

Clustering 2 (Hierarchical Clustering Methods)

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Some parts of this notes are borrowed from LW Chan's notes
XLMiner screenshots captured by Hao Liu
Presented by Raymond Wong
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COMP1942



Clustering Methods

- K-means Clustering
 - Original k-means Clustering
 - Sequential K-means Clustering
 - Forgetful Sequential K-means Clustering
 - How to use the data mining tool
- Hierarchical Clustering Methods
 - Agglomerative methods
 - Divisive methods polythetic approach and monothetic approach
 - How to use the data mining tool

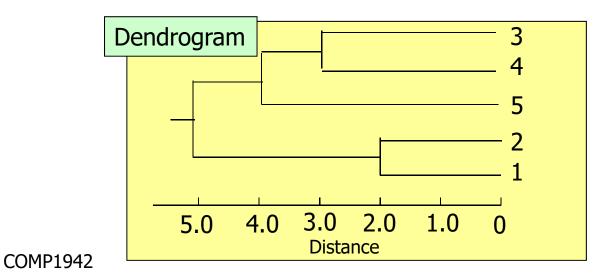


- The partition of data is not done at a single step.
- There are two varieties of hierarchical clustering algorithms
 - Agglomerative successively fusions of the data into groups
 - Divisive separate the data successively into finer groups



Dendrogram

 Hierarchic grouping can be represented by two-dimensional diagram known as a dendrogram.



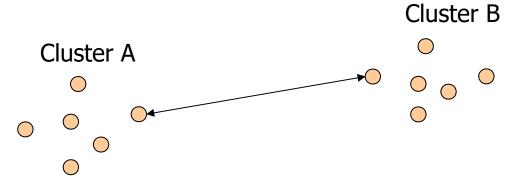


- Single Linkage
- Complete Linkage
- Group Average Linkage
- Centroid Linkage
- Median Linkage



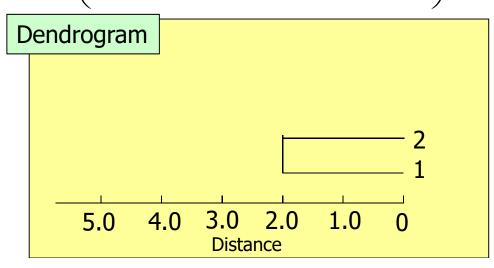
Single Linkage

- Also, known as the nearest neighbor technique
- Distance between groups is defined as that of the closest pair of data, where only pairs consisting of one record from each group are considered

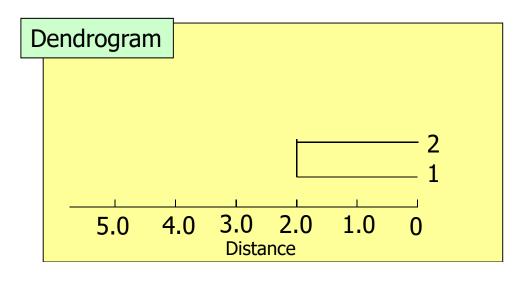


2 3 5 4 0.0 0.0 2 5.0 6.0 0.0 3 10.0 9.0 4.0 0.0 4 8.0 5.0 3.0 0.05 9.0

(12) 3 5 0.0(12) 0.0 5.0 3 9.0 4.0 0.0 4 5.0 3.0 5 8.0



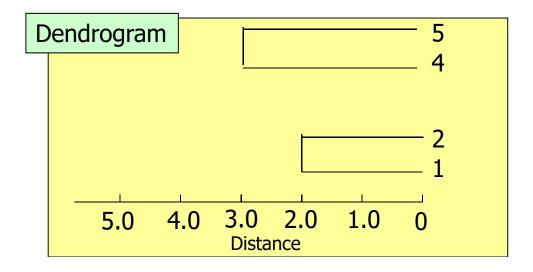




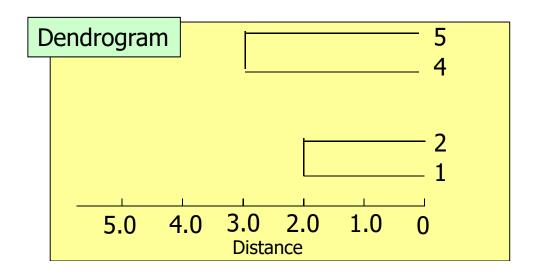


(12)
$$\begin{pmatrix} 0.0 \\ 5.0 & 0.0 \\ 4 & 9.0 & 4.0 & 0.0 \\ 5 & 8.0 & 5.0 & 3.0 & 0.0 \end{pmatrix}$$

$$\begin{array}{cccc}
(12) & 0.0 \\
3 & 5.0 & 0.0 \\
(45) & 8.0 & 4.0 & 0.0
\end{array}$$



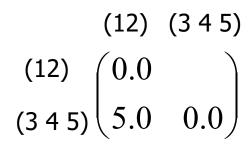


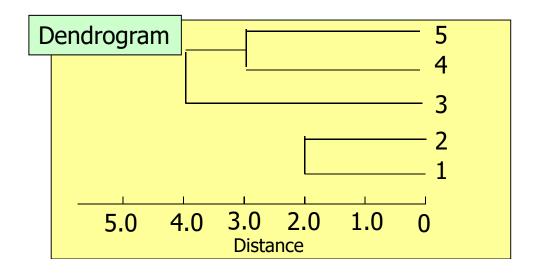




$$(12) \quad 3 \quad (45)$$

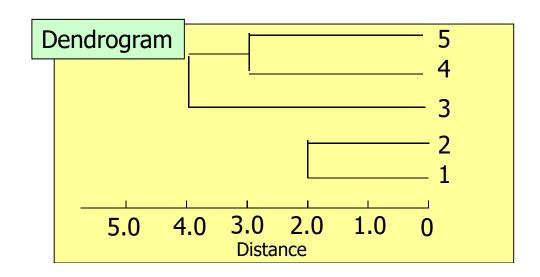
$$(12) \quad \begin{pmatrix} 0.0 \\ 5.0 \quad 0.0 \\ 8.0 \quad 4.0 \end{pmatrix} \quad 0.0$$







$$\begin{array}{c}
 (12) & (3 4 5) \\
 (12) & 0.0 \\
 (3 4 5) & 5.0 & 0.0
 \end{array}$$

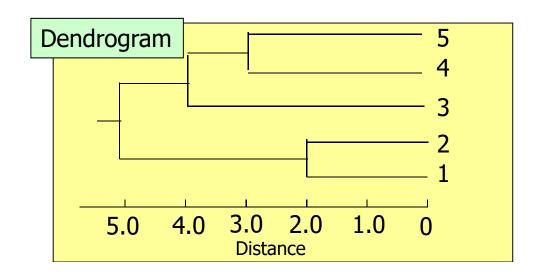




$$(12) (3 4 5)$$

$$(12) (0.0)$$

$$(3 4 5) (5.0) (0.0)$$



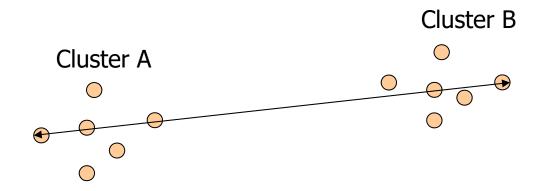


- Single Linkage
- Complete Linkage
- Group Average Linkage
- Centroid Linkage
- Median Linkage



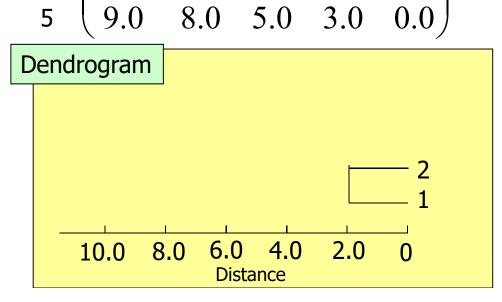
Complete Linkage

 The distance between two clusters is given by the distance between their most distant members

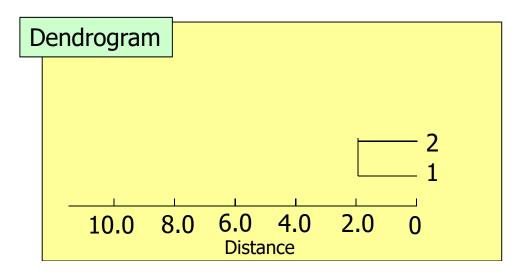


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2 3 5 4 2 0.0 5.0 3 6.0 0.0 10.0 9.0 4.0 0.0 4 5.0 3.0



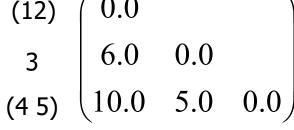


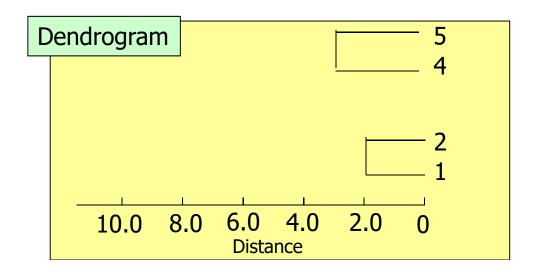




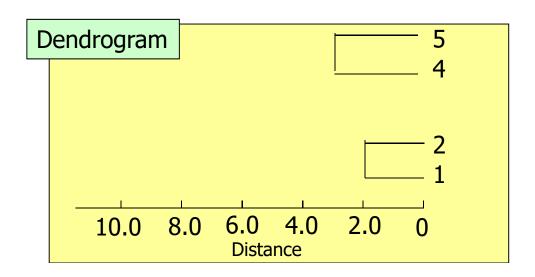
$$\begin{array}{c|cccc}
(12) & 0.0 \\
3 & 6.0 & 0.0 \\
4 & 10.0 & 4.0 & 0.0 \\
5 & 9.0 & 5.0 & 3.0 & 0.0
\end{array}$$

(12) 3 (45) (12)
$$(0.0)$$



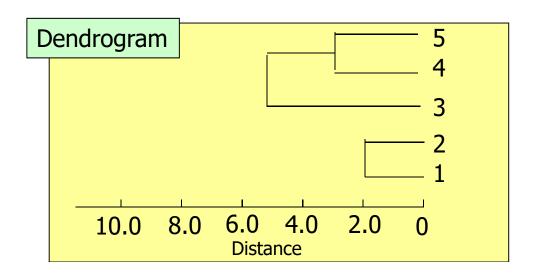






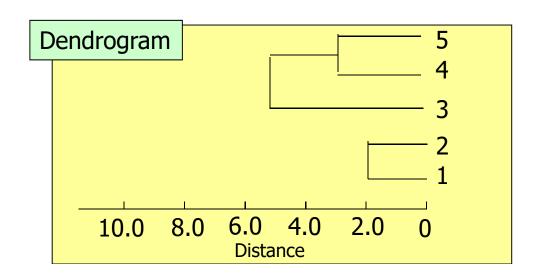


$$\begin{array}{c}
(12) & (3 4 5) \\
(12) & 0.0 \\
(3 4 5) & 10.0 & 0.0
\end{array}$$



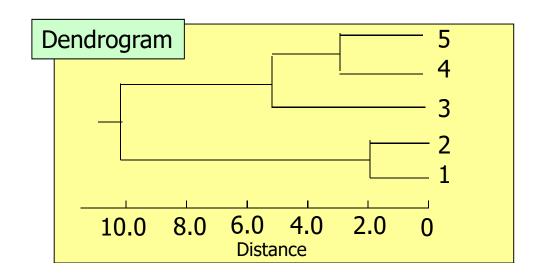


$$\begin{array}{c}
(12) & (3 4 5) \\
(12) & 0.0 \\
(3 4 5) & 10.0 & 0.0
\end{array}$$





$$\begin{array}{c}
(12) & (3 4 5) \\
(12) & 0.0 \\
(3 4 5) & 10.0 \\
\end{array}$$



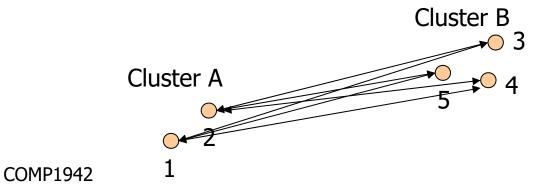


- Single Linkage
- Complete Linkage
- Group Average Linkage
- Centroid Linkage
- Median Linkage



Group Average Clustering

- The distance between two clusters is defined as the average of the distances between all pairs of records (one from each cluster).
- $d_{AB} = 1/6 (d_{13} + d_{14} + d_{15} + d_{23} + d_{24} + d_{25})$



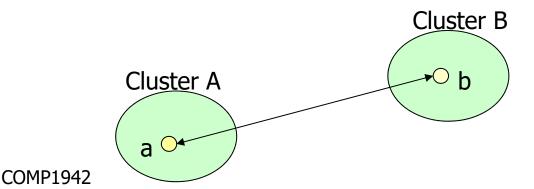


- Single Linkage
- Complete Linkage
- Group Average Linkage
- Centroid Linkage >
- Median Linkage



Centroid Clustering

- The distance between two clusters is defined as the distance between the mean vectors of the two clusters.
- $\mathbf{d}_{AB} = \mathbf{d}_{ab}$
- where a is the mean vector of the cluster A and b is the mean vector of the cluster B.



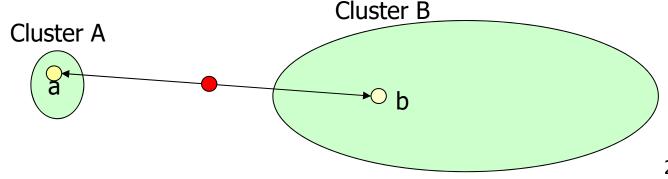


- Single Linkage
- Complete Linkage
- Group Average Linkage
- Centroid Linkage
- Median Linkage



Median Clustering

- Disadvantage of the Centroid Clustering: When a large cluster is merged with a small one, the centroid of the combined cluster would be closed to the large one, ie. The characteristic properties of the small one are lost
- After we have combined two groups, the mid-point of the original two cluster centres is used as the centre of the newly combined group





- Single Linkage
- Complete Linkage
- Group Average Linkage
- Centroid Linkage
- Median Linkage

There are other distance measurements (e.g., McQuitty's linkage/method and Ward's linkage/method).
We will not discuss them.



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 - How to use the data mining tool



Divisive Methods

- In a divisive algorithm, we start with the assumption that all the data is part of one cluster.
- We then use a distance criterion to divide the cluster in two, and then subdivide the clusters until a stopping criterion is achieved.
 - ✓ Polythetic divide the data based on the values by all attributes
 - Monothetic divide the data on the basis of the possession of a single specified attribute



- Distance
 - Single Linkage
 - Complete Linkage
 - Group Average Linkage
 - Centroid Linkage
 - Median Linkage

4

```
1 2 3 4 5 6 7

1 0

2 10 0

3 7 7 0

4 30 23 21 0

5 29 25 22 7 0

6 38 34 31 10 11 0

7 42 36 36 13 17 9 0
```

$$B = \{2, 3, 4, 5, 6, 7\}$$

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$$D(1, *) = 26.0$$

$$D(2, *) = 22.5$$

$$D(3, *) = 20.7$$

$$D(4, *) = 17.3$$

$$D(5, *) = 18.5$$

$$D(6, *) = 22.2$$

$$D(7, *) = 25.5$$

4

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$$D(2, A) = 10$$

$$D(3, A) = 7$$

$$D(4, A) = 30$$

$$D(5, A) = 29$$

$$D(6, A) = 38$$

$$D(7, A) = 42$$

$$B = \{2, 3, 4, 5, 6, 7\}$$

$$COMP1942$$

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$$D(2, A) = 10$$
 $D(2, B) = 25.0$ $D(3, A) = 7$ $D(3, B) = 23.4$

$$D(4, A) = 30$$
 $D(4, B) = 14.8$

$$B = \{2, 3, 4, 5, 6, 7\}$$

$$COMP1942$$

$$D(7, A) = 42$$
 $D(7, B) = 22.2$

4

Polythetic Approach

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1 2 3 4 5 6 7

1 0

2 10 0

3 7 7 0

4 30 23 21 0

5 29 25 22 7 0

6 38 34 31 10 11 0

7 42 36 36 13 17 9 0
```

D(2, A) = 10 D(2, B) = 25.0
$$\Delta_2$$
 = 15.0

$$D(3, A) = 7$$
 $D(3, B) = 23.4$ $\Delta_3 = 16.4$

D(4, A) = 30 D(4, B) = 14.8
$$\Delta_4 = -15.2$$

D(5, A) = 29 D(5, B) = 16.4
$$\Delta_5$$
 = -12.6

D(6, A) = 38 D(6, B) = 19.0
$$\Delta_6 = -19.0$$

D(7, B) = 22.2

$$A = \{1, 3\}$$
 $D(7, A) = 42$

Polythetic Approach

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D(2, A) = 10 D(2, B) = 25.0
$$\Delta_2$$
 = 15.0

D(3, A) = 7 D(3, B) = 23.4
$$\Delta_3$$
 = 16.4

D(4, A) = 30 D(4, B) = 14.8
$$\Delta_4$$
 = -15.2

D(5, A) = 29 D(5, B) = 16.4
$$\Delta_5$$
 = -12.6

D(6, A) = 38 D(6, B) = 19.0
$$\Delta_6$$
 = -19.0

A =
$$\{1, 3\}$$
 D(7, A) = 42 D(7, B) = 22.2 Δ_7 = -19.8

$$B = \{2, 4, 5, 6, 7\}$$

Polythetic Approach

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```

$$D(2, A) = 8.5$$

$$D(4, A) = 25.5$$

$$D(5, A) = 25.5$$

$$D(6, A) = 34.5$$

$$D(7, A) = 39.0$$

$$A = \{1, 3\}$$

$$B = \{2, 4, 5, 6, 7\}$$
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Polythetic Approach

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D(2, A) = 8.5
$$D(2, B) = 29.5$$
 $D(4, A) = 25.5$ $D(4, B) = 13.2$ $D(5, A) = 25.5$ $D(5, B) = 15.0$ $D(6, A) = 34.5$ $D(6, B) = 16.0$

D(7, A) = 39.0

D(7, B) = 18.75

$$B = \{2, 4, 5, 6, 7\}$$
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Polythetic Approach

```
      1
      2
      3
      4
      5
      6
      7

      1
      0
      10
      0

      2
      10
      0
      0

      3
      7
      7
      0

      4
      30
      23
      21
      0

      5
      29
      25
      22
      7
      0

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      31
      10
      11
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      42
      36
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      17
      9
      0
```

D(2, A) = 8.5 D(2, B) = 29.5
$$\Delta_2 = 21.0$$

D(4, A) = 25.5 D(4, B) = 13.2
$$\Delta_4$$
 = -12.3

D(5, A) = 25.5 D(5, B) = 15.0
$$\Delta_5 = -10.5$$

D(6, A) = 34.5 D(6, B) = 16.0
$$\Delta_6$$
 = -18.5

D(7, A) = 39.0 D(7, B) = 18.75
$$\Delta_7$$
 = -20.25

$$A = \{1, 3, 2\}$$

$$B = \{ 4, 5, 6, 7 \}$$

Polythetic Approach

```
1 2 3 4 5 6 7

1 0

2 10 0

3 7 7 0

4 30 23 21 0

5 29 25 22 7 0

6 38 34 31 10 11 0

7 42 36 36 13 17 9 0
```

D(2, A) = 8.5 D(2, B) = 29.5
$$\Delta_2$$
 = 21.0

D(4, A) = 25.5 D(4, B) = 13.2
$$\Delta_4 = -12.3$$

D(5, A) = 25.5 D(5, B) = 15.0
$$\Delta_5 = -10.5$$

D(6, A) = 34.5 D(6, B) = 16.0
$$\Delta_6 = -18.5$$

D(7, A) = 39.0 D(7, B) = 18.75
$$\Delta_7$$
 = -20.25

$$A = \{1, 3, 2\}$$

$$B = \{ 4, 5, 6, 7 \}$$
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Polythetic Approach

```
      1
      2
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      1
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      10
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```

$$D(4, A) = 24.7$$
 $D(5, A) = 25.3$
 $D(6, A) = 34.3$

D(7, A) = 38.0

Polythetic Approach

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      11
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```

$$D(5, A) = 25.3$$
 $D(5, B) = 11.7$

$$D(6, A) = 34.3$$
 $D(6, B) = 10.0$

$$D(7, A) = 38.0 \mid D(7, B) = 13.0$$

$$A = \{1, 3, 2\}$$

$$B = \{4, 5, 6, 7\}$$
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Polythetic Approach

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      1
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D(4, A) = 24.7 D(4, B) = 10.0
$$\Delta_4 = -14.7$$

D(5, A) = 25.3 D(5, B) = 11.7 $\Delta_5 = -13.6$
D(6, A) = 34.3 D(6, B) = 10.0 $\Delta_6 = -24.3$
D(7, A) = 38.0 D(7, B) = 13.0 $\Delta_7 = -25.0$

$$A = \{1, 3, 2\}$$

$$B = \{4, 5, 6, 7\}$$

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All differences are negative. The process would continue on each subgroup separately.



Clustering Methods

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Monothetic

It is usually used when the data consists of **binary** variables.

	Α	В	C
1	0	1	1
2	1	1	0
3	1	1	1
4	1	1	0
5	0	0	1

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Monothetic

It is usually used when the data consists of **binary** variables.

	Α	В	С
1	0	1	1
2	1	1	0
3	1	1	1
4	1	1	0
5	0	0	1

ВА	1	0
1	a=3	b=1
0	c=0	d=1

Chi-Square Measure

$$\chi_{AB}^{2} = \frac{(ad - bc)^{2} N}{(a+b)(a+c)(b+d)(c+d)}$$
$$= \frac{(3-0)^{2} \cdot 5}{4 \cdot 3 \cdot 2 \cdot 1}$$
$$= 1.875$$

ВА	1	0	
1	a=3	b=1	L! -
0	c=0	d=1	etic

It is usually used when the data consists of **binary** variables.

	Α	В	С
1	0	1	1
2	1	1	0
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It is usually used when the data consists of **binary** variables.

	Α	В	С
1	0	1	1
2	1	1	0
3	1	1	1
4	1	1	0
5	0	0	1

Attr.	AB	
a	3	
b	1	
С	0	
d	1	
N	5	
χ^2	1.87	

$$\chi_{AB}^{2} = \frac{(ad - bc)^{2} N}{(a+b)(a+c)(b+d)(c+d)}$$
$$= \frac{(3-0)^{2} \cdot 5}{4 \cdot 3 \cdot 2 \cdot 1}$$
$$= 1.875$$

ВА	1	0	
1	a=3	b=1	L! -
0	c=0	d=1	etic

It is usually used when the data consists of **binary** variables.

	Α	В	С
1	0	1	1
2	1	1	0
3	1	1	1
4	1	1	0
5	0	0	1

Attr.	AB	AC	ВС
a	3	1	2
b	1	2	1
С	0	2	2
d	1	0	0
N	5	5	5
χ^2	1.87	2.22	0.83

For attribute A,
$$\chi_{AB}^2 + \chi_{AC}^2 = 4.09$$

For attribute B,
$$\chi_{AB}^2 + \chi_{BC}^2 = 2.70$$

For attribute C,
$$\chi_{AC}^2 + \chi_{BC}^2 = 3.05$$

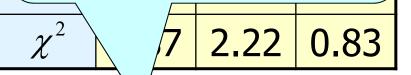
ВА	1	0	
1	a=3	b=1	L! .
0	c=0	d=1	etic

It is usually used when the data consists of **binary** variables.

	Α	В	C
1	0	1	1
2	1	1	0
3	1	1	1
4	1	1	0
5	0	0	1

Attr.	AB	AC	BC
a	3	1	2
b	1	2	1

We choose attribute A for dividing the data into two groups. {2, 3, 4}, and {1, 5}



For attribute A,

$$\chi_{AB}^{2} + \chi_{AC}^{2} = 4.09$$

For attribute B,
$$\chi_{AB}^2 + \chi_{BC}^2 = 2.70$$

For attribute C,
$$\chi_{AC}^2 + \chi_{BC}^2 = 3.05$$



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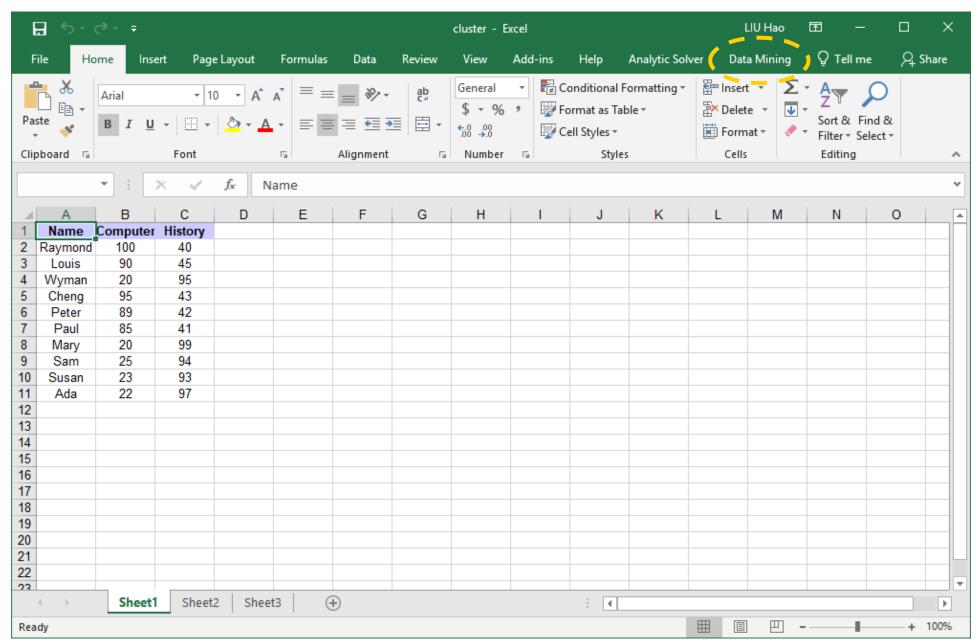
How to use the data mining tool

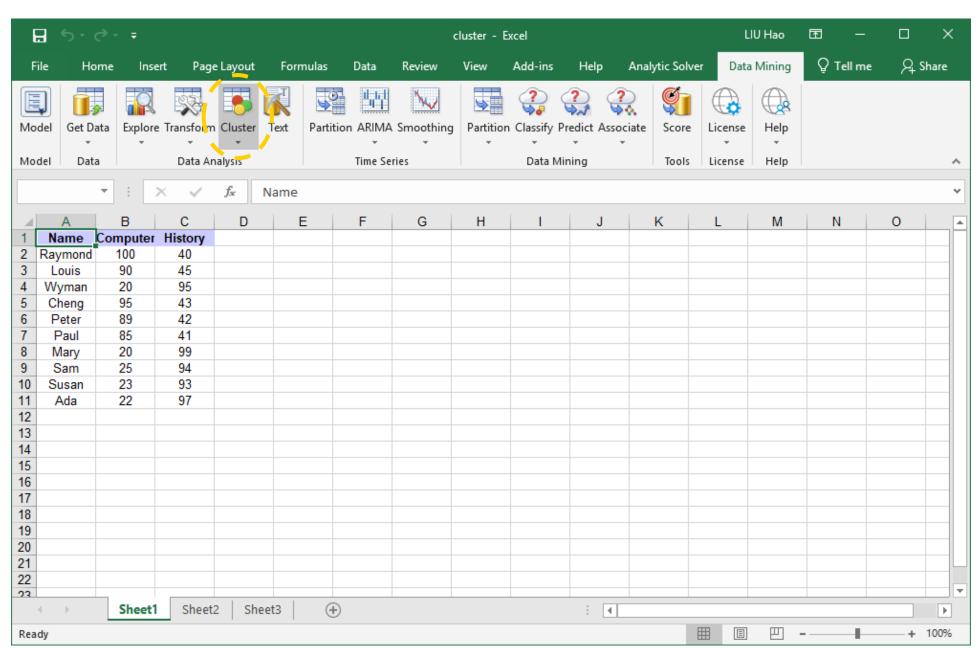
- We have the following 2 versions.
- XLMiner Desktop (installed in either the CSE lab or your computer)
 - XLMiner Cloud (installed as a plugin in your Office 365 Excel)

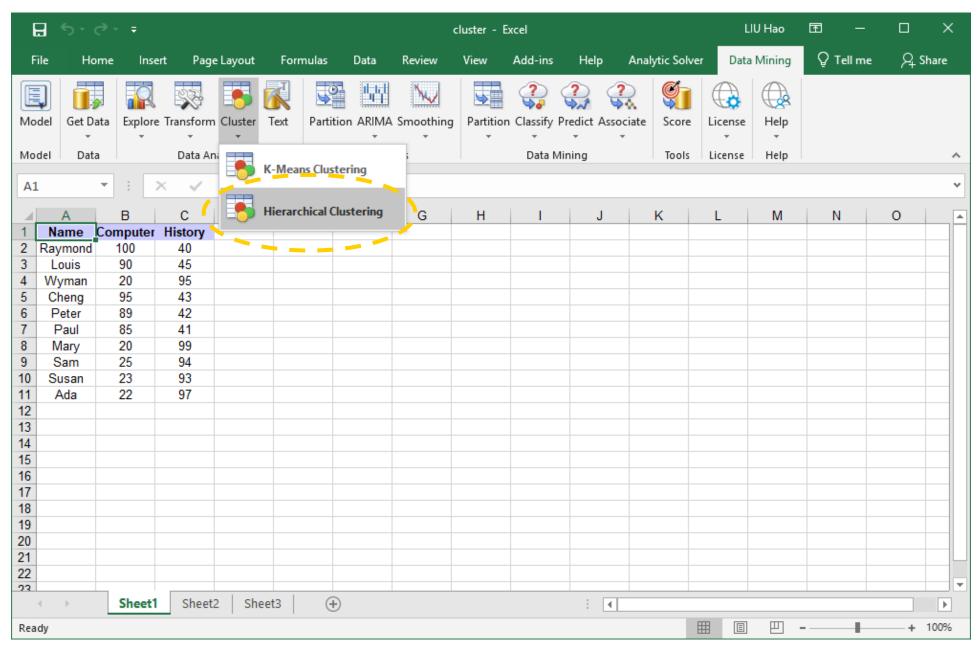


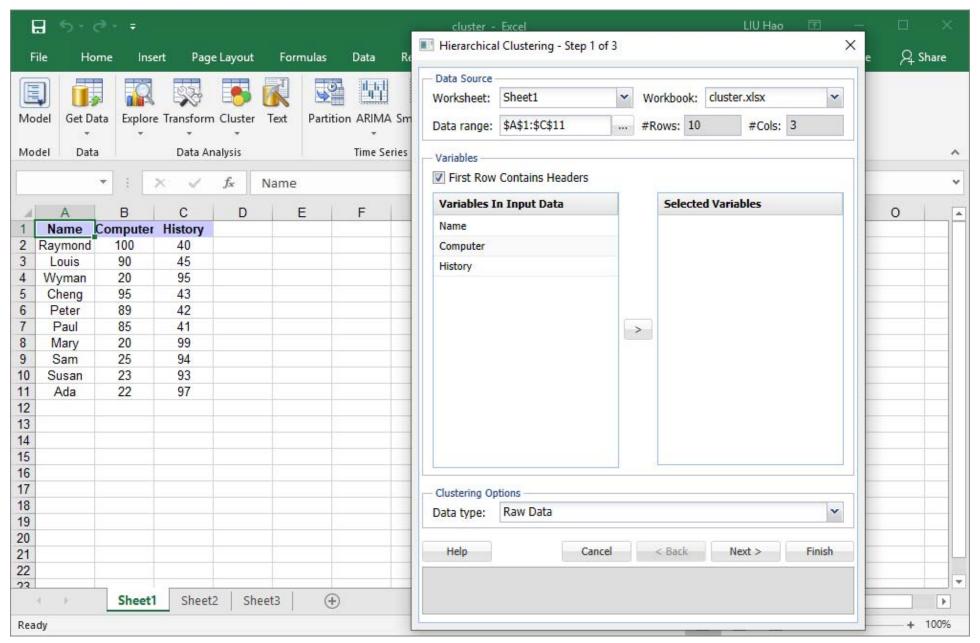
How to use the data mining tool (XLMiner Desktop)

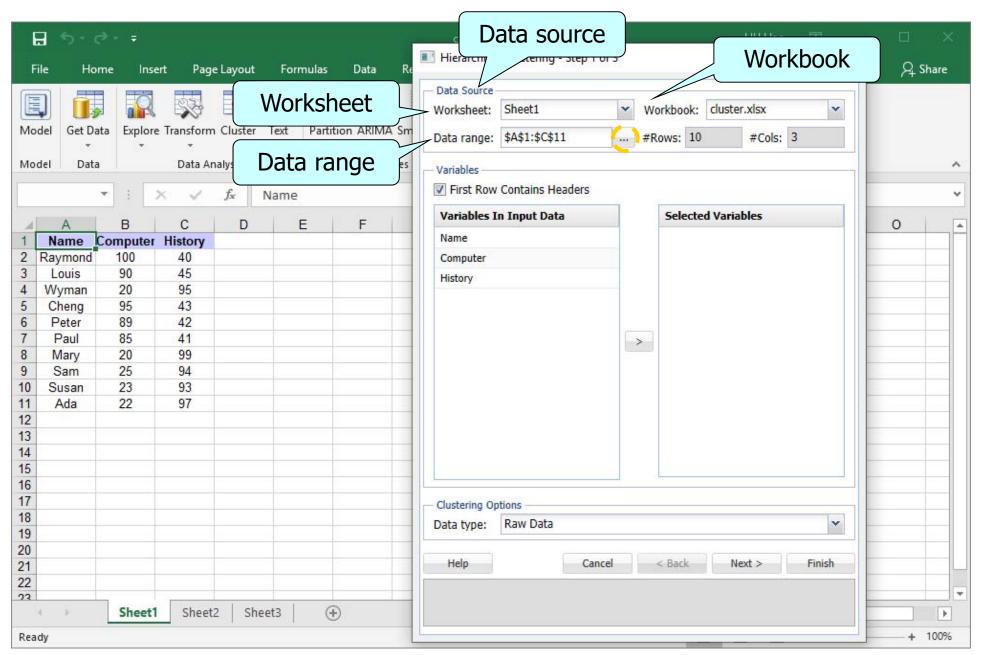
- We can use XLMiner for performing hierarchical clustering
- Open "cluster.xlsx" in MS Excel in a CSE lab machine

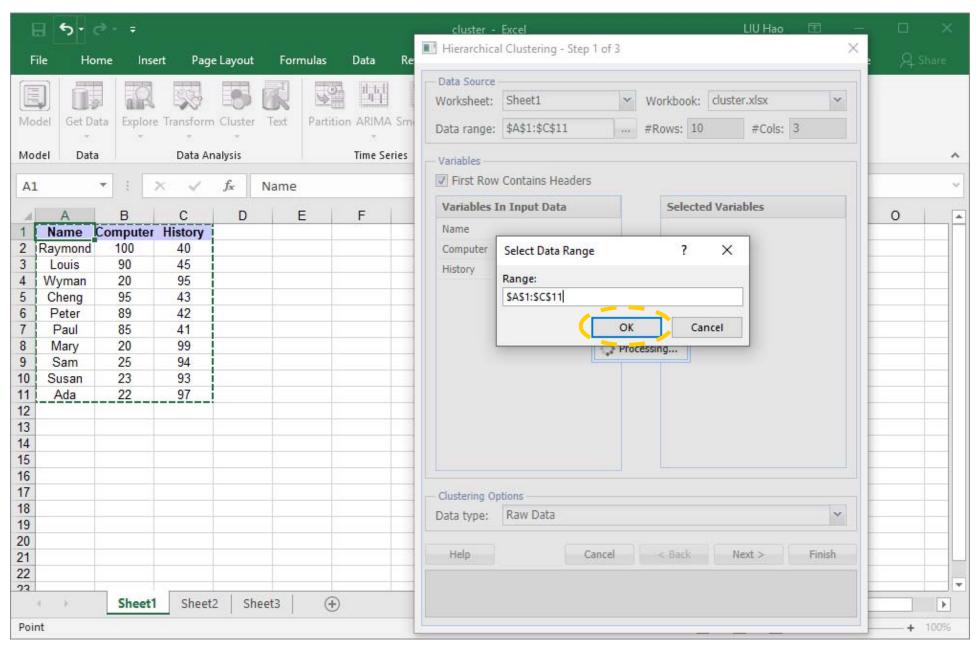


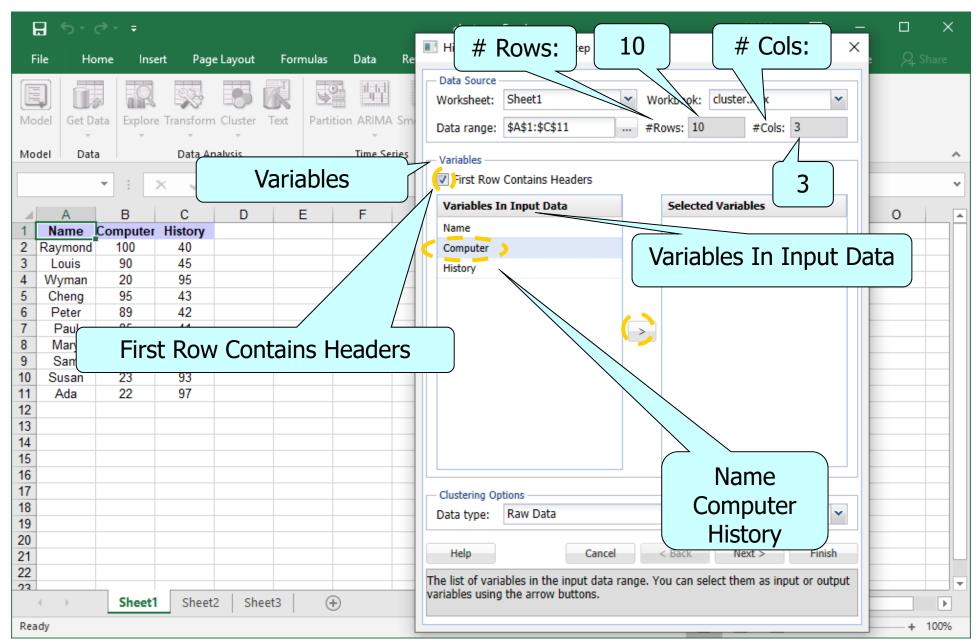


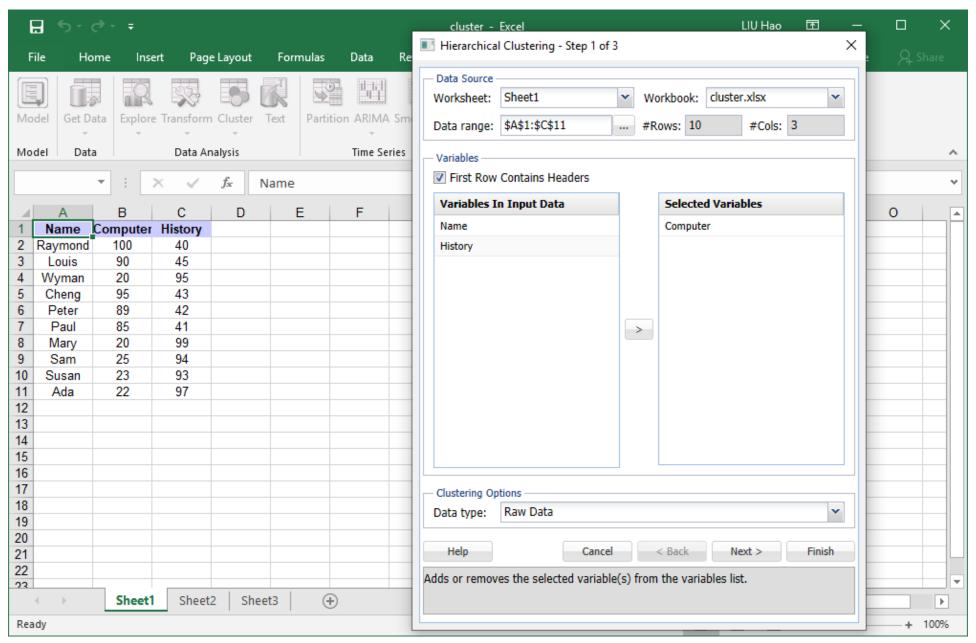


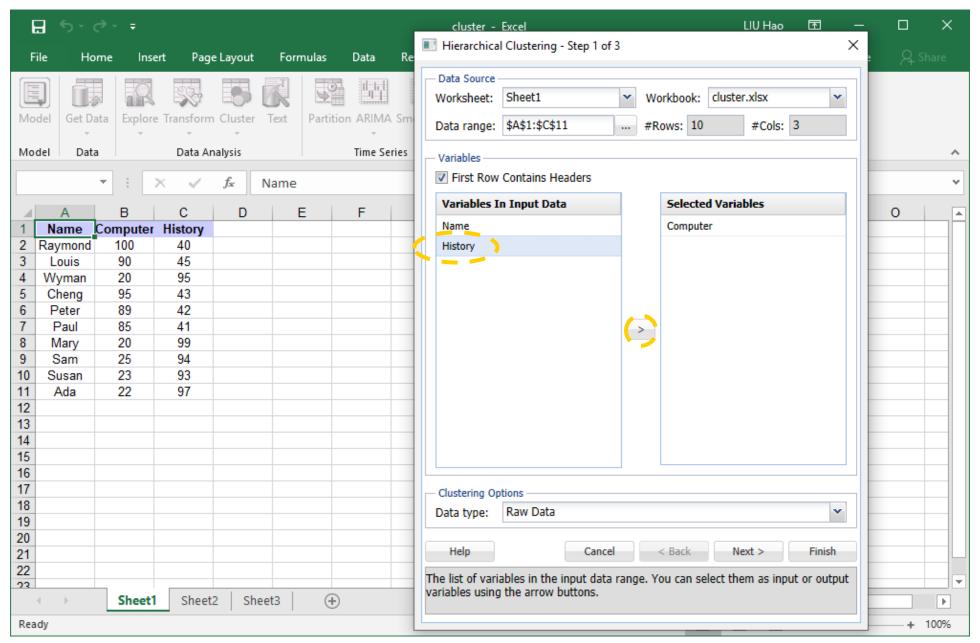


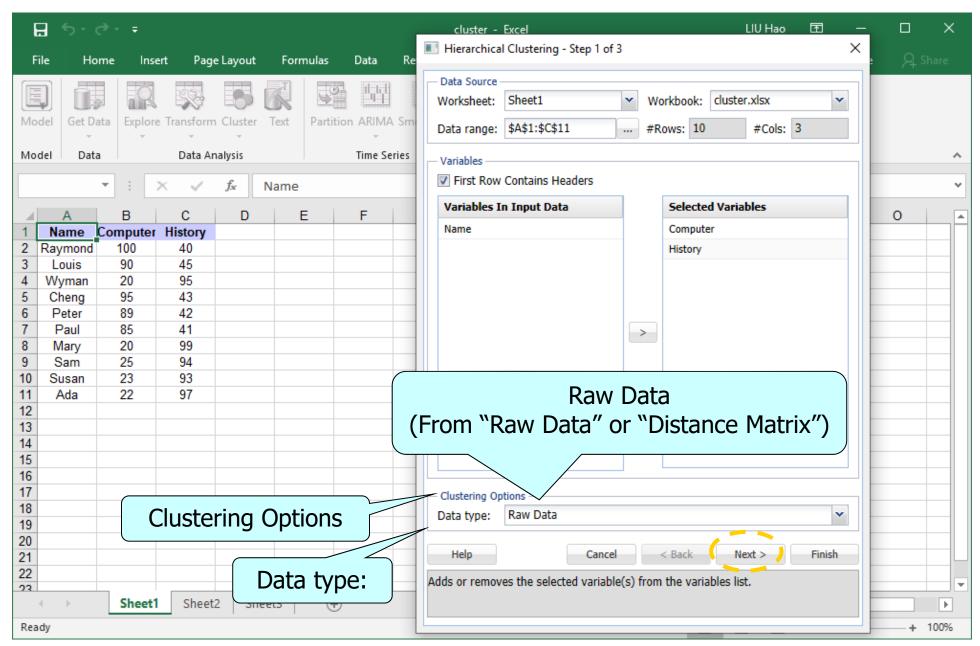


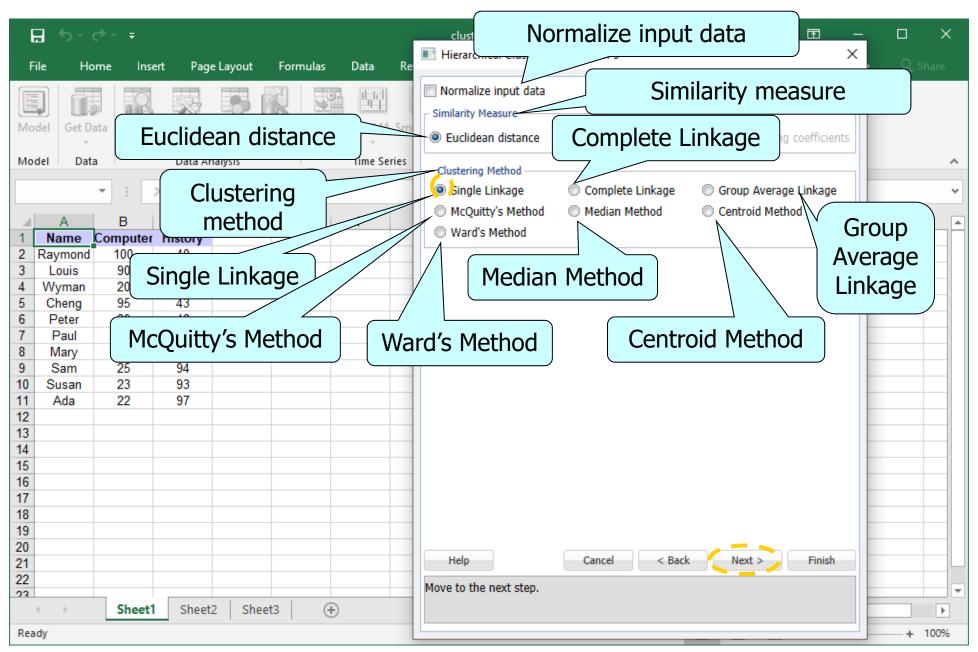


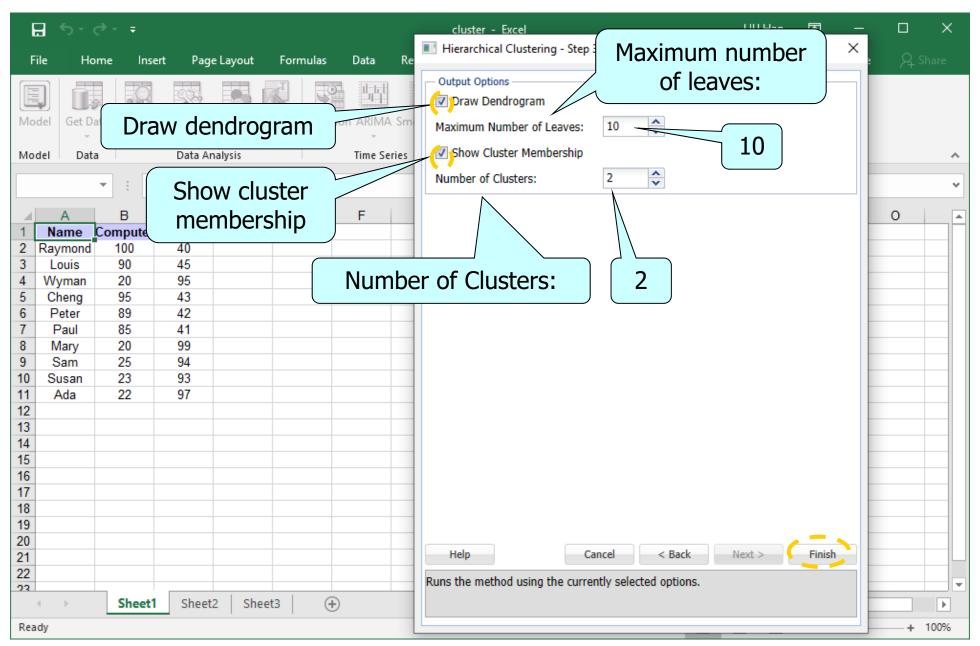


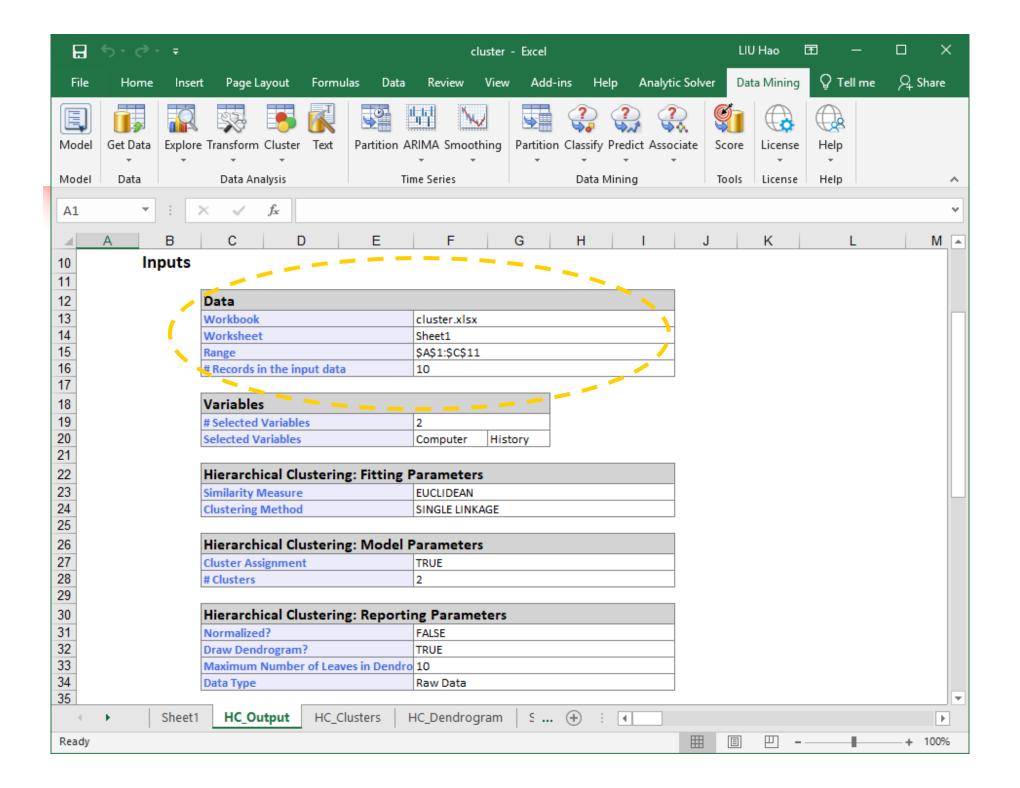


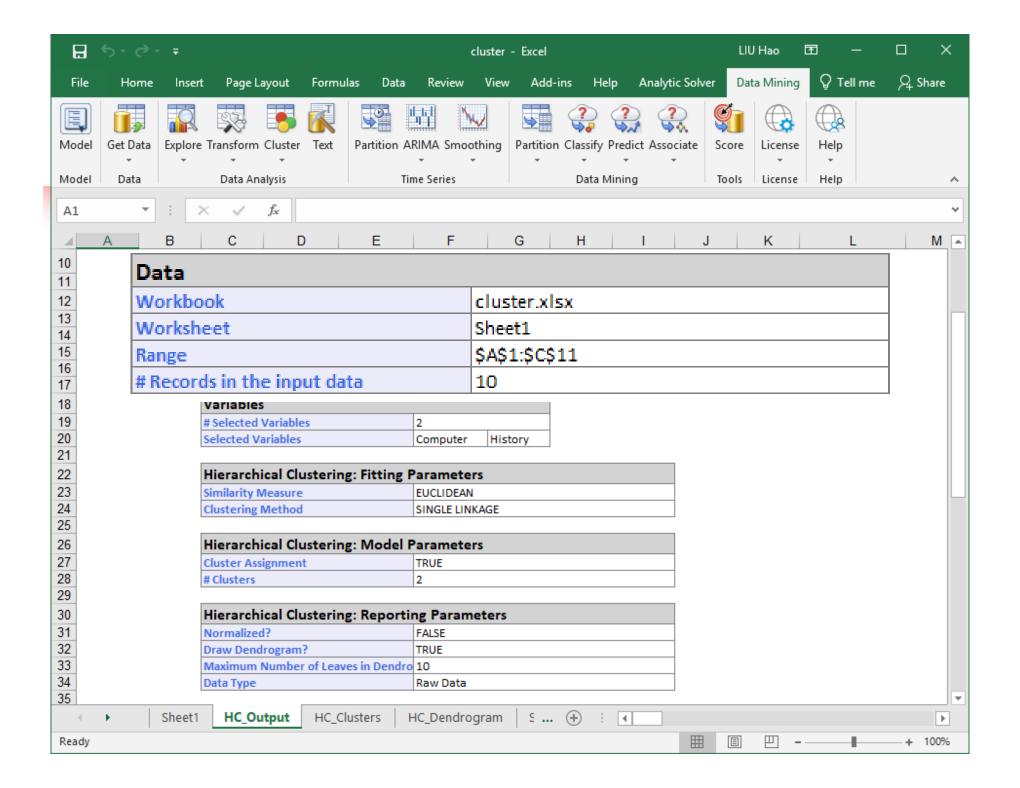


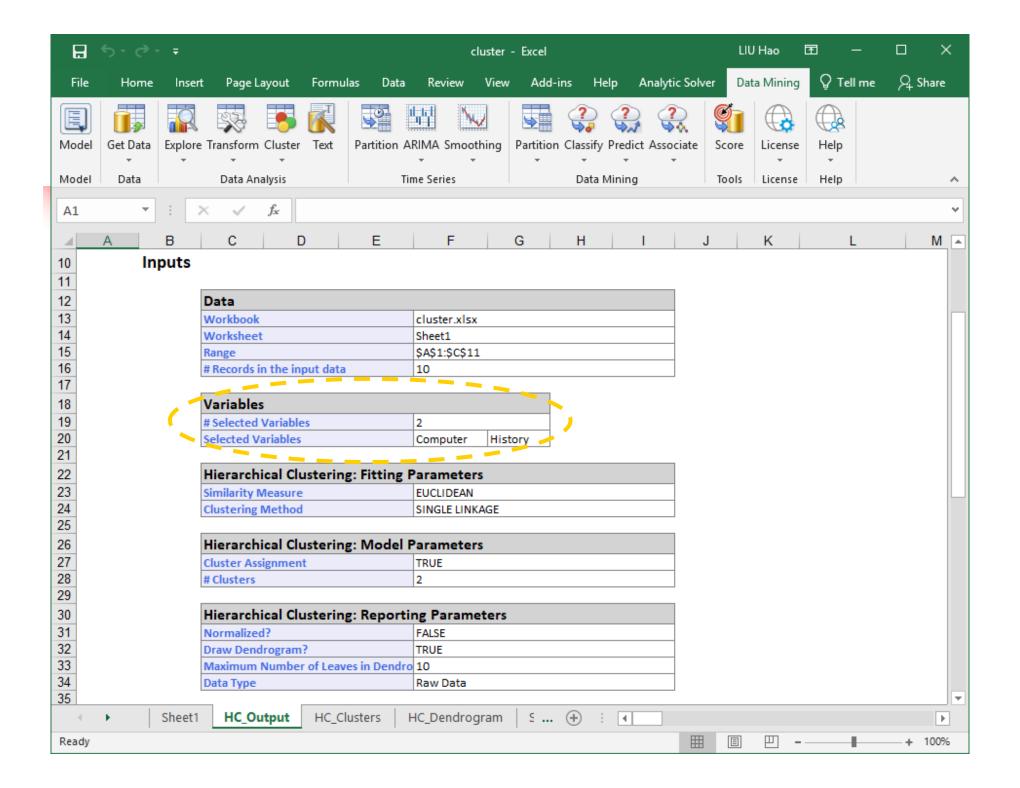


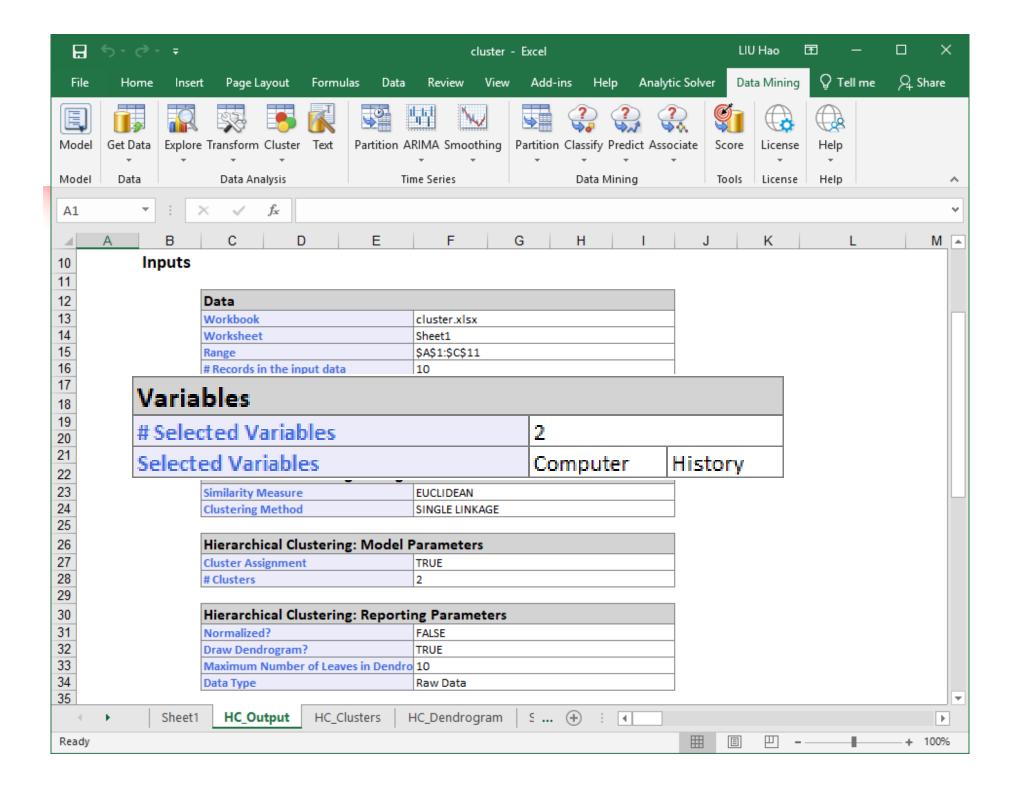


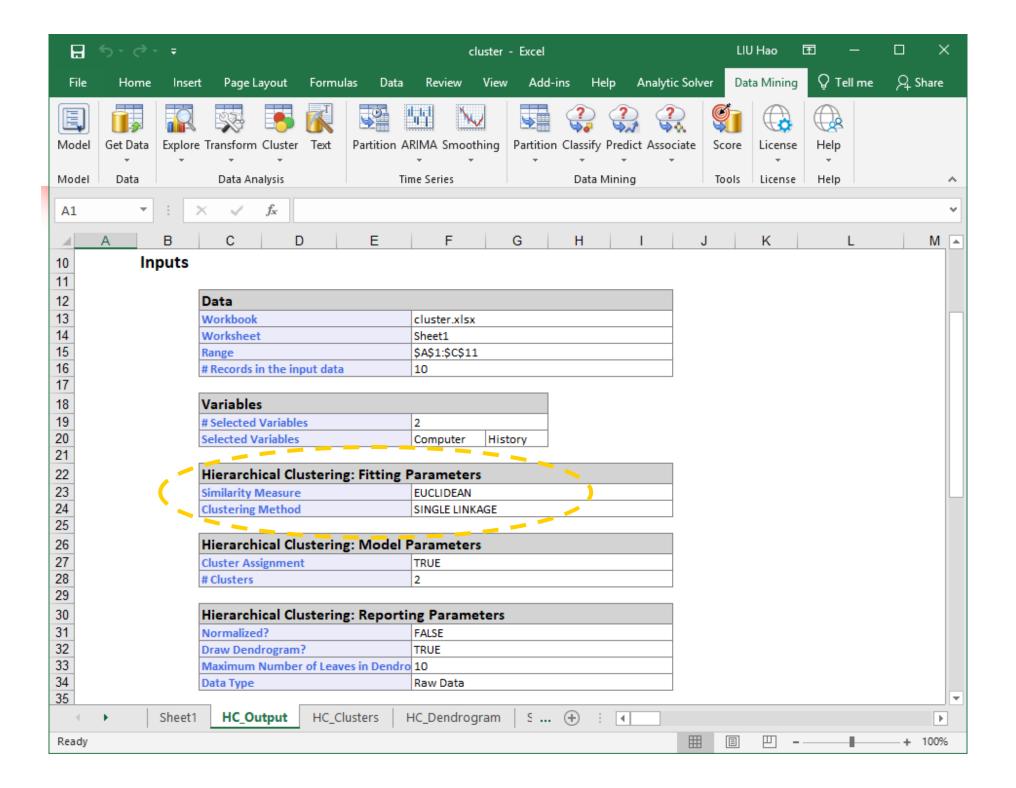


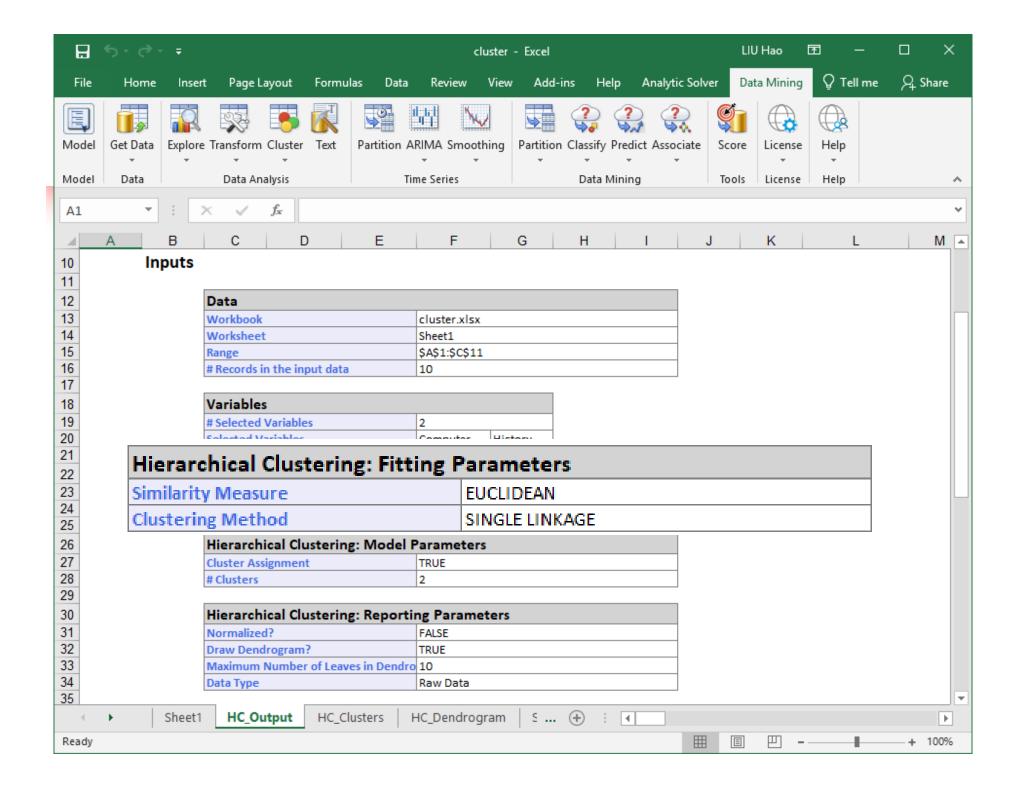


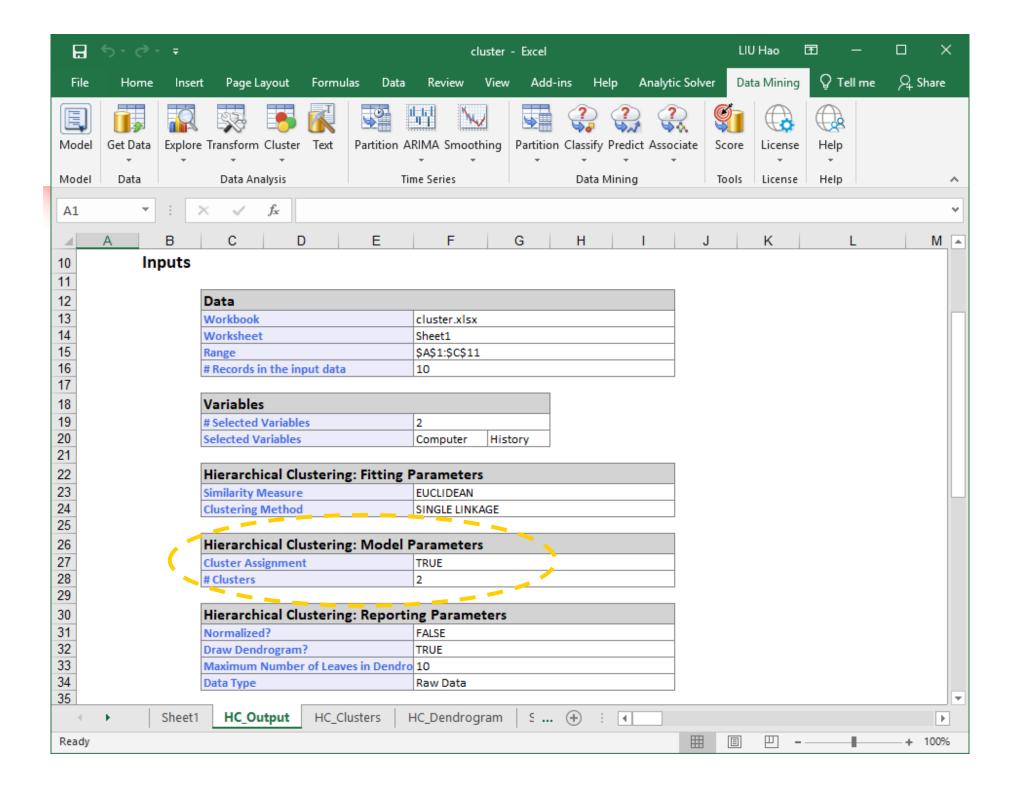


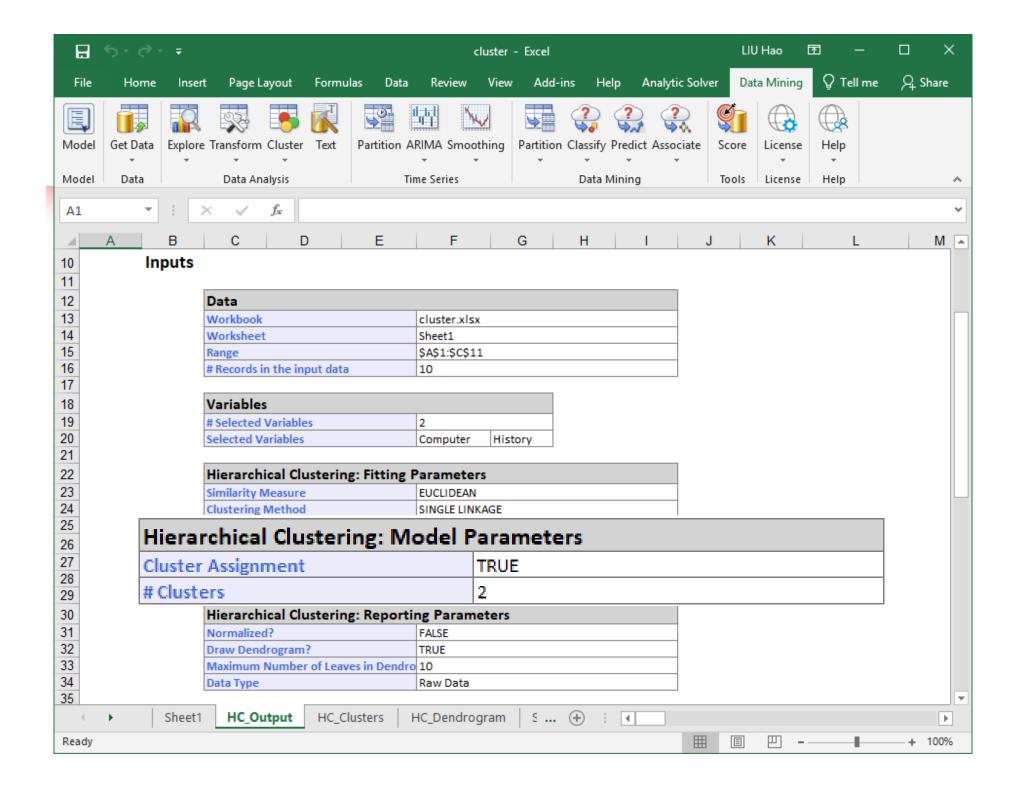


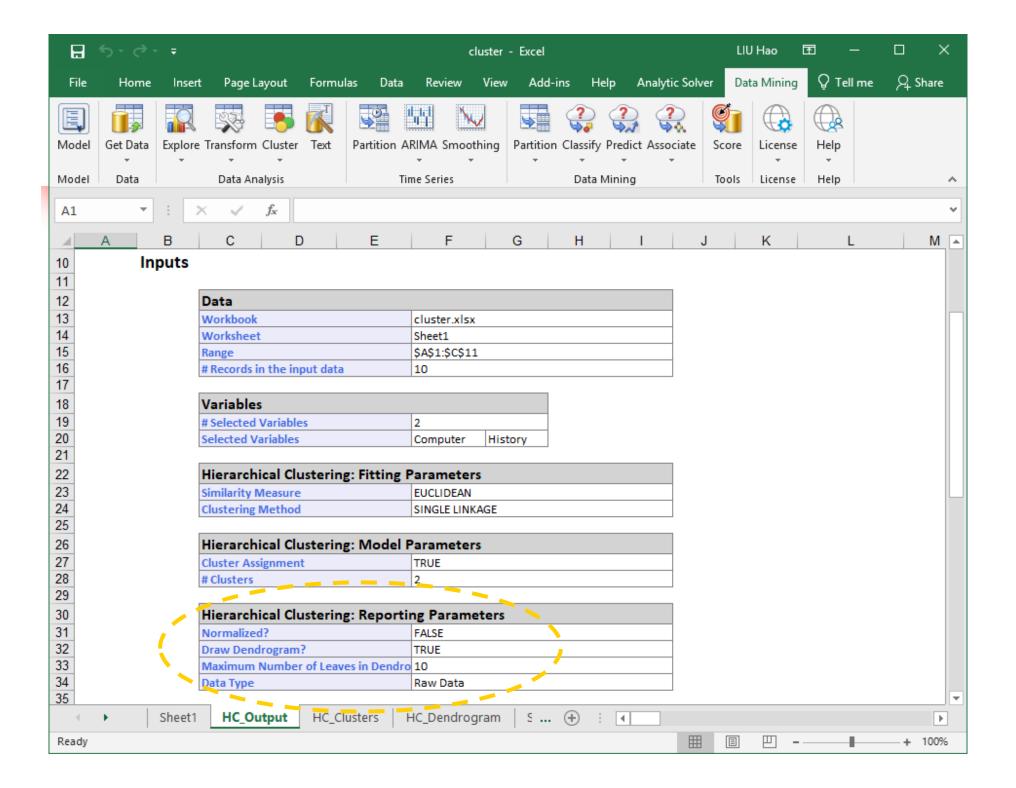




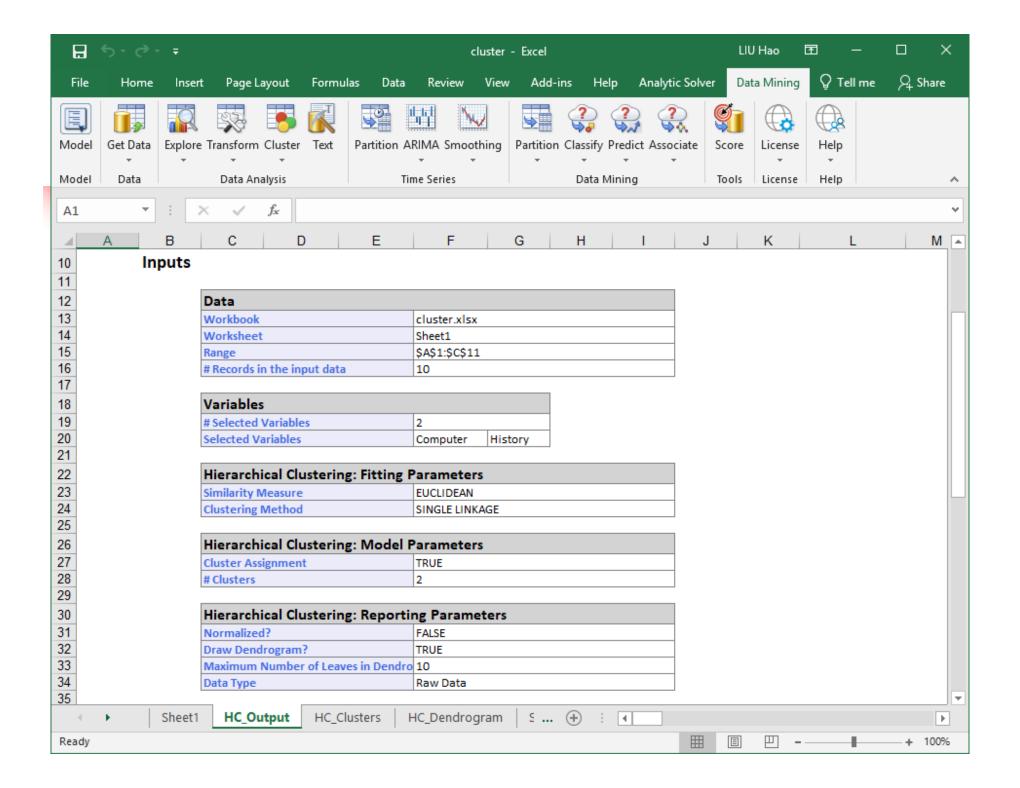


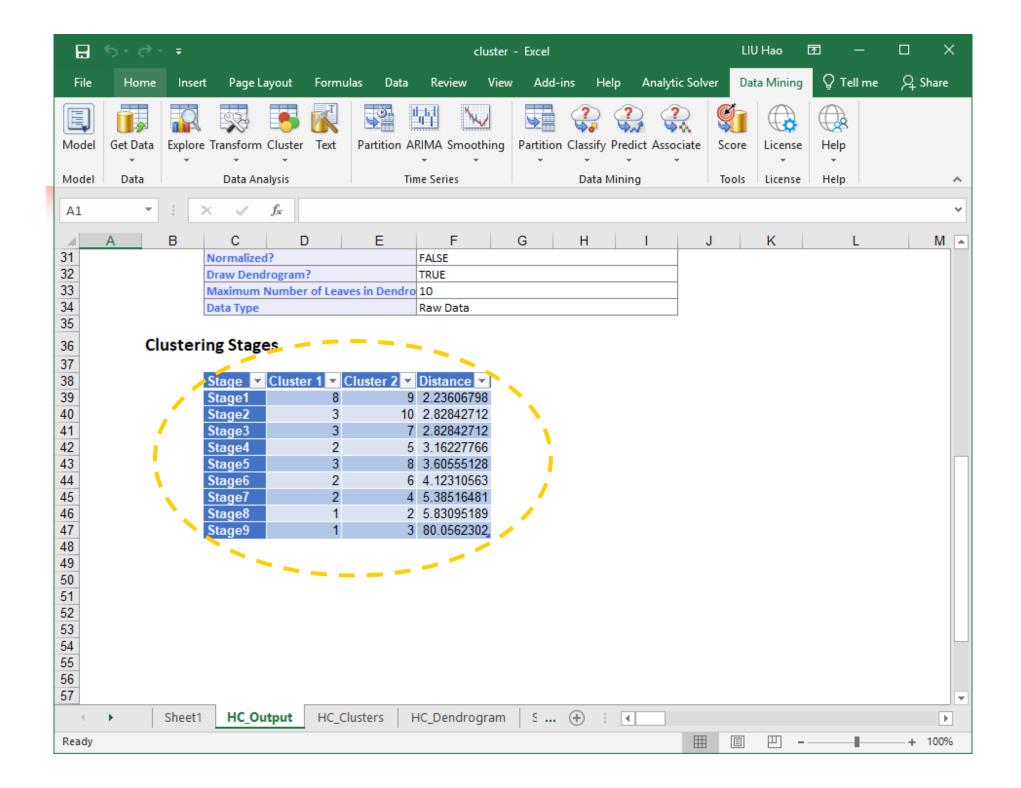


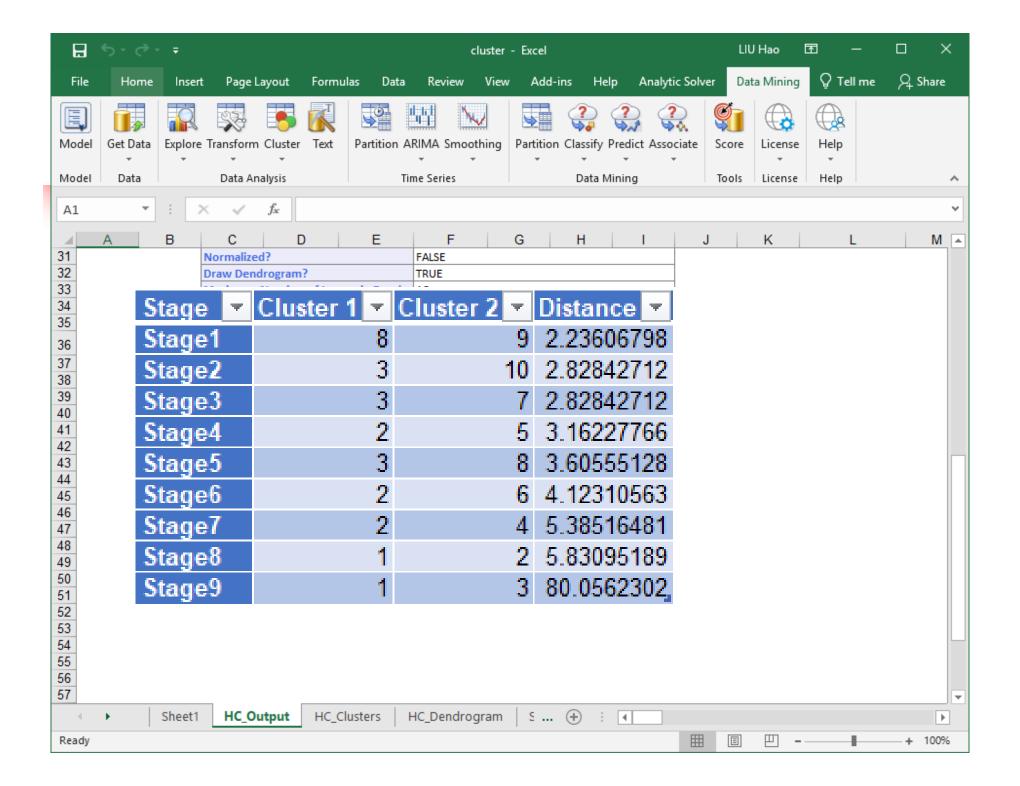


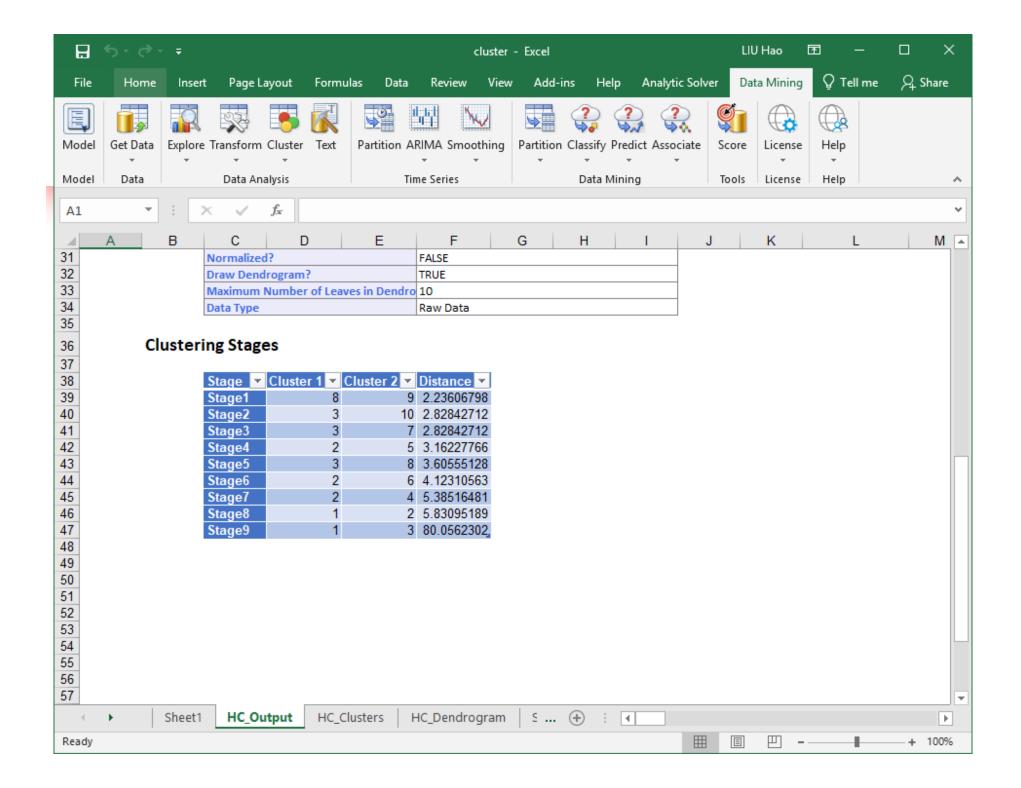


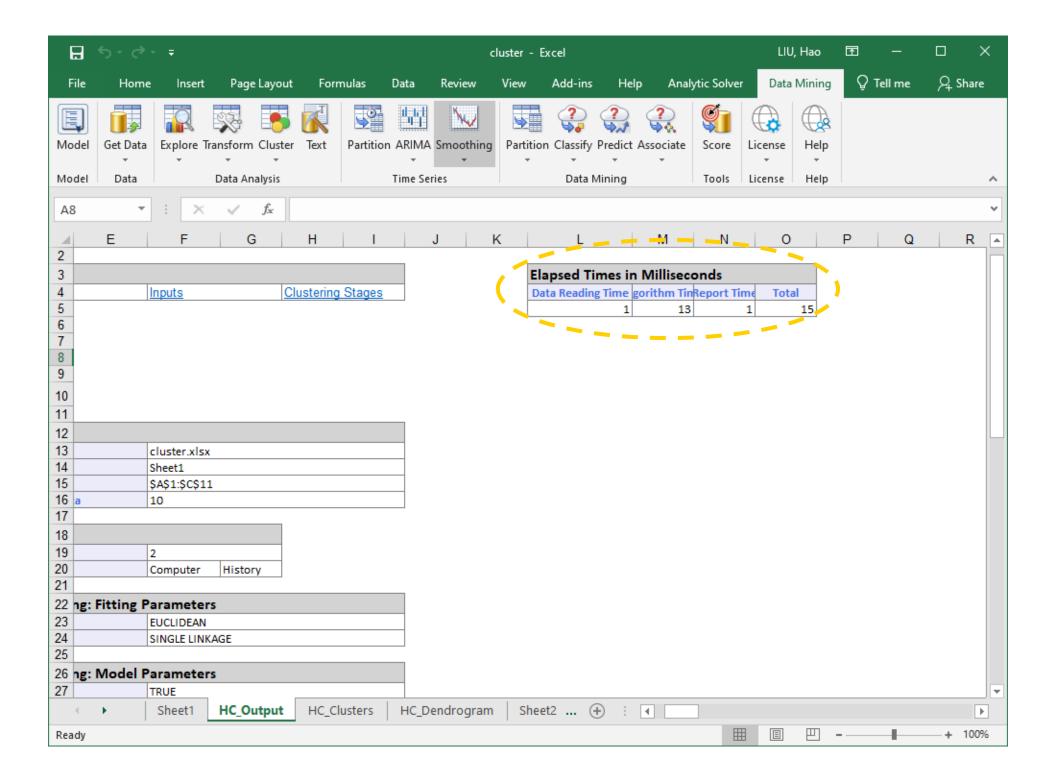


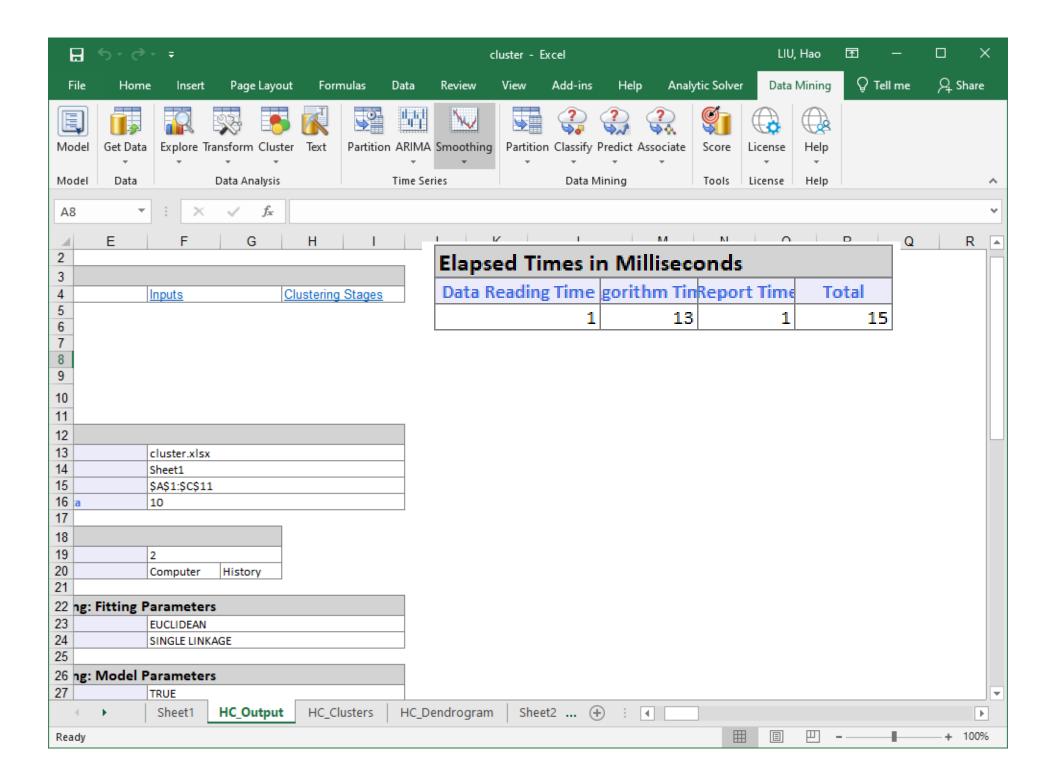


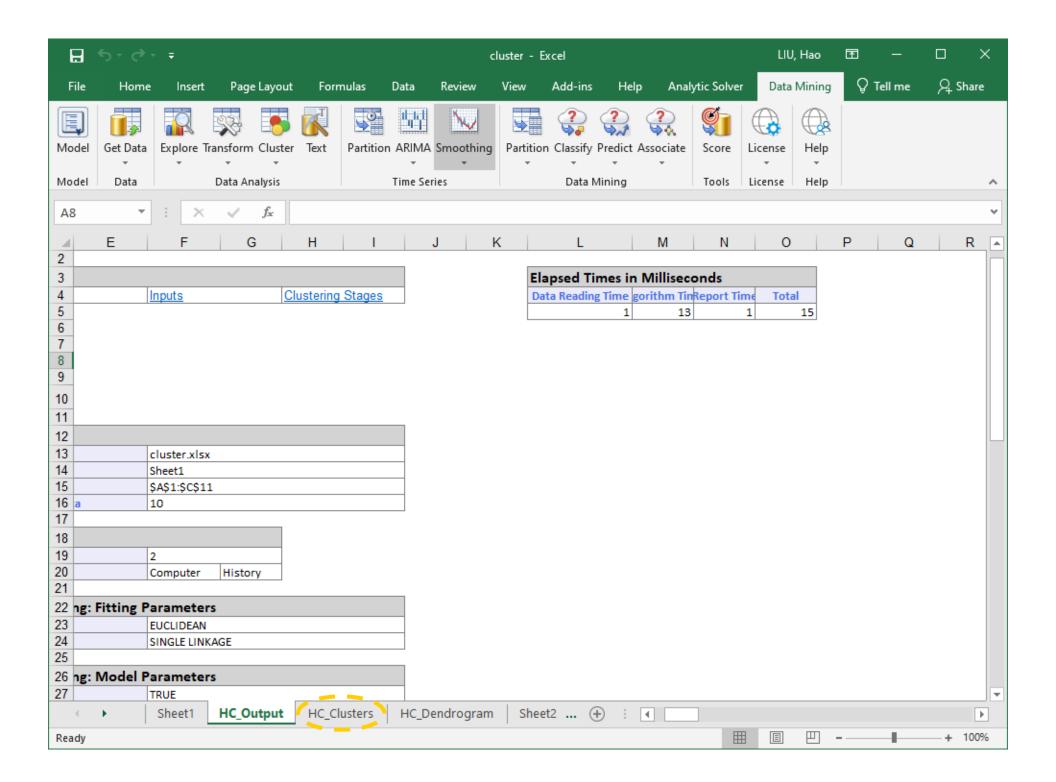


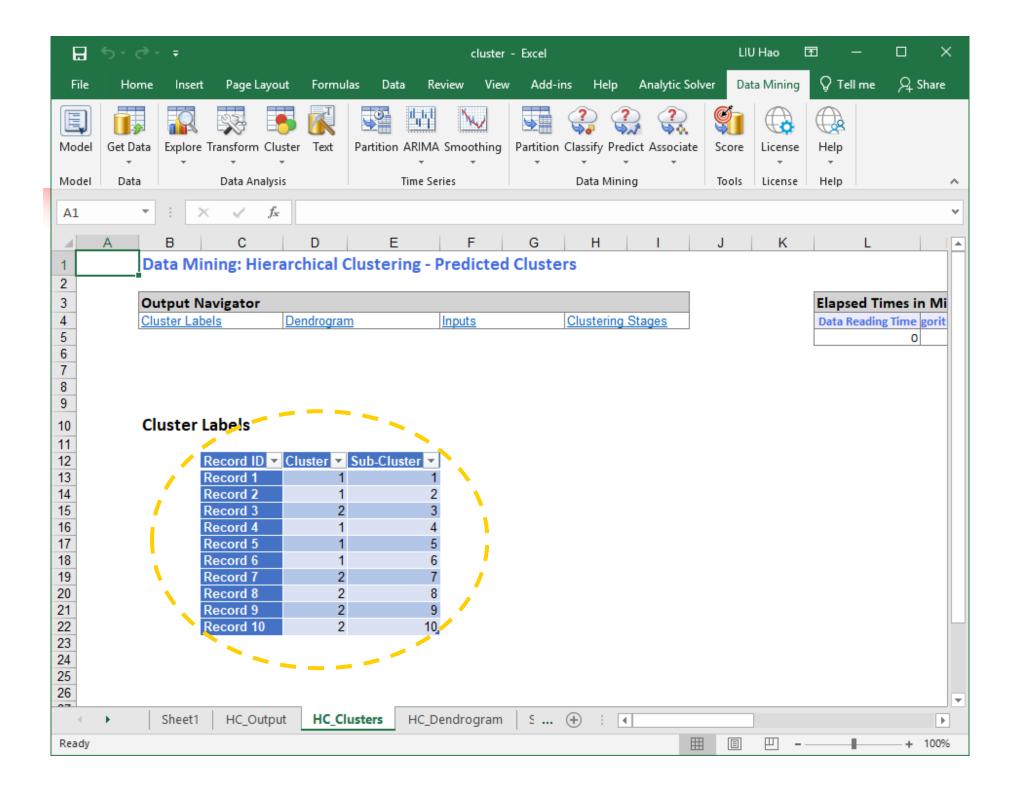


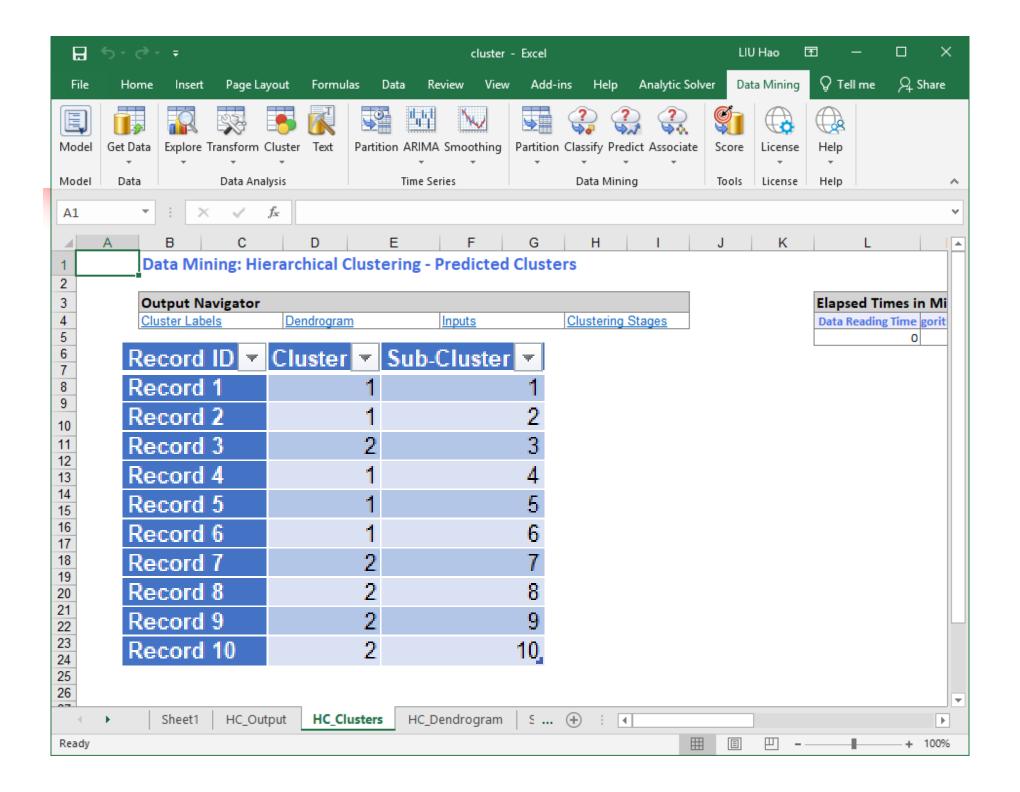


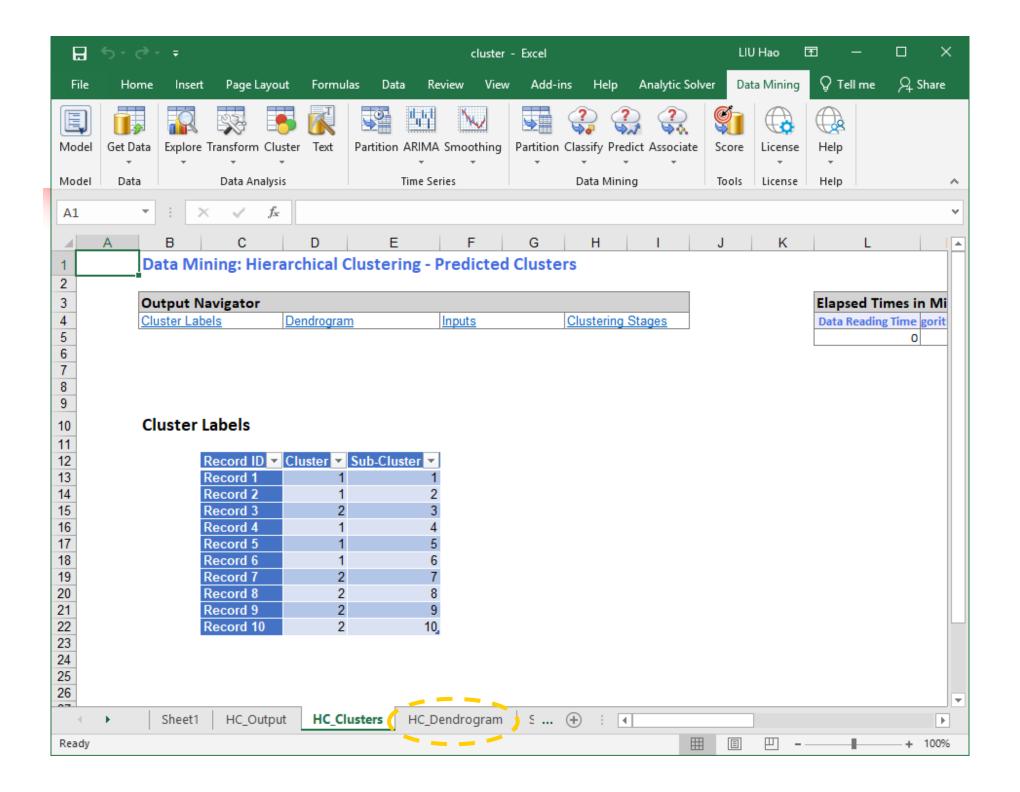


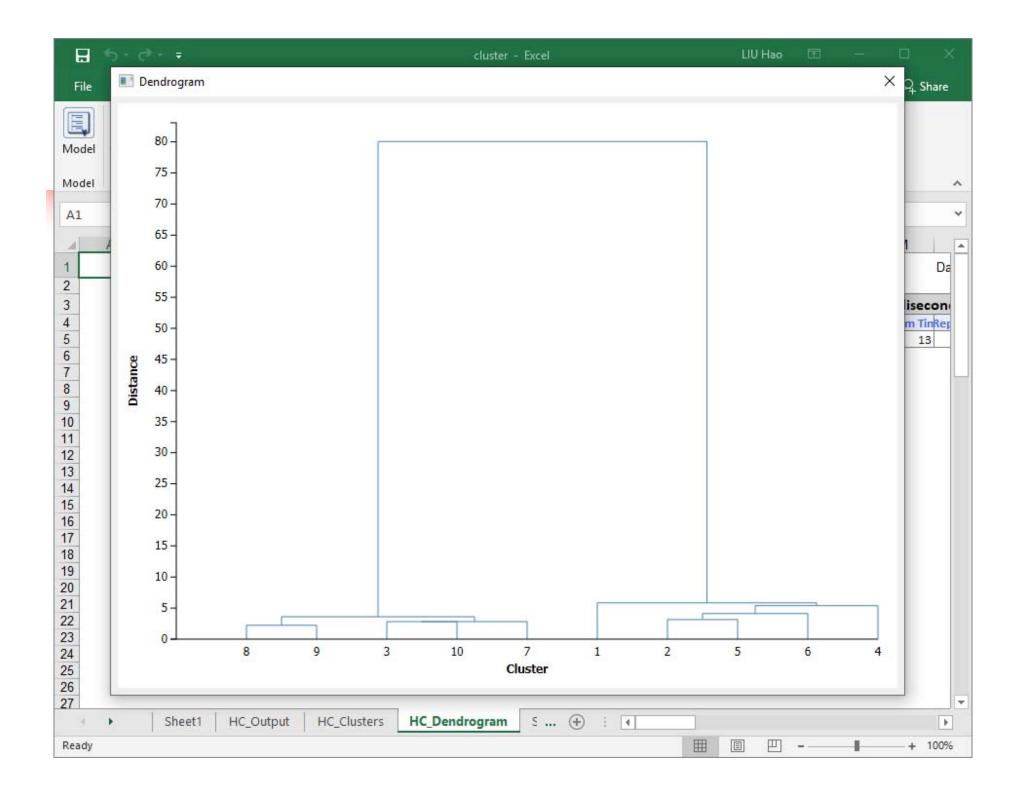






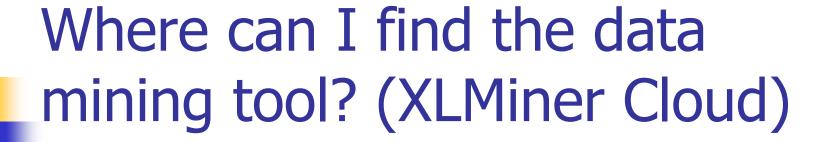




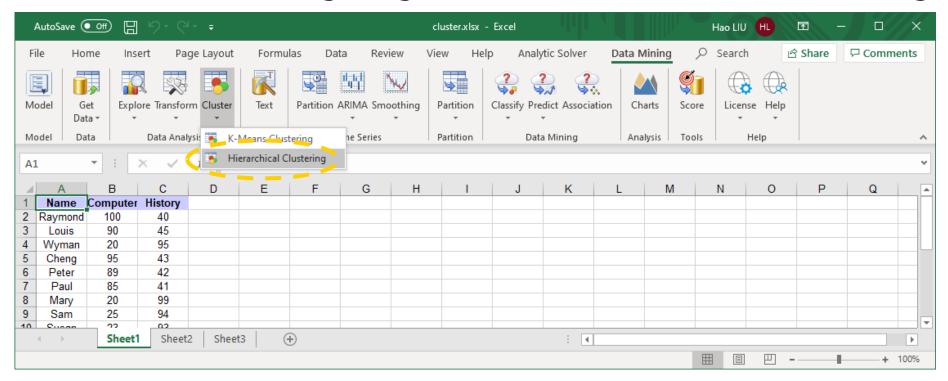


How to use the data mining tool

- We have the following 2 versions.
 - XLMiner Desktop (installed in either the CSE lab machine or your computer)
- XLMiner Cloud (installed as a plugin in your Office 365 Excel)



- The way of opening Hierarchical Clustering in XLMiner Cloud plugin in your Office 365 Excel
 - "Data Mining" Tag → Cluster → Hierarchical Clustering





How to use the data mining tool (XLMiner Cloud)

- The steps of performing "hierarchical clustering" in XLMiner Cloud is similar to the steps in XLMiner Desktop.
- The clustering result of XLMiner Cloud is the same as that from XLMiner Desktop.

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How to use the data mining tool (XLMiner Cloud)

- The output format of XLMiner Cloud is similar to the output in XLMiner Desktop.
- However, to display the dendrogram, you need to call out the "Charts" window.

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