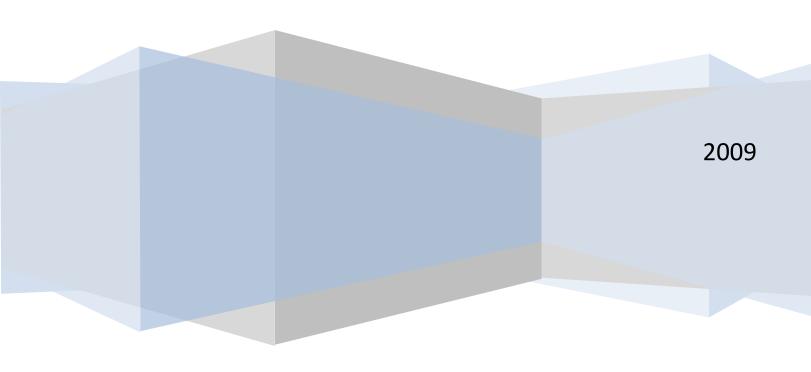
Foundations of Data Mining CS-691

Homework Assignment - 3
Sandipan Dey



1. First the iris text data provided needs to be converted to **weka-compatible attribute relation file format (.arff)** that looks like the following:

% Iris

@RELATION iris

- @ATTRIBUTE Sepal_length NUMERIC
- @ATTRIBUTE Sepal_width NUMERIC
- @ATTRIBUTE Petal_length NUMERIC
- **@ATTRIBUTE Petal width NUMERIC**

@DATA

2	14	33	50
24	56	31	67
23	51	31	69
2	10	36	46
20	52	30	65
19	51	27	58
13	45	28	57
16	47	33	63

As can be seen from above, only the last four attributes from the text data are selected.

If we run KMeans algorithm in Weka with the .arff file as the input file,

weka.clusterers.SimpleKMeans -V -N < numClusters> -A < distanceFunction> -I maxIteration -S seed

- Initial number of clusters is chosen as 3 (since we suspect that specifies_name attribute, or equivalently specifies_no attribute denotes the class labels for the data those already obtained by applying some supervised method and there are exactly 3 different class labels, namely, I.Setosa, I.Verginica, I.Versicolor)
- distanceFunction as Euclidian
- maximum iteration (to converge) as 500
- random seed (to select initial cluster centers) as 10
- display standard deviation option is selected

The following output is obtained after the algorithm terminates in 4 iterations, with MSE 7.12:

=== Run information ===

Scheme: weka.clusterers.SimpleKMeans -V -N 3 -A "weka

Relation: iris Instances: 150 Attributes: 4

> Sepal_length Sepal_width Petal_length Petal_width

Test mode: evaluate on training data

=== Model and evaluation on training set ===

kMeans

Number of iterations: 4

Within cluster sum of squared errors: 7.115548372424189

Missing values globally replaced with mean/mode

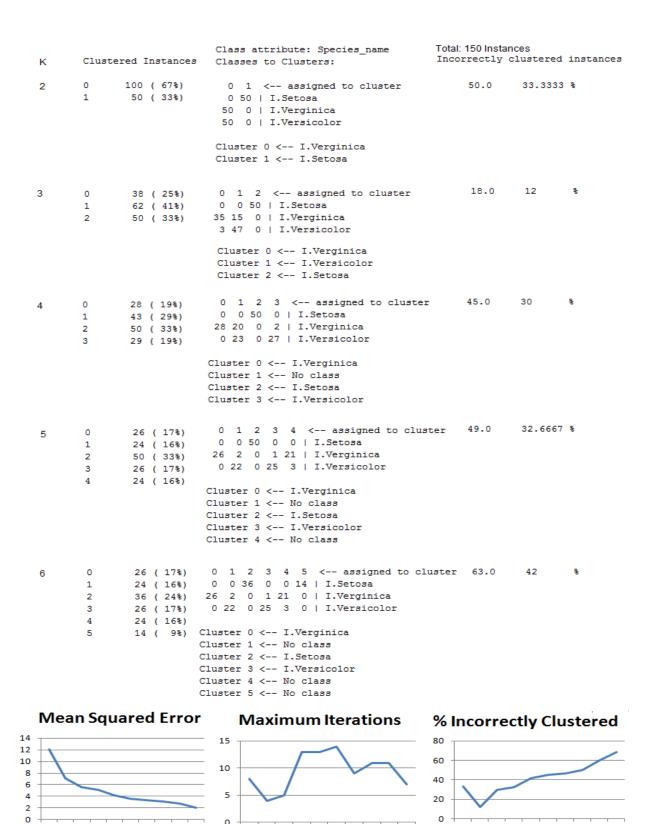
Cluster centroids:

		Cluster#		
Attribute	Full Data	0	1	2
	(150)	(38)	(62)	(50)
Sepal_length	11.9267	20.7368	14.1613	
	+/-7.569	+/-2.8254	+/-2.7051	+/-1.0539
Sepal_width	37.7867	57.1579	44.5968	14.62
	+/-17.7762	+/-5.1963	+/-5.6784	+/-1.7366
Petal_length	30.5533	30.8421	27.371	34.28
_	+/-4.3728	+/-2.8335	+/-2.9266	+/-3.7906
Petal width	58.4467	68.5	59.0161	50.1
_	+/-8.2686	+/-5.0871	+/-4.5682	+/-3.5355

Clustered Instances

0 38 (25%) 1 62 (41%) 2 50 (33%)

If the classes to cluster evaluation option from weka (with class label as specifies_name, that is to be ignored when running KMeans but the resulting cluster-membership for each instance is to be validated against the corresponding class labels) is used to verify the clusters generated, the following output is obtained additionally:

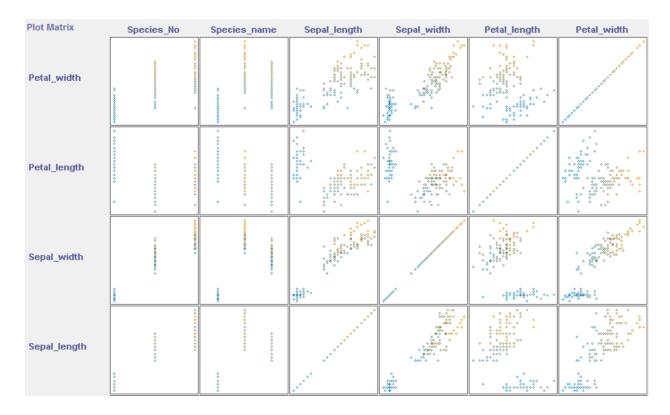


As can be seen from above, the number of incorrectly clustered instances is minimum when K = 3

8

3

7 8 9 10



As seen from the Weka **Visualize**, there are clearly 3 classes (pre-determined labels) in the data, so in unsupervised grouping one can expect 3 clusters and start with $\mathbf{K} = \mathbf{3}$ for KMeans.

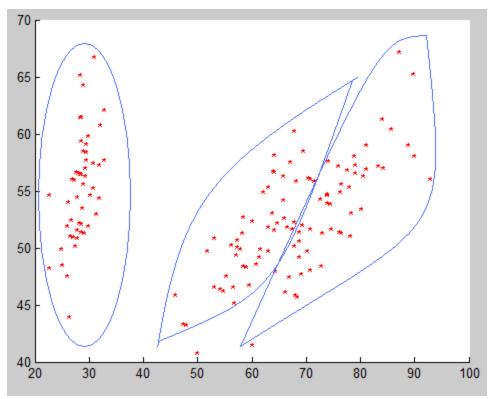
Compression (dimensionality reduction / feature extraction technique)

PCA can be used for compression. For Iris data it's enough to use 2 most dominant Eigen vectors for projection in the feature space, since the Eigen values obtained are 2.9127, 0.9150, 0.1483, 0.0241, the 1st two dominant Eigen Vectors preserve

```
\frac{2.9127 + 0.9150}{2.9127 + 0.9150 + 0.1483 + 0.0241} = 95.69\%  of variance.
```

First we shall be interested to see the direction of maximum variations in the data along the feature space. To find it a **scatter plot** is done in between the data projections along the 2nd most dominant eigen vectors in the transformed feature space, with the following output:

```
% Matlab
% iris data already loaded in X
[COEFF,SCORE,latent] = princomp(X); % PCA
A = COEFF(:, 1:2);
Y = X * A; % Projection on 2 most dominat PCs
scatter(Y(:,1), Y(:, 2), 15, [1,0,0], 'p') % scatter plot in the projected space
```



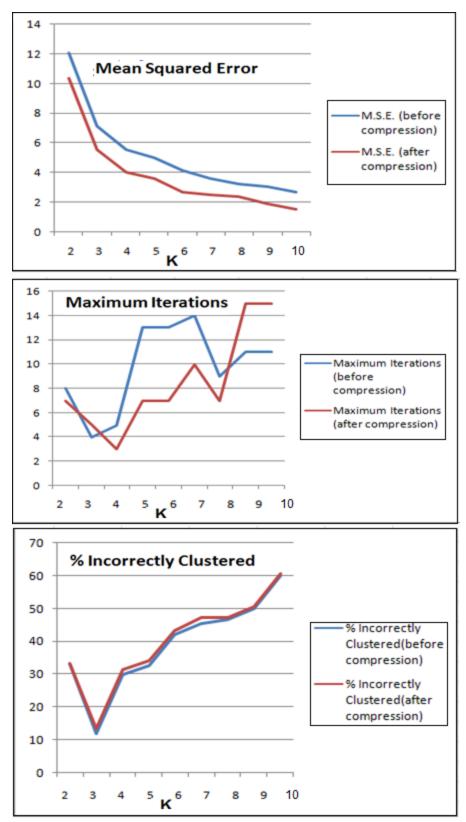
There are clearly **3 different groups** in the data (outlined approximately), hence k = 3 is the best choice for KMeans.

Altrnatively, PCA can be done using weka as well: java weka.filters.AttributeSelectionFilter -S "weka.attributeSelection.Ranker" -E "weka.attributeSelection.PrincipalComponents -R 0.5" -i iris.arff -o fs_iris.arff

Project in the feature space and compress by dimesionality reduction

```
% Matlab
X = zscore(X); % Normalize
[COEFF,SCORE,latent] = princomp(X); % PCA
A = COEFF(:, 1:2);
Y = X * A; % Projection on 2 most dominat PCs
Xc = Y * A'; % Inverse projection
mean(Xc - X); % Nearly Zero
```

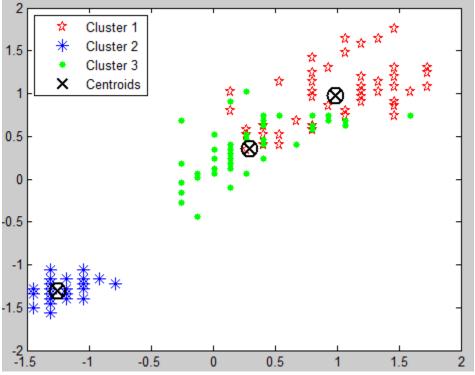
Now, if we compare the KMeans algorithm's output in Weka, in between before and after compression, we get the following results:



Again, it can be seen that even after compression, the # incorrectly-clustered instances are minimized when **K** = **3** (assuming **Specis_name** to be class labels). Also, M.S.E. reduces after PCA compression.

Running KMeans on the compressed data and plotting the output:

```
% matlab
% iris data already loaded in X
opts = statset('Display','final');
k = 3;
                                                      % # clusters
[idx,ctrs] = kmeans(X,k,...
                                                      % kmeans
                    'Distance','sqEuclidean',...
                    'Replicates',5,...
                    'Options', opts);
plot(X(idx==1,1),X(idx==1,2),'rp','MarkerSize',8)
hold on
plot(X(idx==2,1),X(idx==2,2),'b*','MarkerSize',10)
hold on
plot(X(idx==3,1),X(idx==3,2),'g.','MarkerSize',15)
plot(ctrs(:,1),ctrs(:,2),'kx',...
     'MarkerSize',12,'LineWidth',2)
plot(ctrs(:,1),ctrs(:,2),'ko',...
     'MarkerSize', 12, 'LineWidth', 2)
legend('Cluster 1','Cluster 2','Cluster 3','Centroids',...
       'Location','NW')
          Cluster 1
```



Evidently there are 3 clusters (2 overlapping).

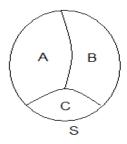
Transaction ID	Items Bought
1	{Milk, Beer, Diapers}
2	{Bread, Butter, Milk}
3	{Milk, Diapers, Cookies}
4	{Bread, Butter, Cookies}
5	{Beer, Cookies, Diapers}
6	{Milk, Diapers, Bread, Butter}
7	{Bread, Butter, Diapers}
8	{Beer, Diapers}
9	{Milk, Diapers, Bread, Butter}
10	{Beer, Cookies}

Table 6.23. Market basket transactions.

- Consider the market basket transactions shown in Table 6.23.
 - (a) What is the maximum number of association rules that can be extracted from this data (including rules that have zero support)?
 - (b) What is the maximum size of frequent itemsets that can be extracted (assuming minsup > 0)?
 - (c) Write an expression for the maximum number of size-3 itemsets that can be derived from this data set.
 - (d) Find an itemset (of size 2 or larger) that has the largest support.
 - (e) Find a pair of items, a and b, such that the rules {a} → {b} and {b} → {a} have the same confidence.

Answer

If $S=\{I_1,I_2,\ldots,I_d\},\ |S|=d$, i.e., with d items, association rules will be of the form $A\to B$, where $A,B\subseteq S,\ A,B\neq \Phi,\ A\cap B=\Phi,\ A\cup B\subseteq S$. This basically implies the division of S into 3 partitions A, B, C s.t. $A,B,C\subseteq S,\ A\cap B\cap C=\Phi,\ A\cup B\cup C=S,\ A,B\neq \Phi$.



Association rules $A \rightarrow B$

A, B may not contain all the elements of S, hence we need to consider another set (possibly non-empty) C, not taking part into association rule formation.

Number of different ways it can be done

= (Total #ways S can be partitioned into A, B, C) – (#ways A is empty) – (#ways B is empty) + (#ways both A, B are empty)

$$=3^{d}-2^{d}-2^{d}+1=3^{d}-2^{d+1}+1$$
.

Thought in slightly different manner, let's consider all possible association rules of the form $A \rightarrow B$. The L.H.S. can consist of any number of items (k) staring from 1 to d – 1 (since both L.H.S and R.H.S. must be non-empty but their intersection is the null set) and has to be chosen from the d-item set and for each of these choices, the R.H.S. can have 1 to d – k items (l) in it.

Hence, total number of different ways

$$= \sum_{k=1}^{d-1} \sum_{l=1}^{d-k} \binom{d}{k} \binom{d-k}{l}$$

$$= \sum_{k=1}^{d-1} \binom{d}{k} \sum_{l=1}^{d-k} \binom{d-k}{l} = \sum_{k=1}^{d-1} \binom{d}{k} (2^{d-k} - 1) = \sum_{k=1}^{d-1} \binom{d}{k} (2^{d-k}) - \sum_{k=1}^{d-1} \binom{d}{k}$$

$$= 3^{d} - 2^{d} - 1 - (2^{d} - 2) = 3^{d} - 2^{d+1} + 1$$

Since by Binomial theorem,

$$(x+1)^{d} - x^{d} - 1 = \sum_{k=1}^{d-1} {d \choose k} (x^{d-k}) \Rightarrow 3^{d} = \sum_{k=0}^{d} {d \choose k} (2^{d-k}) = 2^{d} + 1 + \sum_{k=1}^{d-1} {d \choose k} (2^{d-k})$$

(a) Here, d = 6. Hence, maximum number of association rules $= 3^6 - 2^{6+1} + 1 = 729 - 128 + 1 = 602$

(b)If *minsup* > 0, maximum size of frequent item-sets that can be extracted = maximum width of a record in the transaction = 4 here.

(c) Maximum number of size-k item-sets that can be derived from the dataset containing d items

$$=$$
 $\begin{pmatrix} d \\ k \end{pmatrix}$. Here, we have, d = 6 and k = 3. Hence, maximum # of item-sets $=$ $\begin{pmatrix} 6 \\ 3 \end{pmatrix}$ =20.

(d)

In	Items	#
1	Beer	4
2	Bread	5
3	Butter	5
4	Cookies	4
5	Diapers	7
6	Milk	5

1-itemset

In	Items	#
1	{Beer, Bread}	0
2	{Beer, Butter}	0
3	{Beer, Cookies}	2
4	{Beer, Diapers}	3
5	{Beer, Milk}	1
6	{Bread, Butter}	5
7	{Bread, Cookies}	1
8	{Bread, Diapers}	3
9	{Bread, Milk}	3
10	{Butter, Cookies}	1
11	{Butter, Diapers}	3
12	{Butter, Milk}	3
13	{Cookies, Diapers}	2
14	{Cookies, Milk}	1
15	{Diapers, Milk}	4

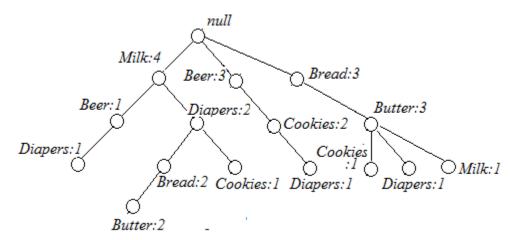
2-itemset

The highest support-count in set of all 2-itemsets = 5, i.e., for {Bread, Butter}. Considering only the item-sets with support count 5 or higher for 3-itemsets (because by anti-monotone property, the support-count for any superset of an item-set is less than or equal to the support count of that item-set). Also, {Beer, Bread} support count is 0, we need not consider its superset. As we can see, support counts for all other 2-item-sets are strictly less than 5, all 3-item sets will have support count strictly less than 5.

In	Items	#
1	{ Bread, Butter, Cookies }	1
2	{Bread, Butter, Diapers}	3
3	{Bread, Butter, Milk}	3

Hence, the item-set (of size-2 or larger) with the largest support count (5) is the 2-item-set {Bread, Butter}.

Let's construct the FP-tree,



From the FP tree it's clear that only {Bread, Butter} is having the support count as high as 5.

(e) ::
$$confidence(\{a\} \rightarrow \{b\}) = \frac{\sigma(\{a\} \ and \ \{b\})}{\sigma(\{a\})}$$
,
$$confidence(\{a\} \rightarrow \{b\}) = confidence(\{b\} \rightarrow \{a\}) \Rightarrow \sigma(\{a\}) = \sigma(\{b\})$$

Consider the following two rules:

$$\begin{aligned} & \{ \text{Bread,Diapers} \} \rightarrow \{ \text{\textit{Butter,Milk}} \} \text{ and } \{ \text{\textit{Butter,Milk}} \} \rightarrow \{ \text{Bread,Diapers} \} \\ & \because \sigma \big(\{ \text{Bread,Diapers}, \text{\textit{Butter,Milk}} \} \big) = 2 \quad \land \quad \sigma \big(\{ \text{Bread,Diapers} \} \big) = \sigma \big(\{ \text{\textit{Butter,Milk}} \} \big) = 3, \\ & \textit{\textit{confidence}} \big(\{ \text{Bread,Diapers} \} \rightarrow \{ \text{\textit{Butter,Milk}} \} \big) = \textit{\textit{confidence}} \big(\{ \text{\textit{Butter,Milk}} \} \rightarrow \{ \text{Bread,Diapers} \} \big) \\ & = \frac{2}{3} \end{aligned}$$

- Consider the training examples shown in Table 4.8 for a binary classification problem.
 - (a) What is the entropy of this collection of training examples with respect to the positive class?

Table 4.8. Data set for Exercise 3.

Instance	a_1	a_2	a_3	Target Class
1	T	T	1.0	+
2	T	\mathbf{T}	6.0	+
3	T	\mathbf{F}	5.0	_
4	F	\mathbf{F}	4.0	+
5	F	\mathbf{T}	7.0	_
6	F	\mathbf{T}	3.0	_
7	F	\mathbf{F}	8.0	_
8	T	\mathbf{F}	7.0	+
9	F	\mathbf{T}	5.0	_

- (b) What are the information gains of a₁ and a₂ relative to these training examples?
- (c) For a₃, which is a continuous attribute, compute the information gain for every possible split.
- (d) What is the best split (among a₁, a₂, and a₃) according to the information gain?
- (e) What is the best split (between a₁ and a₂) according to the classification error rate?
- (f) What is the best split (between a₁ and a₂) according to the Gini index?

Answer

(a) Here the target class is a binary random variable X with the following probability mass function

$$p(x) = P(X = x) = \begin{cases} \frac{4}{9}, & x \text{ is } + ve \\ \frac{5}{9}, & x \text{ is } - ve \end{cases}$$

$$H(X) = \sum_{x \in X} p(x) \log \left(\frac{1}{p(x)}\right)$$

$$= \sum_{x \ge 0} p(x) \log \left(\frac{1}{p(x)}\right) + \sum_{x \le 0} p(x) \log \left(\frac{1}{p(x)}\right)$$

$$= I(4,5) = \frac{4}{9} \log_2 \left(\frac{9}{4}\right) + \frac{5}{9} \log_2 \left(\frac{9}{5}\right) = 0.52 + 0.47 = 0.99$$
where $I(p, n)$ is defined as $-\frac{p}{p+n} \log \left(\frac{p}{p+n}\right) - \frac{n}{p+n} \log \left(\frac{n}{p+n}\right)$.

(b)
$$E(a_1) = \frac{|a_1 = T|}{|a_1|} H(X \mid a_1 = T) + \frac{|a_1 = F|}{|a_1|} H(X \mid a_1 = F)$$

$$= \frac{4}{9} I(3,1) + \frac{5}{9} I(1,4) = \frac{4}{9} \left(\frac{3}{4} \log \left(\frac{4}{3}\right) + \frac{1}{4} \log \left(\frac{4}{1}\right)\right) + \frac{5}{9} \left(\frac{1}{5} \log \left(\frac{5}{1}\right) + \frac{4}{5} \log \left(\frac{5}{4}\right)\right)$$

$$= \frac{4}{9} \times 0.8113 + \frac{5}{9} \times 0.7219 = 0.36057 + 0.40106 = 0.76163$$

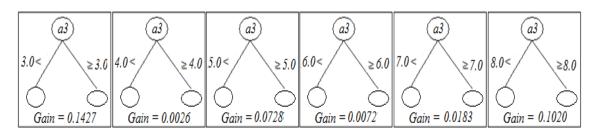
$$\therefore Gain(a_1) = H(X) - E(a_1) = I(4,5) - E(a_1) = 0.9911 - 0.7616 = 0.2294$$

$$E(a_2) = \frac{5}{9} I(2,3) + \frac{4}{9} I(2,2) = 0.9839$$

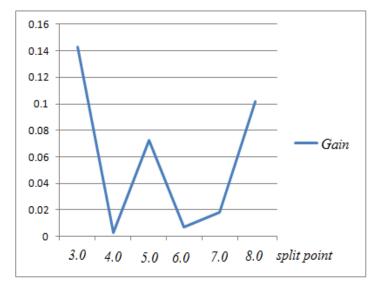
$$\therefore Gain(a_2) = H(X) - E(a_2) = I(4,5) - E(a_2) = 0.9911 - 0.9839 = 0.0072$$

(c) Since *a3* is continuous valued, we try all possible split points, in order to split the set into 2 subsets. For instance, if <6.0 then left subset, ow create right subset. For all different choises of the split-points, the information gain is as follows:

a3						
Split point	3.0	4.0	5.0	6.0	7.0	8.0
Gain	0.1427	0.0026	0.0728	0.0072	0.0183	0.1020

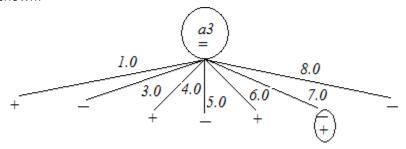


Splitting the data set into 2 subset using different values of the attribute a3 as split point



Splitting the data set into 2 subset using different values of the attribute a3 as split point

If the number of split points is increased, the gain will also increase in general, resulting in **highest gain** in the worst case if there are 5 splits (at the cost of 7 branches in the tree), as shown:

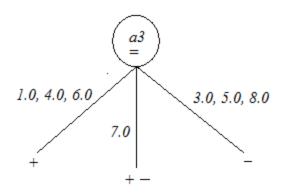


$$E(a_3) = \frac{1}{9}I(1,0) + \frac{1}{9}I(0,1) + \frac{1}{9}I(1,0) + \frac{2}{9}I(0,2) + \frac{1}{9}I(1,0) + \frac{2}{9}I(1,1) + \frac{1}{9}I(0,1)$$

$$= \frac{1}{9}.0 + \frac{1}{9}.0 + \frac{1}{9}.0 + \frac{2}{9}.0 + \frac{1}{9}.0 + \frac{2}{9}.1 + \frac{1}{9}.0 = 0.2222$$

$$\therefore Gain(a_3) = H(X) - E(a_3) = I(4,5) - E(a_3) = 0.9911 - 0.2222 = 0.7689$$

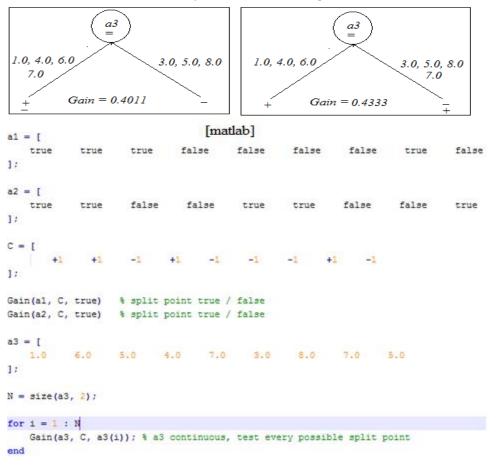
So far the **values** of the attribute a3 were considered in **sorted order**. From the above it can be easily seen that the split can be minimized to 3 and yet the same gain can be achieved (if we get rid of the order in the attribute values)



$$E(a_3) = \frac{3}{9}I(1,0) + \frac{2}{9}I(0,2) + \frac{4}{9}I(0,1)$$
$$= \frac{3}{9}.0 + \frac{2}{9}.1 + \frac{4}{9}.0 = 0.2222$$

:.
$$Gain(a_3) = H(X) - E(a_3) = I(4,5) - E(a_3) = 0.9911 - 0.2222 = 0.7689$$

If the value 7.0 is included in any of the subsets, the gain decreases.



[matlab]

```
* attribute A
% target class C
a split value s
function [G] = Gain(A, C, s)
   nc = size(A, 2); % size of target class labels
    posC = 0;
    for i = 1 : nc
        if (C(i) > 0)
                                                       A
           posC = posC + 1;
                                             A < s
    end
                                                              A \ge s
    G = I(posC, nc - posC) - E(A, C, s);
end
                                           attribute A with split point s
% attribute A
& target class C
* split value s
function [WH] = E(A, C, s)
   WH = 0:
                   % initialize weighted average entropy E(A)
    n = size(A, 2); % size of attribute values
    nc = size(A, 2): % size of corresponding target class labels
                   % must be equal
    if (n - nc)
        % attribute set A to be split into 2 subsets Al, A2: s being the
        % split point: all tuples with values of A < s will fall in A1,
        % otherwise fall into A2.
       nA1 = 0:
        nA2 = 0;
        posA1 = 0; % positive class labels in A1
        posA2 = 0; % positive class labels in A2
        for i = 1 : n
            if (A(i) >= s)
                nA1 = nA1 + 1; % number of tuples in A1
                if (C(i) > 0) % if corresponding class label is positive
                    posA1 = posA1 + 1;
                end
            else
                nA2 = nA2 + 1; % number of tuples in A2; nA2 = N - nA1
                if (C(i) > 0)
                                 % if corresponding class label is positive
                 posA2 = posA2 + 1;
            end
        end
        WH = (nA1 / n) * I(posA1, nA1 - posA1) + (nA2 / n) * I(posA2, nA2 - posA2);
    end
end
% find entropy
function [H] = I(a, b)
   p = a / (a + b);
    n = b / (a + b);
   logp = 0;
   if (p ~= 0)
       logp = log2(p);
    logn = 0;
    if (n ~= 0)
       logn = log2(n);
    end
    H = -p * logp - n * logn
```

(d)The attribute corresponding to the largest information gain should be chosen. If we allow **binary splitting** only (maintaining attribute order), the information gain is highest in case of the attribute a1, we should choose attribute a1 for splitting.

If we allow n-ary splitting without maintaining attribute order, *a3* has the highest gain in the 3-split shown above, hence *a3* should be chosen.

(e)

$$ClassErr(t) = 1 - \max_{i} \left[p(i \mid t) \right]$$

$$ClassErr(X \mid a_{1} = T) = 1 - \max\left(\frac{3}{4}, \frac{1}{4}\right) = \frac{1}{4}$$

$$ClassErr(X \mid a_{1} = F) = 1 - \max\left(\frac{1}{5}, \frac{4}{5}\right) = \frac{1}{5}$$

$$ClassErr(a_{1}) = \frac{|a_{1} = T|}{|a_{1}|} ClassErr(X \mid a_{1} = T) + \frac{|a_{1} = F|}{|a_{1}|} ClassErr(X \mid a_{1} = F)$$

$$= \frac{4}{9} \cdot \frac{1}{4} + \frac{5}{9} \cdot \frac{1}{5} = \frac{2}{9} = 0.2222$$

$$ClassErr(a_{2})$$

$$= \frac{5}{9} \left(1 - \frac{3}{5}\right) + \frac{4}{9} \left(1 - \frac{2}{4}\right) = \frac{5}{9} \left(\frac{2}{5}\right) + \frac{4}{9} \left(\frac{2}{4}\right) = \frac{4}{9} = 0.4444$$

The best split is the attribute with minimum classification error rate, hence a1.

The best split is the attribute with minimum gini index, hence a1.