



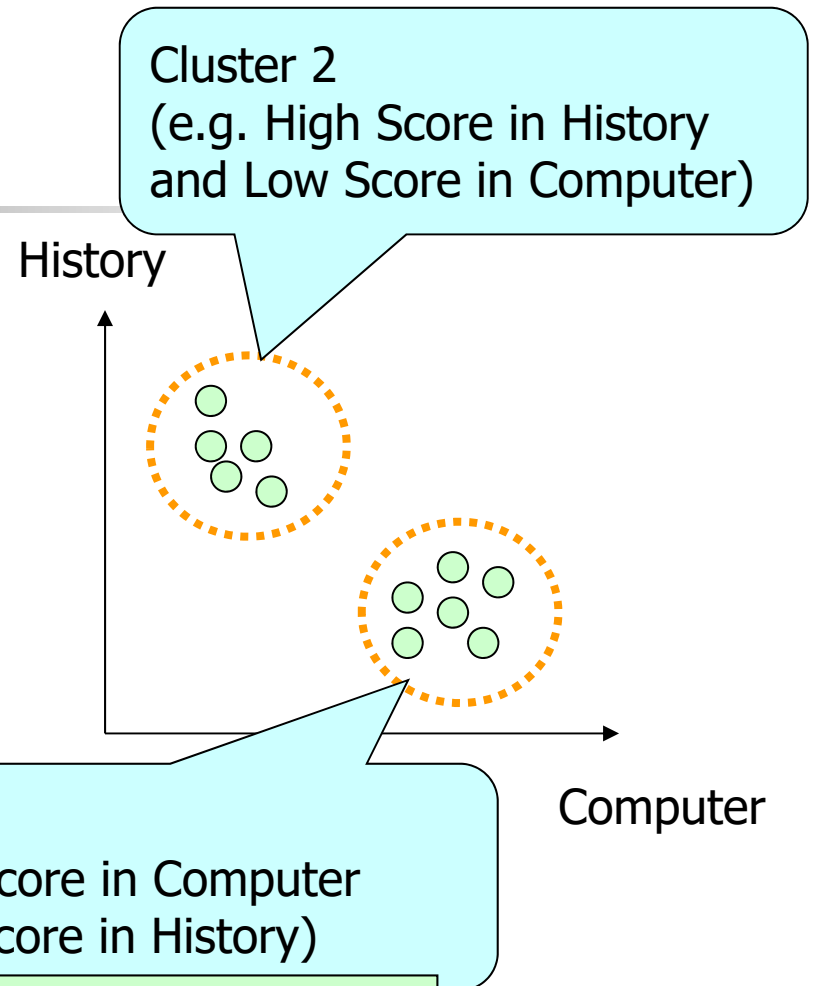
Clustering 1

(Introduction and kmean)

Prepared by Raymond Wong
Some parts of this notes are borrowed from LW Chan's notes
Screenshots of XLMiner Captured by Hao Liu
Presented by Raymond Wong
raywong@cse

Clustering

	Computer	History
Raymond	100	40
Louis	90	45
Wyman	20	95
...



Problem: to find all clusters



Why Clustering?

- Clustering for Utility
 - Summarization
 - Compression



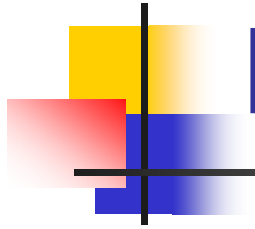
Why Clustering?

- Clustering for Understanding
 - Applications
 - Biology
 - Group different species
 - Psychology and Medicine
 - Group medicine
 - Business
 - Group different customers for marketing
 - Network
 - Group different types of traffic patterns
 - Software
 - Group different programs for data analysis



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



K-mean Clustering

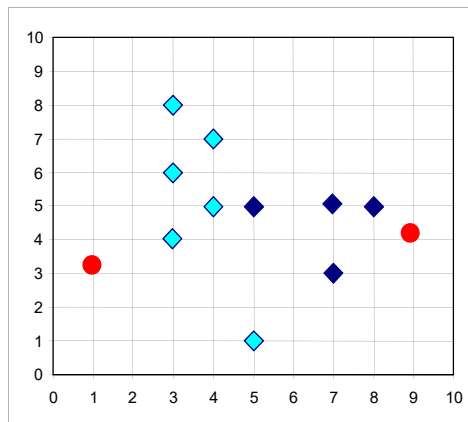
- Suppose that we have n example feature vectors x_1, x_2, \dots, x_n , and we know that they fall into k compact clusters, $k < n$
- Let m_i be the mean of the vectors in cluster i .
- we can say that x is in cluster i if distance from x to m_i is the minimum of all the k distances.



Procedure for finding k-means

- Make initial guesses for the means m_1, m_2, \dots, m_k
- Until there is no change in any mean
 - Assign each data point to the cluster whose mean is the nearest
 - Calculate the mean of each cluster
 - For i from 1 to k
 - Replace m_i with the mean of all examples for cluster i

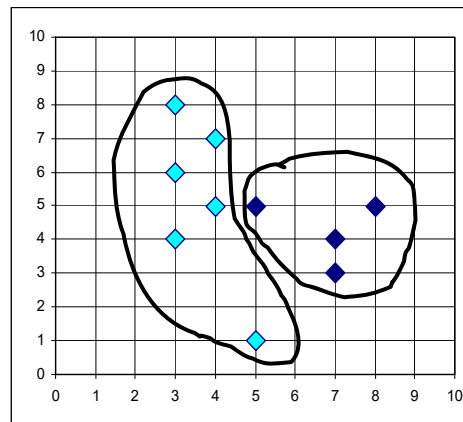
Procedure for finding k-means



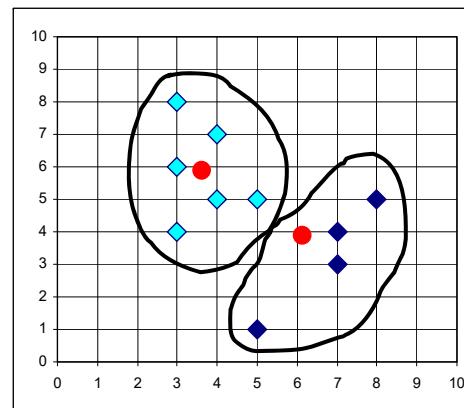
$k=2$

Arbitrarily choose k means

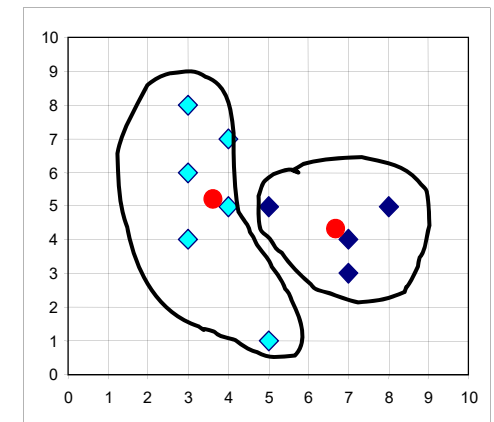
Assign each object to most similar center



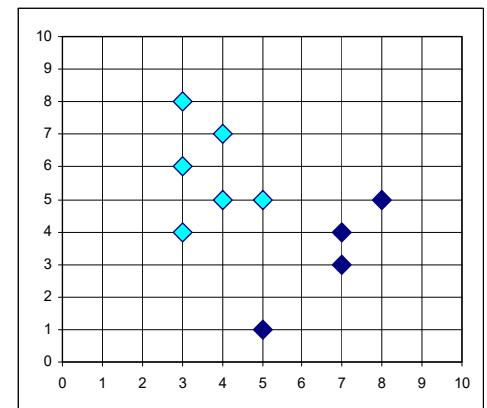
reassign



Update the cluster means



reassign



Update the cluster means



Initialization of k-means

- The way to initialize the means was not specified. One popular way to start is to randomly choose k of the examples
- The results produced depend on the initial values for the means, and it frequently happens that suboptimal partitions are found. The standard solution is to try a number of different starting points



Disadvantages of k-means

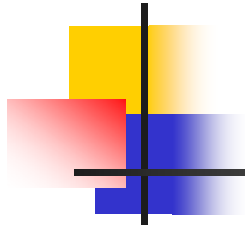
- Disadvantages

- In a “bad” initial guess, there are no points assigned to the cluster with the initial mean m_i .
- The value of k is not user-friendly. This is because we do not know the number of clusters before we want to find clusters.



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Sequential k-Means Clustering

- Another way to modify the k-means procedure is to update the means one example at a time, rather than all at once.
- This is particularly attractive when we acquire the examples over a period of time, and we want to start clustering before we have seen all of the examples
- Here is a modification of the k-means procedure that operates sequentially



Sequential k-Means Clustering

- Make initial guesses for the means m_1, m_2, \dots, m_k
- Set the counts n_1, n_2, \dots, n_k to zero
- Until interrupted
 - Acquire the next example, x
 - If m_i is closest to x
 - Increment n_i
 - Replace m_i by $m_i + (1/n_i) \cdot (x - m_i)$



Clustering Methods

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Forgetful Sequential k-means

- This also suggests another alternative in which we replace the counts by constants. In particular, suppose that a is a constant between 0 and 1, and consider the following variation:
- Make initial guesses for the means m_1, m_2, \dots, m_k
- Until interrupted
 - Acquire the next example x
 - If m_i is closest to x , replace m_i by $m_i + a(x - m_i)$



Forgetful Sequential k-means

- The result is called the “forgetful” sequential k-means procedure.
- It is not hard to show that m_i is a weighted average of the examples that were closest to m_i , where the weight decreases exponentially with the “age” to the example.
- That is, if m_0 is the initial value of the mean vector and if x_j is the j -th example out of n examples that were used to form m_i , then it is not hard to show that

$$m_n = (1-a)^n m_0 + a \sum_{k=1}^n (1-a)^{n-k} x_k$$



Forgetful Sequential k-means

- Thus, the initial value m_0 is eventually forgotten, and recent examples receive more weight than ancient examples.
- This variation of k-means is particularly simple to implement, and it is attractive when the nature of the problem changes over time and the cluster centres “drift”.



Clustering Methods

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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 machine 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 k-mean clustering
- Open “cluster.xlsx” in MS Excel in a CSE lab machine

cluster - Excel

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Paste Font Alignment Number Styles Cells Editing

Name

	A	B	C	D	E	F	G	H	I	J	K	L	M	N	O	P
1	Name	Computer	History													
2	Raymond	100	40													
3	Louis	90	45													
4	Wyman	20	95													
5	Cheng	95	43													
6	Peter	89	42													
7	Paul	85	41													
8	Mary	20	99													
9	Sam	25	94													
10	Susan	23	93													
11	Ada	22	97													
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Sheet1 Sheet2 Sheet3

Ready 100%

cluster - Excel

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Model Data Data Analysis Time Series Data Mining Tools License Help

Name

	A	B	C	D	E	F	G	H	I	J	K	L	M	N	O	P
1	Name	Computer	History													
2	Raymond	100	40													
3	Louis	90	45													
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K-Means Clustering

Hierarchical Clustering

	A	B	C	G	H	I	J	K	L	M	N	O	P
1	Name	Computer	History										
2	Raymond	100	40										
3	Louis	90	45										
4	Wyman	20	95										
5	Cheng	95	43										
6	Peter	89	42										
7	Paul	85	41										
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11	Ada	22	97										
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19													
20													

Sheet1 Sheet2 Sheet3

Ready

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cluster - Excel

k-Means Clustering

Data source

Worksheet

Workbook

Worksheet

Data range

Data Source

Worksheet: Sheet1

Workbook: cluster.xlsx

Data range: \$A\$13

#Rows: 1

#Cols: 1

Variables

☐ First Row Contains Headers

Variables In Input Data

Var1

Selected Variables

Help Cancel < Back Next > Finish

	A	B	C	D	E	F
1	Name	Computer	History			
2	Raymond	100	40			
3	Louis	90	45			
4	Wyman	20	95			
5	Cheng	95	43			
6	Peter	89	42			
7	Paul	85	41			
8	Mary	20	99			
9	Sam	25	94			
10	Susan	23	93			
11	Ada	22	97			
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Sheet1 Sheet2 Sheet3

Ready

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k-Means Clustering - Step 1 of 3

Data Source

Worksheet: Sheet1 Workbook: cluster.xlsx

Data range: \$A\$13 #Rows: 1 #Cols: 1

Variables

☐ First Row Contains Headers

Variables In Input Data

Var1

Select Data Range

Range: \$A\$1:\$C\$11

OK Cancel

Help Cancel < Back Next > Finish

	A	B	C	D	E	F
1	Name	Computer	History			
2	Raymond	100	40			
3	Louis	90	45			
4	Wyman	20	95			
5	Cheng	95	43			
6	Peter	89	42			
7	Paul	85	41			
8	Mary	20	99			
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11	Ada	22	97			
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Sheet1 Sheet2 Sheet3

Point

cluster - Excel

k-Means Clustering - Step 1 of 3

Rows : 10

Cols: 3

3

Variables

First row contains headers

Variables In Input Data

Selected Variables

Name
Computer
History

Name
Computer
History

Help Cancel Finish

The list of variables in the input data range. You can select them as input or output variables using the arrow buttons.

Name	Computer	History
Raymond	100	40
Louis	90	45
Wyman	20	95
Cheng	85	42
Peter	20	99
Paul	25	94
Susan	23	93
Ada	22	97

Sheet1 Sheet2 Sheet3

Ready

cluster - Excel

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k-Means Clustering - Step 1 of 3

Data Source

Worksheet: Sheet1 Workbook: cluster.xlsx

Data range: \$A\$1:\$C\$11 #Rows: 10 #Cols: 3

Variables

☒ First Row Contains Headers

Variables In Input Data

Name

History

Selected Variables

Computer

Help Cancel < Back Next > Finish

Adds or removes the selected variable(s) from the variables list.

	A	B	C	D	E	F
1	Name	Computer	History			
2	Raymond	100	40			
3	Louis	90	45			
4	Wyman	20	95			
5	Cheng	95	43			
6	Peter	89	42			
7	Paul	85	41			
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11	Ada	22	97			
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Sheet1 Sheet2 Sheet3

Ready

cluster - Excel

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k-Means Clustering - Step 1 of 3

Data Source

Worksheet: Sheet1 Workbook: cluster.xlsx

Data range: \$A\$1:\$C\$11 #Rows: 10 #Cols: 3

Variables

☒ First Row Contains Headers

Variables In Input Data		Selected Variables
Name		Computer
History		

Help Cancel < Back Next > Finish

The list of variables in the input data range. You can select them as input or output variables using the arrow buttons.

Ready

Sheet1 Sheet2 Sheet3

	A	B	C	D	E	F
1	Name	Computer	History			
2	Raymond	100	40			
3	Louis	90	45			
4	Wyman	20	95			
5	Cheng	95	43			
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11	Ada	22	97			
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cluster - Excel

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k-Means Clustering - Step 1 of 3

Data Source

Worksheet: Sheet1 Workbook: cluster.xlsx

Data range: \$A\$1:\$C\$11 #Rows: 10 #Cols: 3

Variables

☒ First Row Contains Headers

Variables In Input Data		Selected Variables	
Name			
		Computer	
		History	

>

Help Cancel < Back Next > Finish

Adds or removes the selected variable(s) from the variables list.

Ready

Sheet1 Sheet2 Sheet3

	A	B	C	D	E	F
1	Name	Computer	History			
2	Raymond	100	40			
3	Louis	90	45			
4	Wyman	20	95			
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6	Peter	89	42			
7	Paul	85	41			
8	Mary	20	99			
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10	Susan	23	93			
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cluster - Excel

k-Means Clustering Step 2 of 3

Normalize input data

Parameters

Clusters: 2

Iterations: 10

Options

Centroid Initialization

12345

Help Cancel < Back Next > Finish

Move to the next step.

Clusters:

2

Iterations:

10

	A	B	C	D	E	F
1	Name	Computer	History			
2	Raymond	100	40			
3	Louis	90	45			
4	Wyman	20	95			
5	Cheng	95	43			
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Sheet1 Sheet2 Sheet3

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k-Means Clustering - Step 2 of 3

Options

Fixed Start

Random Starts

Set Seed

No. of Starts:

12345

Help Cancel < Back Next > Finish

The random seed that will be used to generate starting points.

	A	B	C
1	Name	Computer	
2	Raymond	100	
3	Louis	90	
4	Wyman	20	95
5	Cheng	95	43
6	Peter	89	42
7	Paul	85	41
8	Mary	20	99
9	Sam	25	94
10	Susan	23	93
11	Ada	22	97
12			
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20			

Sheet1 Sheet2 Sheet3

Ready

The screenshot displays the Excel interface with a k-Means Clustering dialog box open. The dialog box is titled "k-Means Clustering - Step 3 of 3". Under the "Output Options" section, two options are checked: "Show data summary" and "Show distances from each cluster center". A callout points to "Show data summary" with the text "Show data summary". Another callout points to "Show distances from each cluster center" with the text "Show distances from each cluster center". At the bottom of the dialog box, the "Finish" button is highlighted with a yellow dashed circle. Below the buttons, a text box says "Runs the method using the currently selected options." The background spreadsheet shows a table with columns A, B, and C. Column A is labeled "Name" and column B is labeled "Computer History". The data rows are as follows:

Name	Computer History
Raymond	100
Louis	90
Wyman	20
Cheng	95
Peter	89
Paul	85
Mary	20
Sam	25
Susan	23
Ada	22

cluster - Excel

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E92

Inputs

Data	
Workbook	cluster.xlsx
Worksheet	Sheet1
Range	\$A\$1:\$C\$11
# records in the input data	10

Variables	
# Selected Variables	2
Selected Variables	Computer History

K-Means Clustering: Fitting Parameters	
# Clusters	2
Start type	Random Start
# Iterations	10
Random seed: initial centroids	12345

K-Means Clustering: Reporting Parameters	
Show data summary	TRUE
Show distance from each cluster	TRUE
Normalized?	FALSE

Random Starts Summary

Sheet1 KMC_Output KMC_Clusters Sheet2 Sheet3 ...

Ready

100%

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9101112131415161718192021222324252627282930313233

Data

Workbook	cluster.xlsx
Worksheet	Sheet1
Range	\$A\$1:\$C\$11
# Records in the input data	10

Variables

# Selected Variables	2
Selected Variables	ComputerHistory

K-Means Clustering: Fitting Parameters

# Clusters	2
Start type	Random Start
# Iterations	10
Random seed: initial centroids	12345

K-Means Clustering: Reporting Parameters

Show data summary	TRUE
Show distance from each cluster	TRUE
Normalized?	FALSE

Random Starts Summary

Sheet1KMC_OutputKMC_ClustersSheet2Sheet3...100%

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Inputs

Data	
Workbook	cluster.xlsx
Worksheet	Sheet1
Range	\$A\$1:\$C\$11
# Records in the input data	10

Variables	
# Selected Variables	2
Selected Variables	Computer History

K-Means Clustering: Fitting Parameters	
# Clusters	2
Start type	Random Start
# Iterations	10
Random seed: initial centroids	12345

K-Means Clustering: Reporting Parameters	
Show data summary	TRUE
Show distance from each cluster	TRUE
Normalized?	FALSE

Random Starts Summary

Sheet1 KMC_Output KMC_Clusters Sheet2 Sheet3 ...

Ready

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9101112131415161718192021222324252627282930313233

Inputs

Data	
Workbook	cluster.xlsx
Worksheet	Sheet1
Range	\$A\$1:\$C\$11
# Records in the input data	10

Variables

# Selected Variables	2	
Selected Variables	Computer	History

Start type	Random Start
# Iterations	10
Random seed: initial centroids	12345

K-Means Clustering: Reporting Parameters

Show data summary	TRUE
Show distance from each cluster	TRUE
Normalized?	FALSE

Random Starts Summary

Sheet1KMC_OutputKMC_ClustersSheet2Sheet3

Ready

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Data	
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Worksheet	Sheet1
Range	\$A\$1:\$C\$11
# Records in the input data	10

Variables	
# Selected Variables	2
Selected Variables	Computer History

K-Means Clustering: Fitting Parameters	
# Clusters	2
Start type	Random Start
# Iterations	10
Random seed: initial centroids	12345

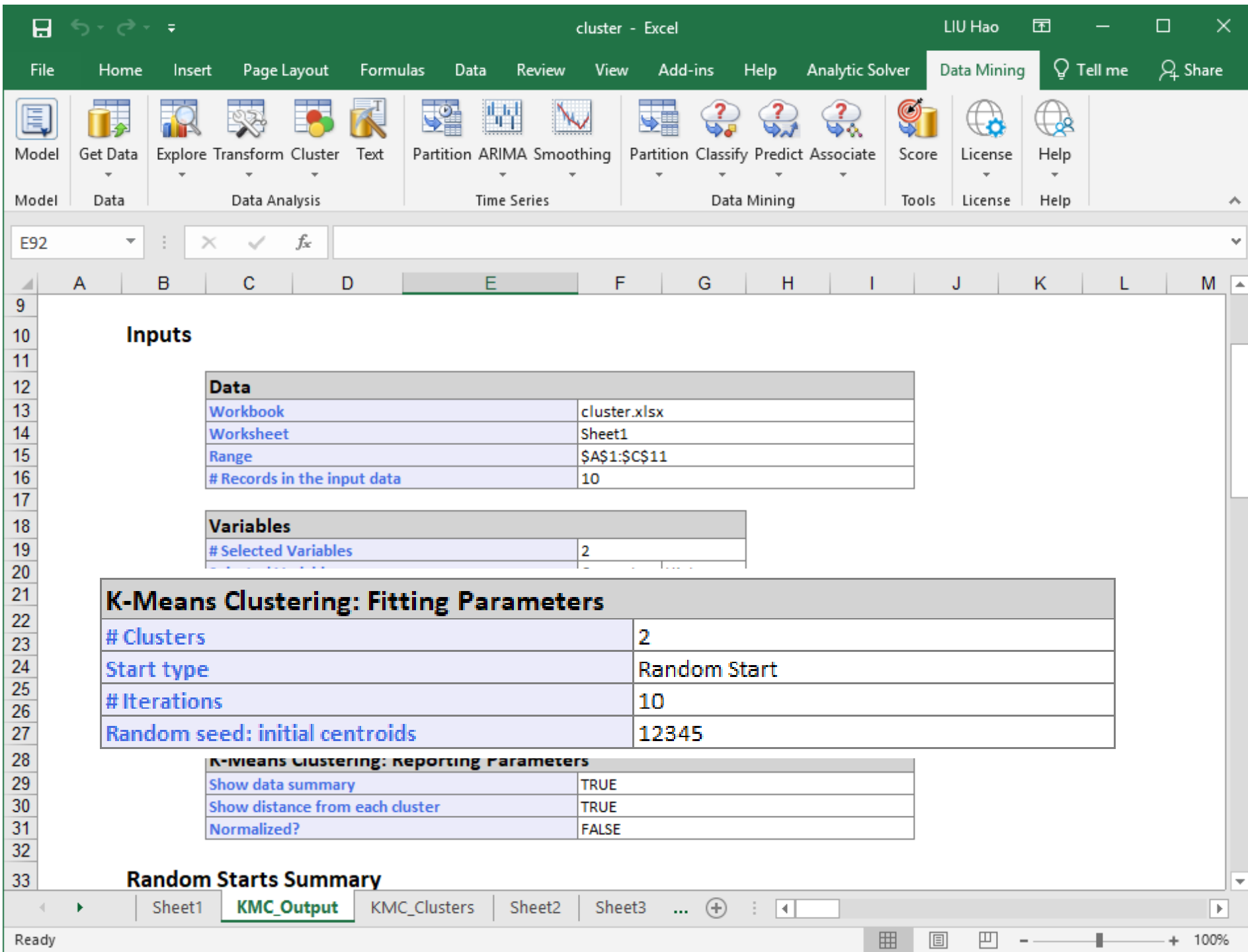
K-Means Clustering: Reporting Parameters	
Show data summary	TRUE
Show distance from each cluster	TRUE
Normalized?	FALSE

Random Starts Summary

Sheet1 KMC_Output KMC_Clusters Sheet2 Sheet3 ...

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Inputs

Data	
Workbook	cluster.xlsx
Worksheet	Sheet1
Range	\$A\$1:\$C\$11
# Records in the input data	10

Variables	
# Selected Variables	2
Selected Variables	Computer History

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Start type	Random Start
# Iterations	10
Random seed: initial centroids	12345

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Random Starts Summary

Sheet1 KMC_Output KMC_Clusters Sheet2 Sheet3 ...

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Inputs

Data	
Workbook	cluster.xlsx
Worksheet	Sheet1
Range	\$A\$1:\$C\$11
# Records in the input data	10

Variables	
# Selected Variables	2
Selected Variables	Computer History

K-Means Clustering: Fitting Parameters	
# Clusters	2
Start type	Random Start
# Iterations	10
Random seed: initial centroids	12345

K-Means Clustering: Reporting Parameters	
Show data summary	TRUE
Show distance from each cluster	TRUE
Normalized?	FALSE

Sheet1 KMC_Output KMC_Clusters Sheet2 Sheet3 ...

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9101112131415161718192021222324252627282930313233

Inputs

Data

Workbook

cluster.xlsx

Worksheet

Sheet1

Range

\$A\$1:\$C\$11

Records in the input data

10

Variables

Selected Variables

2

Selected Variables

ComputerHistory

K-Means Clustering: Fitting Parameters

Clusters

2

Start type

Random Start

Iterations

10

Random seed: initial centroids

12345

K-Means Clustering: Reporting Parameters

Show data summary

TRUE

Show distance from each cluster

TRUE

Normalized?

FALSE

Random Starts Summary

Sheet1KMC_OutputKMC_ClustersSheet2Sheet3

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Random Starts Summary

Start 1. Sum of Squares: 37040.000000

Cluster	Computer	History
Cluster 1	89	42
Cluster 2	89	42

Start 2. Sum of Squares: 35180.000000

Cluster	Computer	History
Cluster 1	85	41
Cluster 2	85	41

Start 3. Sum of Squares: 468.000000

Cluster	Computer	History
Cluster 1	23	93
Cluster 2	85	41

Start 4. Sum of Squares: 303.000000

Cluster	Computer	History
Cluster 1	25	94
Cluster 2	95	43

Best: Start 5. Sum of Squares: 252.000000

Cluster	Computer	History
Cluster 1	20	95
Cluster 2	89	42

Sheet1 KMC_Output KMC_Clusters Sheet2 Sheet3

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Model Data

Start 1. Sum of Squares: 37040.000000

Cluster	Computer	History
Cluster 1	89	42
Cluster 2	89	42

Start 2. Sum of Squares: 35180.000000

Cluster	Computer	History
Cluster 1	85	41
Cluster 2	85	41

Start 3. Sum of Squares: 468.000000

Cluster	Computer	History
Cluster 1	23	93
Cluster 2	85	41

Start 4. Sum of Squares: 303.000000

Cluster	Computer	History
Cluster 1	25	94
Cluster 2	95	43

Best: Start 5. Sum of Squares: 252.000000

Cluster	Computer	History
Cluster 1	20	95
Cluster 2	89	42

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Random Starts Summary

Start 1. Sum of Squares: 37040.000000

Cluster	Computer	History
Cluster 1	89	42
Cluster 2	89	42

Start 2. Sum of Squares: 35180.000000

Cluster	Computer	History
Cluster 1	85	41
Cluster 2	85	41

Start 3. Sum of Squares: 468.000000

Cluster	Computer	History
Cluster 1	23	93
Cluster 2	85	41

Start 4. Sum of Squares: 303.000000

Cluster	Computer	History
Cluster 1	25	94
Cluster 2	95	43

Best: Start 5. Sum of Squares: 252.000000

Cluster	Computer	History
Cluster 1	20	95
Cluster 2	89	42

Sheet1 KMC_Output KMC_Clusters Sheet2 Sheet3

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	A	B	C	D	E	F	G	H	I	J	K	L	M
57			Cluster 1	20	95								
58			Cluster 2	89	42								
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60			Cluster Centers										
61													
62			Cluster	Computer	History								
63			Cluster 1	22	95.6								
64			Cluster 2	91.8	42.2								
65													
66			Inter-Cluster Distances										
67													
68			Cluster	Cluster 1	Cluster 2								
69			Cluster 1	0	87.88401447								
70			Cluster 2	87.88401447	0								
71													
72			Cluster Summary										
73													
74			Cluster	Size	Average Distance								
75			Cluster 1	5	2.723671108								
76			Cluster 2	5	4.965869275								
77			Total	10	3.844770192								
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Sheet1 KMC_Output KMC_Clusters Sheet2 Sheet3

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4Cluster CentersInter-Cluster DistanceCluster Summary

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Elapsed Times in Milliseconds

Data Reading Time	Algorithm Time	Report Time	Total
0	10	2	12

Sheet1KMC_OutputKMC_ClustersSheet2Sheet3

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4Cluster CentersInter-Cluster DistanceCluster Summary

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Elapsed Times in Milliseconds

Data Reading Time

algorithm Time

Report Time

Total

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Sheet1KMC_OutputKMC_ClustersSheet2Sheet3

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Cluster Centers

Inter-Cluster Distance

Cluster Summary

Elapsed Times in Milliseconds

Data Reading Time	Algorithm Time	Report Time	Total
0	10	2	12

Sheet1

KMC_Output

KMC_Clusters

Sheet2

Sheet3

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A1

Data Mining: K-Means Clustering - Predicted Clusters

Date: 2023/10/27

Output Navigator

[Cluster Labels](#) [Inputs](#) [Random Starts Summa](#) [Cluster Centers](#) [Inter-Cluster Distance](#) [Cluster Summary](#)

Cluster Labels

Record ID	Cluster	Cluster 1	Cluster 2
Record 1	2	95.7880995	8.48999411
Record 2	2	84.7606041	3.3286634
Record 3	1	2.0880613	89.1239586
Record 4	2	89.9764414	3.2984845
Record 5	2	85.8018648	2.80713377
Record 6	2	83.3676196	6.9050706
Record 7	1	3.94461658	91.5504233
Record 8	1	3.4	84.5309411
Record 9	1	2.78567766	85.5223947
Record 10	1	1.4	88.7416475

Sheet1 KMC_Output **KMC_Clusters** Sheet2 Sheet3

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Model Data Data Analysis Time Series Data Mining

A1

Data Mining: K-Means Clustering - Predicted Clusters

Record 1 corresponds to the first record

Record ID	Cluster	Cluster 1	Cluster 2
Record 1	2	95.7880995	8.48999411
Record 2	2	84.7606041	3.3286634
Record 3	1	2.0880613	89.1239586
Record 4	2	89.9764414	3.2984845
Record 5	2	85.8018648	2.80713377
Record 6	2	83.3676196	6.9050706
Record 7	1	3.94461658	91.5504233
Record 8	1	3.4	84.5309411
Record 9	1	2.78567766	85.5223947
Record 10	1	1.4	88.7416475

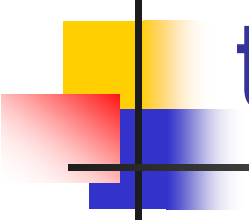
Name	Computer	History
Raymond	100	40
Louis	90	45
Wyman	20	95
Cheng	95	43
Peter	89	42
Paul	85	41
Mary	20	99
Sam	25	94
Susan	23	93
Ada	22	97

Sheet1 KMC_Output KMC_Clusters Sheet2 Sheet3

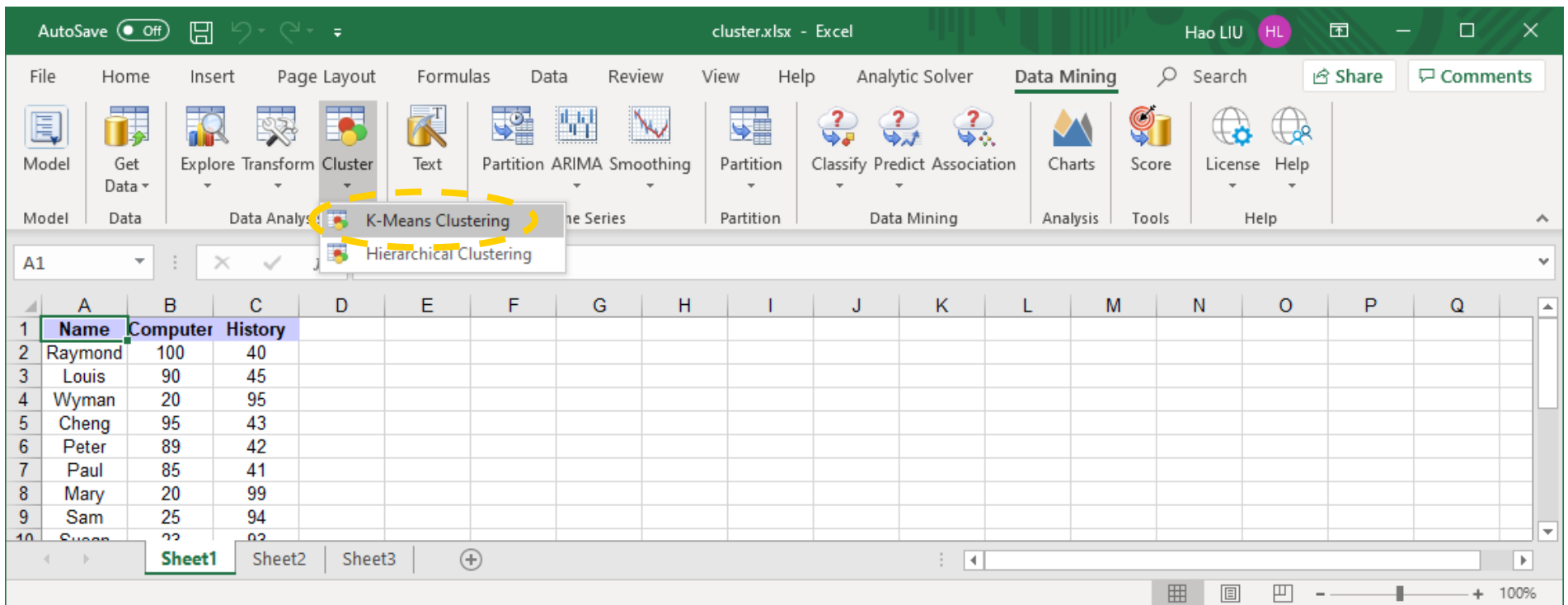
Ready

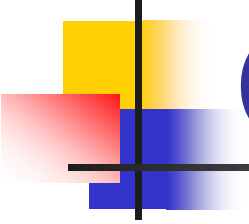
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How to use the data mining tool

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

- “Data Mining” Tag → Cluster → K-Means Clustering





How to use the data mining tool (XLMiner Cloud)

- The steps of performing “k-means clustering” in XLMiner Cloud is similar to the steps in XLMiner Desktop.
- The output format and the clustering result of XLMiner Cloud are the same as that from XLMiner Desktop.