

Data science (Unsupervised learning methods)

Presented By:

Sri Krishnamurthy, CFA, CAP www.QuantUniversity.com sri@quantuniversity.com

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Unsupervised learning Introduction



Unsupervised learning methods

- Are known as methods deal with finding patterns or classes of unlabeled data objects. In other word in such datasets there is no continuous or discrete responds associated with observations.
- Methods include of clustering (partitioning and hierarchical), P.C.A, association rules mining and Kernel density clustering.
- The AdultUCI, iris and inquisition.basket are the sample datasets used in this chapter.
- In python mainly scikit-learn package deals with data mining and machine learning algorithms while there are plenty of packages and functions in R.



Clustering

- ✓ K-Means clustering
- ✓ Linkage methods
- ✓ Distance functions
- ✓ Hierarchical clustering
- ✓ Elbow chart and bend graph
- ✓ Kernel density estimation
- ✓ Kernel density clustering



K-Means clustering

- K-Means is defined as the main partitioning clustering method which divides data into different clusters.
- K-Means randomly assigns initial clusters to observations and tries to modify that at each iteration such a way within clusters distance of objects reaches minimum.
- Final answers in K-Mean depends on initial assignments and are defined as local minima. To reach global minima this process should be repeated over and over for reasonable number of times.
- K-Means calculates the distance of each data object from the center of the cluster while function form can be Euclidean, Manhattan or correlation, etc.



Linkage methods

- In clustering methods to answer how close the data objects and clusters are will be answered by different types of linkage as:
- Complete: The largest distance of inter-clusters by comparing pairwise
- Single: The smallest distance of inter-clusters by comparing pairwise
- Average: The average distance of all inter-clusters pairwise data objects
- Centroid: The distance between centroids of the clusters



Distance functions

- Three main commonly used distance functions in clustering methods are Euclidean, Manhattan and correlation (mostly used in time series analysis) while there are couple of other distance types such as Minkowski, Canberra, etc.
- Euclidean distance: In a simple 2 dimensional space for points A,B is defined as below and it can be easily extended to n dimensional space:

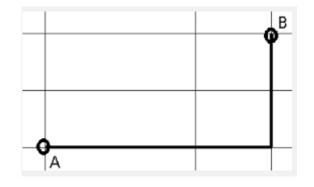
$$D = \sqrt{(X_A - X_B)^2 + (Y_A - Y_B)^2}$$



Distance functions

• Manhattan distance: In a simple 2 dimensional space for points A,B is defined as below and it can be easily extended to n dimensional

space:

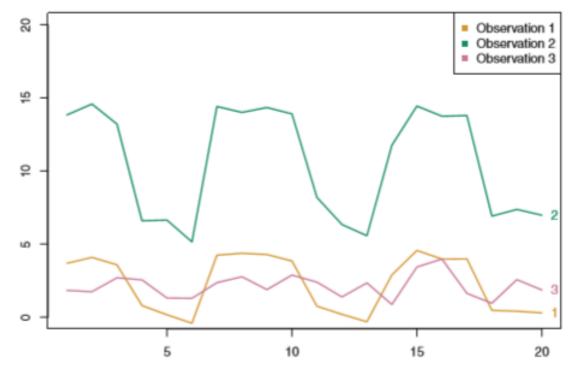


$$D = |X_A - X_B| + |Y_A - Y_B|$$



Distance functions

• Correlation distance: Considers two observations are similar if their features are highly correlated such as observations 1 and 2 in below graph:





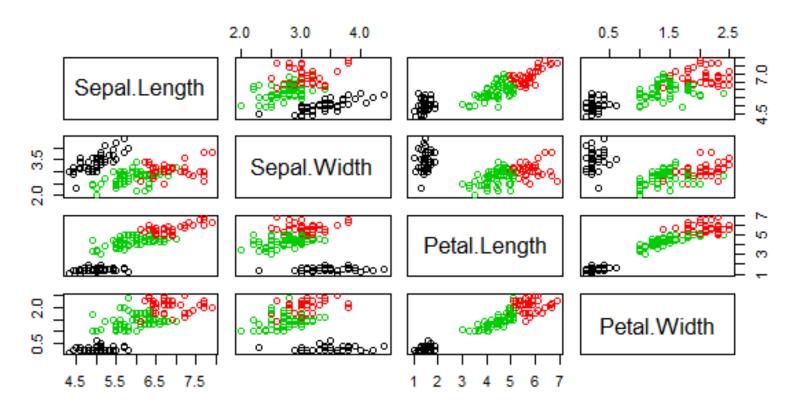
K-Means clustering (R)

```
#### kmeans (Euclidean Distance)
iris # Chosen dataset
iris <- iris[,-5] # Dropping last column</pre>
iris # New dataset
?kmeans # What is kmean?
km.out <- kmeans(iris,3,nstart=10) #nstart tells how many times algorithm</pre>
# starts from beginning since the final answers is related to initial assignments.
names (km. out)
km.out$cluster # kmeans results
plot(iris, col=(km.out$cluster), main="K-mean result with k=3") #Scatterplot matrix
> km.out$cluster # kmeans results
 11111
3 3 3 3 3
2 2 3 2 2
[142] 2 3 2 2 2 3 2 2 3
```



K-Means clustering (R)

K-mean result with k=3





See *Clustering iris.R*

K-Means clustering (R)

```
#### Kmeans (Manhattan Distance)
install.packages("Matrix")
require(amap)
iris
iris <- iris[,-5]
iris
iris <- as.matrix(iris)</pre>
km.out <- Kmeans(iris, 3, iter.max=1000,nstart = 10,method = "manhattan")</pre>
km.out $cluster
iris <- as.data.frame(iris)</pre>
plot(iris, col=(km.out$cluster), main="K-mean result with k=3")
> km.out$cluster
 2 2 2 2 2
3 3 3 3 3
1 1 3 1 1
[142] 1 3 1 1 1 3 1 1 3
> |
```



K-Means clustering (Python)

```
from sklearn import cluster, datasets
In [10]:
         iris=datasets.load_iris()
         x iris=iris.data
In [14]: k means=cluster.KMeans(n clusters=3)
         k means.fit(x iris)
In [15]:
Out[15]: KMeans(copy_x=True, init='k-means++', max_iter=300, n_clusters=3, n_init=10,
             n_jobs=1, precompute_distances='auto', random_state=None, tol=0.0001,
             verbose=0)
         print(k_means.labels_)
In [16]:
          0 0 2 2 0 0 0 0 2 0 2 0 2 0 0 0 2 2 0 0 0 0 0 2 0 0 0 0 2 0 0 0 2 0 0 0 2 0
          0 2]
```



Hierarchical clustering

- Despite K-Means in which initial number of clusters are assigned, in hierarchical we don't need to know about the number of clusters.
- Hierarchical clustering applies bottom-up or agglomerative methods to create the tree-based visualization of clusters which is called Dendrogram.
- By cutting Dendrogram at any specific point we will have different number of clusters.
- Linkage methods which can be used are complete, single, average and centroid while the distance function can be Euclidean, correlation, etc.

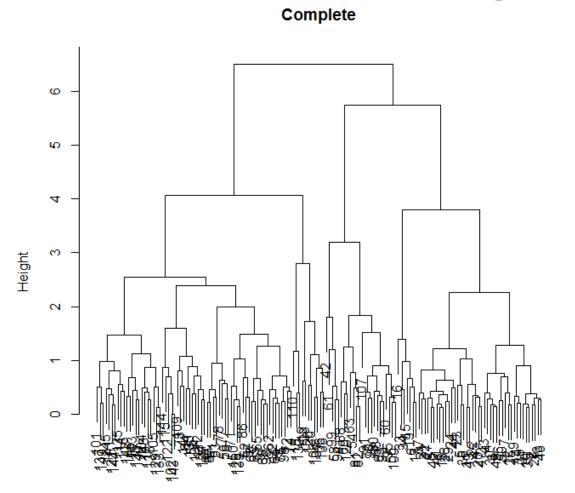


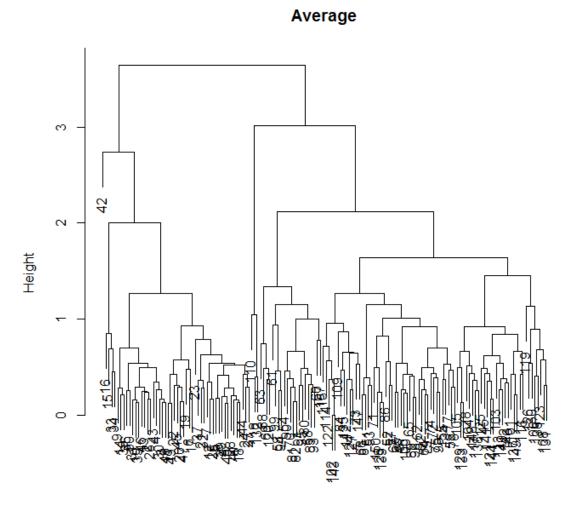
Hierarchical clustering (R)

```
#### Hierarchical clustering
iris=scale(iris) #Scaling the data
hc.complete=hclust(dist(iris),method="complete") # Complete linkage type
hc.average=hclust(dist(iris),method="average") # Average linkage type
par(mfrow=c(1,2)) #Plotting in a matrix form
plot(hc.complete,main='Complete')
plot(hc.average,main='Average')
cutree(hc.complete,3)
cutree(hc.average,3)
> cutree(hc.complete,3)
                           3 3 3 3 3 3 3 3 3 3 3
[124] 3 3 3 3 3 3 3 3 3 3 3 3 3 3 3 3 3
> cutree(hc.average,3)
 [1] 1 1 1 1 1 1 1 1 1 1 1 1 1 1
```



Hierarchical clustering (R)







See **Clustering iris.R**

Hierarchical clustering (Python)

```
In [1]: from sklearn.cluster import AgglomerativeClustering
     from sklearn import datasets, cluster
     iris=datasets.load iris()
     x iris=iris.data
In [2]: complete = AgglomerativeClustering(n clusters=3, linkage='complete').fit(x iris)
     average = AgglomerativeClustering(n clusters=3, linkage='average').fit(x iris)
In [3]: label1=complete.labels
     label1
1, 1, 1, 1, 0, 0, 0, 2, 0, 2, 0, 2, 0, 2, 2, 2, 2, 0, 2, 0, 2, 2, 0,
         2, 0, 2, 0, 0, 0, 0, 0, 0, 0, 2, 2, 2, 0, 2, 0, 0, 0, 0, 2, 2, 2, 0,
         2, 2, 2, 2, 0, 2, 2, 0, 0, 0, 0, 0, 0, 2, 0, 0, 0, 0, 0, 0, 0, 0,
         0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0], dtype=int64)
In [4]: label2=average.labels
     label2
0, 0, 0, 0, 0, 0, 0, 0, 2, 0, 2, 2, 2, 2, 0, 2, 2, 2, 2, 2, 2, 0, 0,
         2, 2, 2, 2, 0, 2, 0, 2, 0, 2, 2, 0, 0, 2, 2, 2, 2, 2, 2, 0, 2, 2, 2, 2,
         0, 2, 2, 2, 0, 2, 2, 0, 2, 2, 0], dtype=int64)
```





Elbow chart and bend graph

- As mentioned in hierarchical clustering, by cutting the Dendrogram at any specific point we may have different number of clusters, but what is the optimum number of clusters?
- Elbow function answers to this question by considering a threshold for explained variance of the dataset.
- Although in K-Means we may initially assign different number of clusters, to answer the same question, we may plot within sum of squared error for different number of clusters and choose the best number of clusters.



Elbow chart (R)

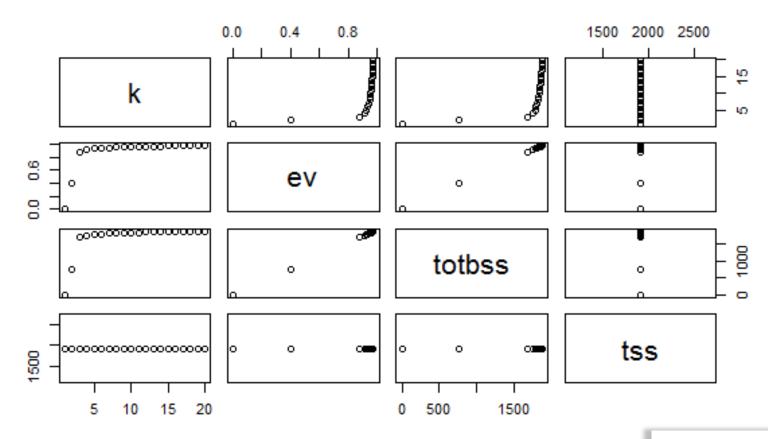
```
iris # Chosen dataset
iris <- iris[.-5]
install.packages("GMD") # Needed package
require("GMD")
dist.obj <- dist(iris[,1:4],method="manhattan") # Defining distance object and method
hclust.obj <- hclust(dist.obj) # Creating clusters</pre>
css.obj <- css.hclust(dist.obj,hclust.obj) # Creating multi object
names(css.obj)
elbow.obj <- elbow.batch(css.obj) # Creating elbow object
print(elbow.obj)
plot(css.obj,elbow.obj=NULL)
#clustering with more relaxed thresholds (resulting a smaller "good" k)
elbow.obj2 <- elbow(css.obj,ev.thres=0.90,inc.thres=0.05)
print(elbow.obj2)
$k
[1] 8
$ev
[1] 0.9498663
$inc.thres
[1] 0.01
$ev.thres
[1] 0.95
attr(,"description")
[1] "A \"good\" k=8 (EV=0.95) is detected when the EV is no less than 0.95\nand the incre
ment of EV is no more than 0.01 for a bigger k.\n"
attr(,"class")
```

css.obj is a multi-object list computing Sum-of-Square for clustering evaluation



See Elbow&Bend Charts iris.R

Elbow chart (R)



See **Elbow&Bend Charts iris.R**

K: number of clusters

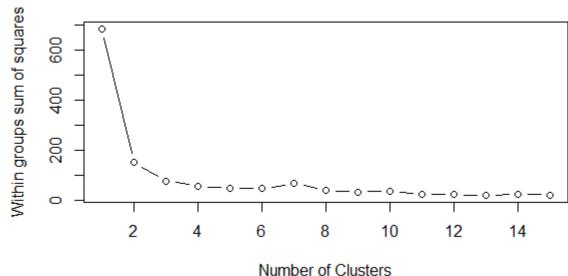
totbss: total between cluster sum-of-square

tss: total sum of square of the data

ev: explained variance given k



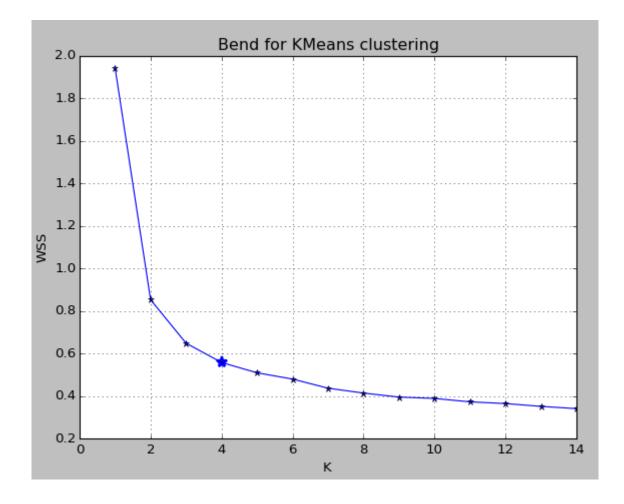
Bend graph (R)





Bend graph (Python)

```
### Needed dataset
from sklearn import *
iris=datasets.load iris()
print iris.data.shape
(150L, 4L)
### Needed modules and functions
import numpy as np
import scipy
from scipy.cluster.vq import kmeans,vq
from scipy.spatial.distance import cdist
import matplotlib.pyplot as plt
### Defining different number of clusters and calculate wss for each of them
K = range(1,15)
KM = [kmeans(iris.data,k) for k in K]
centroids = [cent for (cent, var) in KM] # cluster centroids
avgWithinSS = [var for (cent,var) in KM] # mean within-cluster sum of squares
kIdx = 3
### Bend graph
fig = plt.figure()
ax = fig.add subplot(111)
ax.plot(K, avgWithinSS, 'b*-')
ax.plot(K[kIdx], avgWithinSS[kIdx], marker='*', markersize=10,
   markeredgewidth=2, markeredgecolor='b', markerfacecolor='None')
plt.grid(True)
plt.xlabel('K')
plt.ylabel('WSS')
plt.title('Bend for KMeans clustering')
plt.show()
```





See Bend Charts iris.ipynb

Kernel density estimation

- Density estimation walks the line between unsupervised learning, feature engineering, and data modeling.
- The very basic technique of density estimation is histogram which may lead to different results due to choice of binning problem.
- Gaussian function is the most commonly used one in comparison with the other available kernel forms.
- The main application of kernel density estimation is to know about the distribution of observations by visualizing them.
- Other kernel forms that can be used in kernel density estimation are exponential, linear, etc.



- Kernel density clustering performs cluster analysis based on nonparametric density estimation.
- This method clusters data such a way components with estimated above threshold are maximally connected.
- The number of clusters is automatically selected according to the number of modes of estimated density.
- Kernel density clustering can be applied to either low or high dimensional data.

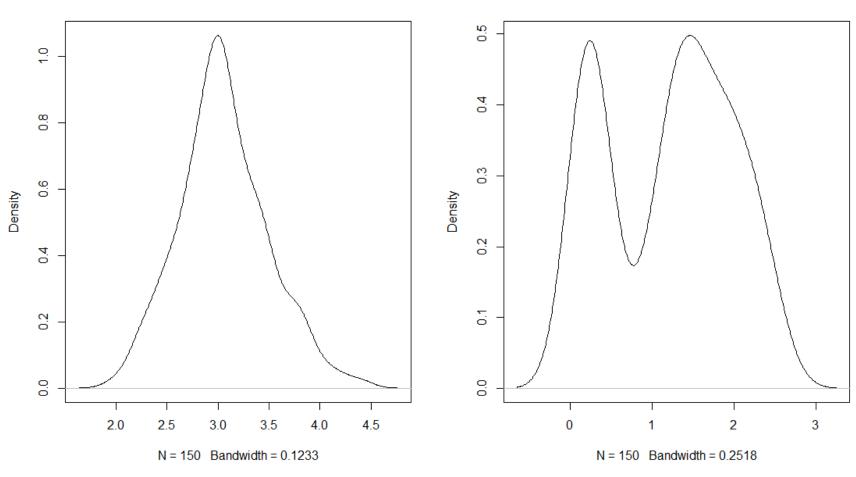


Kernel density estimation (R)

Kernel density estimation (R)

density.default(x = x, xlab = Sepal.Width)

density.default(x = y, xlab = Petal.Width)

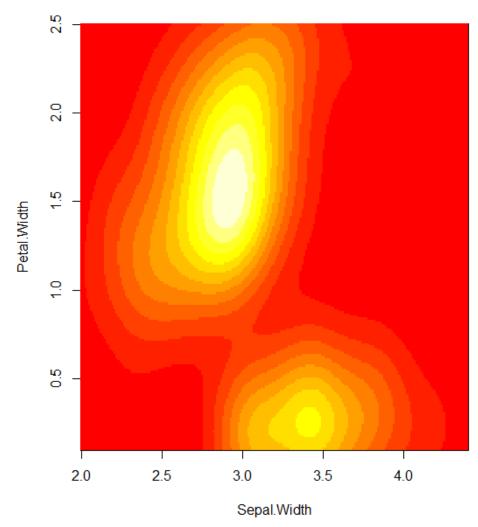




See Kernel Density Estimation iris.R

Kernel density estimation (R)

Two-Dimensional Kernel Density Estimation

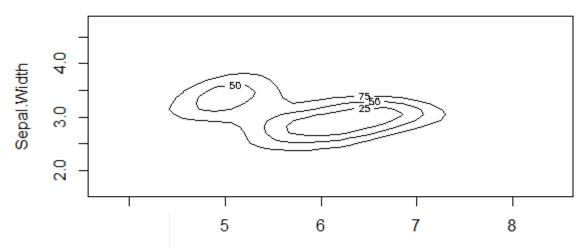




```
### Needed package
install.packages("pdfcluster")
library("pdfcluster")
### Dataset
iris # Chosen dataset
iris <- iris[,-5] # Dropping last column
iris # New dataset
### 2d Clustering
x <- iris[,c(1,2)]
pdf <- kepdf(x)
summary(pdf)
plot(pdf)</pre>
```

Kernel density estimate of data

Sepal.Length



The highest density data point has position 98 in the sample data

Rows of 75 % top density data points: 1 2 3 4 5 7 8 10 11 12 13 18 20 21 22 24 25 26 27 28 29 30 31 32 35 36 37 38 40 41 44 45 46 47 48 49 50 51 52 53 55 56 57 59 62 64 65 66 67 68 70 71 72 73 74 75 76 77 78 79 80 81 82 83 84 85 87 89 90 91 92 93 95 96 97 98 100 101 102 103 104 105 111 112 113 114 115 116 117 121 122 124 125 127 128 129 130 133 134 135 1 38 139 140 141 142 143 144 145 146 147 148 150

Rows of 50 % top density data points: 1 3 5 8 12 18 24 25 27 28 29 30 36 40 41 44 50 52 53 55 56 59 62 64 65 66 67 68 72 74 75 76 78 79 80 83 84 87 89 91 92 93 95 96 97 98 100 1 02 104 105 111 112 113 115 116 117 121 122 124 127 128 129 133 134 135 138 139 140 141 14 2 143 144 146 148 150

Rows of 25 % top density data points: 55 56 59 62 64 66 68 72 74 75 76 78 79 83 84 87 92 97 98 100 102 104 105 113 115 117 127 128 129 133 134 138 139 141 143 146 148 150

Kepdf (kernel estimate of a probability density function) estimates density of univariate or multivariate data by the kernel method.



See Kernel Density Clustering iris.R

```
### 3d Clustering
y <- iris[,c(1,2,3)]
pdf <- kepdf(y)
summary(pdf)
plot(pdf)</pre>
```

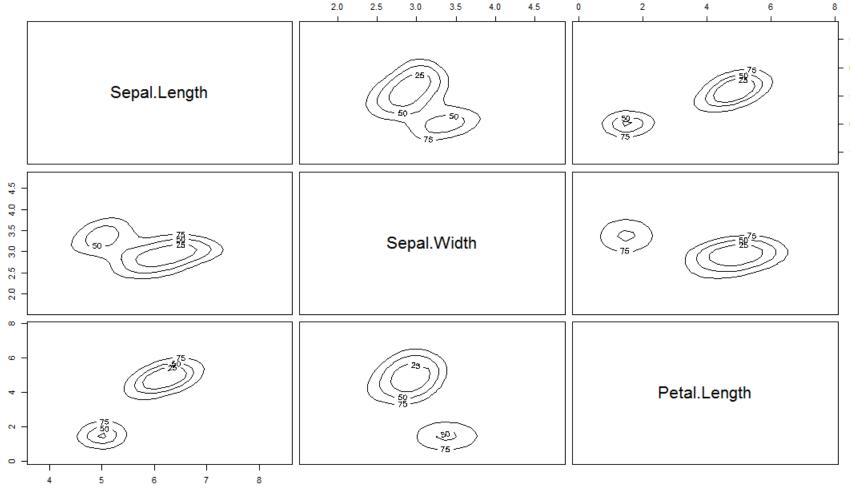
The highest density data point has position 64 in the sample data

Rows of 75 % top density data points: 1 2 3 4 5 7 8 10 11 12 13 18 20 21 22 24 25 26 27 28 29 30 31 32 35 36 37 38 40 41 43 44 45 46 47 48 49 50 51 52 53 55 56 57 59 62 64 65 66 67 68 70 71 72 73 74 75 76 77 78 79 80 81 83 84 85 87 89 90 91 92 93 95 96 97 98 100 101 102 103 104 105 111 112 113 114 115 116 117 121 122 124 125 127 128 129 130 133 134 135 1 38 139 140 141 142 143 144 145 146 147 148 150

Rows of 50 % top density data points: 1 3 5 8 10 12 18 22 24 25 27 28 29 30 31 35 36 38 40 41 44 48 50 52 53 55 56 59 62 64 66 67 68 72 74 75 76 78 79 83 84 87 92 93 95 96 97 98 100 102 104 105 111 112 113 115 116 117 121 122 124 127 128 129 133 134 138 139 140 141 1 42 143 146 148 150

Rows of 25 % top density data points: 1 8 18 27 40 41 44 50 55 56 59 64 68 74 75 78 79 8 4 87 92 97 98 100 104 111 113 115 117 124 127 128 134 138 139 141 146 148 150







See Kernel Density Clustering iris.R

```
### 4d Clustering
pdf <- kepdf(iris)
summary(pdf)
plot(pdf)</pre>
```

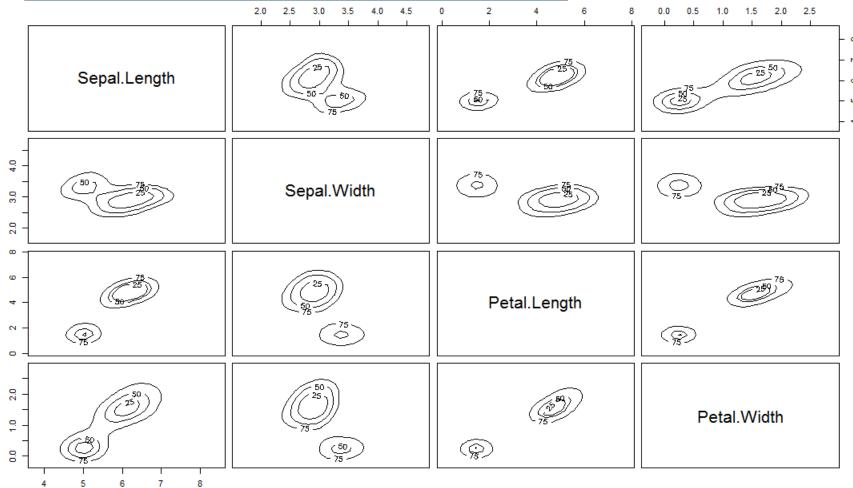
The highest density data point has position 8 in the sample data

Rows of 75 % top density data points: 1 2 3 4 5 6 7 8 10 11 12 13 17 18 20 21 22 23 24 2 5 26 27 28 29 30 31 32 35 36 37 38 39 40 41 43 44 45 46 47 48 49 50 52 53 55 56 57 59 60 62 64 65 66 67 68 70 71 72 73 74 75 76 77 78 79 80 81 82 83 84 85 87 89 90 91 92 93 95 96 97 98 100 102 103 104 105 111 112 113 116 117 121 122 124 125 127 128 129 133 134 135 138 139 140 141 142 143 144 145 146 148 150

Rows of 50 % top density data points: 1 2 3 4 5 7 8 10 11 12 13 18 21 22 24 25 27 28 29 30 31 32 35 36 37 38 40 41 44 46 48 49 50 55 56 59 62 64 67 68 72 74 75 76 78 79 83 84 87 89 91 92 93 95 96 97 98 100 104 105 111 112 113 117 124 127 128 129 134 138 139 140 146 1 48 150

Rows of 25 % top density data points: 1 3 5 8 12 18 25 27 28 29 30 31 35 36 40 41 48 50 55 56 62 64 72 74 78 79 84 92 97 98 100 104 117 127 128 134 139 148







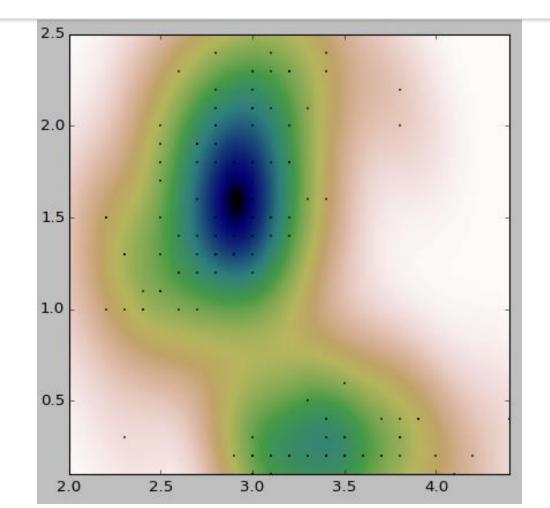
See Kernel Density Clustering iris.R

Kernel density estimation (Python)

```
In [89]: ### Needed packages and dataset
         from sklearn import datasets
         import numpy as np
         from scipy import stats
         iris = datasets.load iris()
         m1= iris.data[:,1:2]
         m2= iris.data[:,3:]
         m1 = m1[\sim np.isnan(m1)]
         m2 = m2[\sim np.isnan(m2)]
         xmin = m1.min()
         xmax = m1.max()
         ymin = m2.min()
         ymax = m2.max()
In [90]: ### Creating meshgrid and kernel function
         X, Y = np.mgrid[xmin:xmax:100j, ymin:ymax:100j]
         positions = np.vstack([X.ravel(), Y.ravel()])
         values = np.vstack([m1, m2])
         kernel = stats.gaussian_kde(values)
         Z = np.reshape(kernel(positions).T, X.shape)
In [93]: ###Plotting
         import matplotlib.pyplot as plt
         fig = plt.figure()
         ax = fig.add subplot(111)
         ax.imshow(np.rot90(Z), cmap=plt.cm.gist_earth_r
         ax.plot(m1, m2, 'k.', markersize=2)
         ax.set_xlim([xmin, xmax])
         ax.set_ylim([ymin, ymax])
         plt.show()
```

See Kernel Density Estimation iris.ipynb

Two dimensional kernel density estimation plot for iris dataset (X: Sepal width and Y: Petal width)





Association Rules



Association rules

- Is known as method of finding if-else type relationship (X => Y) among variables called as rule.
- There are three main criterion of customizing and sorting rules as:
- ✓ Support (X => Y) = $\frac{frequency(X \ and \ Y)}{N}$
- ✓ Confidence (X => Y) = $\frac{frequency(X \ and \ Y)}{frequency(X)}$
- ✓ lift (X => Y) = $\frac{Support(X \ and \ Y)}{Support(X)*Support(Y)}$
- Association rule method applies Apriori algorithm(https://en.wikipedia.org/wiki/Apriori_algorithm) to find the rules.
- The main application of association rule method is market basket analysis for point-of-sales datasets.

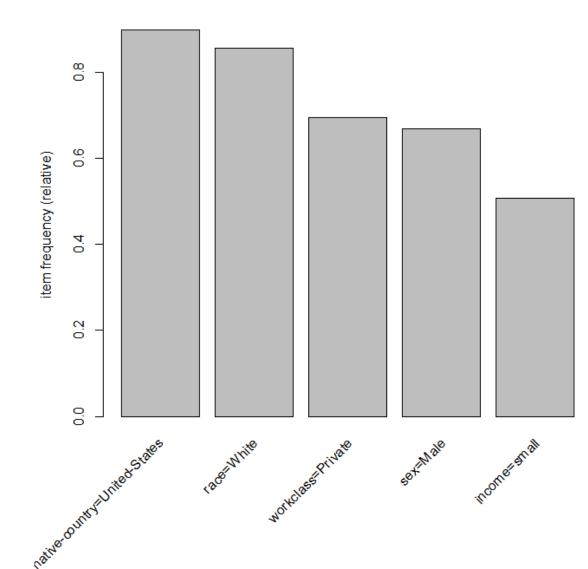


```
### Needed package, library and dataset
install.packages("arules")
library(arules)
require(arules)
data("AdultUCI")
Adult <- AdultUCI[,-c(1,3,5,11,12,13)]
Adult = as(Adult, "transactions")
Adult
#### Association rules
inspect(Adult[1:5,]) # First 5 rows
itemFrequencyPlot(Adult, support=0.5) # Items having at least support of 0.5
itemFrequencyPlot(Adult,topN=5) # Top 5 support items
### Finding rules
r1 <- apriori(Adult) # Primary search for rules
r1
r2 <- apriori(Adult, parameter=list(support=0.5, confidence=0.5, minlen=2))
r2 # Customized search for rules
inspect(r2[1:5]) # First 5 rules
```

Apriori function mines frequent item sets, association rules or association hyper edges using the Apriori algorithm. The Apriori algorithm employs level-wise search for frequent item sets.



```
> r2 # Customized search for rules
set of 16 rules
> inspect(r2[1:5]) # First 5 rules
  1hs
                                    rhs
                                                                   support
1 {sex=Male}
                                 => {race=White}
                                                                   0.5883256
2 {race=White}
                                 => {sex=Male}
                                                                   0.5883256
3 {sex=Male}
                                 => {native-country=United-States} 0.5983170
4 {native-country=United-States}
                                => {sex=Male}
                                                                   0.5983170
5 {workclass=Private}
                                 => {race=White}
                                                                   0.5942427
  confidence lift
1 0.8800919 1.0292957
2 0.6880657 1.0292957
3 0.8950383 0.9973412
4 0.6667047 0.9973412
5 0.8560137 1.0011355
```





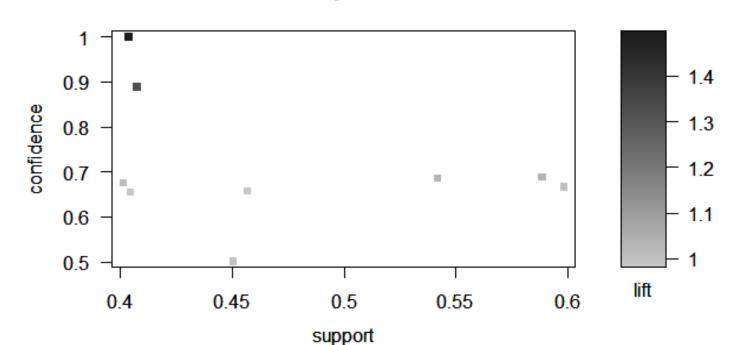
See arule AdultUCI.R

```
> inspect(sort(r2, by="support")[1:5]) # Sorting rules by support(Top 5)
   1hs
                                    rhs
                                                                  support
                                                                            confidence lift
                                 => {native-country=United-States} 0.7881127 0.9217231 1.0270761
9 {race=White}
10 {native-country=United-States} => {race=White}
                                                                  0.7881127 0.8781940 1.0270761
7 {workclass=Private}
                                 => {native-country=United-States} 0.6171942 0.8890757 0.9906971
 {native-country=United-States} => {workclass=Private}
                                                                  0.6171942 0.6877396 0.9906971
                                 => {native-country=United-States} 0.5983170 0.8950383 0.9973412
3 {sex=Male}
> inspect(sort(r2, by="lift")[1:5]) # Sorting rules by lift(Top 5)
  1hs
                                                   support confidence
                                                                          lift
1 {sex=Male,
   native-country=United-States > {race=White} 0.5415421 0.9051090 1.058554
2 {workclass=Private,
   native-country=United-States } => {race=White} 0.5433848  0.8804113  1.029669
3 {sex=Male}
                                 => {race=white} 0.5883256  0.8800919 1.029296
4 {race=White}
                                 => {sex=Male} 0.5883256 0.6880657 1.029296
5 {race=White,
   native-country=United-States > {sex=Male} 0.5415421 0.6871379 1.027908
```



```
> inspect(sort(r3, by="lift")[1:5])
  1hs
                                         rhs
                                                      support confidence
                                                                             lift
                                      => {sex=Male} 0.4036485 0.9999493 1.495851
1 {relationship=Husband}
2 {marital-status=Married-civ-spouse,
   relationship=Husband}
                                      => {sex=Male} 0.4034028 0.9999492 1.495851
3 {marital-status=Married-civ-spouse} => {sex=Male} 0.4074157  0.8891818 1.330151
4 {race=White}
                                      => {sex=Male} 0.5883256  0.6880657  1.029296
5 {race=White,
   native-country=United-States}
                                      => {sex=Male} 0.5415421
                                                               0.6871379 1.027908
```

Scatter plot for 10 rules







Association rules (Python)

```
In [7]: import Orange # Needed package
         import Orange.data
         data = Orange.data.Table("inquisition.basket") # Orange data object for association rules
In [34]: rules = Orange.associate.AssociationRulesSparseInducer(data, confidence=.8) # Default support is at least 0.3
                                                                                  # and confidence greater than 0.8
         print "%5s %5s" % ("supp", "conf") # Customized rules
In [35]:
         for r in rules[:10]:
             print "%5.3f %5.3f %s" % (r.support, r.confidence, r)
                 conf
          supp
                1.000
         0.300
                        amongst -> our
                1.000
                        efficiency -> ruthless
         0.300
                        ruthless -> efficiency
         0.300
                1.000
                        efficiency -> ruthless are
         0.300
                1.000
                1.000 efficiency ruthless -> are
         0.300
                        efficiency are -> ruthless
         0.300
                1.000
                        ruthless -> efficiency are
         0.300
                1.000
         0.300 1.000 ruthless are -> efficiency
               1.000
                        efficiency -> ruthless are fear
         0.300
                        efficiency ruthless -> are fear
         0.300 1.000
```



Association rules (Python)

rules = Orange.associate.AssociationRulesSparseInducer(data, support = 0.5, confidence=0.8) # Support is at least 0.5 # and confidence greater than 0.8

```
for r in rules[:10]:
   print "%5.3f %5.3f %s" % (r.support, r.confidence, r)
supp
       conf
0.500
      1.000
            fear -> surprise
            surprise -> fear
0.500
      1.000
0.500
      1.000
            fear -> surprise our
            fear surprise -> our
0.500
      1.000
0.500
      1.000
            fear our -> surprise
0.500
     1.000
            surprise -> fear our
0.500
      1.000
            surprise our -> fear
            fear -> our
0.500
      1.000
0.500
      1.000
            surprise -> our
```



Summary

We have covered	Unsupervised learning methods
Clustering methods	 ✓ Definition of unsupervised learning methods ✓ K-Means clustering and its features such as linkage methods and distance function form ✓ Hierarchical clustering and its property as Dendrogram ✓ How to choose number of clusters by using elbow chart and bend graph ✓ To evaluate the density of the data by Kernel method ✓ Clustering based on Kernel density estimation
Association rules mining	 ✓ The rules (relationships) between variables as well as support, confidence and lift indices ✓ How to customize, sort and limit rules



Q&A







Thank you!

Contact

Sri Krishnamurthy, CFA, CAP Founder and CEO QuantUniversity LLC.

Linked in srikrishnamurthy

www.QuantUniversity.com