

**Solutions for Tutorial exercises
Association Rule Mining.**

Exercise 1. Apriori

Trace the results of using the Apriori algorithm on the grocery store example with support threshold $s=33.34\%$ and confidence threshold $c=60\%$. Show the candidate and frequent itemsets for each database scan. Enumerate all the final frequent itemsets. Also indicate the association rules that are generated and highlight the strong ones, sort them by confidence.

| Transaction ID | Items |
|----------------|------------------------|
| T1 | HotDogs, Buns, Ketchup |
| T2 | HotDogs, Buns |
| T3 | HotDogs, Coke, Chips |
| T4 | Chips, Coke |
| T5 | Chips, Ketchup |
| T6 | HotDogs, Coke, Chips |

Solution:

Support threshold = 33.34% \Rightarrow threshold is at least 2 transactions.

Applying Apriori

| Pass (k) | Candidate k-itemsets and their support | Frequent k-itemsets |
|----------|---|--|
| k=1 | HotDogs(4), Buns(2), Ketchup(2), Coke(3), Chips(4) | HotDogs, Buns, Ketchup, Coke, Chips |
| k=2 | {HotDogs, Buns}(2), {HotDogs, Ketchup}(1), {HotDogs, Coke}(2), {HotDogs, Chips}(2), {Buns, Ketchup}(1), {Buns, Coke}(0), {Buns, Chips}(0), {Ketchup, Coke}(0), {Ketchup, Chips}(1), {Coke, Chips}(3) | {HotDogs, Buns}, {HotDogs, Coke}, {HotDogs, Chips}, {Coke, Chips} |
| k=3 | {HotDogs, Coke, Chips}(2) | {HotDogs, Coke, Chips} |
| k=4 | {} | |

Note that {HotDogs, Buns, Coke} and {HotDogs, Buns, Chips} are not candidates when k=3 because their subsets {Buns, Coke} and {Buns, Chips} are not frequent.

Note also that normally, there is no need to go to k=4 since the longest transaction has only 3 items.

All Frequent Itemsets: {HotDogs}, {Buns}, {Ketchup}, {Coke}, {Chips}, {HotDogs, Buns}, {HotDogs, Coke}, {HotDogs, Chips}, {Coke, Chips}, {HotDogs, Coke, Chips}.

Association rules:

{HotDogs, Buns} would generate: HotDogs \rightarrow Buns ($2/6=0.33$, $2/4=0.5$) and
Buns \rightarrow HotDogs ($2/6=0.33$, $2/2=1$);

{HotDogs, Coke} would generate: HotDogs \rightarrow Coke (0.33 , 0.5) and
Coke \rightarrow HotDogs ($2/6=0.33$, $2/3=0.66$);

{HotDogs, Chips} would generate: HotDogs \rightarrow Chips (0.33 , 0.5) and
Chips \rightarrow HotDogs ($2/6=0.33$, $2/4=0.5$);

{Coke, Chips} would generate:
Coke \rightarrow Chips ($3/6=0.5$, $3/3=1$) and
Chips \rightarrow Coke ($3/6=0.5$, $3/4=0.75$);

{HotDogs, Coke, Chips} would generate: HotDogs \rightarrow Coke \wedge Chips ($2/6=0.33$, $2/4=0.5$),
Coke \rightarrow Chips \wedge HotDogs ($2/6=0.33$, $2/3=0.66$),
Chips \rightarrow Coke \wedge HotDogs ($2/6=0.33$, $2/4=0.5$),
HotDogs \wedge Coke \rightarrow Chips ($2/6=0.33$, $2/2=1$),
HotDogs \wedge Chips \rightarrow Coke ($2/6=0.33$, $2/2=1$) and
Coke \wedge Chips \rightarrow HotDogs ($2/6=0.33$, $2/3=0.66$).

With the confidence threshold set to 60%, the Strong Association Rules are (sorted by confidence):

| | |
|---|---|
| 1. Coke \rightarrow Chips (0.5, 1) | 5. Chips \rightarrow Coke (0.5, 0.75), |
| 2. Buns \rightarrow HotDogs (0.33, 1); | 6. Coke \rightarrow HotDogs (0.33, 0.66); |
| 3. HotDogs \wedge Coke \rightarrow Chips(0.33, 1) | 7. Coke \rightarrow Chips \wedge HotDogs (0.33, 0.66) |
| 4. HotDogs \wedge Chips \rightarrow Coke(0.33, 1) | 8. Coke \wedge Chips \rightarrow HotDogs(0.33, 0.66). |

Exercise 2. FP-tree and FP-Growth

- Use the transactional database from the previous exercise with same support threshold and build a frequent pattern tree (FP-Tree). Show for each transaction how the tree evolves.
- Use FP-Growth to discover the frequent itemsets from this FP-tree.

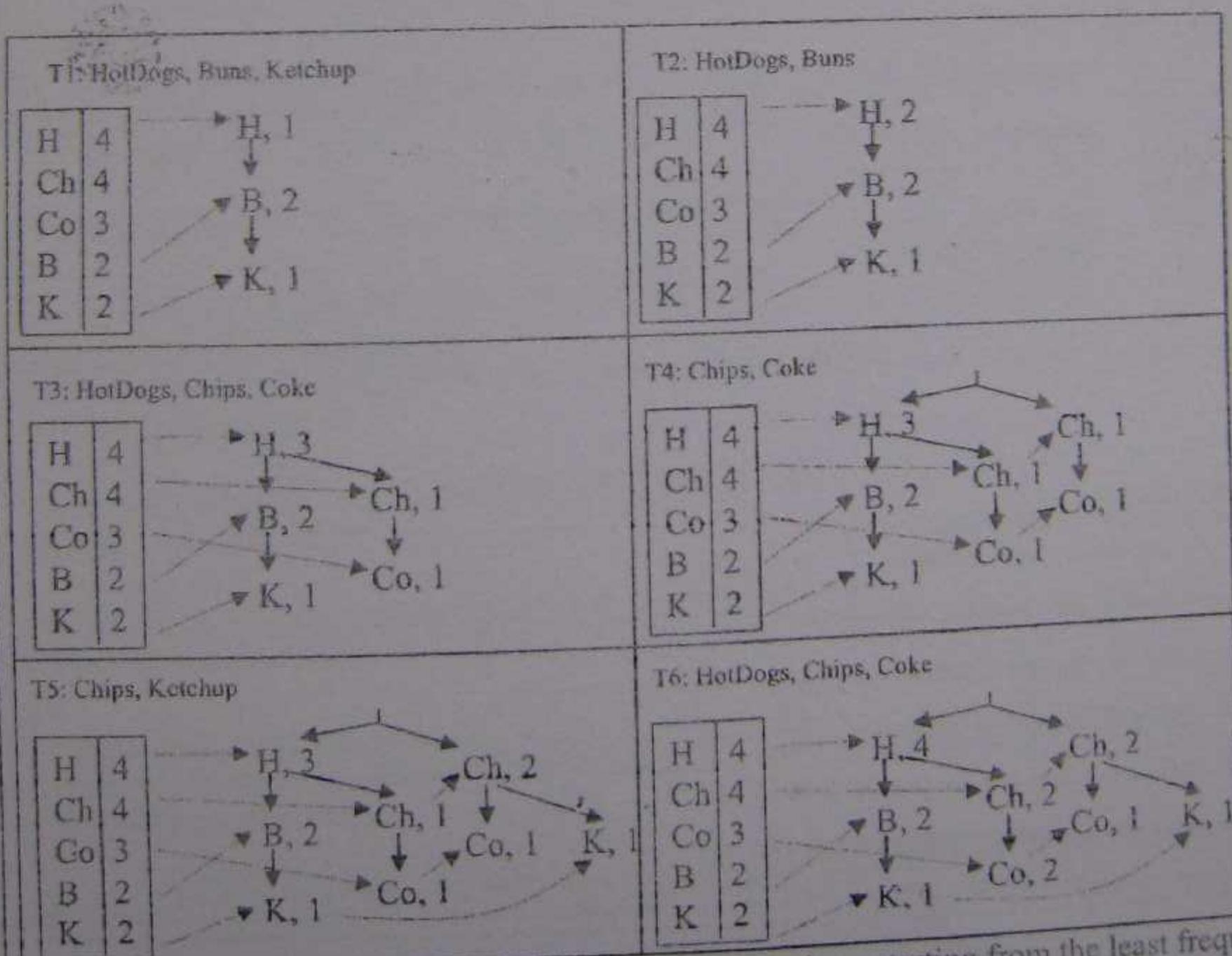
Solution:

- The first scan of the database generates the list of frequent 1-itemsets and builds the header table where the items are sorted by frequency.

Error!

| Item | Code | Support |
|---------|------|---------|
| HotDogs | H | 4 = 66% |
| Chips | Ch | 4 = 66% |
| Coke | Co | 3 = 50% |
| Buns | B | 2 = 33% |
| Ketchup | K | 2 = 33% |

The second scan is used to create the FP-tree. Each transaction is sorted by item support.



- We need to build a conditional tree for each frequent item starting from the least frequent.
- For Ketchup (K), we have two branches H-B-K and Ch-K but since K has a support of 1 in each branch, this would eliminate all items (since support threshold is 2) leaving only <K:2>. This leads to the

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- discovery of {Ketchup} (2) as frequent item.
- For Buns (B), we have only one branch H-B. The sub-transaction {HotDogs, Buns} appears twice. We have thus the patterns <B:2, H:2> and <B:2>. This leads to the discovery of {HotDogs, Buns} (2) and {Buns}(2) as frequent itemsets.
 - For Coke (Co), we have two branches: H-Ch-Co and Ch-Co resulting in the tree Co(3) → Ch(3) → H(2). We have thus 3 patterns: <Co:2, Ch:2, H:2>, <Co:3, Ch:3> and <Co:3>. This leads to the discovery of the following frequent itemsets: {Coke, Chips, HotDogs}(2), {Coke, Chips}(3) and {Coke}(3).
 - For Chips (Ch), we have two paths H-Ch and Ch, giving the following tree Ch(4) → H(2). This gives the patterns <Ch:2, H:2> and <Ch:4>. Thus, the itemsets {Chips, HotDogs}(2) and {Chips}(4) are frequent.
 - For HotDogs (H), The only and obvious pattern is <H:4> leading to the discovery of {HotDogs}(4) as frequent itemset.

All Frequent Itemsets (like in previous exercise): {HotDogs}, {Buns}, {Ketchup}, {Coke}, {Chips}, {HotDogs, Buns}, {HotDogs, Coke}, {HotDogs, Chips}, {Coke, Chips}, {HotDogs, Coke, Chips}.

Notice that there was no candidacy generation. Frequent itemsets were generated directly.

Exercise 3: Using WEKA

Load a dataset described with nominal attributes, e.g. weather.nominal. Run the Apriori algorithm to generate association rules.

Solution:

Running Weka with the default parameters:

Apriori -N 10 -T 0 -C 0.9 -D 0.05 -U 1.0 -M 0.1 -S -1.0

```
==== Run information ====
Scheme:      weka.associations.Apriori -N 10 -T 0 -C 0.9 -D 0.05 -U 1.0 -M 0.1 -S -
1.0
Relation:    weather.symbolic
Instances:   14
Attributes:  5
              outlook
              temperature
              humidity
              windy
              play
==== Associator model (full training set) ====
Apriori
=====
Minimum support: 0.15
Minimum metric <confidence>: 0.9
Number of cycles performed: 17
Generated sets of large itemsets:
Size of set of large itemsets L(1): 12
Size of set of large itemsets L(2): 47
Size of set of large itemsets L(3): 39
Size of set of large itemsets L(4): 6
Best rules found:
1. humidity=normal windy=FALSE 4 => play=yes 4    conf: (1)
2. temperature=cool 4 => humidity=normal 4 ,    conf: (1)
3. outlook=overcast 4 => play=yes 4    conf: (1)
```

| | | | | |
|-----|--|------------|----------------------------|-----------|
| 4. | temperature=cool play=yes 3 | \implies | humidity=normal 3 | conf: (1) |
| 5. | outlook=rainy windy=FALSE 3 | \implies | play=yes 3 | conf: (1) |
| 6. | outlook=rainy play=yes 3 | \implies | windy=FALSE 3 | conf: (1) |
| 7. | outlook=sunny humidity=high 3 | \implies | play=no 3 | conf: (1) |
| 8. | outlook=sunny play=no 3 | \implies | humidity=high 3 | conf: (1) |
| 9. | temperature=cool windy=FALSE 2 | \implies | humidity=normal play=yes 2 | conf: (1) |
| 10. | temperature=cool humidity=normal windy=FALSE 2 | \implies | play=yes 2 | conf: (1) |

Exercise 4: Apriori and FP-Growth (to be done at your own time, not in class)

Giving the following database with 5 transactions and a minimum support threshold of 60% and a minimum confidence threshold of 80%, find all frequent itemsets using (a) Apriori and (b) FP-Growth. (c) Compare the efficiency of both processes. (d) List all strong association rules that contain "A" in the antecedent (Constraint). (e) Can we use this constraint in the frequent itemset generation phase?

| TID | Transaction |
|-----|--------------------|
| T1 | {A, B, C, D, E, F} |
| T2 | {B, C, D, E, F, G} |
| T3 | {A, D, E, H} |
| T4 | {A, D, F, I, J} |
| T5 | {B, D, E, K} |

Solutions for Tutorial exercises

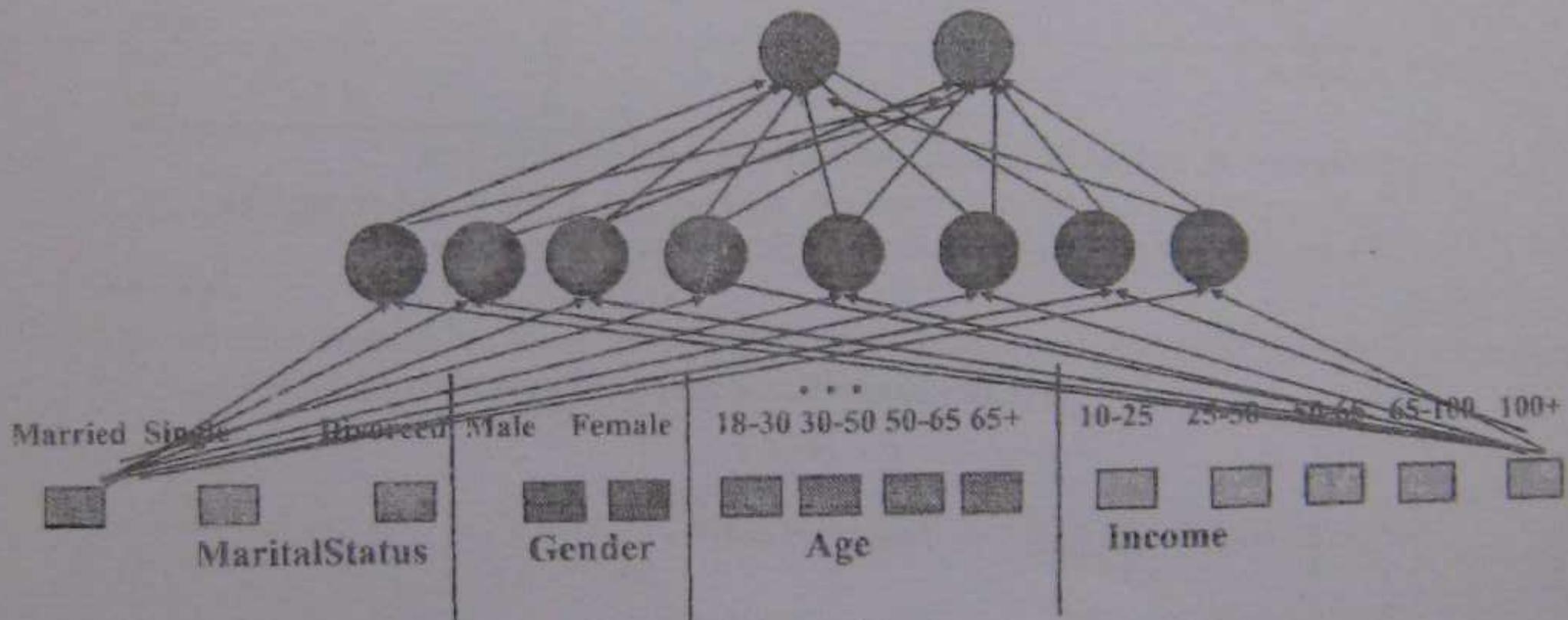
Backpropagation neural networks, Naïve Bayes, Decision Trees, k-NN, Associative Classification.

Exercise 1.

Suppose we want to classify potential bank customers as good creditors or bad creditors for loan applications. We have a training dataset describing past customers using the following attributes: Marital status {married, single, divorced}, Gender {male, female}, Age {[18..30], [30..50], [50..65], [65+]}, Income {[10K..25K], [25K..50K], [50K..65K], [65K..100K], [100K+]}. Design a neural network that could be trained to predict the credit rating of an applicant.

Solution:

We have 2 classes, good creditor and bad creditor. This means we would need two nodes in the output layer. There are 4 variables: Marital Status, Gender, Age and Income. However, since we have 3 values for Marital status, 2 values for Gender, 4 intervals for Age and 5 intervals for Income, we would have 14 neuron units in the input layer. In the hidden layer we can have $(14+2)/2=8$ neurons. The architecture of the neural networks could look like this.

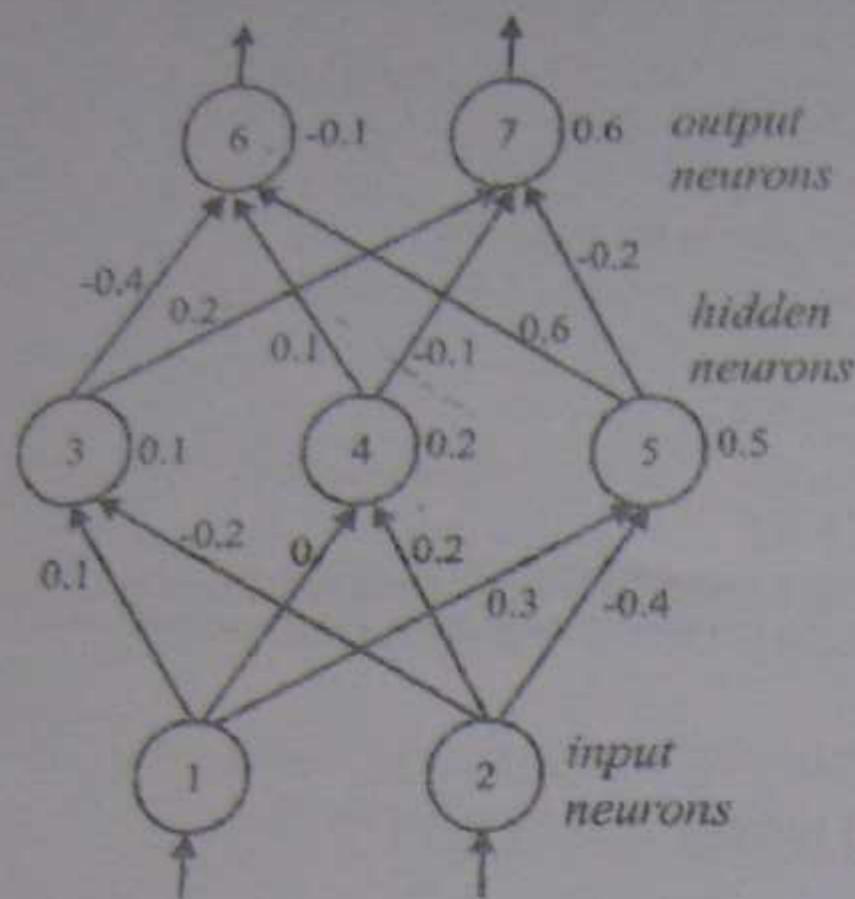


The weights are initialized with random values.

Are there other possible architectures?

Exercise 2.

Given the following neural network with initialized weights as in the picture, explain the network architecture knowing that we are trying to distinguish between nails and screws and an example of training tuples is as follows: T1 {0.6, 0.1, nail}, T2 {0.2, 0.3, screw}.



Let the learning rate η be 0.1 and the weights be as indicated in the figure above. Do the forward propagation of the signals in the network using T1 as input, then perform the back propagation of the error. Show the changes of the weights.

Solution:

What encoding of the outputs?

10 for class "nail", 01 for class "screw"

Forward pass for T1 - calculate the outputs o_6 and o_7

$$o_1 = 0.6, o_2 = 0.1, \text{ target output } 10, \text{ i.e. class "nail"}$$

Activations of the hidden units:

$$\text{net}_3 = o_1 * w_{13} + o_2 * w_{23} + b_3 = 0.6 * 0.1 + 0.1 * (-0.2) + 0.1 = 0.14$$

$$o_3 = 1/(1+e^{-\text{net}_3}) = 0.53$$

$$\text{net}_4 = o_1 * w_{14} + o_2 * w_{24} + b_4 = 0.6 * 0 + 0.1 * 0.2 + 0.2 = 0.22$$

$$o_4 = 1/(1+e^{-\text{net}_4}) = 0.55$$

$$\text{net}_5 = o_1 * w_{15} + o_2 * w_{25} + b_5 = 0.6 * 0.3 + 0.1 * (-0.4) + 0.5 = 0.64$$

$$o_5 = 1/(1+e^{-\text{net}_5}) = 0.65$$

Activations of the output units:

$$\text{net}_6 = o_3 * w_{36} + o_4 * w_{46} + o_5 * w_{56} + b_6 = 0.53 * (-0.4) + 0.55 * 0.1 + 0.65 * 0.6 - 0.1 = 0.13$$

$$o_6 = 1/(1+e^{-\text{net}_6}) = 0.53$$

$$\text{net}_7 = o_3 * w_{37} + o_4 * w_{47} + o_5 * w_{57} + b_7 = 0.53 * 0.2 + 0.55 * (-0.1) + 0.65 * (-0.2) + 0.6 = 0.52$$

$$o_7 = 1/(1+e^{-\text{net}_7}) = 0.63$$

Backward pass for T1 - calculate the output errors δ_6 and δ_7

(note that $d_6=1, d_7=0$ for class "nail")

$$\delta_6 = (d_6 - o_6) * o_6 * (1-o_6) = (1-0.53)*0.53*(1-0.53)=0.12$$
$$\delta_7 = (d_7 - o_7) * o_7 * (1-o_7) = (0-0.63)*0.63*(1-0.63)=-0.15$$

Calculate the new weights between the hidden and output units ($\eta=0.1$)

$$\Delta w_{36} = \eta * \delta_6 * o_3 = 0.1 * 0.12 * 0.53 = 0.006$$
$$w_{36\text{new}} = w_{36\text{old}} + \Delta w_{36} = -0.4 + 0.006 = -0.394$$

$$\Delta w_{37} = \eta * \delta_7 * o_3 = 0.1 * -0.15 * 0.53 = -0.008$$
$$w_{37\text{new}} = w_{37\text{old}} + \Delta w_{37} = 0.2 - 0.008 = -0.19$$

Similarly for $w_{46\text{new}}$, $w_{47\text{new}}$, $w_{56\text{new}}$ and $w_{57\text{new}}$

For the biases b_6 and b_7 (remember: biases are weights with input 1):

$$\Delta b_6 = \eta * \delta_6 * 1 = 0.1 * 0.12 = 0.012$$
$$b_{6\text{new}} = b_{6\text{old}} + \Delta b_6 = -0.1 + 0.012 = -0.012$$

Similarly for b_7

Calculate the errors of the hidden units δ_3 , δ_4 and δ_5

$$\delta_3 = o_3 * (1-o_3) * (w_{36} * \delta_6 + w_{37} * \delta_7) = 0.53 * (1-0.53) * (-0.4 * 0.12 + 0.2 * (-0.15)) = -0.019$$

Similarly for δ_4 and δ_5

Calculate the new weights between the input and hidden units ($\eta=0.1$)

$$\Delta w_{13} = \eta * \delta_3 * o_1 = 0.1 * (-0.019) * 0.6 = -0.0011$$
$$w_{13\text{new}} = w_{13\text{old}} + \Delta w_{13} = 0.1 - 0.0011 = 0.0989$$

Similarly for $w_{23\text{new}}$, $w_{14\text{new}}$, $w_{24\text{new}}$, $w_{15\text{new}}$ and $w_{25\text{new}}$; b_3 , b_4 and b_6

Repeat the same procedure for the other training examples

Forward pass for T2...backward pass for T2...

Exercise 3.

Why is the Naïve Bayesian classification called “naïve”?

Answer: Naïve Bayes assumes that all attributes are: 1) equally important and 2) independent of one another given the class.

Exercise 4. Naïve Bayes for data with nominal attributes

Given the training data in the table below (*Buy Computer* data), predict the class of the following new example using Naïve Bayes classification: age<=30, income=medium, student=yes, credit-rating=fair

| RID | age | income | student | credit_rating | Class: buys_computer |
|-----|---------|--------|---------|---------------|----------------------|
| 1 | <=30 | high | no | fair | no |
| 2 | <=30 | high | no | excellent | no |
| 3 | 31...40 | high | no | fair | yes |
| 4 | >40 | medium | no | fair | yes |
| 5 | >40 | low | yes | fair | yes |
| 6 | >40 | low | yes | excellent | no |
| 7 | 31...40 | low | yes | excellent | yes |
| 8 | <=30 | medium | no | fair | no |
| 9 | <=30 | low | yes | fair | yes |
| 10 | >40 | medium | yes | fair | yes |
| 11 | <=30 | medium | yes | excellent | yes |
| 12 | 31...40 | medium | no | excellent | yes |
| 13 | 31...40 | high | yes | fair | yes |
| 14 | >40 | medium | no | excellent | no |

Solution:

$E = \text{age} \leq 30, \text{income} = \text{medium}, \text{student} = \text{yes}, \text{credit-rating} = \text{fair}$

E_1 is age<=30, E_2 is income=medium, E_3 is student=yes, E_4 is credit-rating=fair

We need to compute $P(\text{yes}|E)$ and $P(\text{no}|E)$ and compare them.

$$P(\text{yes}|E) = \frac{P(E_1|\text{yes})P(E_2|\text{yes})P(E_3|\text{yes})P(E_4|\text{yes})P(\text{yes})}{P(E)}$$

$$P(\text{yes}) = 9/14 = 0.643$$

$$P(\text{no}) = 5/14 = 0.357$$

$$P(E_1|\text{yes}) = 2/9 = 0.222$$

$$P(E_1|\text{no}) = 3/5 = 0.6$$

$$P(E_2|\text{yes}) = 4/9 = 0.444$$

$$P(E_2|\text{no}) = 2/5 = 0.4$$

$$P(E_3|\text{yes}) = 6/9 = 0.667$$

$$P(E_3|\text{no}) = 1/5 = 0.2$$

$$P(E_4|\text{yes}) = 6/9 = 0.667$$

$$P(E_4|\text{no}) = 2/5 = 0.4$$

$$P(\text{yes}|E) = \frac{0.222 \ 0.444 \ 0.667 \ 0.668 \ 0.443}{P(E)} = \frac{0.028}{P(E)} \quad P(\text{no}|E) = \frac{0.6 \ 0.4 \ 0.2 \ 0.4 \ 0.357}{P(E)} = \frac{0.007}{P(E)}$$

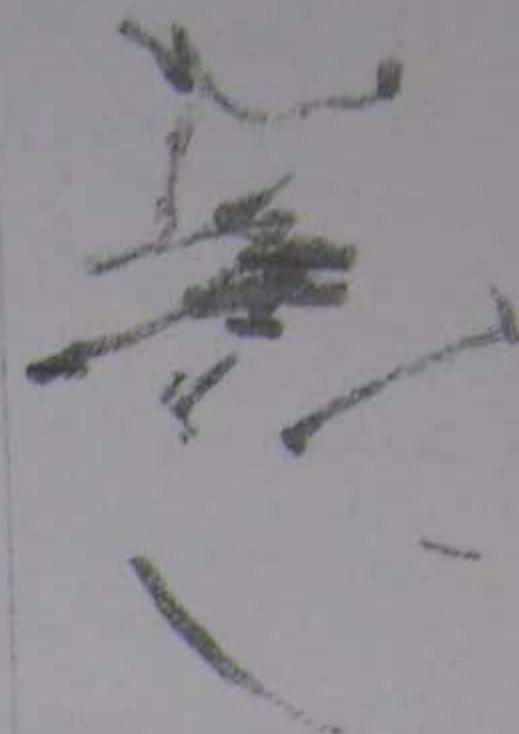
Hence, the Naïve Bayes classifier predicts buys_computer=yes for the new example.

Exercise 5. Applying Naïve Bayes to data with numerical attributes and using the Laplace correction (to be done at your own time, not in class)

Given the training data in the table below (*Tennis* data with some numerical attributes), predict the class of the following new example using Naïve Bayes classification:
outlook=overcast, temperature=60, humidity=62, windy=false.

Tip: You can use Excel or Matlab for the calculations of logarithm, mean and standard deviation. Matlab is installed on our undergraduate machines. The following Matlab functions can be used: log2 – logarithm with base 2, mean – mean value, std – standard deviation. Type help <function name> (e.g. help mean) for help on how to use the functions and examples.

| outlook | temperature | humidity | windy | play |
|----------|-------------|----------|-------|------|
| sunny | 85 | 85 | false | no |
| sunny | 80 | 90 | true | no |
| overcast | 83 | 86 | false | yes |
| rainy | 70 | 96 | false | yes |
| rainy | 68 | 80 | false | yes |
| rainy | 65 | 70 | true | yes |
| overcast | 64 | 65 | true | no |
| sunny | 72 | 95 | false | yes |
| sunny | 69 | 70 | false | no |
| rainy | 75 | 80 | false | yes |
| sunny | 75 | 70 | true | yes |
| overcast | 72 | 90 | true | yes |
| overcast | 81 | 75 | false | yes |
| rainy | 71 | 91 | true | no |



Solution:

First, we need to calculate the mean μ and standard deviation σ values for the numerical attributes. X_i , $i=1..n$ – the i -th measurement, n – number of measurements

$$\mu = \frac{\sum_{i=1}^n X_i}{n}$$

$$\sigma^2 = \frac{\sum_{i=1}^n (X_i - \mu)^2}{n-1}$$

$$\mu_{\text{temp_yes}} = 73, \sigma_{\text{temp_yes}} = 6.2;$$

$$\mu_{\text{temp_no}} = 74.6, \sigma_{\text{temp_no}} = 8.0$$

$$\mu_{\text{hum_yes}} = 79.1, \sigma_{\text{temp_yes}} = 10.2;$$

$$\mu_{\text{hum_no}} = 86.2, \sigma_{\text{temp_no}} = 9.7$$

Second, to calculate $f(\text{temperature}=60|\text{yes})$, $f(\text{temperature}=60|\text{no})$, $f(\text{humidity}=62|\text{yes})$ and $f(\text{humidity}=62|\text{no})$ using the probability density function for the normal distribution:

$$f(x) = \frac{1}{\sigma\sqrt{2\pi}} e^{-\frac{(x-\mu)^2}{2\sigma^2}}$$

(b)

$$f(\text{temperature} = 60 \mid \text{yes}) = \frac{1}{6.2\sqrt{2\pi}} e^{-\frac{(60-73)^2}{2(6.2)^2}} = 0.071$$

$$f(\text{temperature} = 60 \mid \text{no}) = \frac{1}{8\sqrt{2\pi}} e^{-\frac{(60-74.6)^2}{2(8)^2}} = 0.0094$$

$$f(\text{humidity} = 62 \mid \text{yes}) = \frac{1}{10.2\sqrt{2\pi}} e^{-\frac{(62-79.1)^2}{2(10.2)^2}} = 0.0096$$

$$f(\text{humidity} = 62 \mid \text{no}) = \frac{1}{9.7\sqrt{2\pi}} e^{-\frac{(62-86.2)^2}{2(9.7)^2}} = 0.0018$$

Third, we can calculate the probabilities for the nominal attributes:

$$P(\text{yes}) = 9/14 = 0.643$$

$$P(\text{no}) = 5/14 = 0.357$$

$$P(\text{outlook} = \text{overcast} \mid \text{yes}) = 4/14 = 0.286$$

$$P(\text{windy} = \text{false} \mid \text{yes}) = 6/9 = 0.667$$

$$P(\text{outlook} = \text{overcast} \mid \text{no}) = 0/5 = 0$$

$$P(\text{windy} = \text{false} \mid \text{no}) = 2/5 = 0.4$$

As $P(\text{outlook} = \text{overcast} \mid \text{no}) = 0$, we need to use a Laplace estimator for the attribute outlook. We assume that the three values (sunny, overcast, rainy) are equally probable and set $\mu = 3$:

$$P(\text{outlook} = \text{overcast} \mid \text{yes}) = \frac{4+1}{9+3} = \frac{5}{12} = 0.4167$$

$$P(\text{outlook} = \text{overcast} \mid \text{no}) = \frac{0+1}{5+3} = \frac{1}{8} = 0.125$$

Fourth, we can calculate the final probabilities:

$$P(\text{yes} \mid E) = \frac{0.4167 * 0.0071 * 0.0096 * 0.667 * 0.643}{P(E)} = \frac{1.22 * 10^{-5}}{P(E)}$$

$$P(\text{no} \mid E) = \frac{0.125 * 0.0094 * 0.0018 * 0.4 * 0.357}{P(E)} = \frac{3.02 * 10^{-7}}{P(E)}$$

Therefore, the Naïve Bayes classifier predicts play=yes for the new example.

Exercise 6. Using Weka (to be done at your own time, not in class)

Load iris data (iris.arff). Choose 10-fold cross validation. Run the Naïve Bayes and Multi-layer perceptron (trained with the backpropagation algorithm) classifiers and compare their performance. Which classifier produced the most accurate classification? Which one learns faster?

Exercise 7. k-Nearest neighbours

Given the training data in Exercise 4 (*Buy Computer* data), predict the class of the following new example using k-Nearest Neighbour for k=5: age<=30, income=medium, student=yes, credit-rating=fair. For similarity measure use a simple match of attribute values: $\text{Similarity}(A, B) =$

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$$\sum_{i=1}^4 w_i * \delta(a_i, b_i) / 4 \text{ where } \delta(a_i, b_i) \text{ is 1 if } a_i \text{ equals } b_i \text{ and 0 otherwise. } a_i \text{ and } b_i \text{ are either age, income, student or credit_rating. Weights are all 1 except for income it is 2.}$$

Solution:

| RID | age | income | student | credit_rating | Class: buys_computer |
|-----|---------|--------|---------|---------------|----------------------|
| 1 | <=30 | high | no | fair | no |
| 2 | <=30 | high | no | excellent | no |
| 3 | 31...40 | high | no | fair | yes |
| 4 | >40 | medium | no | fair | yes |
| 5 | >40 | low | yes | fair | yes |
| 6 | >40 | low | yes | excellent | no |
| 7 | 31...40 | low | yes | excellent | yes |
| 8 | <=30 | medium | no | fair | no |
| 9 | <=30 | low | yes | fair | yes |
| 10 | >40 | medium | yes | fair | yes |
| 11 | <=30 | medium | yes | excellent | yes |
| 12 | 31...40 | medium | no | excellent | yes |
| 13 | 31...40 | high | yes | fair | yes |
| 14 | >40 | medium | no | excellent | no |

| RID | Class | Distance to New |
|-----|-------|------------------|
| 1 | No | (1+0+0+1)/4=0.5 |
| 2 | No | (1+0+0+0)/4=0.25 |
| 3 | Yes | (0+0+0+1)/4=0.25 |
| 4 | Yes | (0+2+0+1)/4=0.75 |
| 5 | Yes | (0+0+1+1)/4=0.5 |
| 6 | No | (0+0+1+0)/4=0.25 |
| 7 | Yes | (0+0+1+0)/4=0.25 |
| 8 | No | (1+2+0+1)/4=1 |
| 9 | Yes | (1+0+1+1)/4=0.75 |
| 10 | Yes | (0+2+1+1)/4=1 |
| 11 | Yes | (1+2+1+0)/4=1 |
| 12 | Yes | (0+2+0+0)/4=0.5 |
| 13 | Yes | (0+0+1+1)/4=0.5 |
| 14 | No | (0+2+0+0)/4=0.5 |

Among the five nearest neighbours four are from class Yes and one from class No. Hence, the k-NN classifier predicts buys_computer=yes for the new example.

Exercise 8. Decision trees

Given the training data in Exercise 4 (*Buy Computer* data), build a decision tree and predict the class of the following new example: age<=30, income=medium, student=yes, credit-rating=fair.

Solution:

First check which attribute provides the highest Information Gain in order to split the training set based on that attribute. We need to calculate the expected information to classify the set and the entropy of each attribute. The information gain is this mutual information minus the entropy.

The mutual information of the two classes $I(S_{14}, S_{15}) = 1(9,5) = -9/14 \log_2(9/14) - 5/14 \log_2(5/14) = 0.94$

- For Age we have three values age_{<=30} (2 yes and 3 no), age_{31..40} (4 yes and 0 no) and age_{>40} (3 yes 2 no)

$$\begin{aligned}\text{Entropy}(\text{age}) &= 5/14 (-2/5 \log(2/5) - 3/5 \log(3/5)) + 4/14 (0) + 5/14 (-3/5 \log(3/5) - 2/5 \log(2/5)) \\ &= 5/14(0.9709) + 0 + 5/14(0.9709) \\ &\approx 0.6935\end{aligned}$$

$$\text{Gain}(\text{age}) = 0.94 - 0.6935 = 0.2465$$

- For Income we have three values income_{high} (2 yes and 2 no), income_{medium} (4 yes and 2 no) and income_{low} (3 yes 1 no)

$$\begin{aligned}\text{Entropy}(\text{income}) &= 4/14(-2/4 \log(2/4) - 2/4 \log(2/4)) + 6/14 (-4/6 \log(4/6) - 2/6 \log(2/6)) \\ &\quad + 4/14 (-3/4 \log(3/4) - 1/4 \log(1/4)) \\ &\approx 4/14 (1) + 6/14 (0.918) + 4/14 (0.811) \\ &= 0.285714 + 0.393428 + 0.231714 = 0.9108\end{aligned}$$

$$\text{Gain}(\text{income}) = 0.94 - 0.9108 = 0.0292$$

- For Student we have two values student_{yes} (6 yes and 1 no) and student_{no} (3 yes 4 no)

$$\begin{aligned}\text{Entropy}(\text{student}) &= 7/14(-6/7 \log(6/7)) + 7/14(-3/7 \log(3/7) - 4/7 \log(4/7)) \\ &\approx 7/14(0.5916) + 7/14(0.9852) \\ &= 0.2958 + 0.4926 = 0.7884\end{aligned}$$

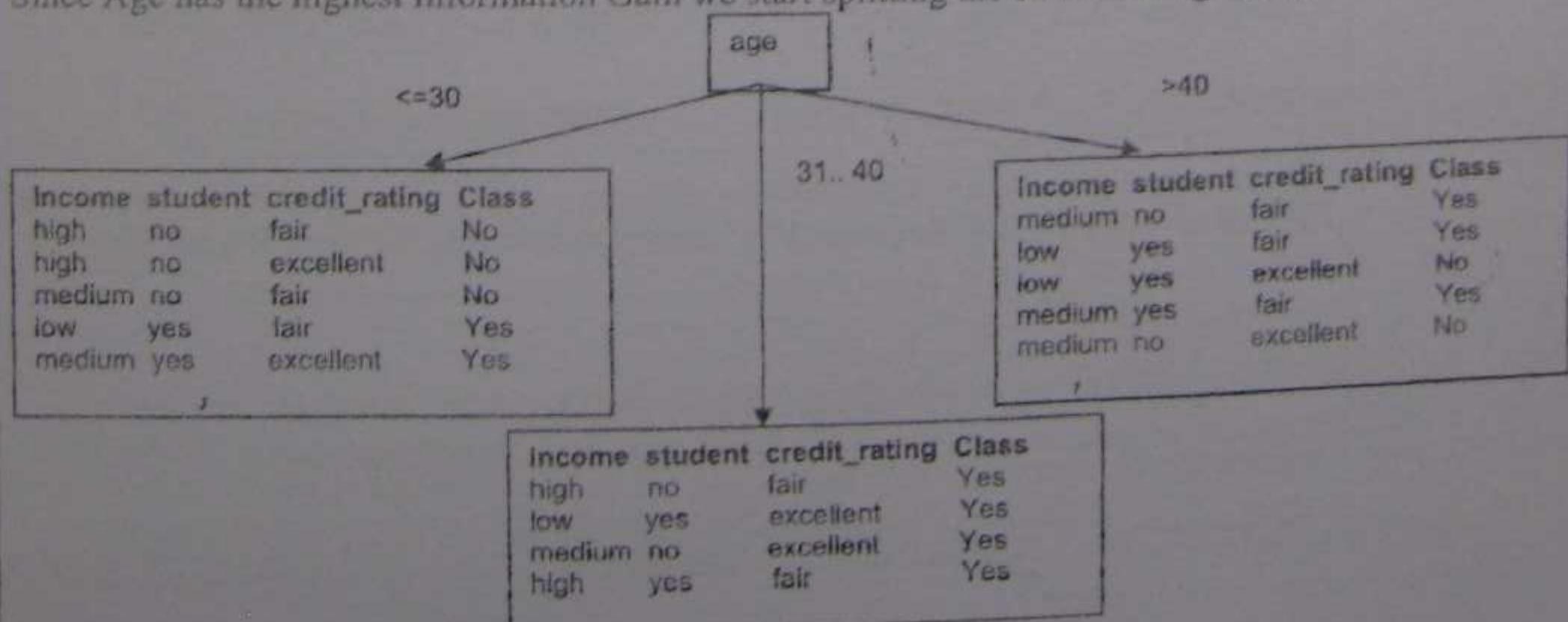
$$\text{Gain}(\text{student}) = 0.94 - 0.7884 = 0.1516$$

- For Credit_Rating we have two values credit_rating_{fair} (6 yes and 2 no) and credit_rating_{excellent} (3 yes 3 no)

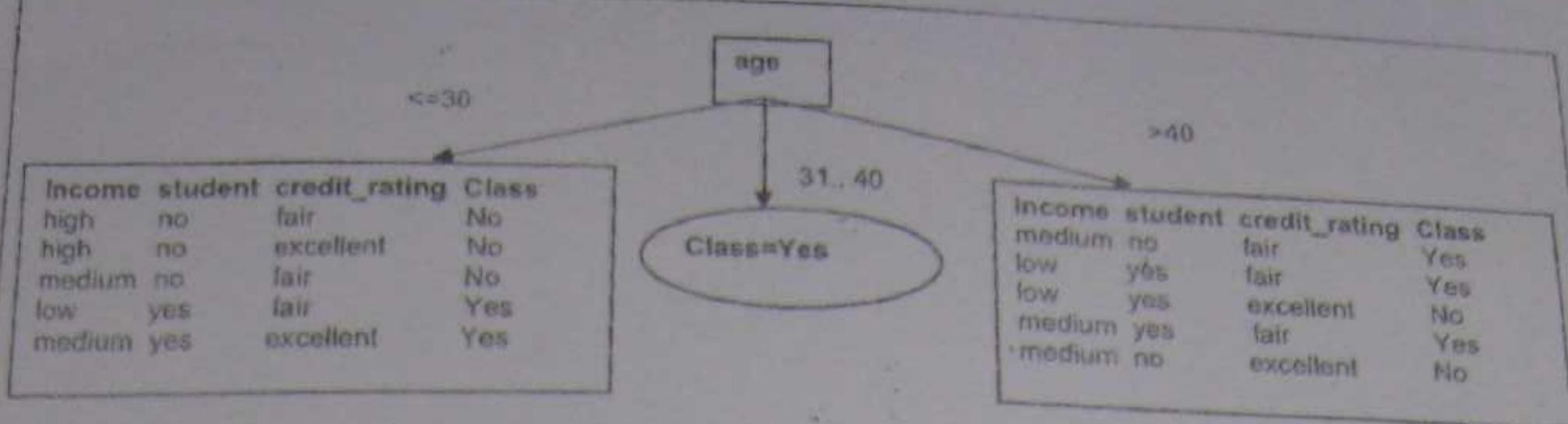
$$\begin{aligned}\text{Entropy}(\text{credit_rating}) &= 8/14(-6/8 \log(6/8) - 2/8 \log(2/8)) + 6/14(-3/6 \log(3/6) - 3/6 \log(3/6)) \\ &= 8/14(0.8112) + 6/14(1) \\ &= 0.4635 + 0.4285 = 0.8920\end{aligned}$$

$$\text{Gain}(\text{credit_rating}) = 0.94 - 0.8920 = 0.479$$

Since Age has the highest Information Gain we start splitting the dataset using the age attribute



Since all records under the branch age_{31..40} are all of class Yes, we can replace the leaf with Class=Yes



The same process of splitting has to happen for the two remaining branches. For branch $age \leq 30$ we still have attributes income, student and credit_rating. Which one should be used to split the partition?

The mutual information is $I(S_{Yes}, S_{No}) = I(2,3) = -2/5 \log_2(2/5) - 3/5 \log_2(3/5) = 0.97$

- For Income we have three values income_{high} (0 yes and 2 no), income_{medium} (1 yes and 1 no) and income_{low} (1 yes and 0 no)

$$\begin{aligned} \text{Entropy(income)} &= 2/5(0) + 2/5(-1/2\log(1/2)-1/2\log(1/2)) + 1/5(0) \\ &= 2/5(1) = 0.4 \end{aligned}$$

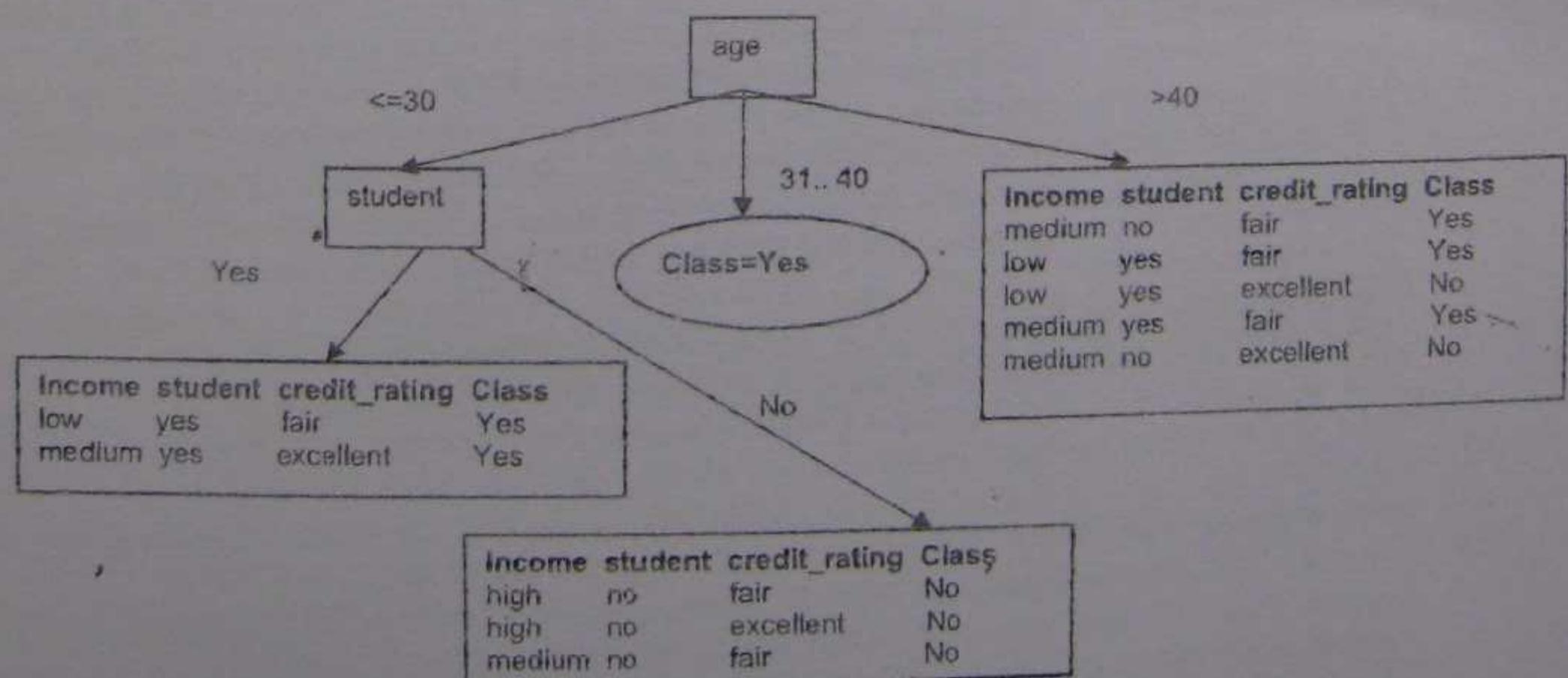
$$\text{Gain(income)} = 0.97 - 0.4 = 0.57$$

- For Student we have two values student_{yes} (2 yes and 0 no) and student_{no} (0 yes 3 no)

$$\text{Entropy(student)} = 2/5(0) + 3/5(0) = 0$$

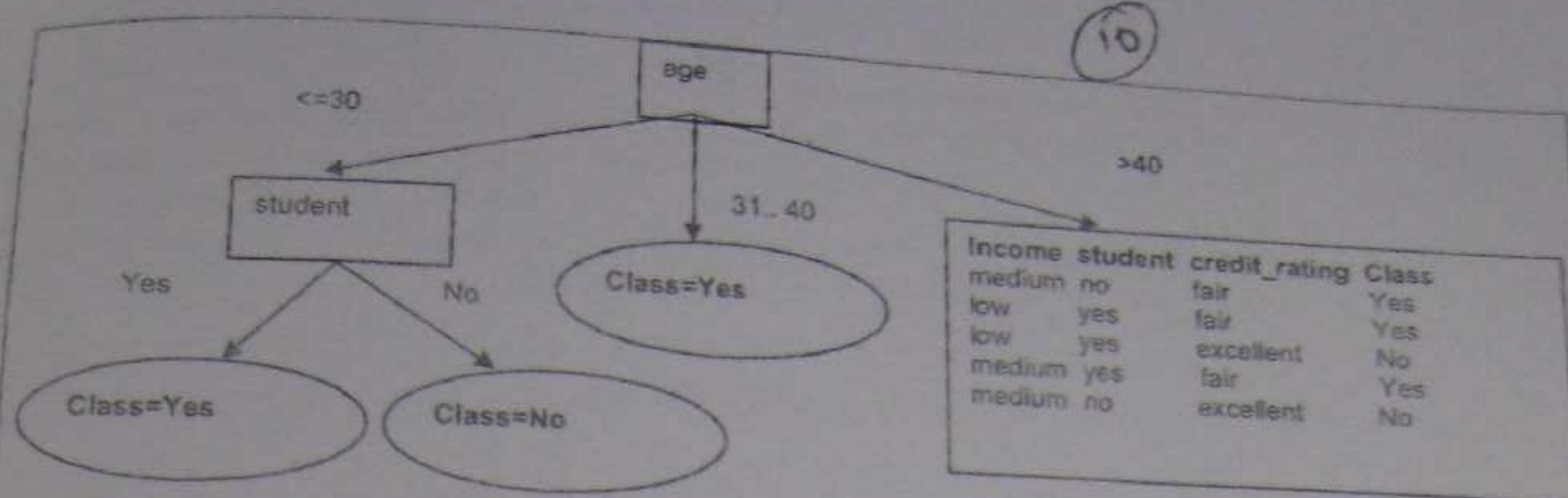
$$\text{Gain(student)} = 0.97 - 0 = 0.97$$

We can then safely split on attribute student without checking the other attributes since the information gain is maximized.



Since these two new branches are from distinct classes, we make them into leaf nodes with their respective class as label:

10



Again the same process is needed for the other branch of age.

The mutual information is $I(S_{\text{Yes}}, S_{\text{No}}) = I(3,2) = -3/5 \log_2(3/5) - 2/5 \log_2(2/5) = 0.97$

- For Income we have two values income_{medium} (2 yes and 1 no) and income_{low} (1 yes and 1 no)

$$\begin{aligned} \text{Entropy}(\text{income}) &= 3/5(-2/3 \log(2/3) - 1/3 \log(1/3)) + 2/5(-1/2 \log(1/2) - 1/2 \log(1/2)) \\ &= 3/5(0.9182) + 2/5(1) = 0.55 + 0.4 = 0.95 \end{aligned}$$

$$\text{Gain}(\text{income}) = 0.97 - 0.95 = 0.02$$

- For Student we have two values student_{yes} (2 yes and 1 no) and student_{no} (1 yes and 1 no)

$$\text{Entropy}(\text{student}) = 3/5(-2/3 \log(2/3) - 1/3 \log(1/3)) + 2/5(-1/2 \log(1/2) - 1/2 \log(1/2)) = 0.95$$

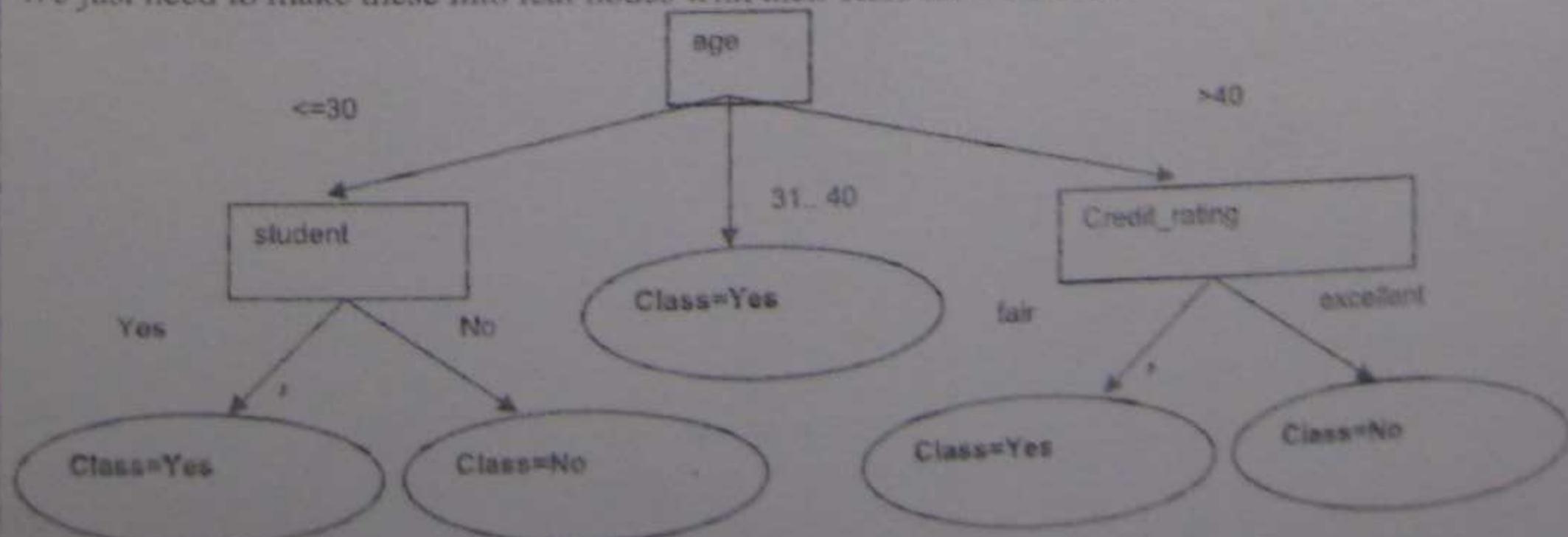
$$\text{Gain}(\text{student}) = 0.97 - 0.95 = 0.02$$

- For Credit_Rating we have two values credit_rating_{fair} (3 yes and 0 no) and credit_rating_{excellent} (0 yes and 2 no)

$$\text{Entropy}(\text{credit_rating}) = 0$$

$$\text{Gain}(\text{credit_rating}) = 0.97 - 0 = 0.97$$

We then split based on credit_rating. These splits give partitions each with records from the same class. We just need to make these into leaf nodes with their class label attached:



New example: age ≤ 30 , income=medium, student=yes, credit-rating=fair
Follow branch(age ≤ 30) then student=yes we predict Class=yes \rightarrow Buys_computer = yes

Tutorial exercises
Clustering – K-means, Nearest Neighbor and Hierarchical.

①

Exercise 1. K-means clustering

Use the k-means algorithm and Euclidean distance to cluster the following 8 examples into 3 clusters:
 $A_1 = (2, 10)$, $A_2 = (2, 5)$, $A_3 = (8, 4)$, $A_4 = (5, 8)$, $A_5 = (7, 5)$, $A_6 = (6, 4)$, $A_7 = (1, 2)$, $A_8 = (4, 9)$.
 The distance matrix based on the Euclidean distance is given below:

| | A_1 | A_2 | A_3 | A_4 | A_5 | A_6 | A_7 | A_8 |
|-------|-------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|
| A_1 | 0 | $\sqrt{25}$ | $\sqrt{36}$ | $\sqrt{13}$ | $\sqrt{50}$ | $\sqrt{52}$ | $\sqrt{65}$ | $\sqrt{5}$ |
| A_2 | | 0 | $\sqrt{37}$ | $\sqrt{18}$ | $\sqrt{25}$ | $\sqrt{17}$ | $\sqrt{10}$ | $\sqrt{20}$ |
| A_3 | | | 0 | $\sqrt{25}$ | $\sqrt{2}$ | $\sqrt{2}$ | $\sqrt{53}$ | $\sqrt{41}$ |
| A_4 | | | | 0 | $\sqrt{13}$ | $\sqrt{17}$ | $\sqrt{52}$ | $\sqrt{2}$ |
| A_5 | | | | | 0 | $\sqrt{2}$ | $\sqrt{45}$ | $\sqrt{25}$ |
| A_6 | | | | | | 0 | $\sqrt{29}$ | $\sqrt{29}$ |
| A_7 | | | | | | | 0 | $\sqrt{58}$ |
| A_8 | | | | | | | | 0 |

Suppose that the initial seeds (centers of each cluster) are A_1 , A_4 and A_7 . Run the k-means algorithm for 1 epoch only. At the end of this epoch show:

- The new clusters (i.e. the examples belonging to each cluster)
- The centers of the new clusters
- Draw a 10 by 10 space with all the 8 points and show the clusters after the first epoch and the new centroids.
- How many more iterations are needed to converge? Draw the result for each epoch.

Solution:

a)

$d(a,b)$ denotes the Euclidean distance between a and b . It is obtained directly from the distance matrix or calculated as follows: $d(a,b) = \sqrt{(x_b - x_a)^2 + (y_b - y_a)^2}$
 $seed1 = A_1 = (2, 10)$, $seed2 = A_4 = (5, 8)$, $seed3 = A_7 = (1, 2)$

epoch1 – start:

A_1 :

$$d(A_1, seed1) = 0 \text{ as } A_1 \text{ is seed1}$$

$$d(A_1, seed2) = \sqrt{13} > 0$$

$$d(A_1, seed3) = \sqrt{65} > 0$$

$\rightarrow A_1 \in \text{cluster1}$

A_2 :

$$d(A_2, seed1) = \sqrt{25} = 5.$$

$$d(A_2, seed2) = \sqrt{18} = 4.24$$

$$d(A_2, seed3) = \sqrt{10} = 3.16 \leftarrow \text{smaller}$$

$\rightarrow A_2 \in \text{cluster3}$

A_3 :

$$d(A_3, seed1) = \sqrt{36} = 6$$

$$d(A_3, seed2) = \sqrt{25} = 5 \leftarrow \text{smaller}$$

$$d(A_3, seed3) = \sqrt{53} = 7.28$$

$\rightarrow A_3 \in \text{cluster2}$

A_4 :

$$d(A_4, seed1) = \sqrt{13}$$

$$d(A_4, seed2) = 0 \text{ as } A_4 \text{ is seed2}$$

$$d(A_4, seed3) = \sqrt{52} > 0$$

$\rightarrow A_4 \in \text{cluster2}$

A_5 :

$$d(A_5, seed1) = \sqrt{50} = 7.07$$

A_6 :

$$d(A_6, seed1) = \sqrt{52} = 7.21$$

$$d(A5, \text{seed}2) = \sqrt{13} = 3.60 \leftarrow \text{smaller}$$

$$d(A5, \text{seed}3) = \sqrt{45} = 6.70$$

$\rightarrow A5 \in \text{cluster}2$

$$d(A6, \text{seed}2) = \sqrt{17} = 4.12 \leftarrow \text{smaller}$$

$$d(A6, \text{seed}3) = \sqrt{29} = 5.38$$

$\rightarrow A6 \in \text{cluster}2$

A7:

$$d(A7, \text{seed}1) = \sqrt{65} > 0$$

$$d(A7, \text{seed}2) = \sqrt{52} > 0$$

$$d(A7, \text{seed}3) = 0 \text{ as } A7 \text{ is seed}3$$

$\rightarrow A7 \in \text{cluster}3$

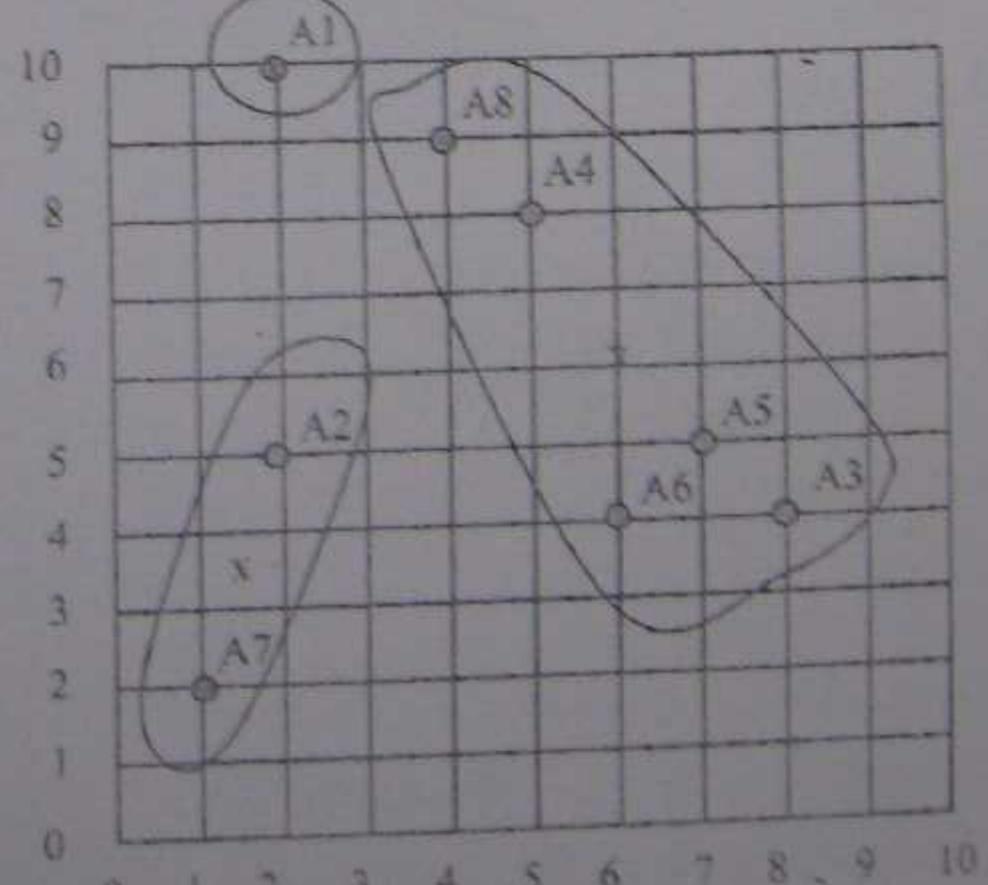
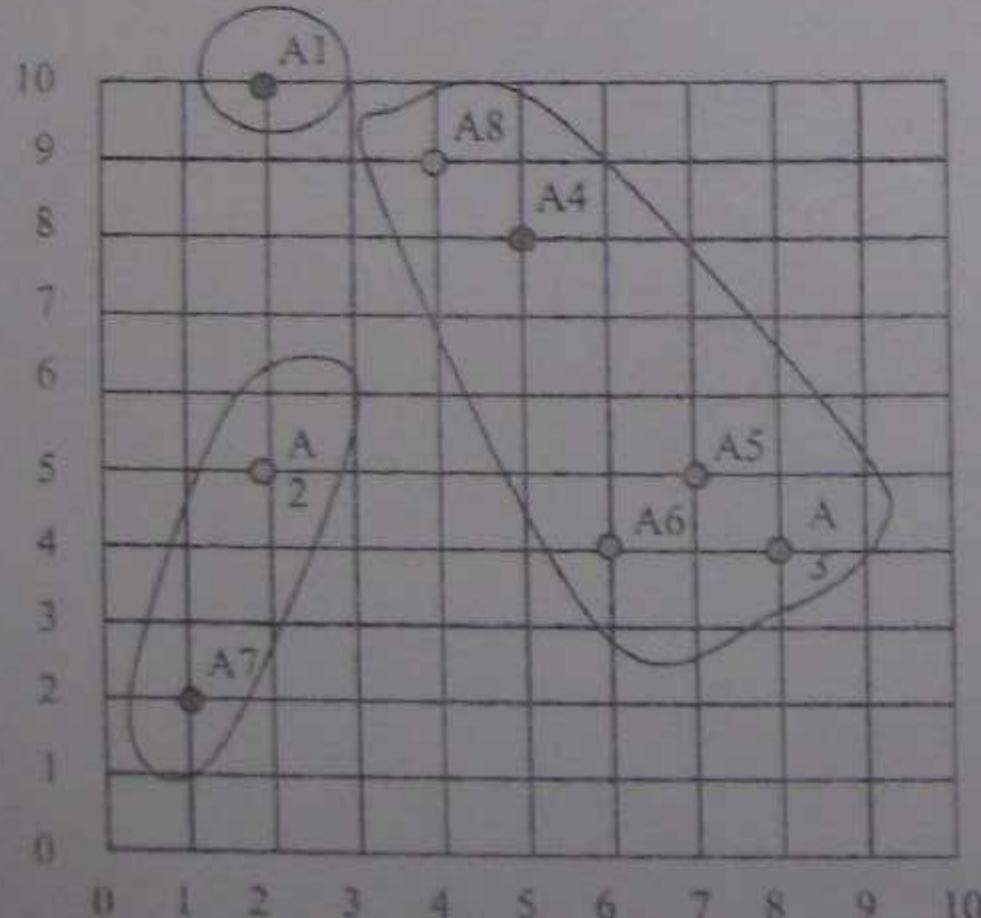
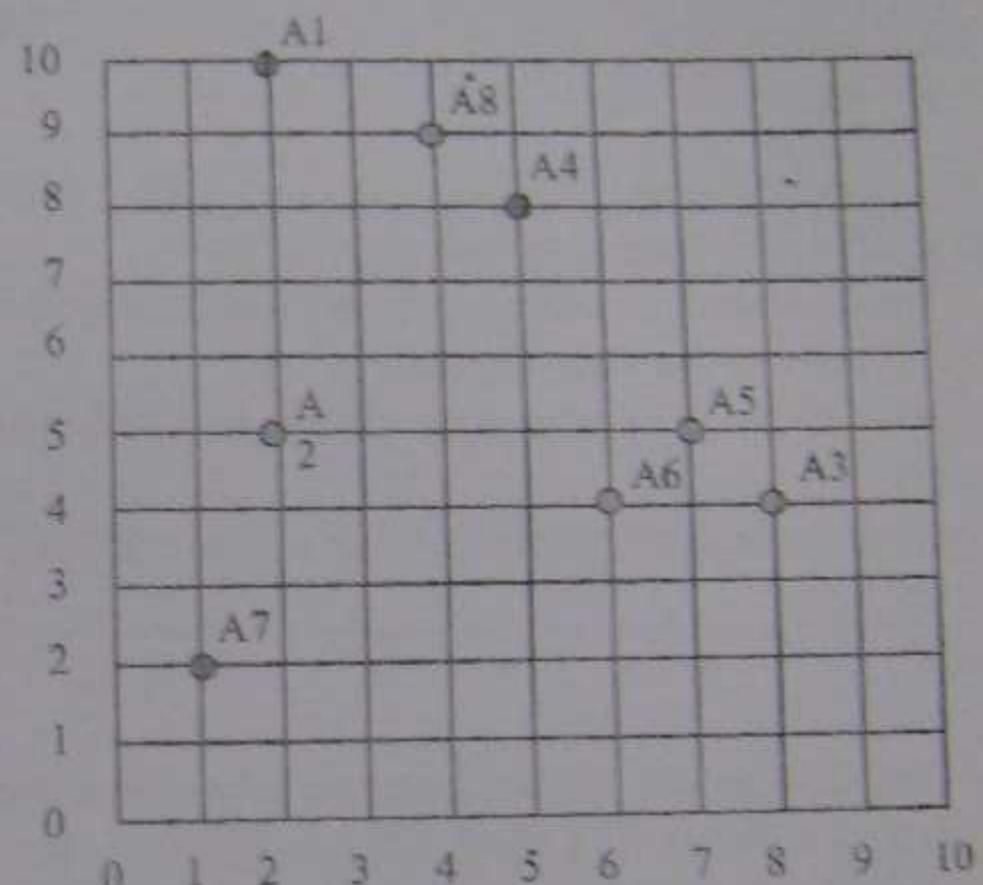
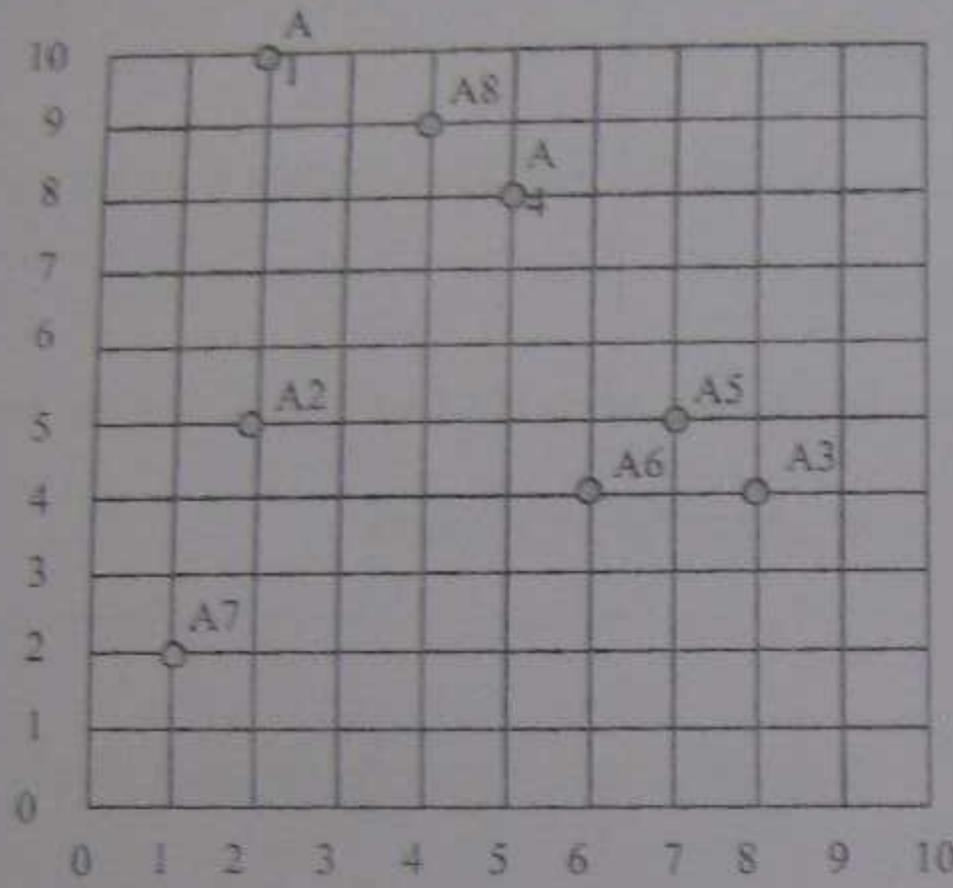
end of epoch1

new clusters: 1: {A1}, 2: {A3, A4, A5, A6, A8}, 3: {A2, A7}

b) centers of the new clusters:

$$C1 = (2, 10), C2 = ((8+5+7+6+4)/5, (4+8+5+4+9)/5) = (6, 6), C3 = ((2+1)/2, (5+2)/2) = (1.5, 3.5)$$

c)



We would need two more epochs. After the 2nd epoch the results would be:

1: {A1, A8}, 2: {A3, A4, A5, A6}, 3: {A2, A7}

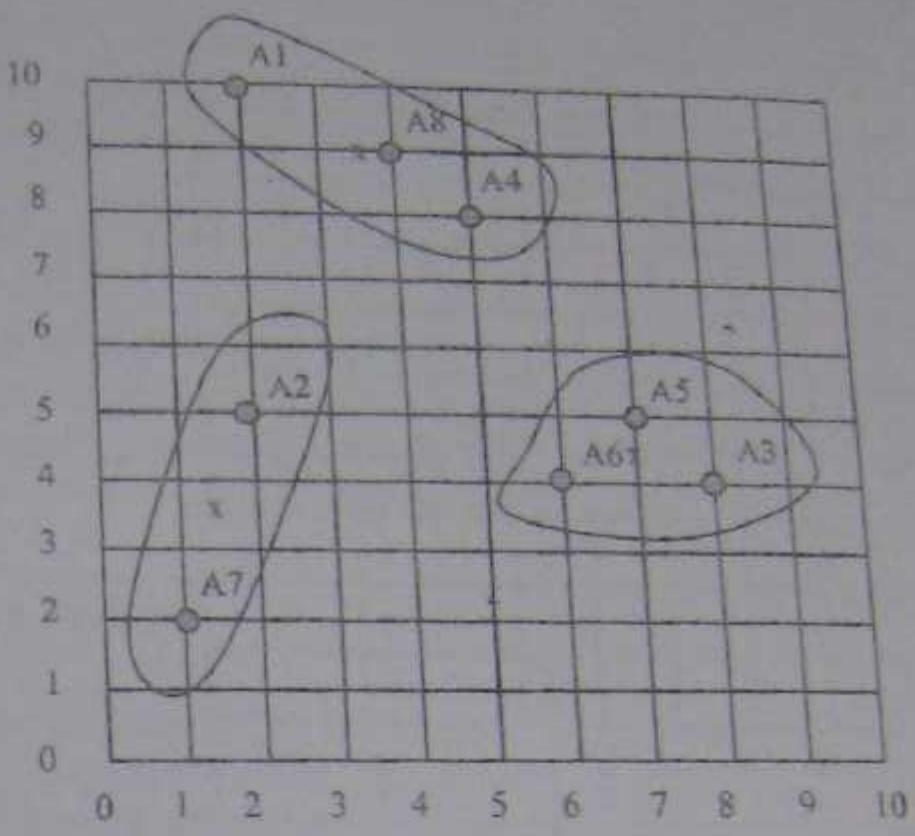
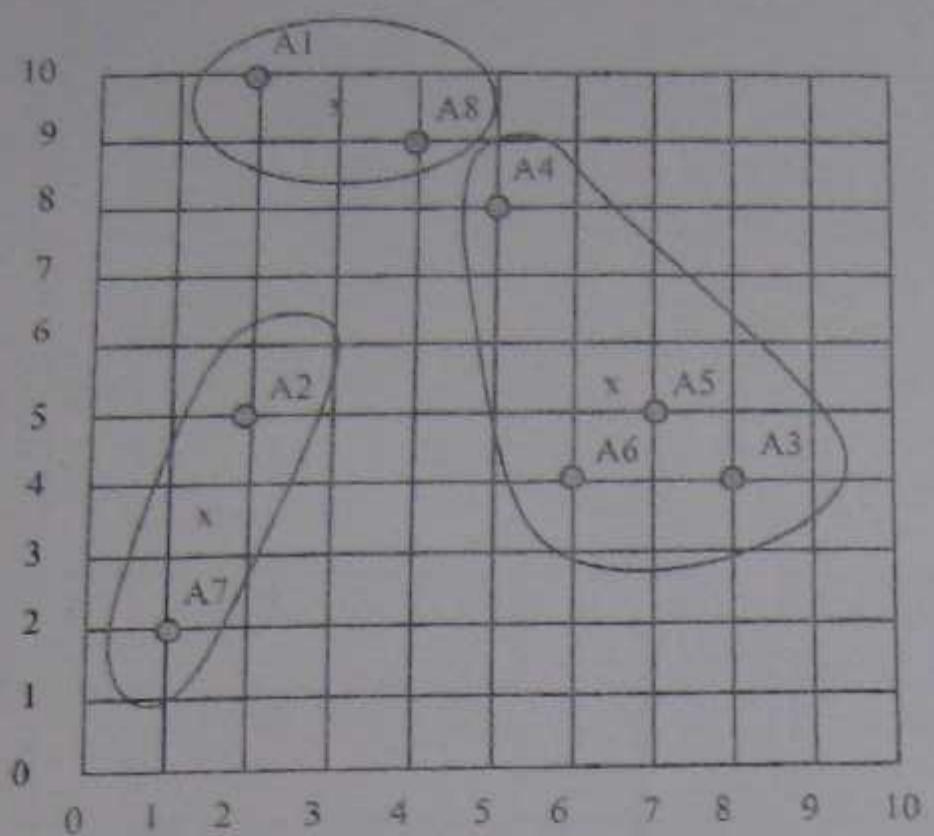
with centers C1=(3, 9.5), C2=(6.5, 5.25) and C3=(1.5, 3.5).

After the 3rd epoch, the results would be:

1: {A1, A4, A8}, 2: {A3, A5, A6}, 3: {A2, A7}

with centers C1=(3.66, 9), C2=(7, 4.33) and C3=(1.5, 3.5).

3



Exercise 2. Nearest Neighbor clustering

Use the Nearest Neighbor clustering algorithm and Euclidean distance to cluster the examples from the previous exercise: A1=(2,10), A2=(2,5), A3=(8,4), A4=(5,8), A5=(7,5), A6=(6,4), A7=(1,2), A8=(4,9). Suppose that the threshold t is 4.

Solution:

A1 is placed in a cluster by itself, so we have K1={A1}.

We then look at A2 if it should be added to K1 or be placed in a new cluster.

$$d(A1, A2) = \sqrt{25} = 5 > t \rightarrow K2 = \{A2\}$$

A3: we compare the distances from A3 to A1 and A2.

$$A3 \text{ is closer to } A2 \text{ and } d(A3, A2) = \sqrt{36} > t \rightarrow K3 = \{A3\}$$

A4: We compare the distances from A4 to A1, A2 and A3.

$$A1 \text{ is the closest object and } d(A4, A1) = \sqrt{13} < t \rightarrow K1 = \{A1, A4\}$$

A5: We compare the distances from A5 to A1, A2, A3 and A4.

$$A3 \text{ is the closest object and } d(A5, A3) = \sqrt{2} < t \rightarrow K3 = \{A3, A5\}$$

A6: We compare the distances from A6 to A1, A2, A3, A4 and A5.

$$A3 \text{ is the closest object and } d(A6, A3) = \sqrt{2} < t \rightarrow K3 = \{A3, A5, A6\}$$

A7: We compare the distances from A7 to A1, A2, A3, A4, A5, and A6.

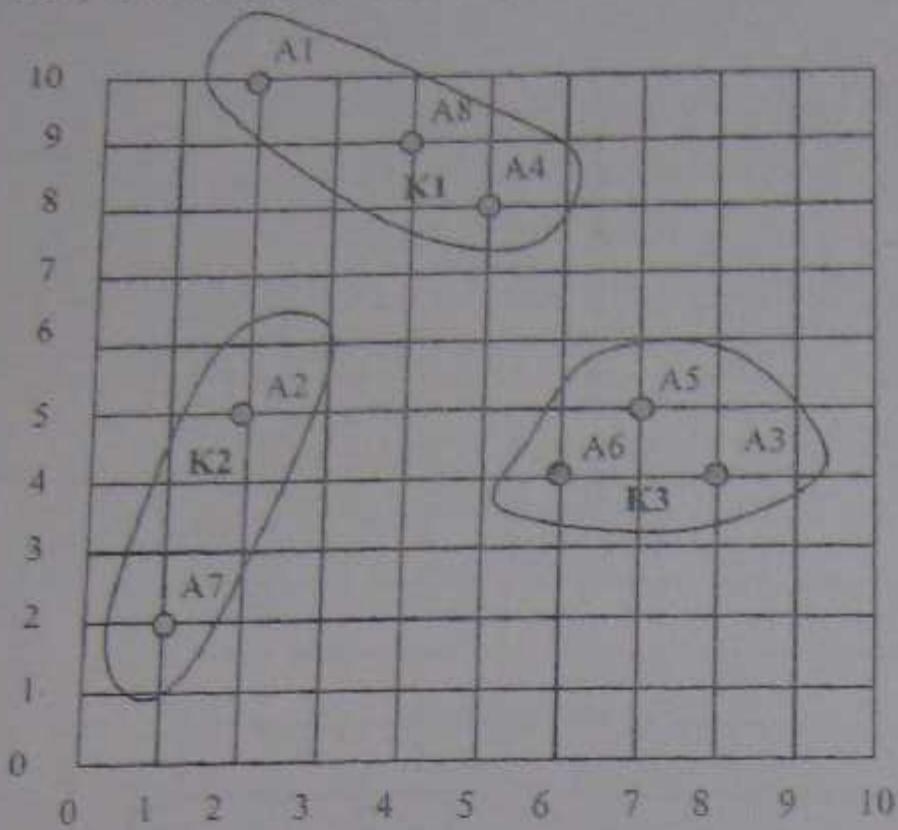
$$A2 \text{ is the closest object and } d(A7, A2) = \sqrt{10} < t \rightarrow K2 = \{A2, A7\}$$

A8: We compare the distances from A8 to A1, A2, A3; A4, A5, A6 and A7.
 A4 is the closest object and $d(A8, A4) = \sqrt{2} < t \rightarrow K1 = \{A1, A4, A8\}$

4

Thus: $K1 = \{A1, A4, A8\}$, $K2 = \{A2, A7\}$, $K3 = \{A3, A5, A6\}$

Yes, it is the same result as with K-means.



Exercise 3. Hierarchical clustering

Use single and complete link agglomerative clustering to group the data described by the following distance matrix. Show the dendrograms.

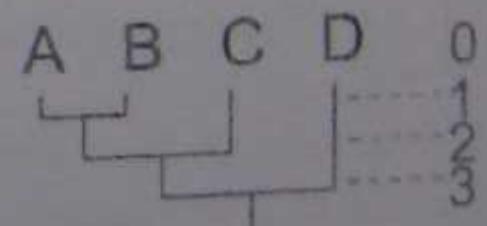
| | A | B | C | D |
|---|---|---|---|---|
| A | 0 | 1 | 4 | 5 |
| B | | 0 | 2 | 6 |
| C | | | 0 | 3 |
| D | | | | 0 |

Solution:

Agglomerative \rightarrow initially every point is a cluster of its own and we merge cluster until we end-up with one unique cluster containing all points.

a) single link: distance between two clusters is the shortest distance between a pair of elements from the two clusters.

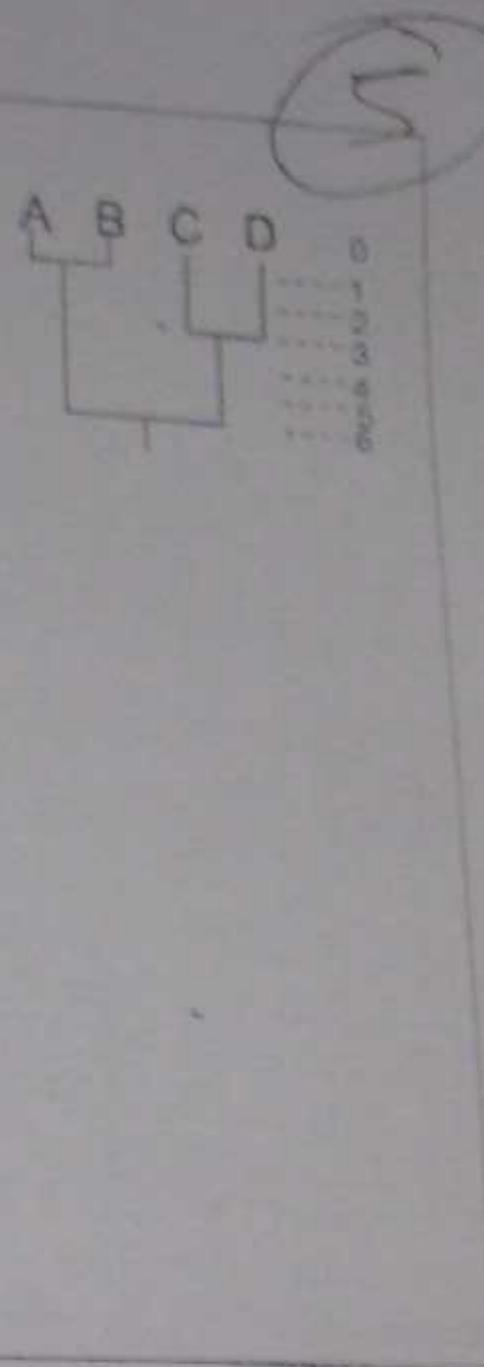
| d | k | K | Comments |
|---|---|--------------------|---|
| 0 | 4 | {A}, {B}, {C}, {D} | We start with each point = cluster |
| 1 | 3 | {A, B}, {C}, {D} | Merge {A} and {B} since A & B are the closest: $d(A, B) = 1$ |
| 2 | 2 | {A, B, C}, {D} | Merge {A, B} and {C} since B & C are the closest: $d(B, C) = 2$ |
| 3 | 1 | {A, B, C, D} | Merge D |



b) complete link: distance between two clusters is the longest distance between a pair of elements from

the two clusters

| d | k | K | Comments |
|---|---|--------------------|---|
| 0 | 4 | {A}, {B}, {C}, {D} | We start with each point = cluster |
| 1 | 3 | {A, B}, {C}, {D} | $d(A,B)=1 \leq 1 \rightarrow$ merge {A} and {B} |
| 2 | 3 | {A, B}, {C}, {D} | $d(A,C)=4 > 2$ so we can't merge C with {A, B} |
| | | | $d(A,D)=5 > 2$ and $d(B,D)=6 > 2$ so we can't merge D with {A, B} |
| 3 | 2 | {A, B}, {C, D} | $d(C,D)=3 > 2$ so we can't merge C and D - $d(A,C)=4 > 3$ so we can't merge C with {A, B} - $d(A,D)=5 > 3$ and $d(B,D)=6 > 3$ so we can't merge D with {A, B} - $d(C,D)=3 \leq 3$ so merge C and D |
| 4 | 2 | {A, B}, {C, D} | {C, D} cannot be merged with {A, B} as $d(A,D)=5 > 4$ (and also $d(B,D)=6 > 4$) although $d(A,C)=4 \leq 4$, $d(B,C)=2 \leq 4$ |
| 5 | 2 | {A, B}, {C, D} | {C, D} cannot be merged with {A, B} as $d(B,D)=6 > 5$ |
| 6 | 1 | {A, B, C, D} | {C, D} can be merged with {A, B} since $d(B,D)=6 \leq 6$, $d(A,D)=5 \leq 6$, $d(A,C)=4 \leq 6$, $d(B,C)=2 \leq 6$ |



Exercise 4: Hierarchical clustering (to be done at your own time, not in class)

Use single-link, complete-link, average-link agglomerative clustering as well as medoid and centroid to cluster the following 8 examples:

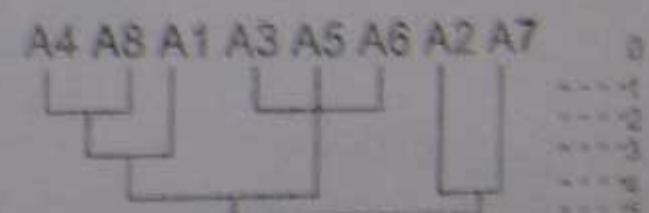
A1=(2,10), A2=(2,5), A3=(8,4), A4=(5,8), A5=(7,5), A6=(6,4), A7=(1,2), A8=(4,9).

The distance matrix is the same as the one in Exercise 1. Show the dendograms.

Solution:

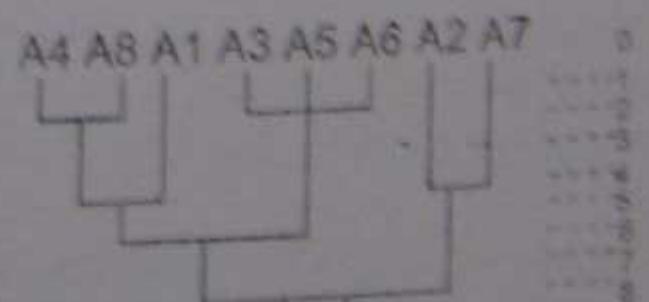
Single Link:

| d | k | K |
|---|---|--|
| 0 | 8 | {A1}, {A2}, {A3}, {A4}, {A5}, {A6}, {A7}, {A8} |
| 1 | 8 | {A1}, {A2}, {A3}, {A4}, {A5}, {A6}, {A7}, {A8} |
| 2 | 5 | {A4, A8}, {A1}, {A3, A5, A6}, {A2}, {A7} |
| 3 | 4 | {A4, A8, A1}, {A3, A5, A6}, {A2}, {A7} |
| 4 | 2 | {A1, A3, A4, A5, A6, A8}, {A2, A7} |
| 5 | 1 | {A1, A3, A4, A5, A6, A8, A2, A7} |



Complete Link:

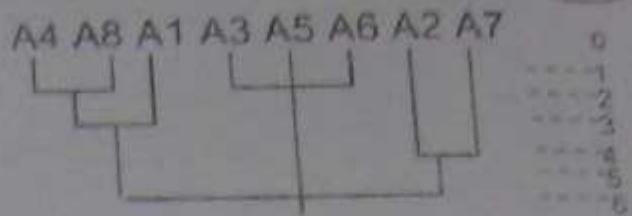
| d | k | K |
|---|---|--|
| 0 | 8 | {A1}, {A2}, {A3}, {A4}, {A5}, {A6}, {A7}, {A8} |
| 1 | 8 | {A1}, {A2}, {A3}, {A4}, {A5}, {A6}, {A7}, {A8} |
| 2 | 5 | {A4, A8}, {A1}, {A3, A5, A6}, {A2}, {A7} |
| 3 | 5 | {A4, A8}, {A1}, {A3, A5, A6}, {A2}, {A7} |
| 4 | 3 | {A4, A8, A1}, {A3, A5, A6}, {A2, A7} |
| 5 | 3 | {A4, A8, A1}, {A3, A5, A6}, {A2, A7} |
| 6 | 2 | {A4, A8, A1, A3, A5, A6}, {A2, A7} |
| 7 | 2 | {A4, A8, A1, A3, A5, A6}, {A2, A7} |
| 8 | 1 | {A4, A8, A1, A3, A5, A6, A2, A7} |



(6)

Average Link

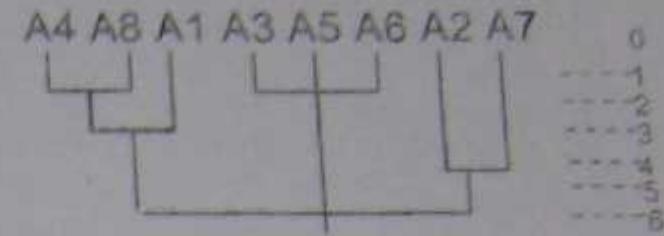
| d | k | K |
|---|---|--|
| 0 | 8 | {A1}, {A2}, {A3}, {A4}, {A5}, {A6}, {A7}, {A8} |
| 1 | 8 | {A1}, {A2}, {A3}, {A4}, {A5}, {A6}, {A7}, {A8} |
| 2 | 5 | {A4, A8}, {A1}, {A3, A5, A6}, {A2}, {A7} |
| 3 | 4 | {A4, A8, A1}, {A3, A5, A6}, {A2}, {A7} |
| 4 | 3 | {A4, A8, A1}, {A3, A5, A6}, {A2, A7} |
| 5 | 3 | {A4, A8, A1}, {A3, A5, A6}, {A2, A7} |
| 6 | 1 | {A4, A8, A1, A3, A5, A6, A2, A7} |



Average distance from {A3, A5, A6} to {A1, A4, A8} is 5.53 and is 5.75 to {A2, A7}

Centroid

| D | k | K |
|---|---|--|
| 0 | 8 | {A1}, {A2}, {A3}, {A4}, {A5}, {A6}, {A7}, {A8} |
| 1 | 8 | {A1}, {A2}, {A3}, {A4}, {A5}, {A6}, {A7}, {A8} |
| 2 | 5 | {A4, A8}, {A1}, {A3, A5, A6}, {A2}, {A7} |
| 3 | 5 | {A4, A8}, {A1}, {A3, A5, A6}, {A2}, {A7} |
| 4 | 3 | {A4, A8, A1}, {A3, A5, A6}, {A2, A7} |
| 5 | 3 | {A4, A8, A1}, {A3, A5, A6}, {A2, A7} |
| 6 | 1 | {A4, A8, A1, A3, A5, A6, A2, A7} |



Centroid of {A4, A8} is B=(4.5, 8.5) and centroid of {A3, A5, A6} is C=(7, 4.33)

distance(A1, B) = 2.91 Centroid of {A1, A4, A8} is D=(3.66, 9) and of {A2, A7} is E=(1.5, 3.5)

distance(D,C)= 5.74 distance(D,E)= 5.90

Medoid

This is not deterministic. It can be different depending upon which medoid in a cluster we chose.

| d | k | K |
|---|---|--|
| 0 | 8 | {A1}, {A2}, {A3}, {A4}, {A5}, {A6}, {A7}, {A8} |
| 1 | 8 | {A1}, {A2}, {A3}, {A4}, {A5}, {A6}, {A7}, {A8} |
| 2 | 5 | {A4, A8}, {A1}, {A3, A5, A6}, {A2}, {A7} |
| 3 | 4 | {A4, A8, A1}, {A3, A5, A6}, {A2}, {A7} |
| 4 | 2 | {A1, A3, A4, A5, A6, A8}, {A2, A7} |
| 5 | 1 | {A1, A3, A4, A5, A6, A8, A2, A7} |

Exercise 5: DBScan

If Epsilon is 2 and minpoint is 2, what are the clusters that DBScan would discover with the following 8 examples: A1=(2,10), A2=(2,5), A3=(8,4), A4=(5,8), A5=(7,5), A6=(6,4), A7=(1,2), A8=(4,9).

The distance matrix is the same as the one in Exercise 1. Draw the 10 by 10 space and illustrate the discovered clusters. What if Epsilon is increased to $\sqrt{10}$?

Solution:

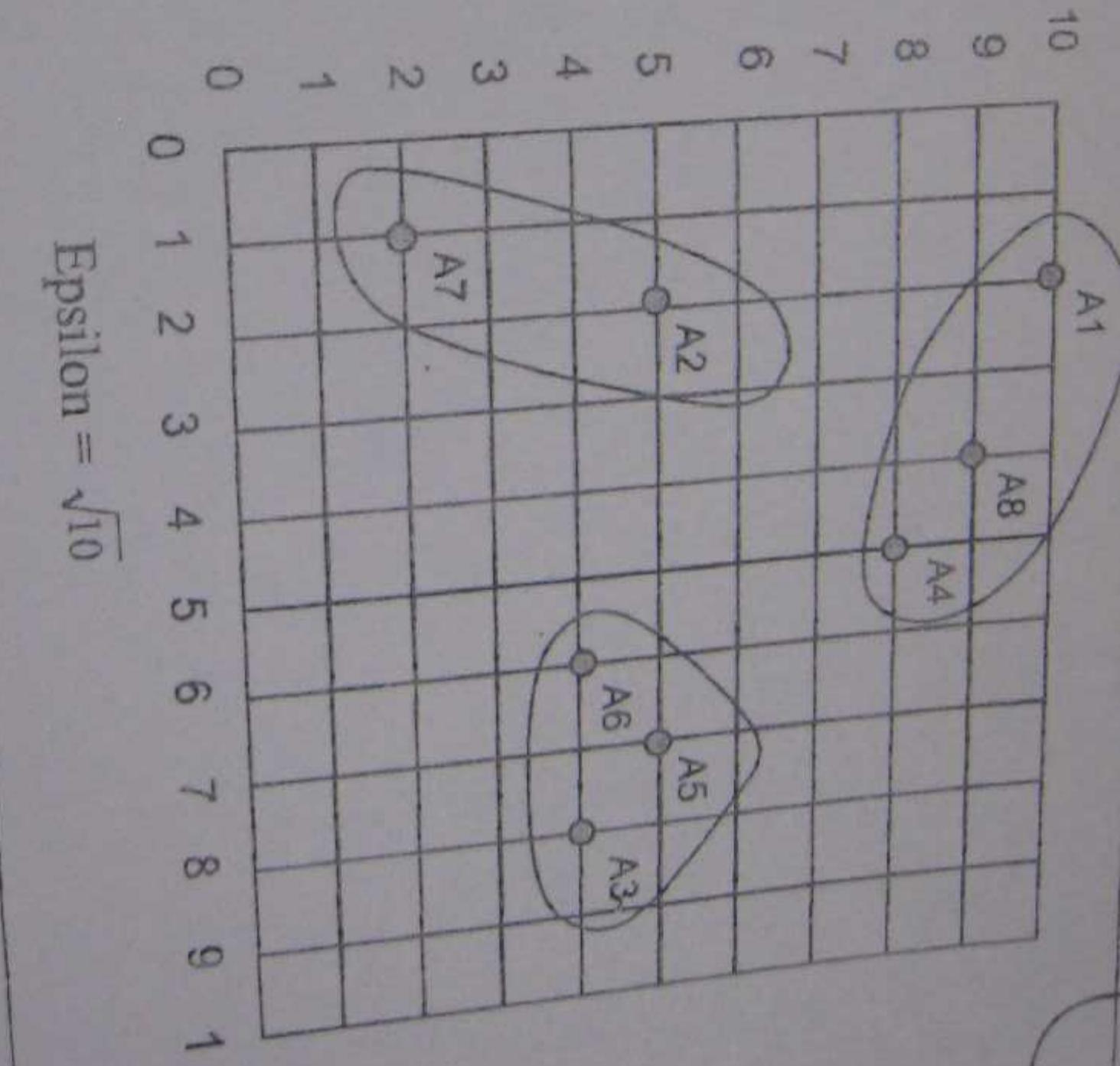
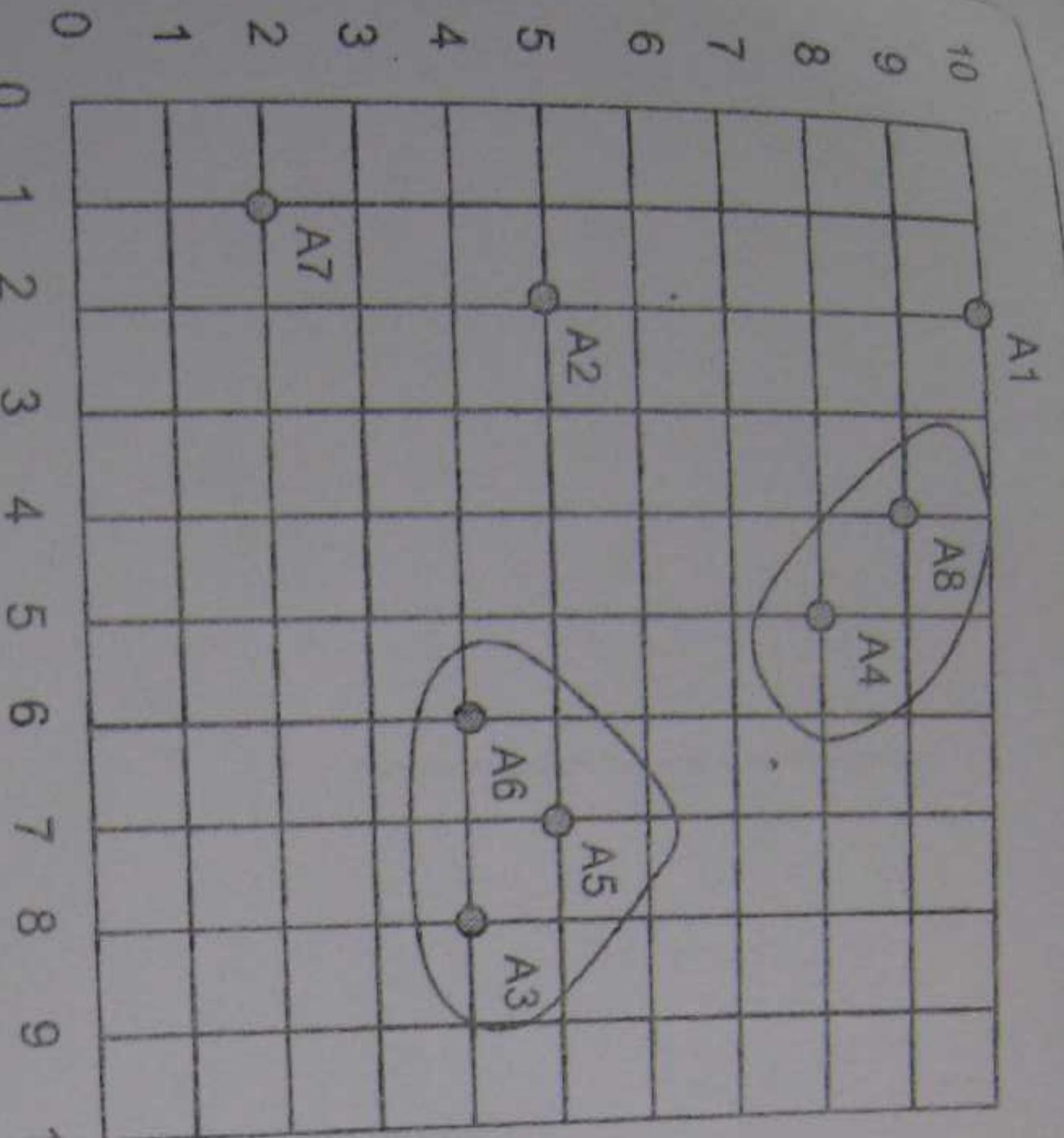
What is the Epsilon neighborhood of each point?

$N_2(A1)=\{\}$; $N_2(A2)=\{\}$; $N_2(A3)=\{A5, A6\}$; $N_2(A4)=\{A8\}$; $N_2(A5)=\{A3, A6\}$;
 $N_2(A6)=\{A3, A5\}$; $N_2(A7)=\{\}$; $N_2(A8)=\{A4\}$

So A1, A2, and A7 are outliers, while we have two clusters $C1=\{A4, A8\}$ and $C2=\{A3, A5, A6\}$

If Epsilon is $\sqrt{10}$ then the neighborhood of some points will increase:

A1 would join the cluster C1 and A2 would join with A7 to form cluster $C3=\{A2, A7\}$.



Epsilon = 2

Epsilon = $\sqrt{10}$