivalence of the model
18 table(iris$Species, predict(m, iris, type="class"))
19 # setosa versicolor virginica
20 # setosa 50 0 0
21 # versicolor 0 49 1
22 # virginica 0 5 45
23 table(iris$Species == predict(m, iris, type="class")) / nrow(iris) # show fraction of predictions
24 # FALSE TRUE
25 # 0.04 0.96
```

Machine Learning with Python

- Recommended package: `scikit-learn`²
- Provides classification, regression, clustering, dimensionality reduction
- Supports via model selection and preprocessing

Example: Decision tree

```
1 from sklearn.datasets import load_iris
2 from sklearn import tree
3 iris = load_iris()
4 m = tree.DecisionTreeClassifier()
5 m = m.fit(iris.data, iris.target)
6
7 # export the tree for graphviz
8 with open("iris.dot", 'w') as f:
9     tree.export_graphviz(m, out_file=f)
10
11 # To plot run: dot -Tpdf iris.dot
```



Sklearn decision tree

²<http://scikit-learn.org/stable/>

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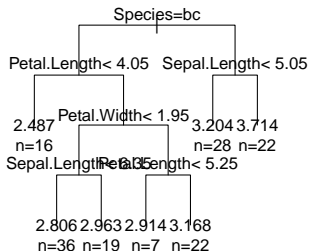
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Regression Trees

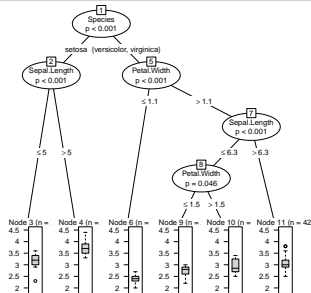
- Regression trees predict numeric values
 - They usually optimize mean-squared error
- Party package uses statistical stopping rules (no pruning needed)

```

1 # Create a regression tree for Sepal.Width which optimizes mean-squared error
2 m = rpart( Sepal.Width ~ Species + Petal.Length + Petal.Width + Sepal.Length, data=iris, method="anova")
3 plot(m, compress=T, uniform=T, margin=0.7) # plot the tree
4 text(m, use.n=T) # add text to the tree
5
6 library(party) # package for recursive partitioning using nonparametric regression
7 m = ctree( Sepal.Width ~ Species + Petal.Length + Petal.Width + Sepal.Length, data=iris)
  
```



Regression tree for Sepal.Width



Regression tree with party

Model Trees [1, p. 202ff, 214ff]

- Problem: CART trees can predict only one class/value per leaf
 - This is suboptimal for regression trees as the accuracy depends on the leafs
- Model trees add a linear regression model on the leaf node
 - Especially unused attributes can be used to predict the numerical value
- M5-prime (M5P) algorithm is state of the art

Example for the Iris data and starting to compare model quality

```
1 library(RWeka)
2 m5 = MSP( Sepal.Width ~ Species + Petal.Length +
3         ↪ Petal.Width + Sepal.Length, data=iris)
4 #M5 pruned model tree:
5 #(using smoothed linear models)
6 #Species=setosa <= 0.5 : LM1 (100/55.118%)
7 #Species=setosa > 0.5 : LM2 (50/57.858%)
8 #
9 #LM num: 1
10 #Sepal.Width =
11 # -0.2457 * Species=virginica,setosa
12 # + 0.4834 * Petal.Width
13 # + 0.1839 * Sepal.Length
14 # + 1.0373
15 #LM num: 2
16 #Sepal.Width =
17 # 0.0896 * Species=virginica,setosa
18 # - 0.0987 * Petal.Width
19 # + 0.6784 * Sepal.Length
20 # - 0.0485
21 # Number of Rules : 2
```

```
1 # Compare the error of CART (rpart), party and MSP
2 MAEi = function (p){
3   return (mean(abs(iris$Sepal.Width - p)))
4 }
5 print(sprintf("rpart: %f party: %f m5p: %f", MAEi(pm),
6             ↪ MAEi(pp), MAEi(p5)))
7 #MAE rpart: 0.203207 party: 0.206693 m5p: 0.189899
8
9 MSEi = function (p){
10  return (sqrt(sum((iris$Sepal.Width - p)^2)/nrow(iris)))
11 }
12 print(sprintf("MSE rpart: %f party: %f m5p: %f", MSEi(pm),
13             ↪ MSEi(pp), MSEi(p5)))
14 #MSE rpart: 0.260416 party: 0.265323 m5p: 0.246495
15
16 MAPEi = function (p){
17  return (100*sum(abs((iris$Sepal.Width -
18             ↪ p)/iris$Sepal.Width))/nrow(iris))
19 }
20 print(sprintf("MAPE rpart: %.1f%% party: %.1f%% m5p:
21             ↪ %.1f%%", MAPEi(pm), MAPEi(pp), MAPEi(p5)))
22 #MAPE rpart: 6.8% party: 6.9% m5p: 6.4%
```

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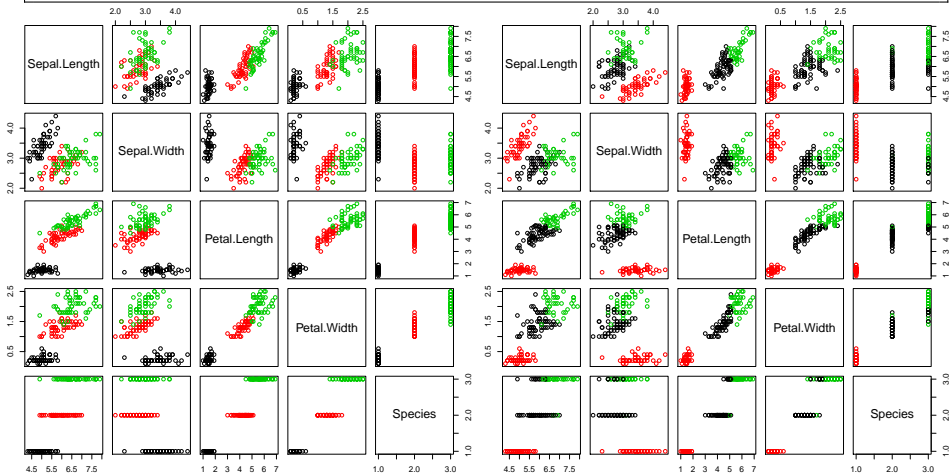
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Clustering

- Partition data into “similar” observations
- Allows prediction of a class for new observations
- Unsupervised learning strategy
- Clustering based on distance metrics to a center (usually euclidean)
 - Can identify regular (convex) shapes
 - k-means: k-clusters, start with a random center, iterative refinement
- Hierarchical clustering: distance based methods
 - Usually based on distance matrix (N^2 elements)
 - Agglomerative (start with individual points) or divisive
- Density based clustering uses proximity to cluster members
 - Can identify any shape
 - DBSCAN: requires the density parameter (eps)
 - OPTICS: nonparametric
- Model-based: automatic selection of the model and clusters
- Normalization of variable ranges is mandatory
 - One dimension with values in 0 to 1 is always dominated by one of 10 to 100

K-means Clustering

```
1 p = kmeans(iris[,1:4], centers=3) # cluster in 4 dimensions, exclude species
2 plot(iris, col=p$cluster)
```

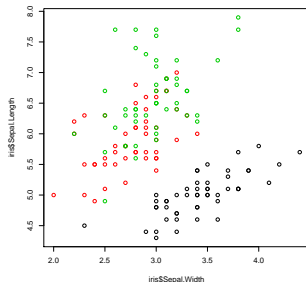


Real species

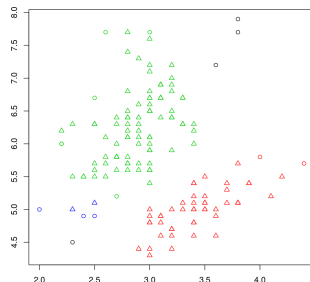
Kmeans in 4D

Density-Based Clustering

```
1 library(fpc) # for dbSCAN
2 # For illustration purpose, we cluster the 4D feature set only using two variables
3
4 # 2D plot coloring the species
5 plot(iris$Sepal.Width, iris$Sepal.Length, col=iris$Species)
6
7 # Create a 2D matrix as input for dbSCAN
8 d = cbind(iris$Sepal.Width, iris$Sepal.Length)
9
10 # try to identify classes, showplot illustrates the process
11 p = dbSCAN(d, eps=0.35, showplot=1)
```



Real species (classes)

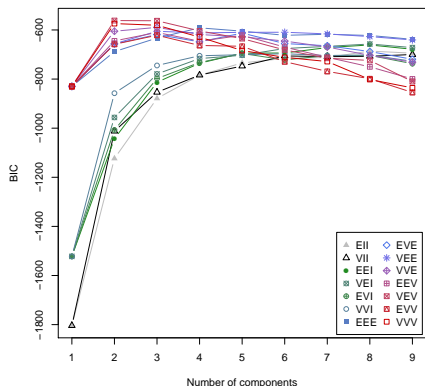
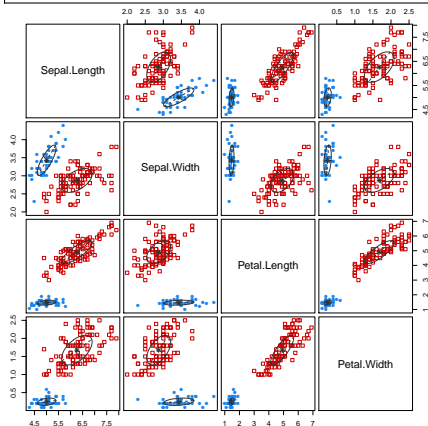


Output of dbSCAN

Model Based Clustering

- Automatic selection of model and cluster number
- Uses bayesian information criterion (BIC) and expectation-maximization

```
1 library(mclust)
2 m = Mclust(iris[,1:4]) # chooses a ellipsoidal model
```



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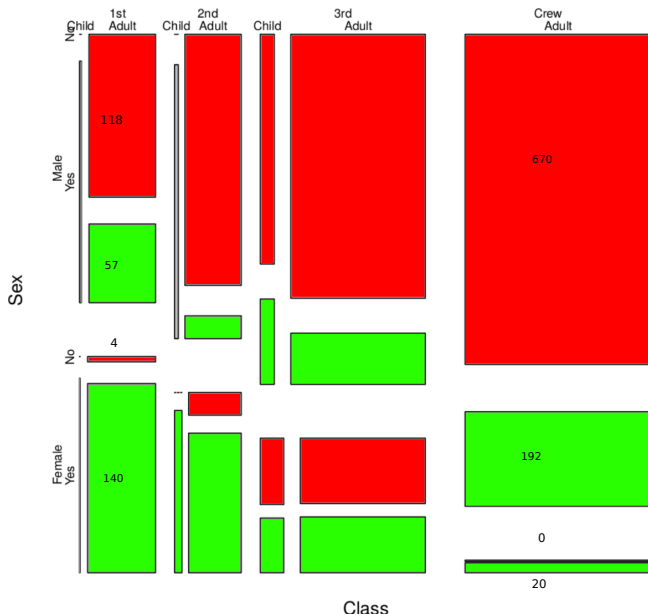
7 Meta-Learning

8 Summary

Association Rule Mining [44]

- Discover interesting relations in correlated facts and extract rules
- Identify frequent item sets “likes HR, likes BigData”
- Example association rule: “likes HR, likes BigData \Rightarrow likes NTHR”
- Data are individual transactions, e.g., purchases, with items
 - Items $I = i_1, \dots, i_n$
 - Transactions $T = t_1, \dots, t_n$
 - Each t_i is a subset of I , e.g., items bought together in a market basket
- Several algorithms exist, e.g., APRIORI, RELIM
- Relevance of rules is defined by support and confidence
 - Assume $X \Rightarrow Y$ be an association rule, X, Y are item-sets
 - $\text{support}(X)$: number of transactions which contains item-set X
 - $\text{confidence}(X \Rightarrow Y) = \text{support}(X \cup Y) / \text{support}(X)$: fraction of transactions which contain X and Y . Indicates if the rule is good

Titanic Dataset Shows the Classes of Survivors



Association Analysis with Python Using Pyming³

```
1 from pymining import itemmining, assocrules
2 import csv
3 with open('titanic2.csv', 'r') as csvfile:
4     reader = csv.reader(csvfile)
5     data = [ r for r in reader ]
6
7 # apply relim algorithm
8 r = itemmining.get_relim_input(data)
9 # find frequent items (more than 1000 instances)
10 itemsets = itemmining.relim(r, min_support=1000)
11 # {frozenset(['No']): 1490, frozenset(['Male', 'Adult', 'No']): 1329, frozenset(['Adult', 'No']): 1438, frozenset(['Adult']):
    ↳ 2092, frozenset(['Male', 'Adult']): 1667, frozenset(['Male', 'No']): 1364, frozenset(['Male']): 1731}
12
13 # mine the association rules
14 r = itemmining.get_relim_input(data)
15 itemsets = itemmining.relim(r, min_support=1)
16 rules = assocrules.mine_assoc_rules(itemsets, min_support=2, min_confidence=0.7)
17 # [(['Adult', 'No']), (['Male']), 1329, 0.9242002781641169], (['No']), (['Male', 'Adult']), 1329, 0.8919463087248322), ...
18 # identify only survival-relevant rules with two or one items/attributes
19 relevant = [ (p, "Yes" in c,supp,conf) for p, c, supp, conf in rules if (c == frozenset(['No']) or c == frozenset(['Yes']))
    ↳ and len(p) <= 2]
20 relevant.sort(key=lambda x : x[1]) # sort based on the survival
21 for p, c, supp, conf in relevant:
22     print(("%.2f: %s <= %s" % (supp, conf, c, p)).replace("frozenset", ""))
23 #1329,0.80: False <= (['Male', 'Adult'])
24 #476,0.76: False <= (['Adult', '3rd'])
25 #154,0.86: False <= (['Male', '2nd'])
26 #422,0.83: False <= (['Male', '3rd'])
27 #344,0.73: True <= (['Female'])
28 #316,0.74: True <= (['Adult', 'Female'])
29 #6,1.00: True <= (['1st', 'Child'])
30 #24,1.00: True <= (['2nd', 'Child'])
```

³<https://github.com/bartdag/pymining>

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Meta-Learning [1, p.359ff]

- Idea: combine multiple (weak) models to improve model performance
- **Ensemble**: team of models used by a meta-model
- Approach: take data subset to train each model and combine prediction
 - Allocation function: defines which training data each model receives
 - Combination function: resolves disagreement
 - Stacking: learn the combination function (as a ML model)
- Advantage of meta-learning:
 - Generalizability: prevents overfitting of training data
 - Performance: small models are faster to train, parallel training is possible
 - Nuanced understanding: subtle patterns are better covered than in a global model

Bagging [1, p. 362]

- Bagging == bootstrap aggregation
- Approach:
 - 1 Generate many training datasets by sampling the training data
 - 2 Train a model for each training dataset (using the same learning algorithm)
 - 3 Combine predictions
 - Voting (for classification problems)
 - Averaging (for prediction problems)
- Particularly useful on unstable learners
 - Unstable learners: training algorithms depending heavily on the input data
- Random forest
 - Build many decision trees (\Rightarrow forest)
 - Increase variety by choosing a small set of features for each tree randomly

Boosting [1, p.366ff]

- Differences to bagging
 - Generate complementary learners
 - Weight vote of learner based on past performance
- Adaptive boosting: learn the difficult-to-classify examples
 - First classifier: train on all data
 - Subsequent rounds: remove correct predictions (with a high probability)
 - Stop after desired accuracy is reached or classifier does not improve
 - Weight vote based on accuracy on the training data on which it was built
 - In R: AdaBoost.M1 algorithm / C5.0 algorithm
- Alternative approach: predictor for predicting the error

Summary

- Data preprocessing normalizes data / treats missing data
- Machine learning problems:
 - Classification, regression, clustering, association rule mining
- Holdout method: strategy to assess model quality
- Evaluation of model performance is crucial
 - Categorical data: confusion matrix + metrics
 - Numerical data: residual, MAE, MSE, MAPE
- Classification: K-NN, Naive Bayes, trees
- Regression: linear models, regression trees
- Clustering: k-means, density-based
- Association rule mining: market basket analysis with APRIORI

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