데이터 마이닝 특강
Practice session

[Clustering]

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Clustering

Introduction review

- **Datamining applications**
- **Datamining tool installation**
  - Orange3
  - Anaconda
  - Pycharm
- **Practice lecture resources**
  - https://github.com/junseokpark/resources/datamining
- **Cloud datamining tools**
  - Cloudera data science workbench
    - https://www.cloudera.com/products/data-science-and-engineering/data-science-workbench.html
  - Amazon machine learning (ML)
    - https://aws.amazon.com/ko/machine-learning/
  - Google cloud AI
    - https://cloud.google.com/products/ai/
  - Databricks unified analytic platform
    - https://databricks.com/product/unified-analytics-platform

Overview

- **Concept of Clustering**

- **Practice of Clustering algorithms on toy data**
  - k-mean
  - Hierarchical-culstering
  - Self Organizing Map

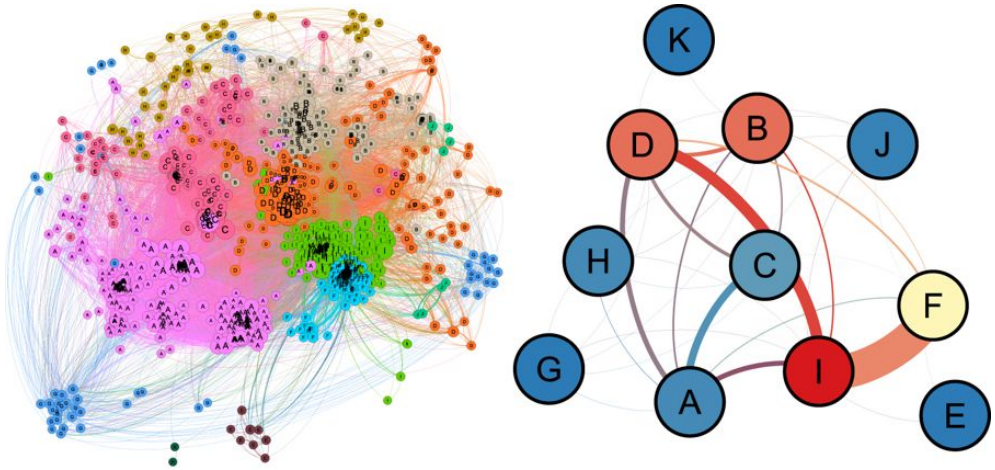
- **Practice of Clustering algorithms on realworld data**
  - Data introduction
  - Data preprocessing
  - k-mean
  - Hierarchical-clustering

Introduction

- **Cluster: a collection of data objects**
  - Similar (or related) to one another within the same group
  - Dissimilar (or unrelated) to the objects in other groups

- **Cluster analysis (or clustering, data segmentation, …)**
  - Finding similarities between data according to the characteristics found in the data and grouping similar data objects into clusters

- **Example[1]**



(a) Effect-Size network (b) Induced network

[1] Valenzuela JF, Monterola C, Tong VJC, Ng TP, Larbi A, 2017. Health and disease phenotyping in old age using a cluster network analysis. *Scientific Reports 7, 1 (2017/11/15), 15608. DOI= http://dx.doi.org/10.1038/s41598-017-15753-3.*

Considerations for Cluster Analysis

- **Partitioning criteria**
  - Single level vs. hierarchical partitioning (often, multi-level hierarchical partitioning is desirable)
- **Separation of clusters**
  - Exclusive (e.g., one customer belongs to only one region) vs. non-exclusive (e.g., one document may belong to more than one class)
- **Similarity measure**
  - Distance-based (e.g., Euclidian, road network, vector) vs. connectivity-based (e.g., density or contiguity)
- **Clustering space**
  - Full space (often when low dimensional) vs. subspaces (often in high-dimensional clustering)

k-Means Clustering

1. Arbitrarily choose *k* objects from D as the initial cluster centers
2. (Re)assign each object to the cluster to which the object is the most similar, based on the mean value of the objects in the cluster
3. Update the cluster means, i.e., calculate the mean value of the objects for each cluster
4. Repeat 2~3 until the criterion function converges

Evaluation Criterion

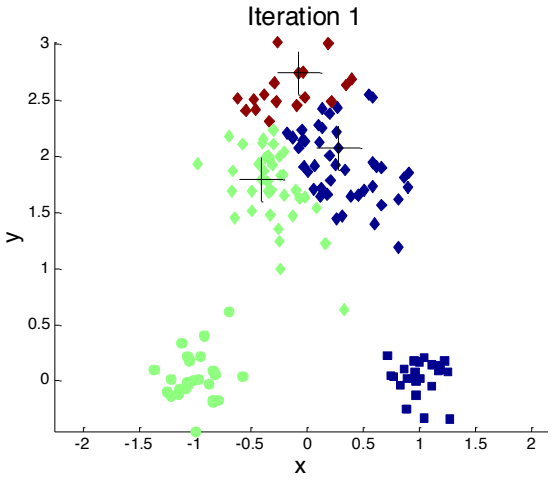
- **The algorithm attempts to determine *k* partitions that minimizes the sum of the square error**

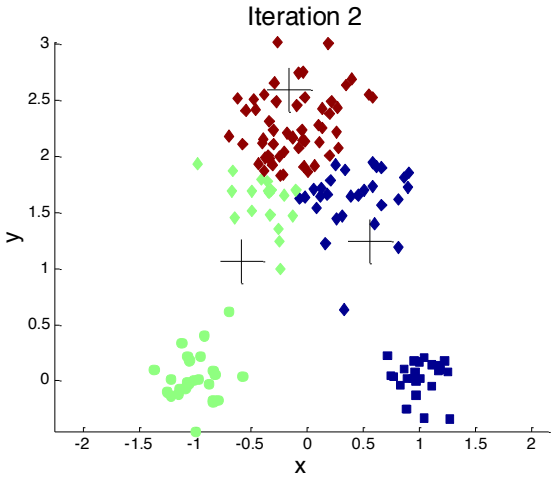
  - p: a point in a cluster C_i
  - m_i: the mean of a cluster C_i

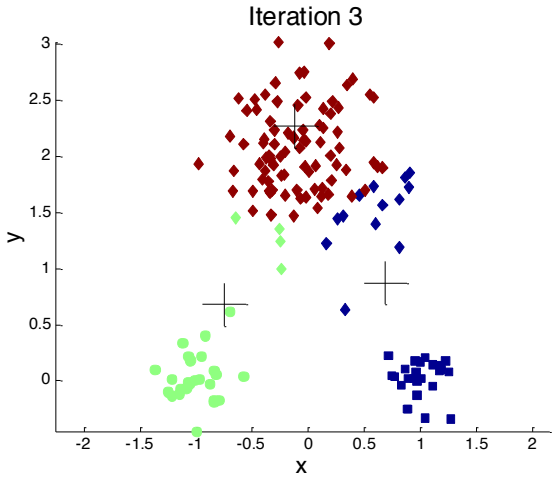
$$SSE = \sum_{i=1}^{k} \sum_{p \in C_i} dist^2(m_i, p)$$

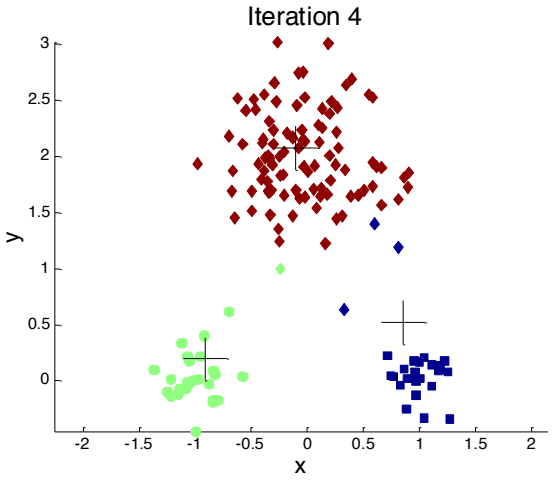
- **This criterion tries to make the resulting *k* clusters as compact as and as separate as possible**

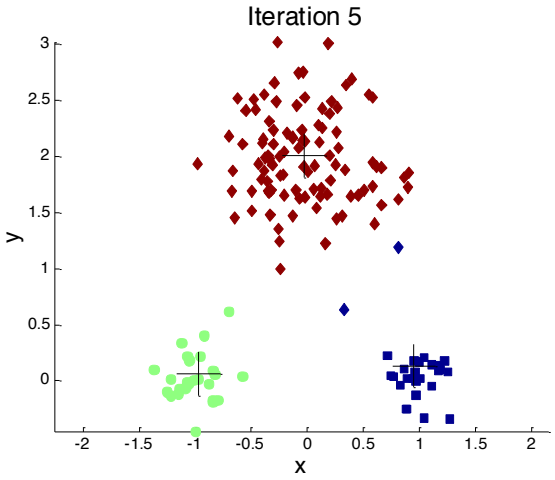
Example of K-Means

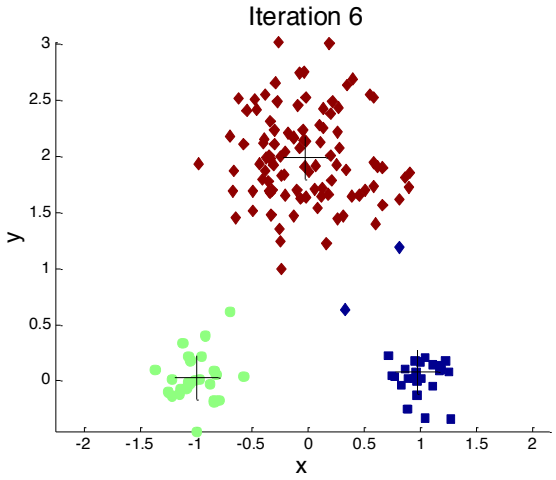




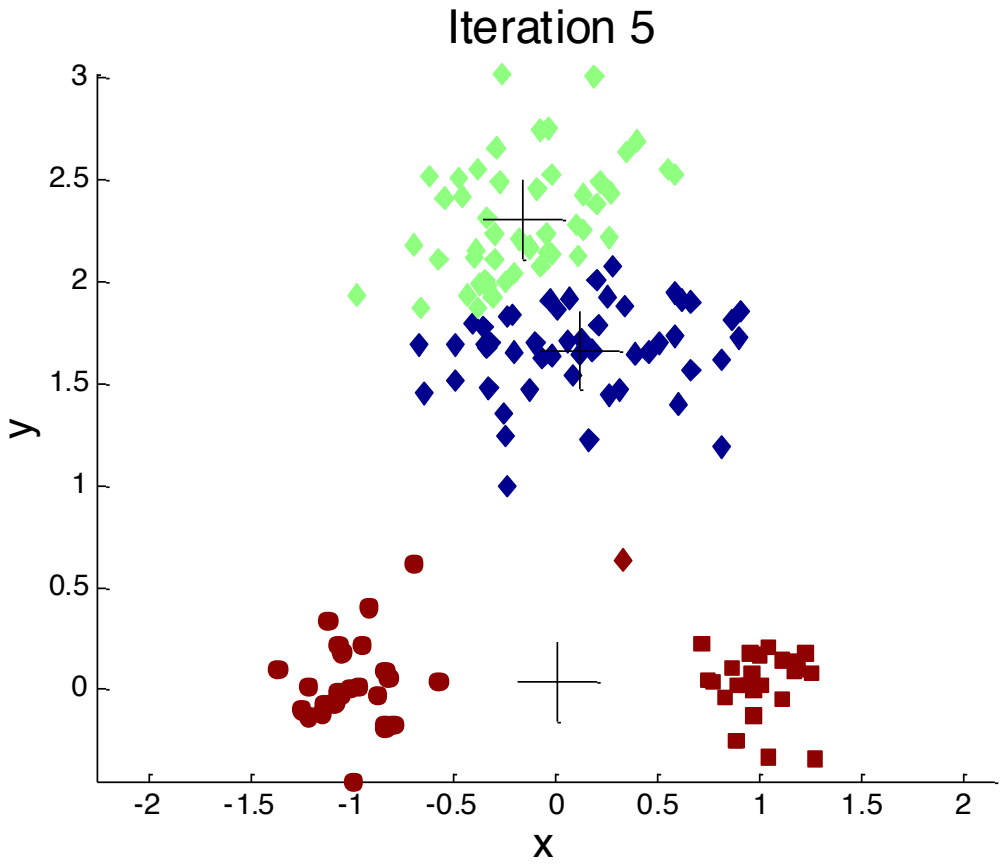








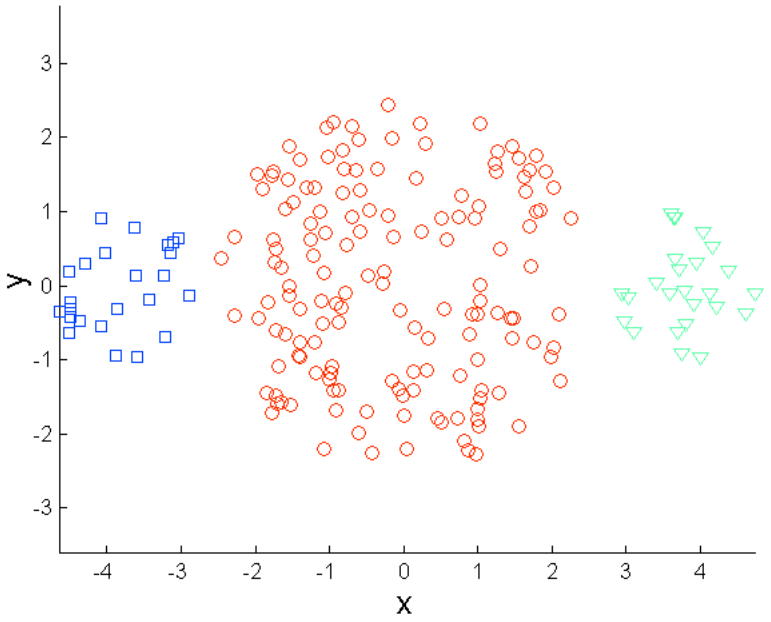
Effects of Choosing Initial Centroids



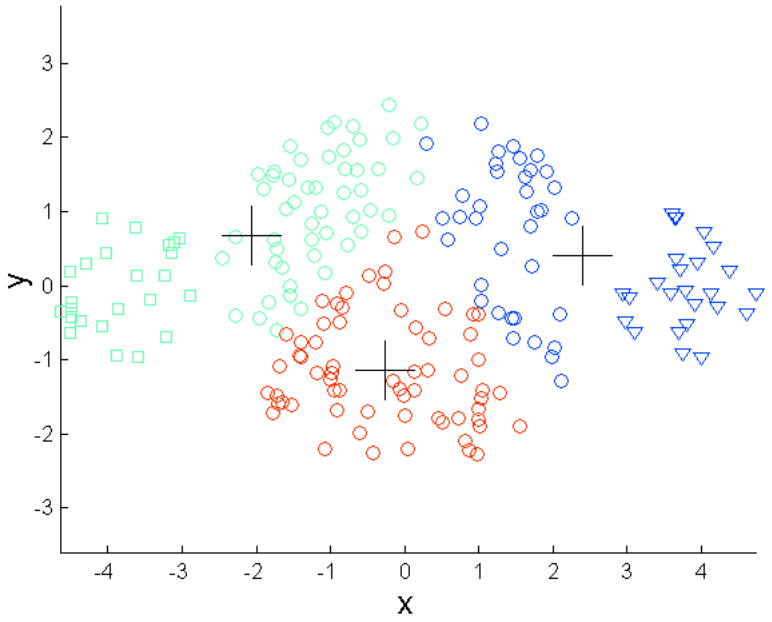
Remarks

- **Strength: efficient**
  - O(*tkn*), where *n* is # of objects, *k* is # of clusters, and *t* is # of iterations; usually, *k*, *t* << *n*
- **Comment: often terminates at a local optimal**
- **Limitations**
  - Applicable only to objects in a continuous space
  - Need to specify *k*, the number of clusters, in advance
  - Not suitable to discover clusters with non-convex shapes or clusters of very different sizes or density
  - Sensitive to noisy data and outliers

Limitations of k-Means: Different Sizes

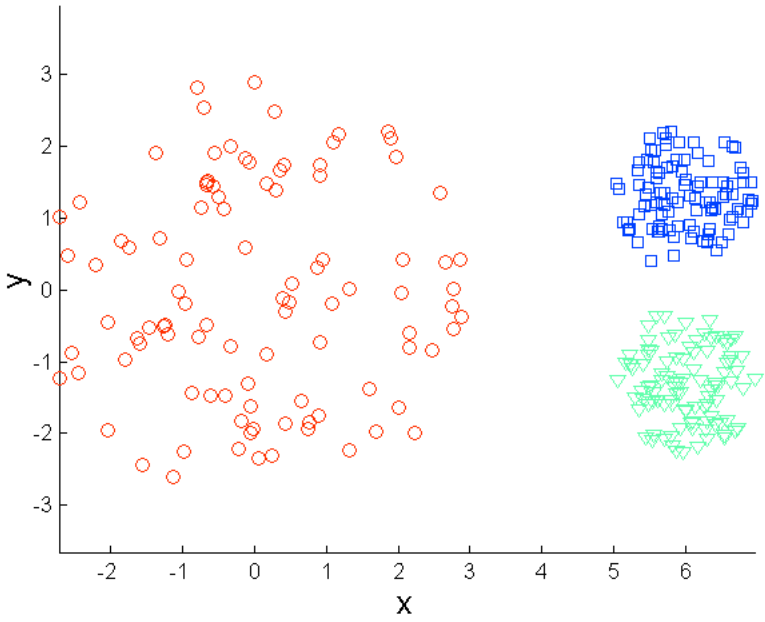


Original Points

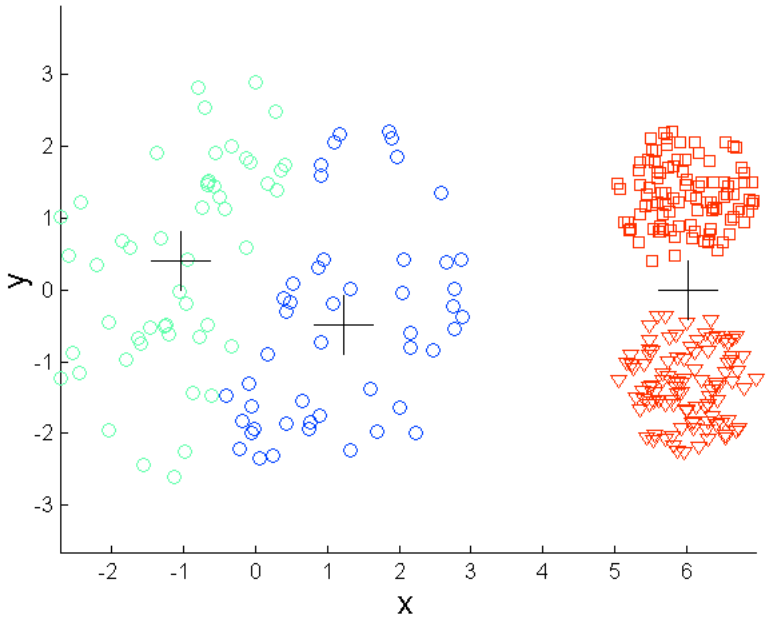


K-means (3 Clusters)

Limitations of k-Means: Different Density

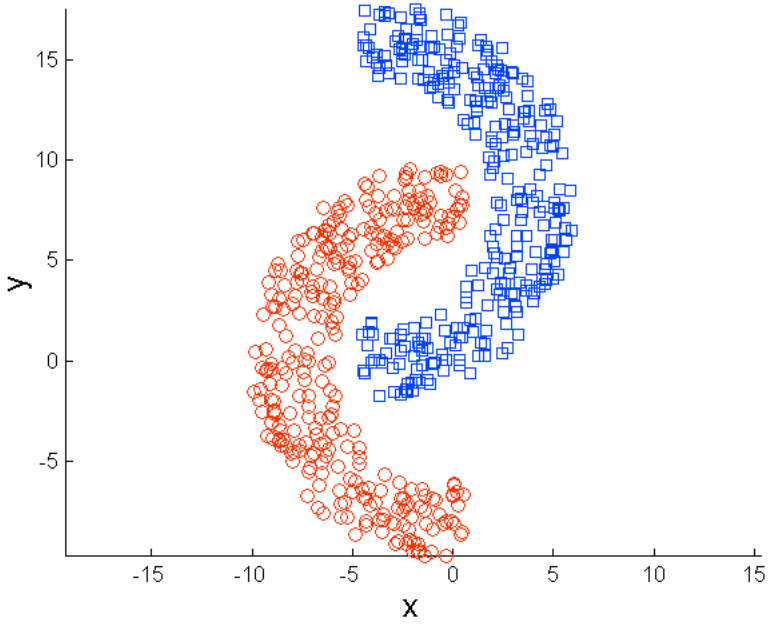


Original Points

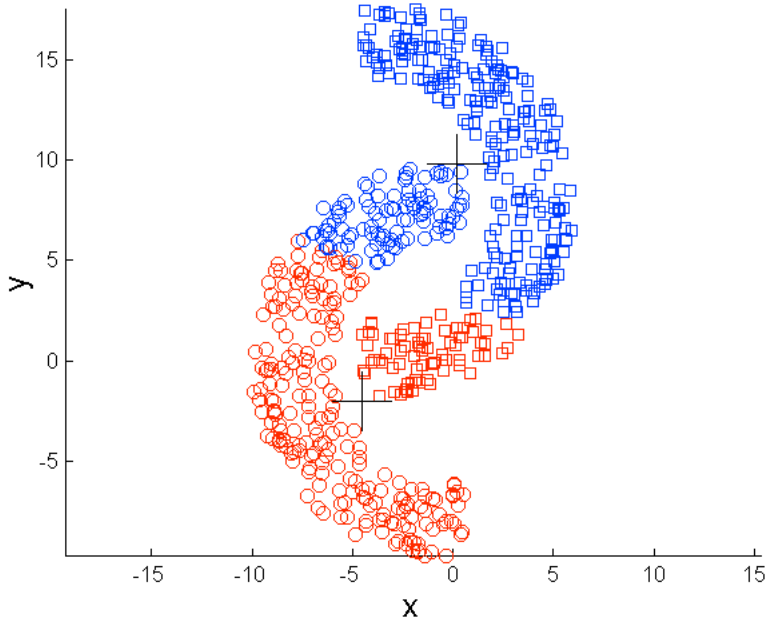


K-means (3 Clusters)

Limitations of k-Means: Non-Convex Shapes



Original Points



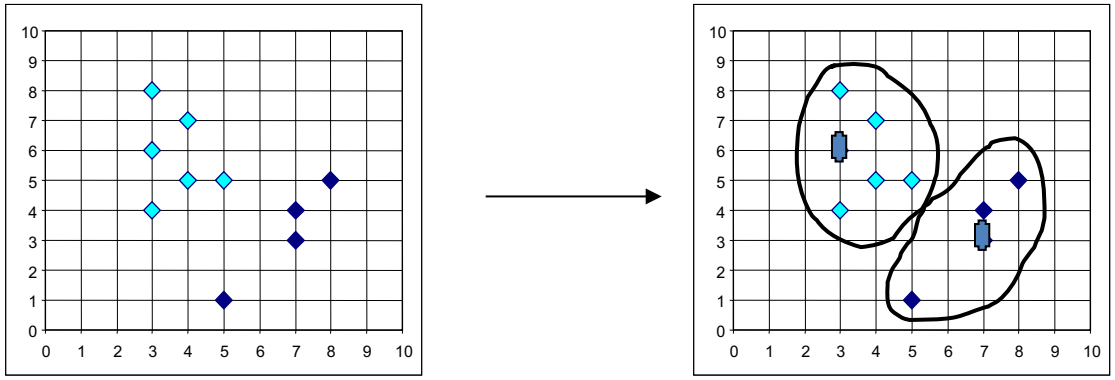
K-means (2 Clusters)

Problem of the k-Means Method

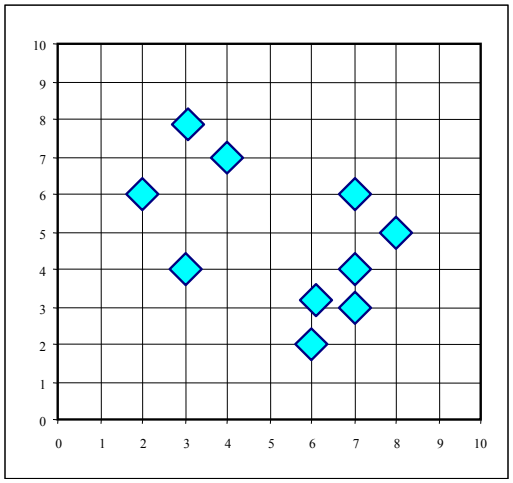
- **Sensitive to outliers**
  - Since an object with an extremely large value may substantially distort the distribution of the data

⇒ **A solution: k-Medoids**

- Instead of taking the **mean** value of the objects in a cluster as a reference point, **medoids** can be used
  - Medoid: the most centrally located **object** in a cluster

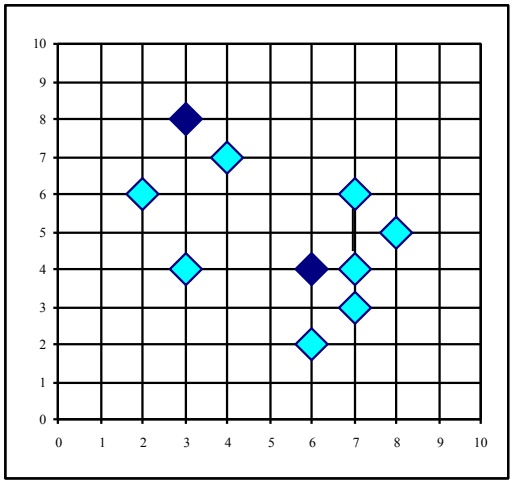


PAM: A Typical k-Medoids Algorithm

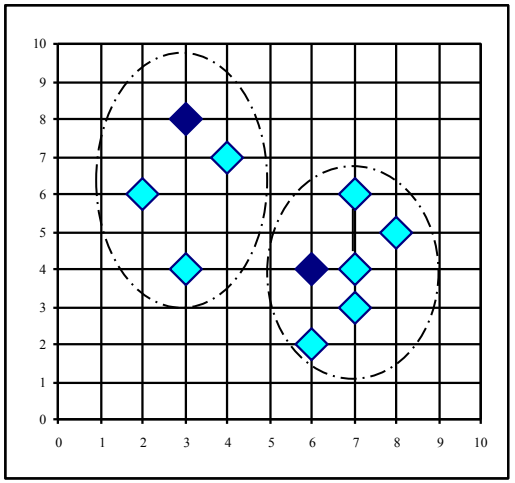


k=2

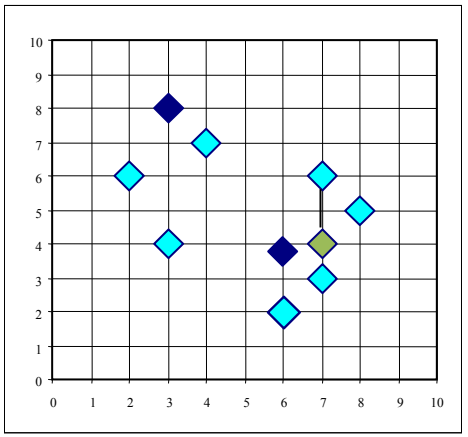
Arbitrary choose k objects as initial medoids



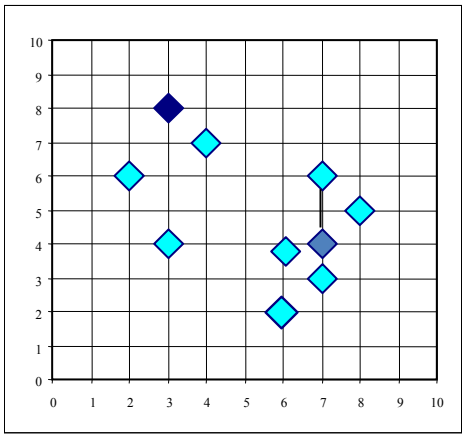
Assign each remaining object to nearest medoids



Randomly select a nonmedoid object, O_{ramdom}



Compute total cost of swapping



Swapping O and O_{ramdom} if quality is improved

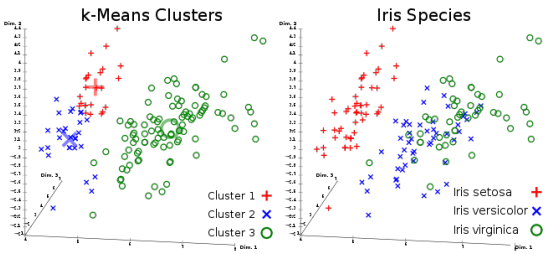
Do loop until no change

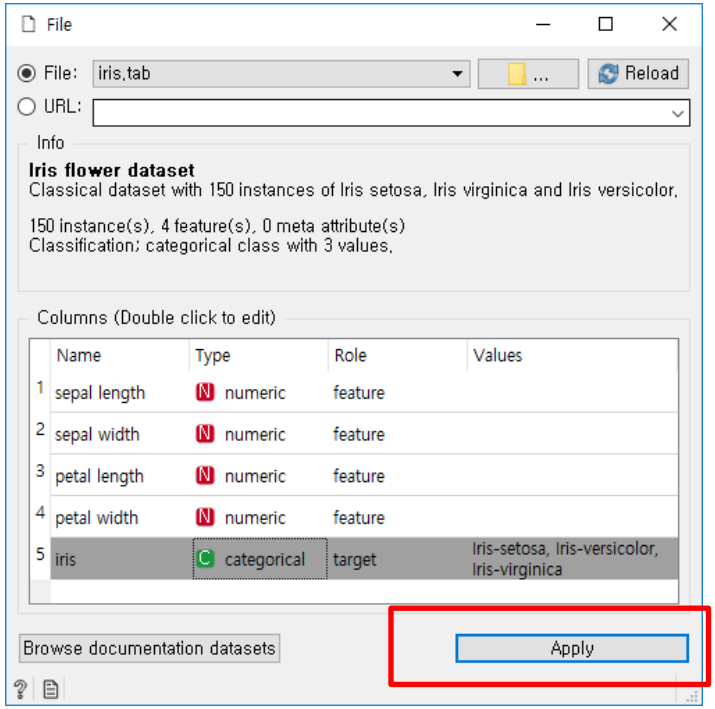
k-Medoids Clustering Method

- ***k*-Medoids clustering: find representative objects (medoids) in clusters**
  - PAM (Partitioning Around Medoids, Kaufmann & Rousseeuw 1987): starts from an initial set of medoids and iteratively replaces one of the medoids by one of the non-medoids if it improves the total distance of the resulting clustering
- **PAM works effectively for small data sets, but does not scale well for large data sets (due to the computational complexity)**
- **Efficiency improvement on PAM**
  - CLARA (Kaufmann & Rousseeuw, 1990): PAM on samples
  - CLARANS (Ng & Han, 1994): randomized re-sampling

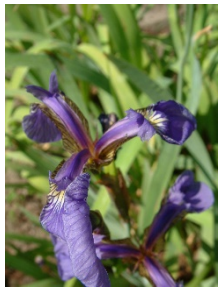
Dataset

- **iris flower data set**
  - multivariate data set
  - introduced by Ronald Fisher in 1936
    - Statistician and Biologist





  - the data to quantify the morphologic variation of *Iris* flowers of three related species



Iris setosa

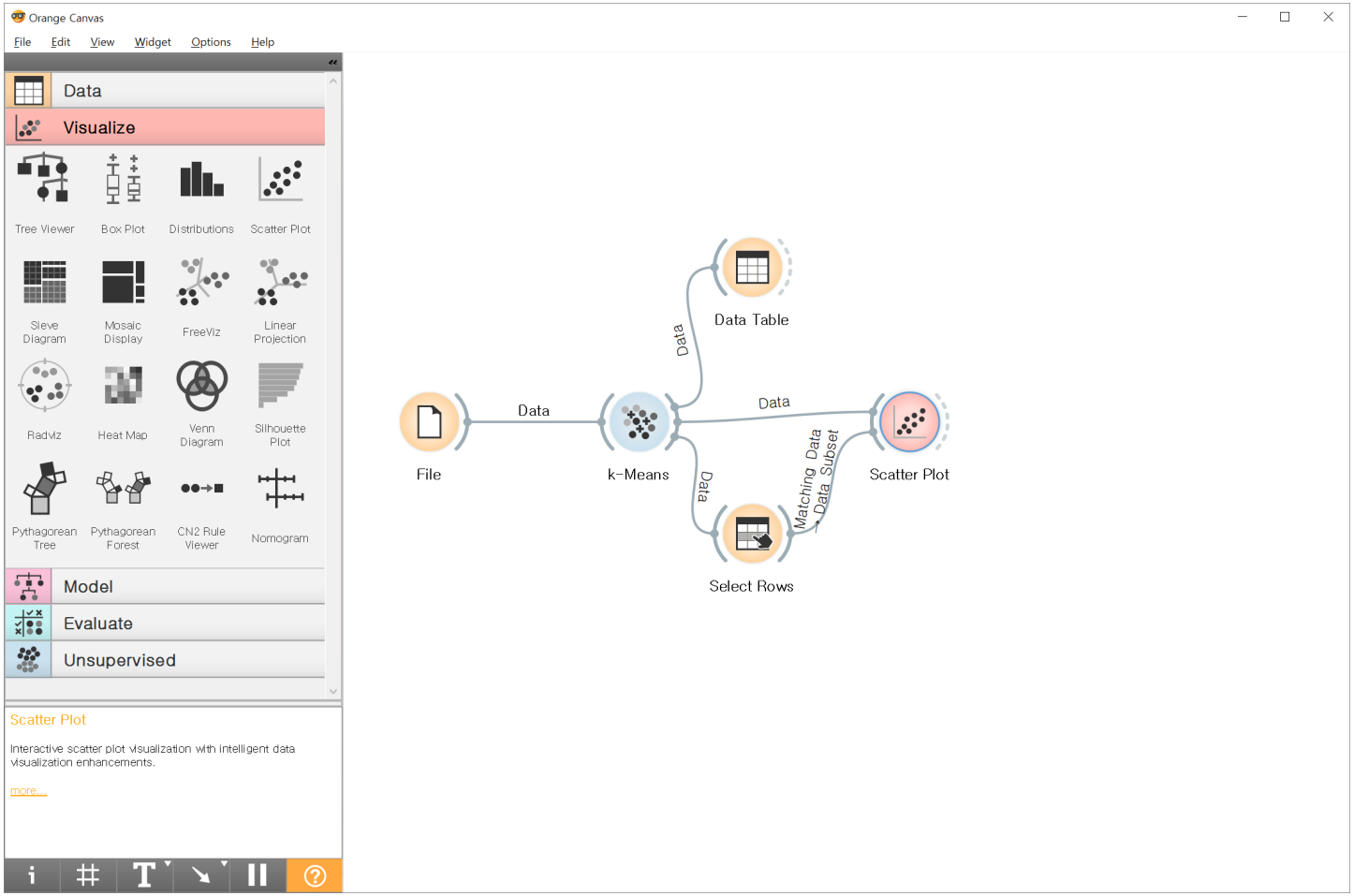
Iris veriscolor

Iris virginica

ref : https://en.wikipedia.org/wiki/Iris_flower_data_set

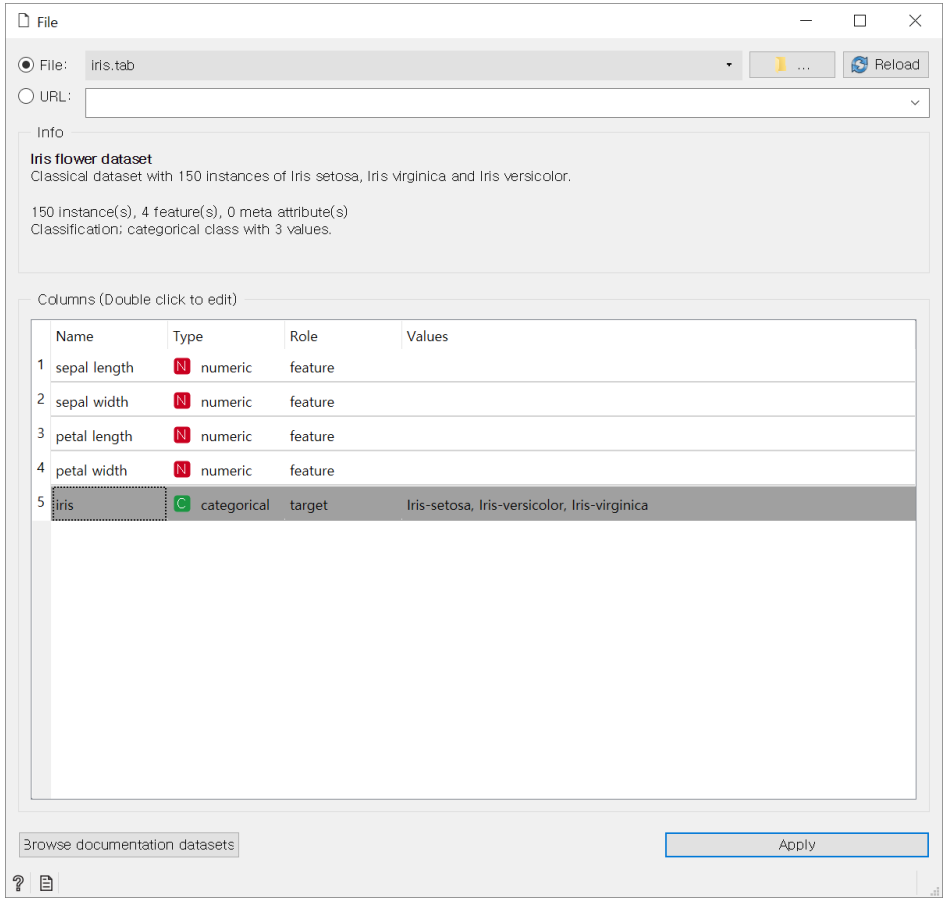
k-means (Cont'd)

- **Build schema**



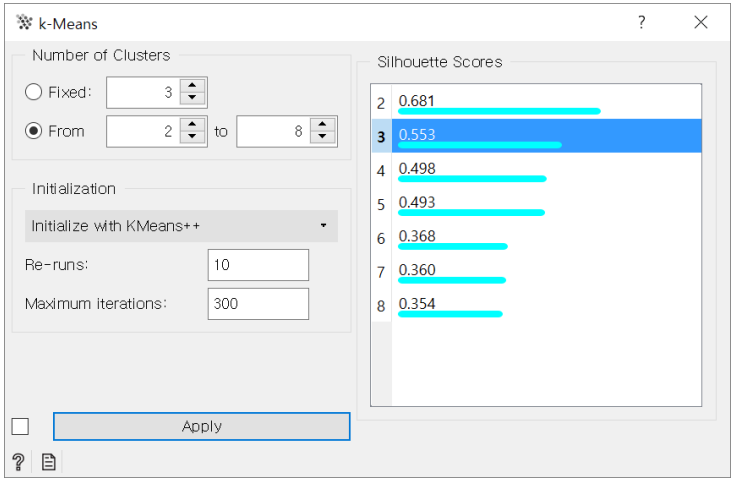
k-means (Cont'd)

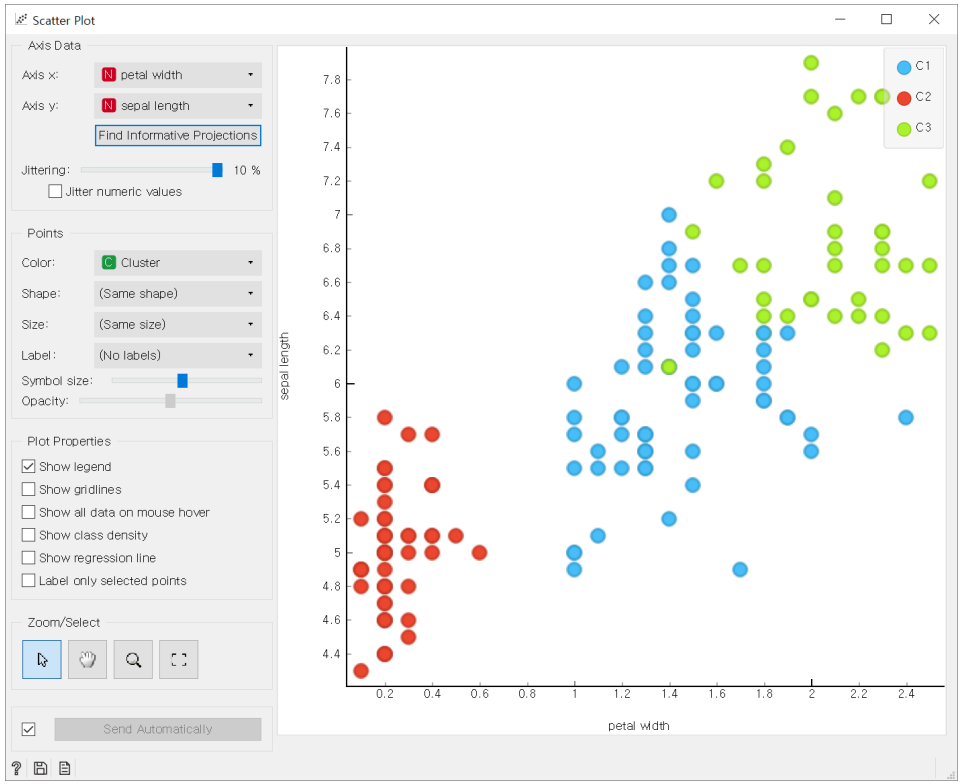
- **Load data**
  - Iris dataset into three clusters



k-means (Cont'd)

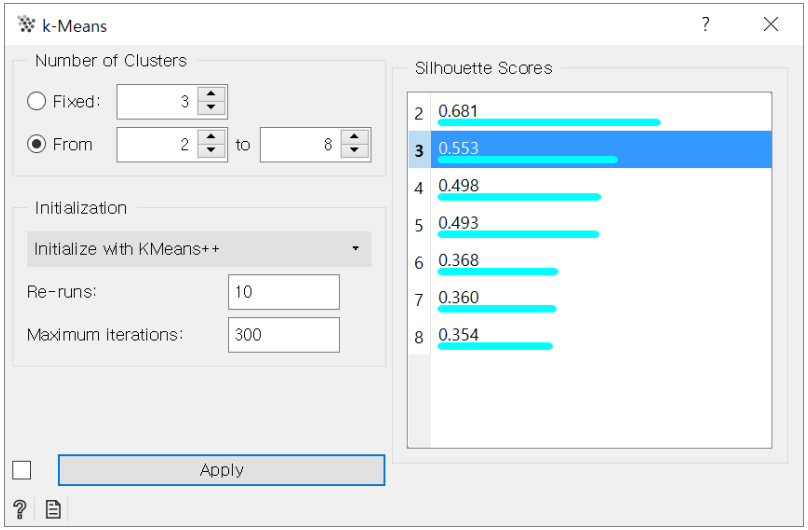
- **Observation of k-means**
  - k-means added the cluster index as a class attribute
  - the scatter plot will color the points according to the clusters they are in





k-means (Cont'd)

- **Hyperparameters and configuration**
  - Fixed : algorithm clusters data in a specified number of clusters.
  - From : widget shows clustering scores for the selected cluster range
  - Silhouette scores : contrasts average distance to elements in the same cluster with the average distance to elements in other clusters
  - initialization
    - Kmeans++ : first center is selected randomly, subsequent are chosen from the remaining points with probability proportioned to squared distance from the closest center
    - Random : clusters are assigned randomly at first and then updated with further iterations
  - Re-runs : how many times the algorithm is run
  - Maximum iterations : the maximum number of iteration within each algorithm run



K-means (Cont'd)

- **Silhouette scores**
  - a method of interpretation and validation of consistency within clusters of data[1]
  - a succinct graphical representation of how well each object lies within its cluster[2]
- **Silhouette value**
  - a measure of how similar an object is to its own cluster (cohesion) compared to other cluster s (separation)
  - ranges from −1 to +1
- **Calculation methods**
  - Euclidian distance
  - Manhattan distance[3]
- **Definition**

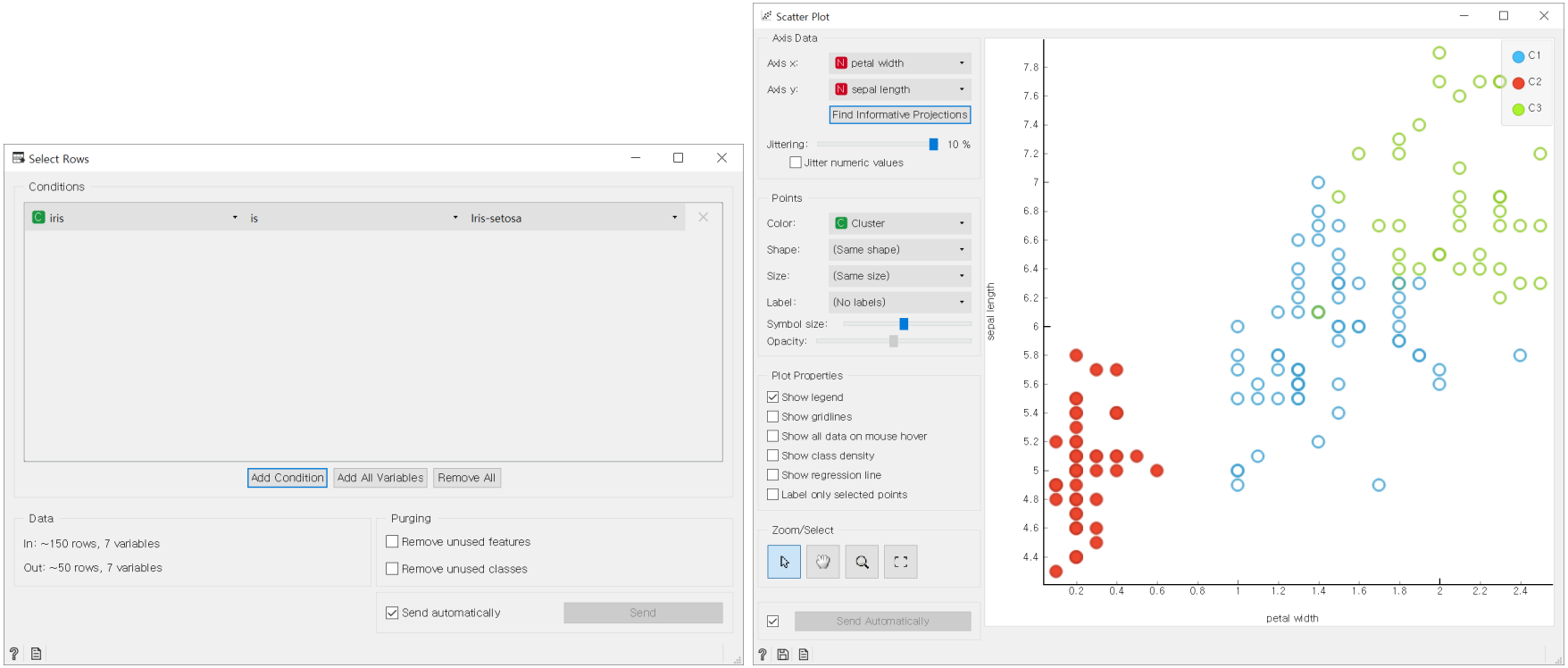
a(i) be the average distance between *i* and all other data within the same cluster.
b(i) be the highest average distance of *i* to all points in any other cluster

- $s(i) = \frac{b(i)-a(i)}{\max\{a(i),b(i)\}}$, which can be also written as $s(i) = \begin{cases} 1 - a(i)/b(i) & if\ a(i) < b(i) \\ 0 & if\ a(i) = b(i) \\ b(i)/a(i) - 1 & if\ a(i) > b(i) \end{cases}$
- $-1 \leq s(i) \leq 1$

[1] https://en.wikipedia.org/wiki/Silhouette_(clustering)
[2] Peter J. Rousseeuw (1987). "Silhouettes: a Graphical Aid to the Interpretation and Validation of Cluster Analysis". *Computational and Applied Mathematics*. **20**: 53–65 . doi:10.1016/0377-0427(87)90125-7.
[3] Paul E. Black, "Manhattan distance", in *Dictionary of Algorithms and Data Structures* [online], Vreda Pieterse and Paul E. Black, eds. 31 May 2006

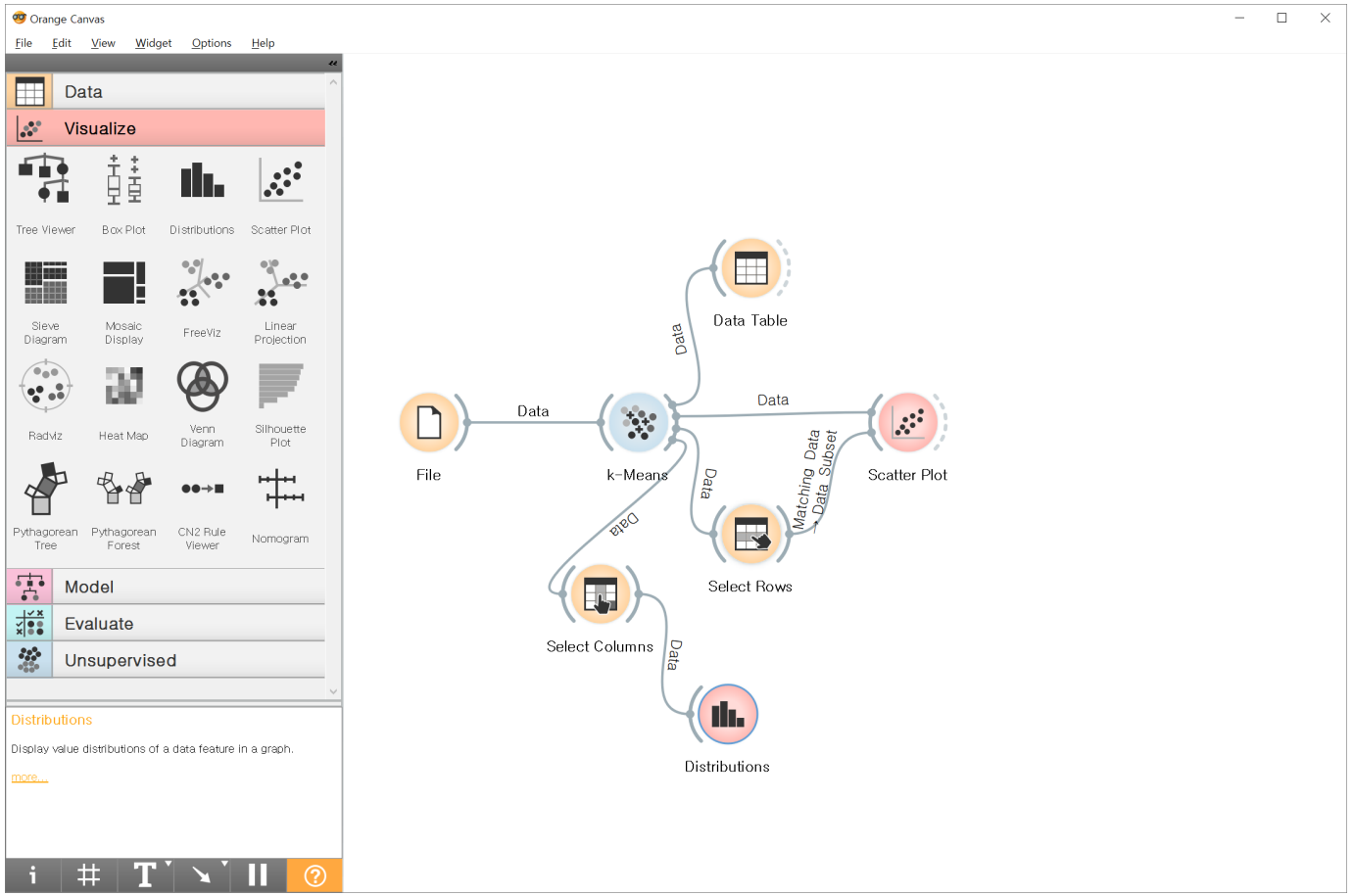
k-means (Cont'd)

- **Evaluation**
  - how well the clusters induced by the (unsupervised) clustering algorithm match the actual classes in the data
  - select individual classes and have the corresponding points marked in the scatter plot



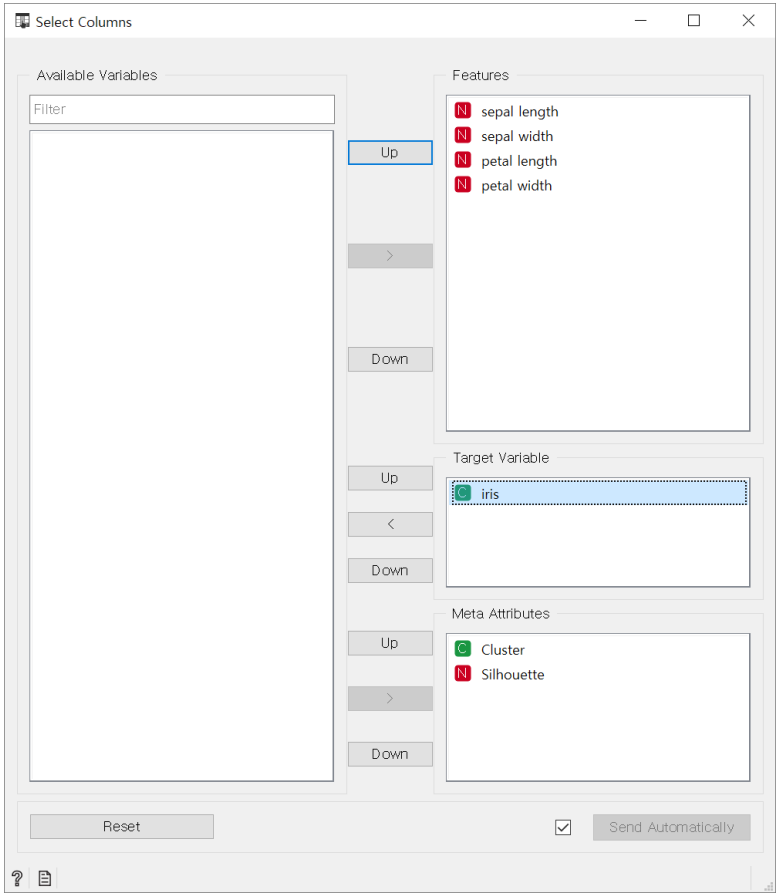
k-means (Cont'd)

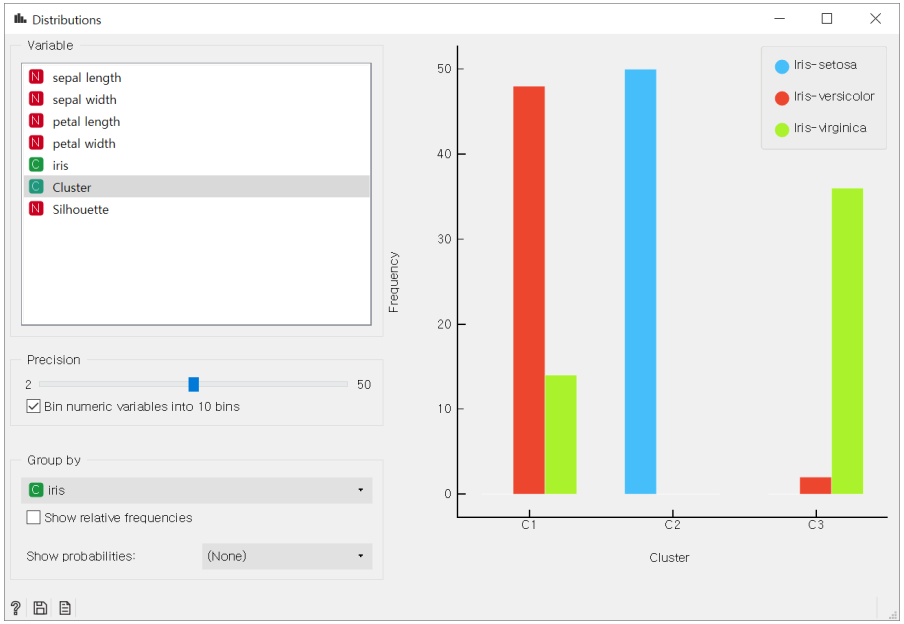
- **Distribution widget**
  - test the match between clusters and the original classes



k-means

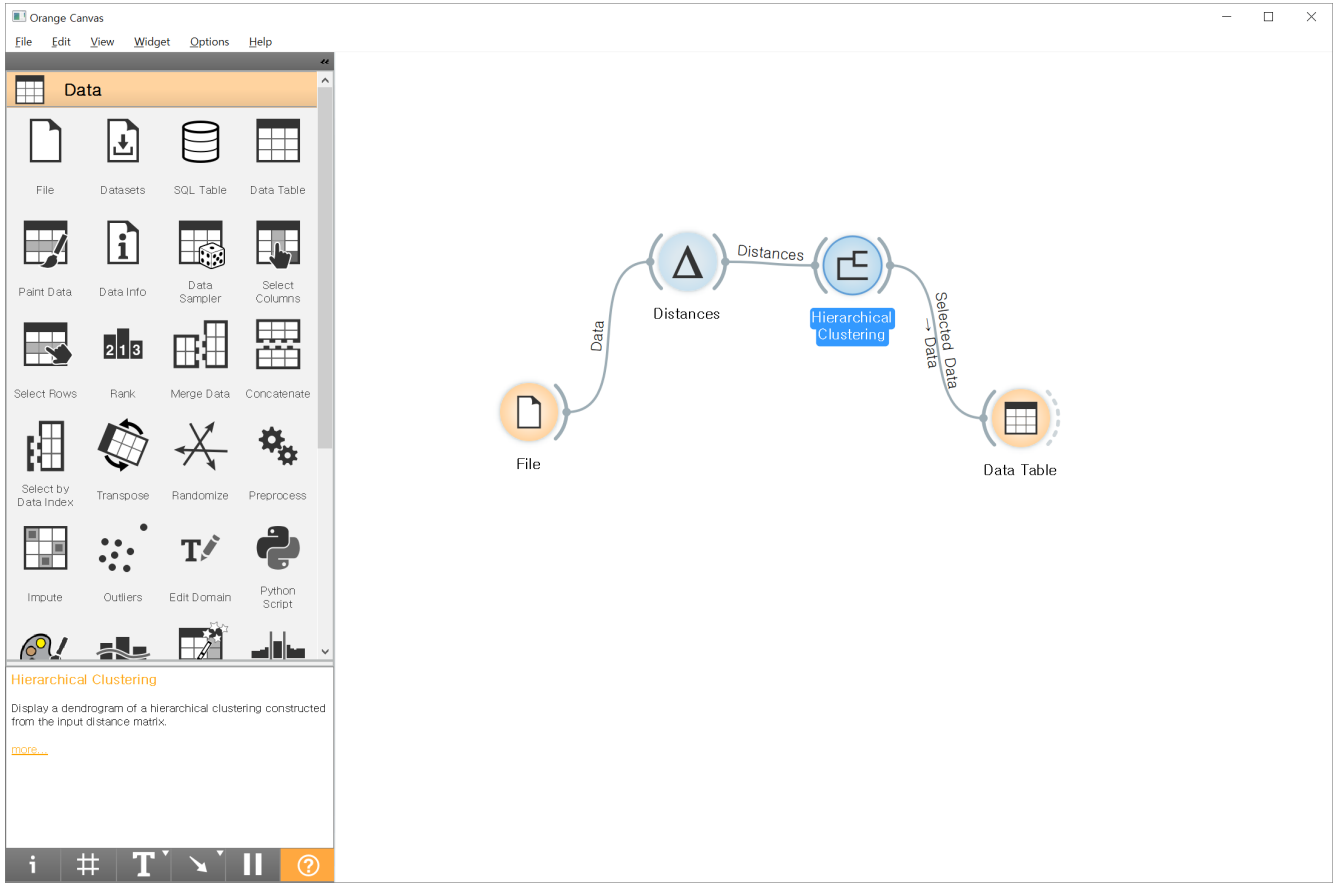
- **Select columns widget**
  - reinstate the original class Iris as the class and put the cluster index among the attributes





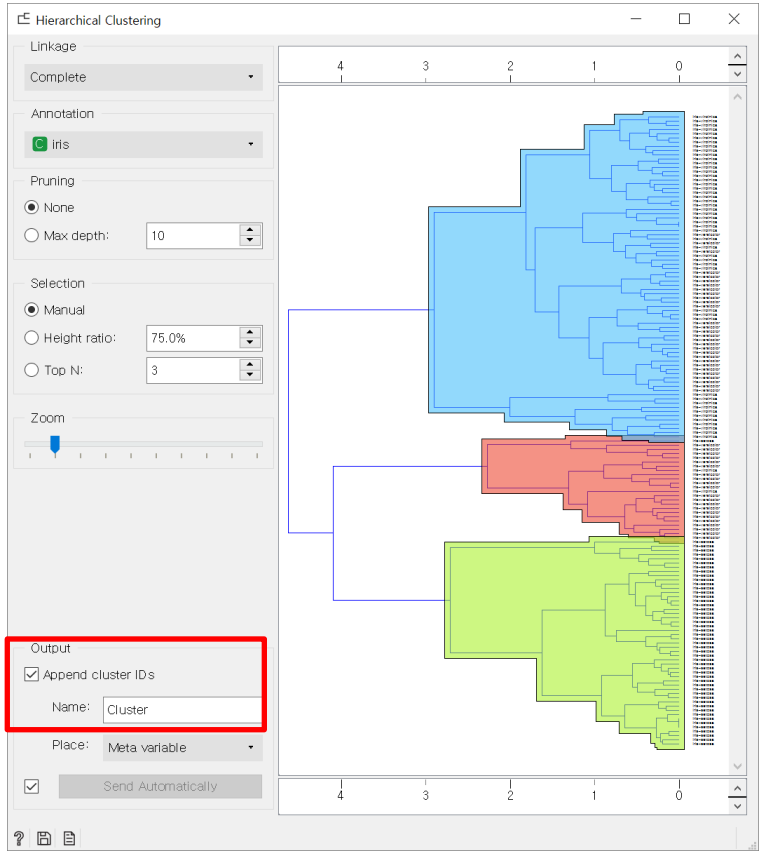
Hierarchical Clustering (Cont'd)

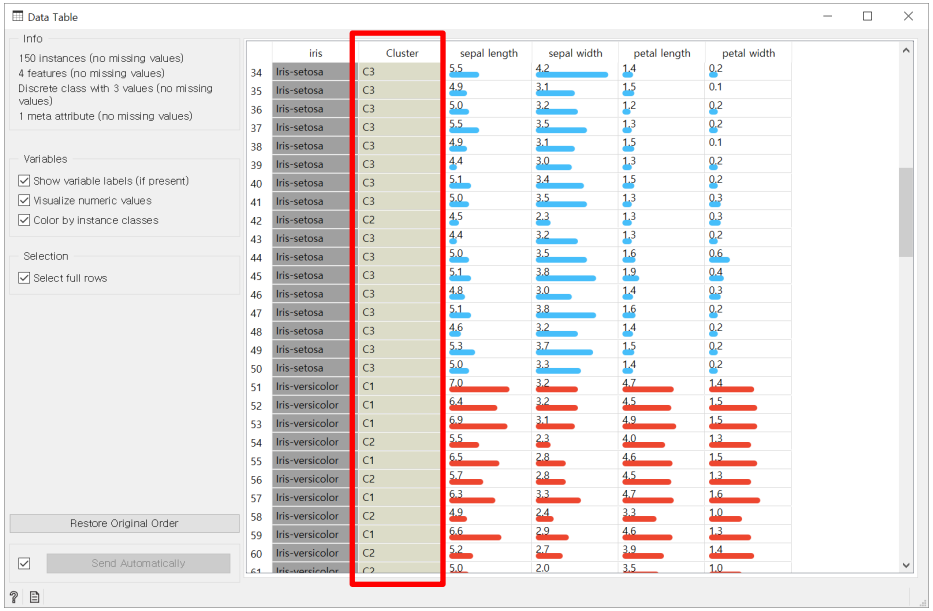
- **Build schema**
  - skip load data (default is iris data)



Hierarchical Clustering (Cont'd)

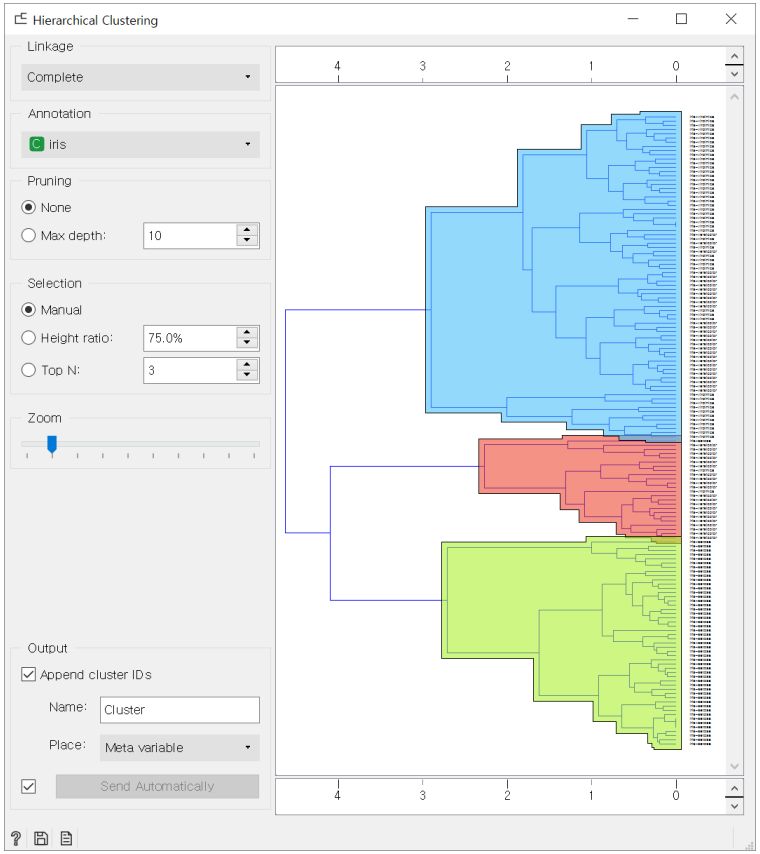
- **Observation of H-Clustering**
  - a way to check how hierarchical clustering clustered individual instance





Hierarchical Clustering (Cont'd)

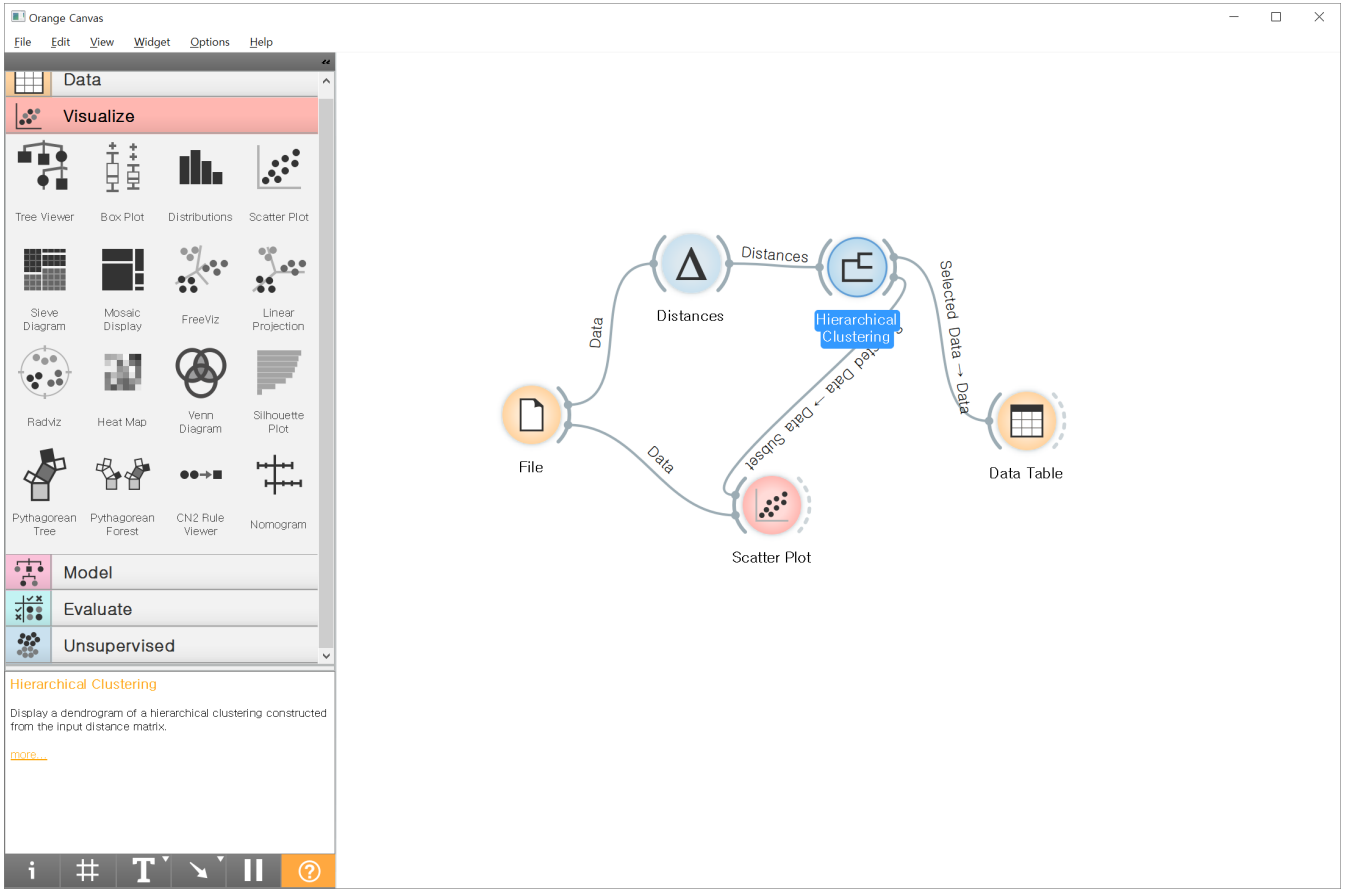
- **Hyperparameters and configuration**
  - Linkage
    - Single : computes the distance between the closest elements of the two clusters
    - Average : computes the average distance between elements of the two clusters
    - Weighted : uses the WPGMA* method
    - Complete : computes the distance between the clusters' most distant elements
  - Annotation
    - Labels of nodes in the dendrogram
  - Pruning
    - Huge dendrograms can be pruned in the Pruning box by selecting the maximum depth of the dendrogram
    - This only affects the display, not the actual clustering
  - Selection methods
    - Manual : Clicking inside the dendrogram will select a cluster
    - Height ratio : Clicking on the bottom or top ruler of the dendrogram places a cutoff line in the graph
    - Top N : Selects the number of top nodes



*WPGMA : **W**eighted **P**air **G**roup **M**ethod with **A**rithmetic Mean. It is a simple agglomerative (bottom-up) hierarchical clustering method, generally attributed to Sokal and Michene

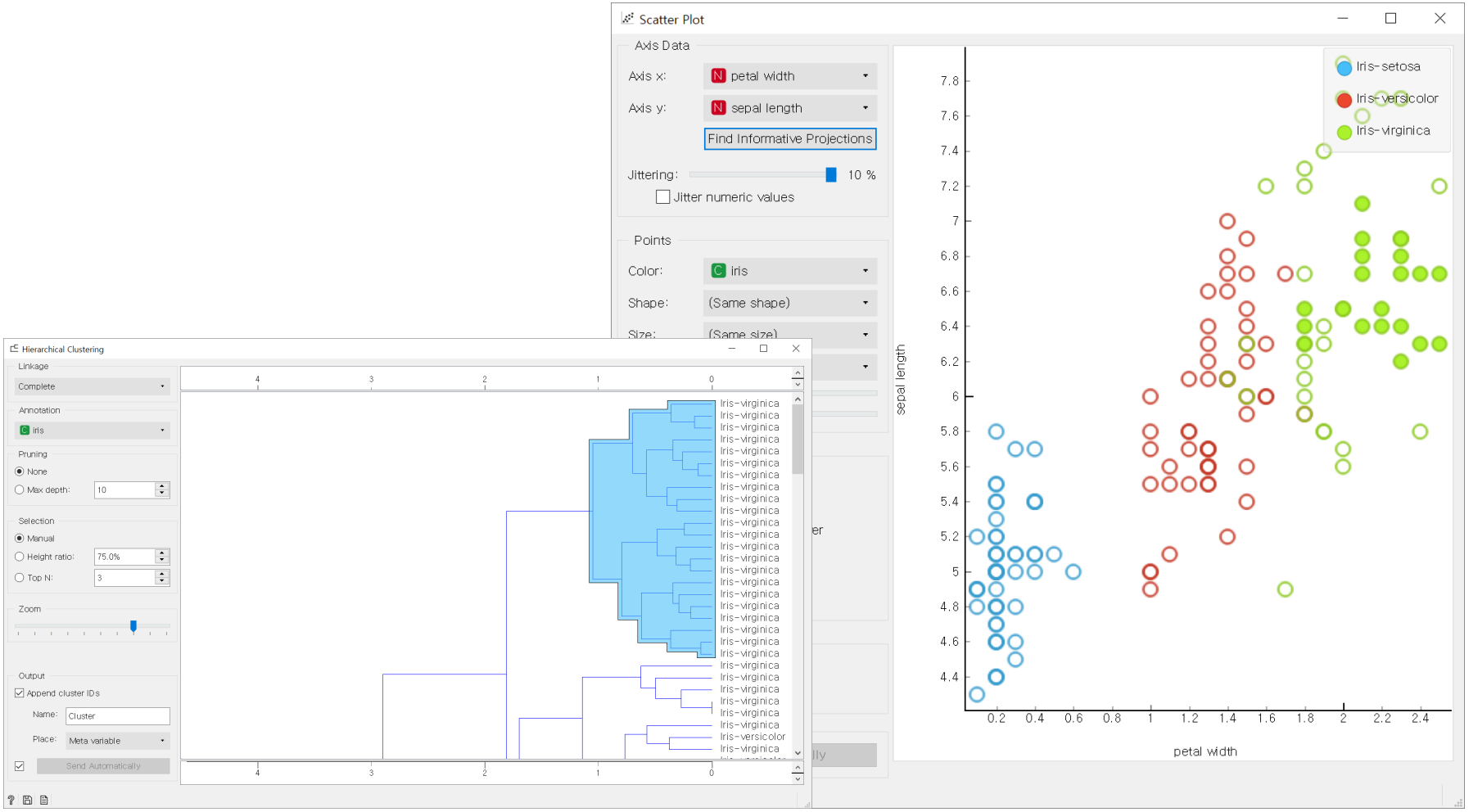
Hierarchical Clustering (Cont'd)

- **Build schema for another observation**



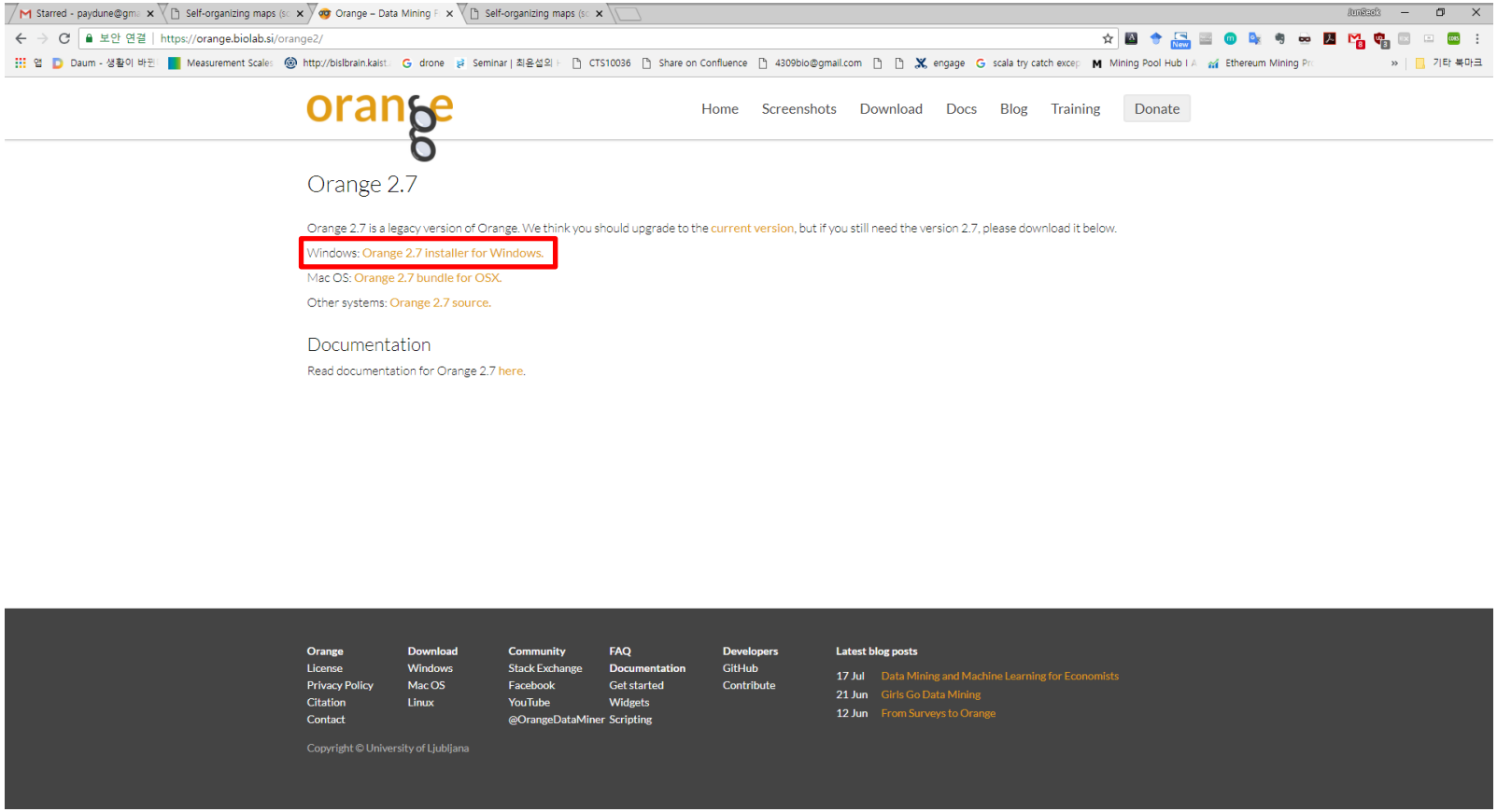
Hierarchical Clustering

- **Observation of the position of the selected clusters in the projection**



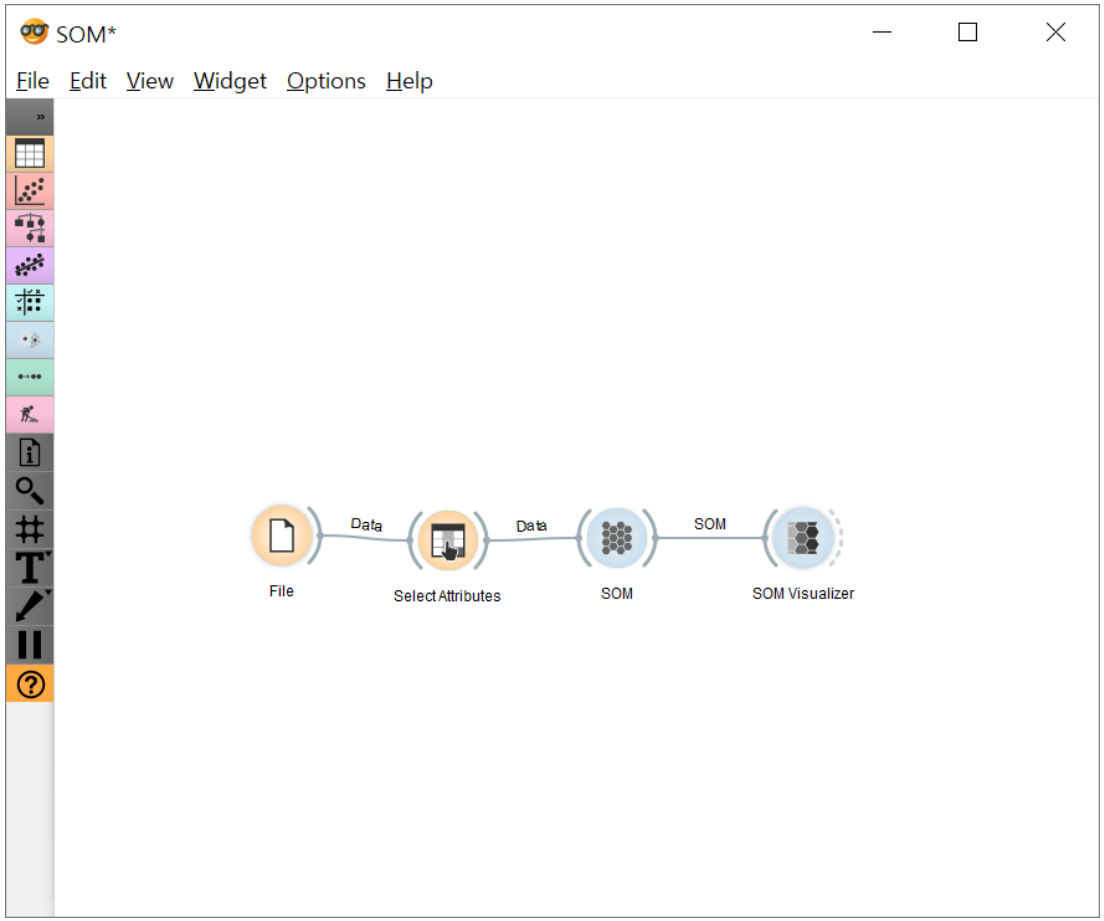
Self-organizing map Preparation

- **Install Orange 2.7 for SOM**
  - https://orange.biolab.si/orange2/



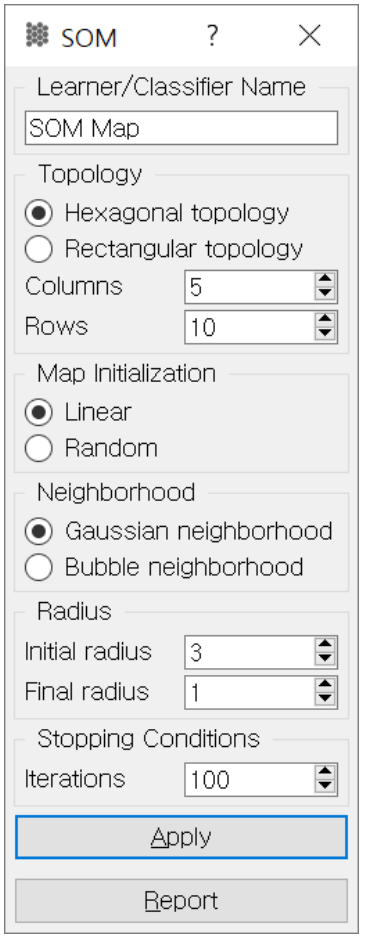
Self-organizing map (Cont'd)

- **Build schema (Orange 2.7)**
  - Default file is *iris.tab*



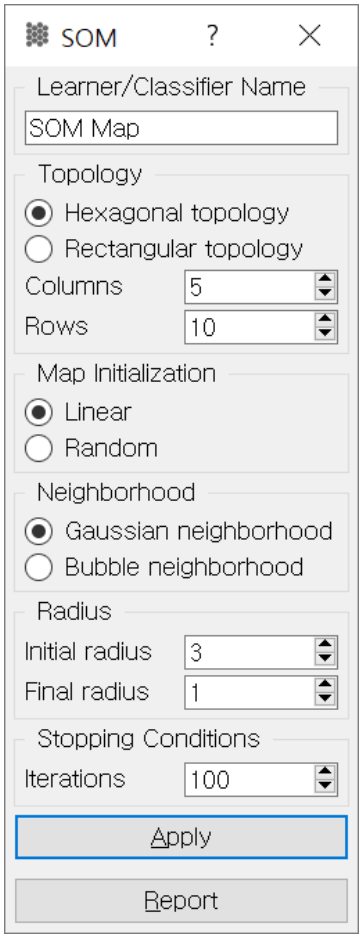
Self-organizing map (Cont'd)

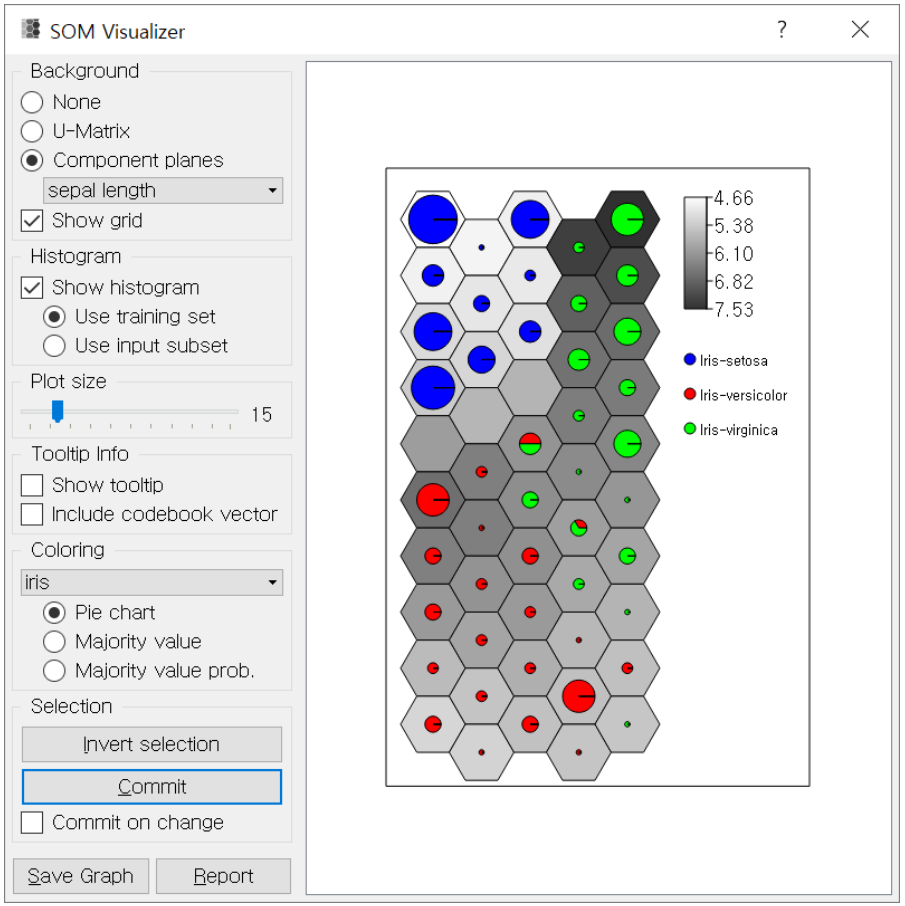
- **Hyperparameters and configuration**
  - Topology : topology type id and map sizes
    - Hexagonal : cells are hexagon-shaped
    - Rectangular : cells are square-shaped
  - Map initialization
    - Linear : Data instances are initially assigned to cells according to their two-dimensional PCA projection
    - Random : Data instances are initially randomly assigned to cells
  - Neighborhood
    - Gaussian : smoothed neighborhood
    - Bubble : crisp neighborhood
  - Radius : initial and final radius
  - Iterations : iterations of a training steps



Self-organizing map

- **Observation from SOM to SOM Visualizer**





Practice with Realdata

Dataset

- **Realworld data**
  - Online Retail Data Set[1]

Data Set Characteristics:	Multivariate, Sequential, Time-Series	**Number of Instances:**	541909	**Area:**	Business
Attribute Characteristics:	Integer, Real	**Number of Attributes:**	8	**Date Donated**	2015-11-06
Associated Tasks:	Classification, Clustering	**Missing Values?**	N/A	**Number of Web Hits:**	231361

  - a transnational data set which contains all the transactions occurring between 01/12/2010 and 09/12/2011 for a UK-based and registered non-store online retail.
  - https://archive.ics.uci.edu/ml/datasets/Online+Retail#
  - Attribute Information

Attributes	Description
InvoiceNo	Invoice number. Nominal, a 6-digit integral number uniquely assigned to each transaction. If this code starts with letter 'c', it indicates a cancellation
StockCode	Product (item) code. Nominal, a 5-digit integral number uniquely assigned to each distinct product
Description	Product (item) name. Nominal.
Quantity	The quantities of each product (item) per transaction. Numeric.
InvoiceDate	Invice Date and time. Numeric, the day and time when each transaction was generated.
UnitPrice	Unit price. Numeric, Product price per unit in sterling.
CustomerID	Customer number. Nominal, a 5-digit integral number uniquely assigned to each customer.
Country	Country name. Nominal, the name of the country where each customer resides.

[1] Dr Daqing Chen, Director: Public Analytics group. chend '@' lsbu.ac.uk, School of Engineering, London South Bank University, London SE1 0AA, UK

Overview

- **Objective**
  - to identify high- and low-value customers for marketing purposes
- **Feature selection**
  - each customer's recency of last purchase
  - frequency of purchase
  - monetary value
- **Preprocessing**
  - Cleansing and generate features from raw data
- **Develop a model**
  - the k-means clustering technique

Preprocessing

- **Python code**
  - https://www.dropbox.com/s/kci0p07jcqkjzj4/PreprocessingForClustering.py?dl=0

- **Overall process of preprocessing**

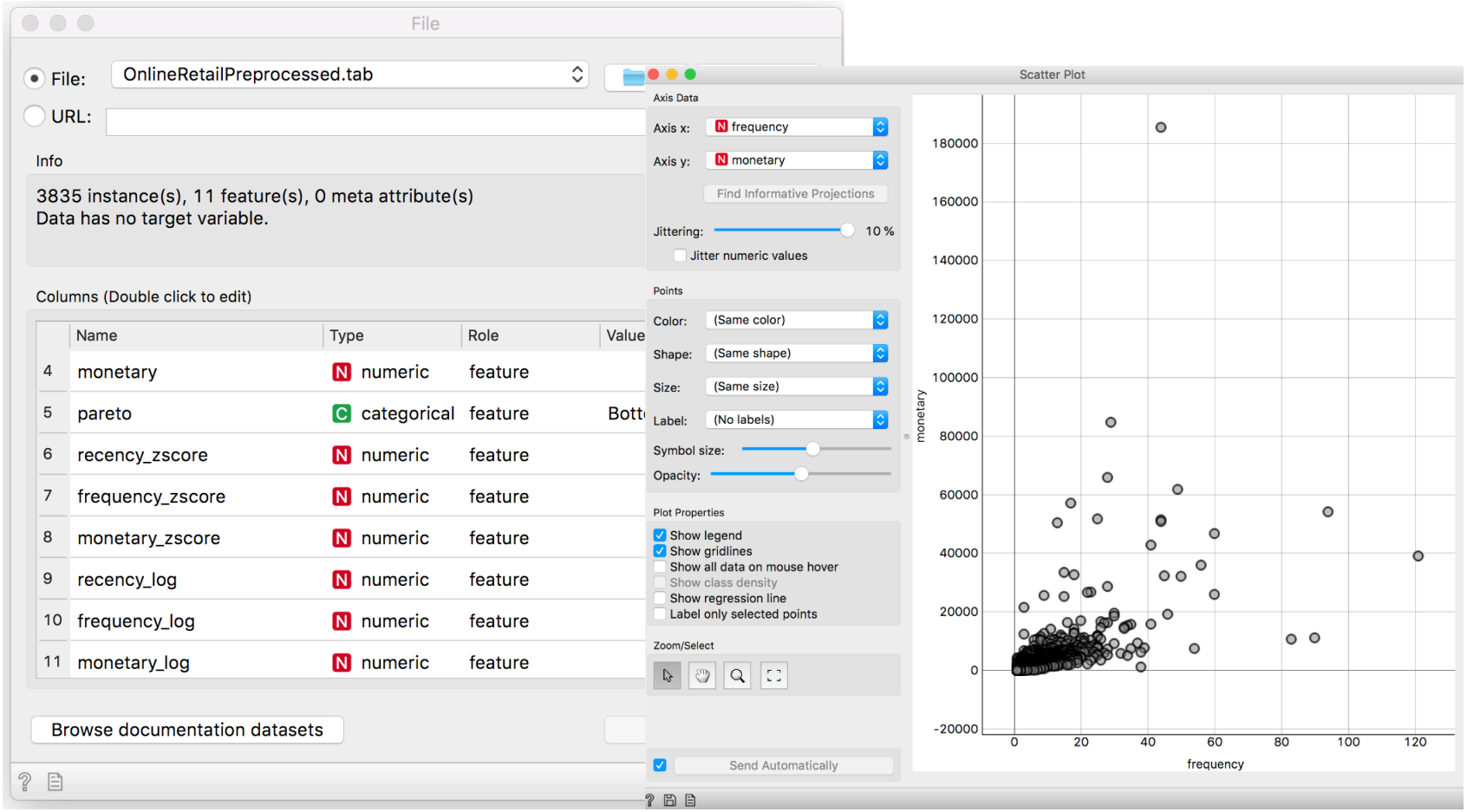
- delete null values
- Restrict country and date

- Frequency
- Recency
- Monetary

- log transform
- z-score

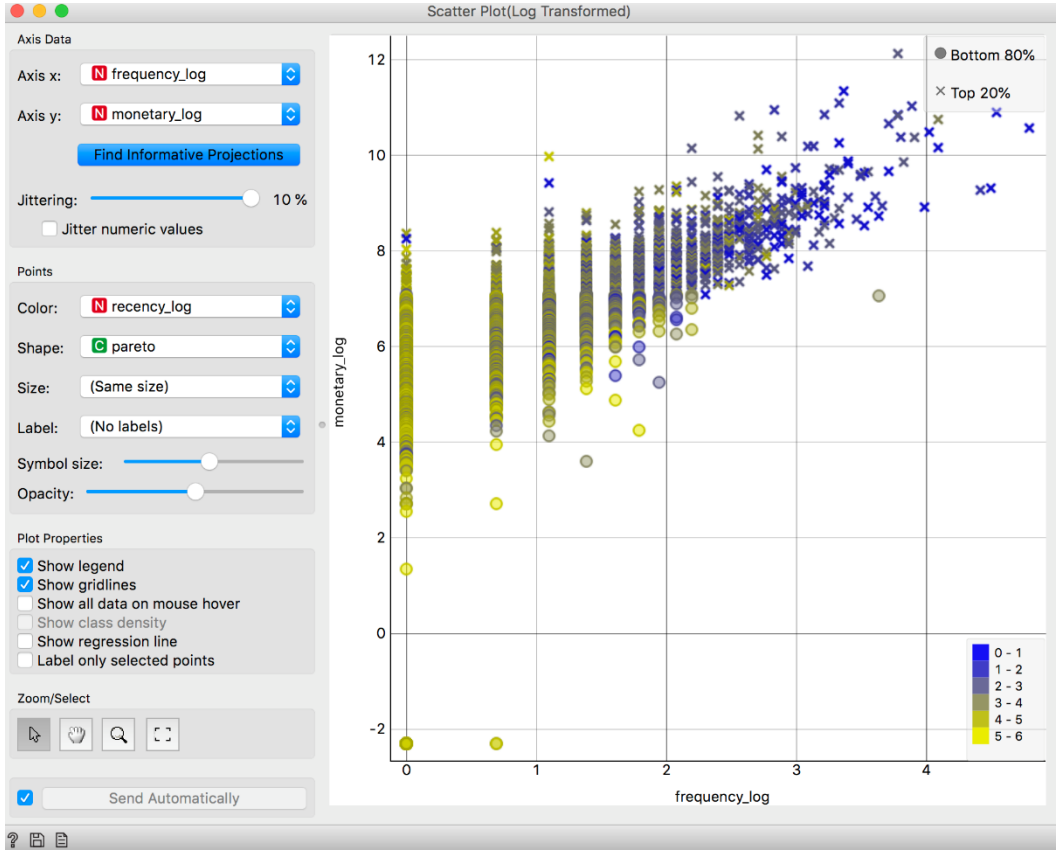
Load data

- **Load preprocessed data**
  - Analysis data for getting insights



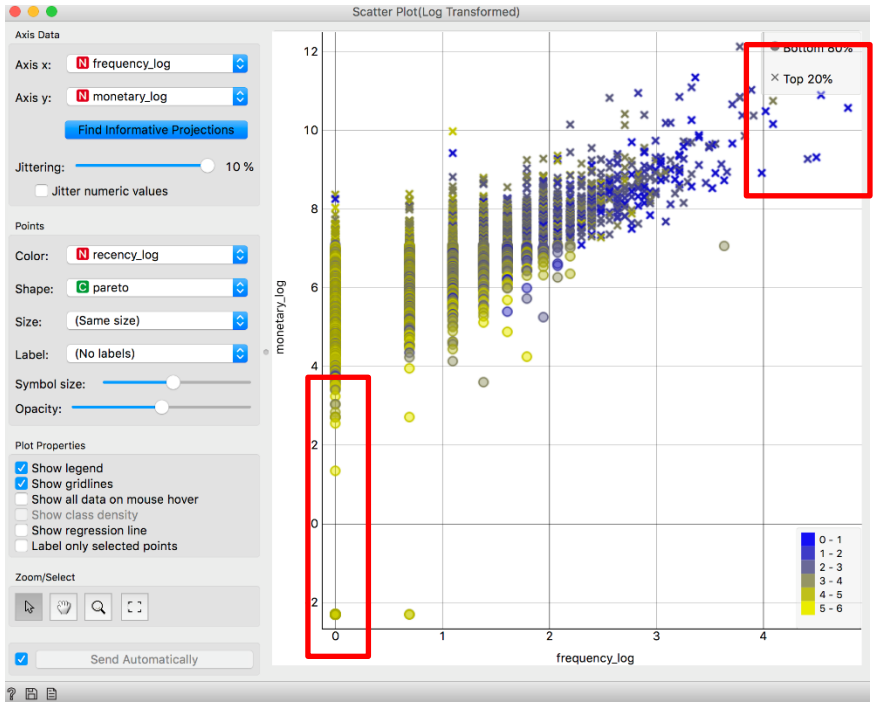
Visualize data

- **Analysis data**
  - a scattering of high-value, high-frequency customers in the top, right-hand corner of the gr aph
  - data points are dark, indicating that they've purchased something recently



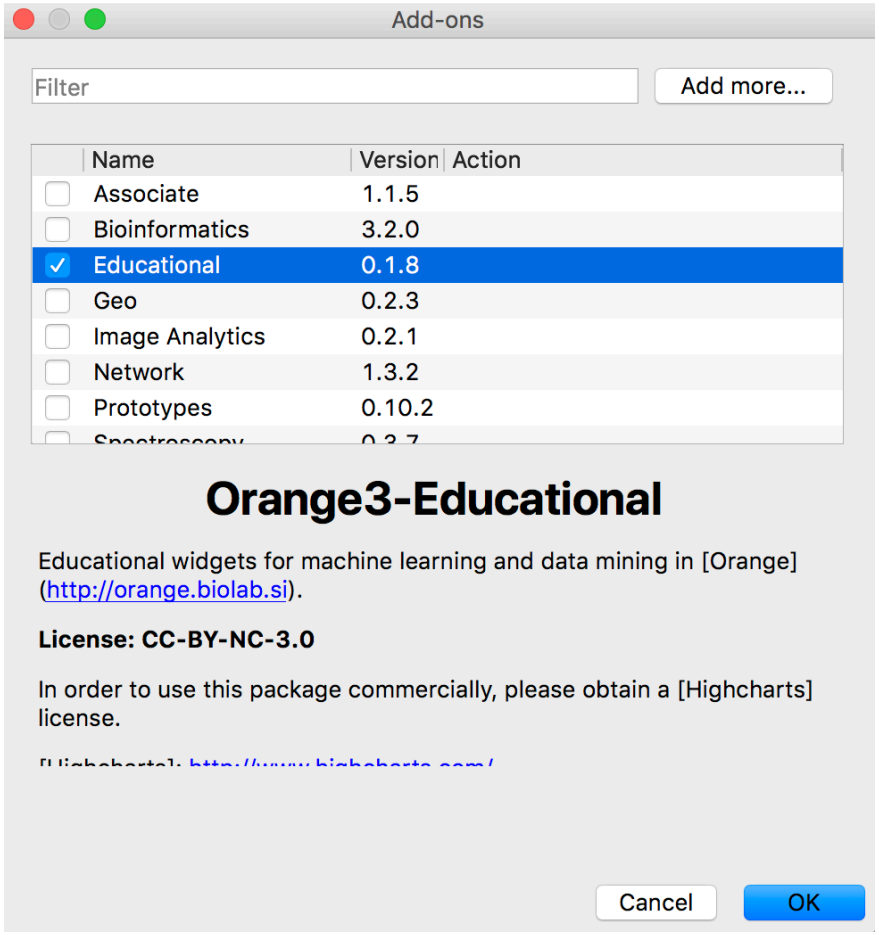
Handling outliers

- **Analysis outliers**
  - The eighteen, no-value customers we just investigated are all customers who returned every thing they bought
  - the outliers may be the most important customers to understand
  - right-hand corner, we have customers who are outliers in terms of being extraordinarily hig h-value, high-frequency shoppers
    - they're the customers we most want



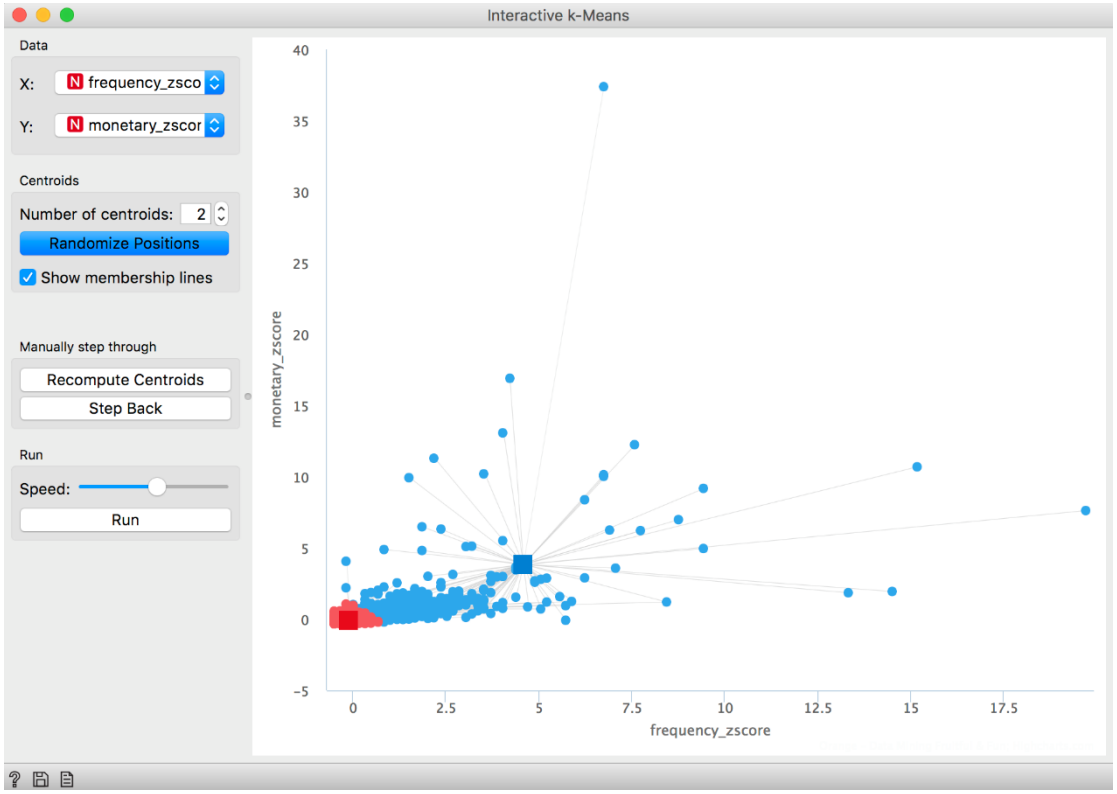
Install add-on

- **Educational add-on**
  - interactive k-mean



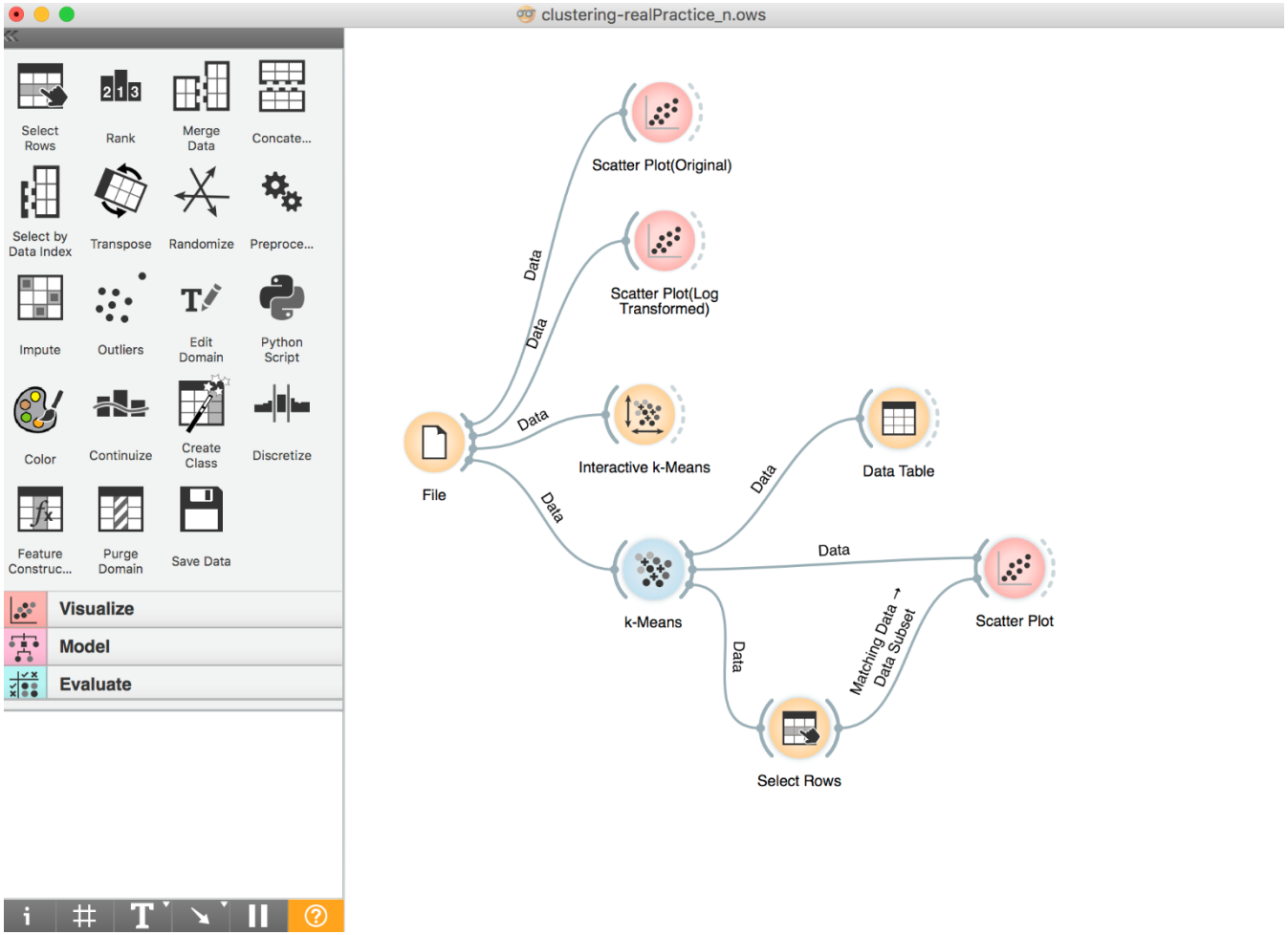
K-means (Cont'd)

- **Determine number of clusters / run *k*-means**
  - the data didn't suggest an obvious choice for the number of clusters
  - to determine how many clusters to extract (Judgement call)
  - identifying high- and low-value customers for the business
  - i.e. k=2 to 10



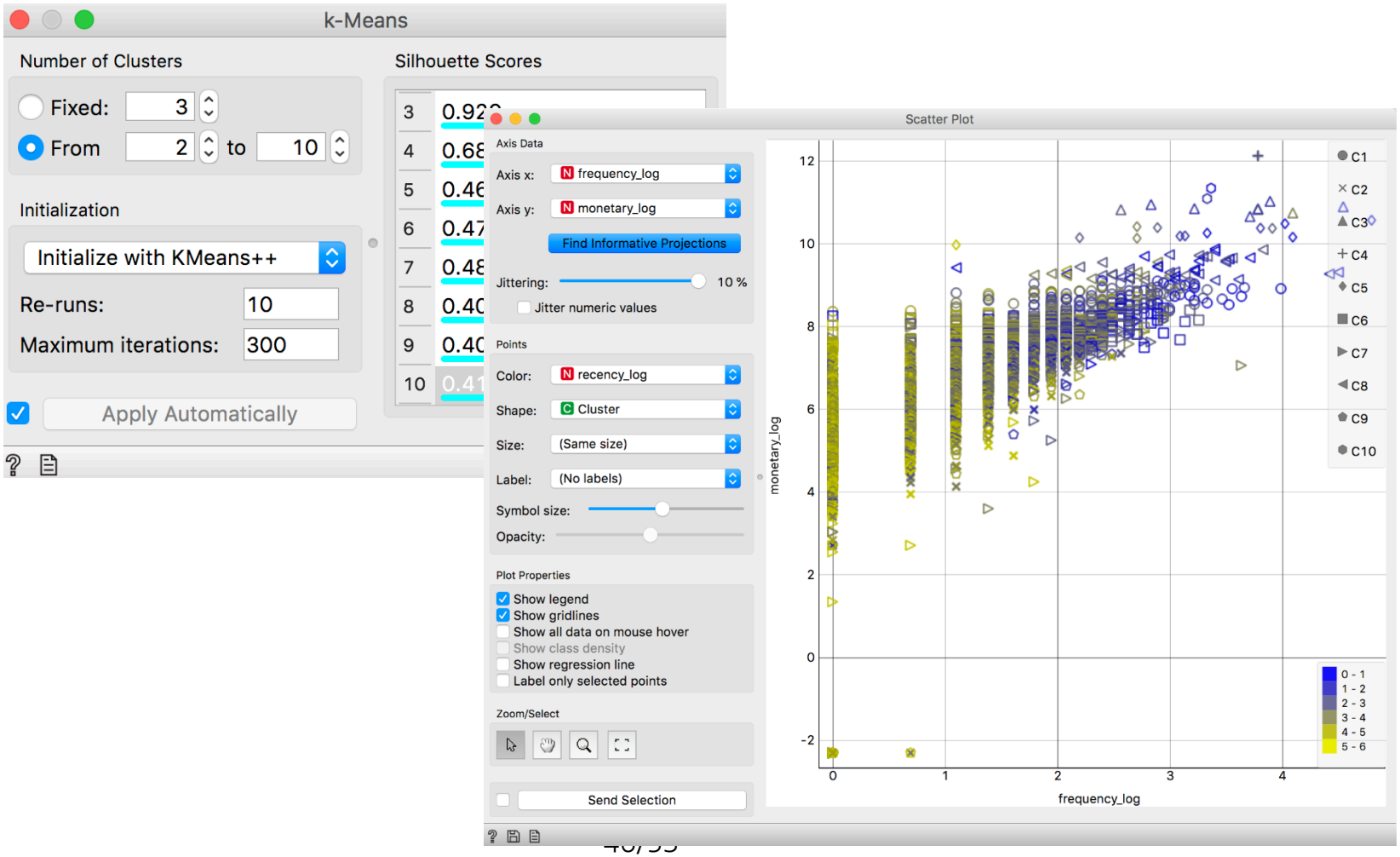
K-mean (Cont'd)

- **K-mean Analysis**
  - Customer segmentation



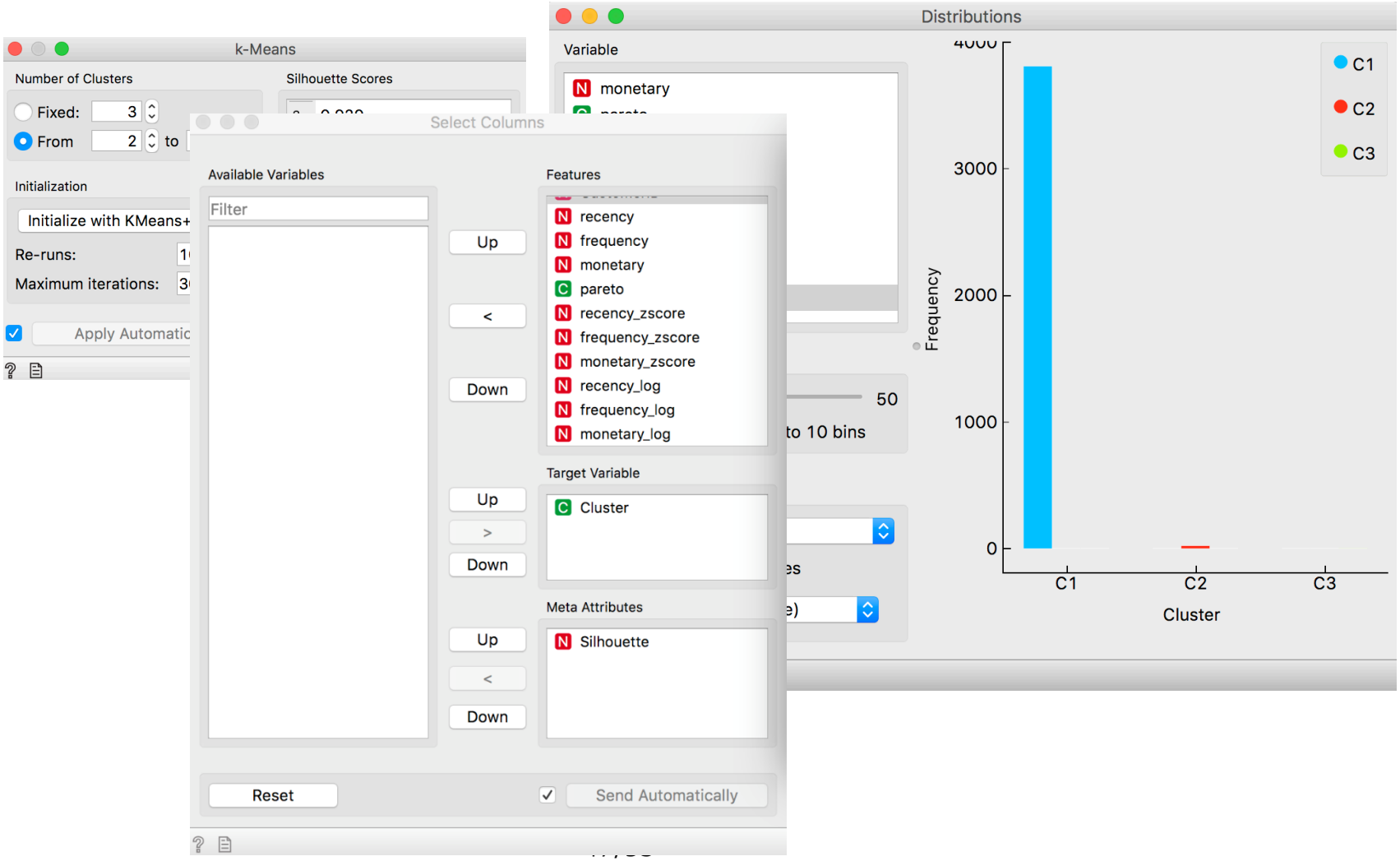
K-mean (Cont'd)

- **K-mean Analysis**
  - Customer segmentation



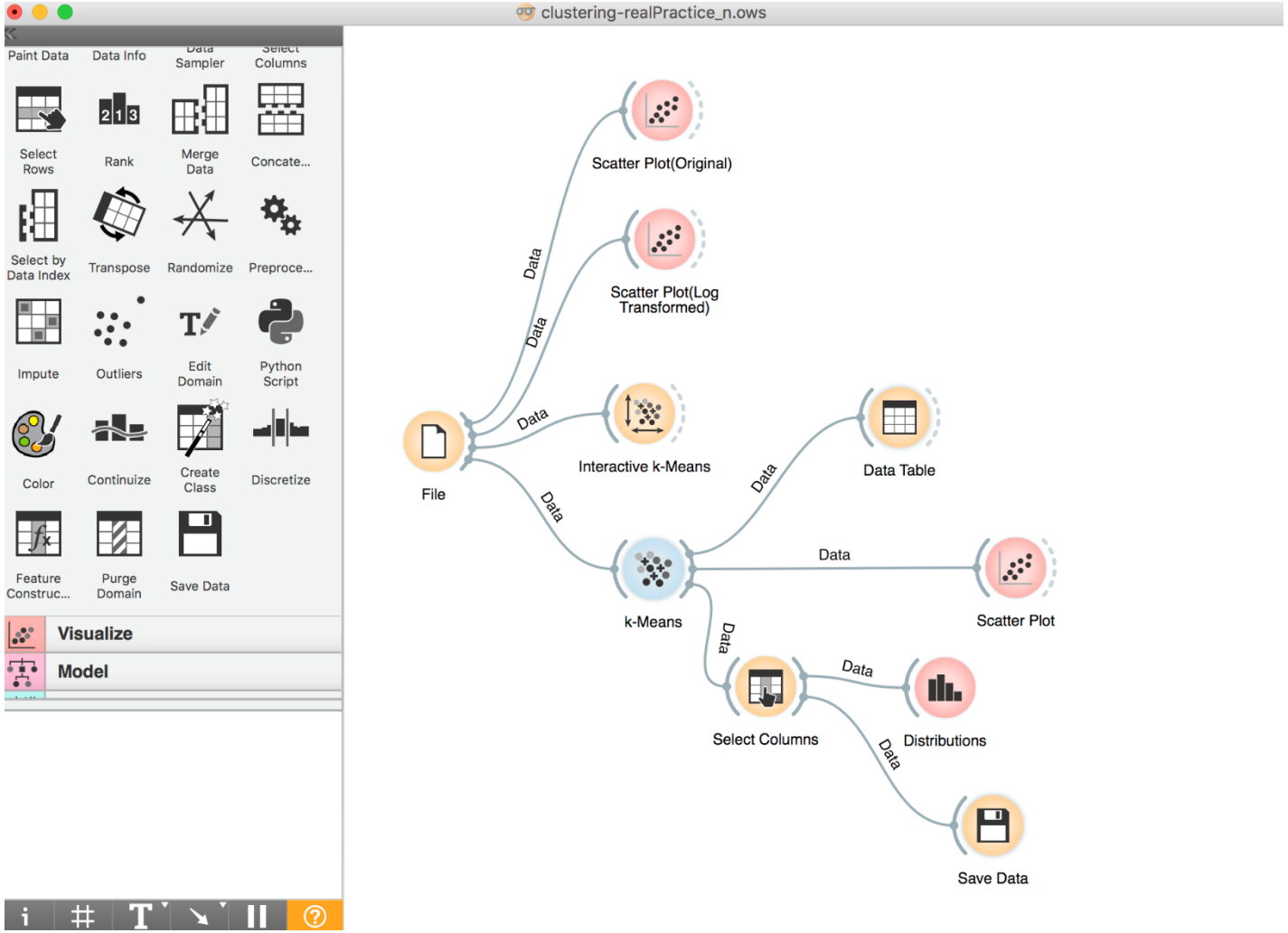
K-mean (Cont'd)

- **K-mean Analysis**
  - Customer segmentation



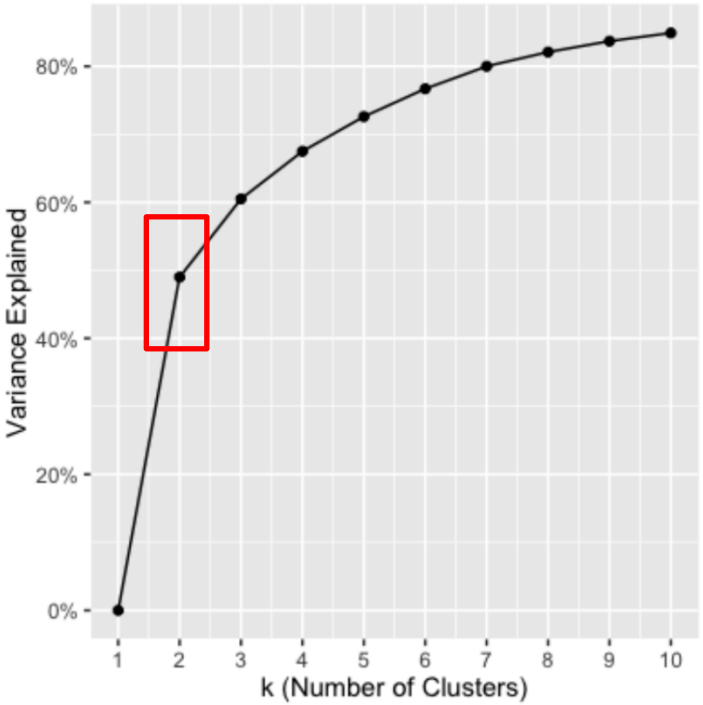
K-mean (Cont'd)

- **Save result then further analysis**

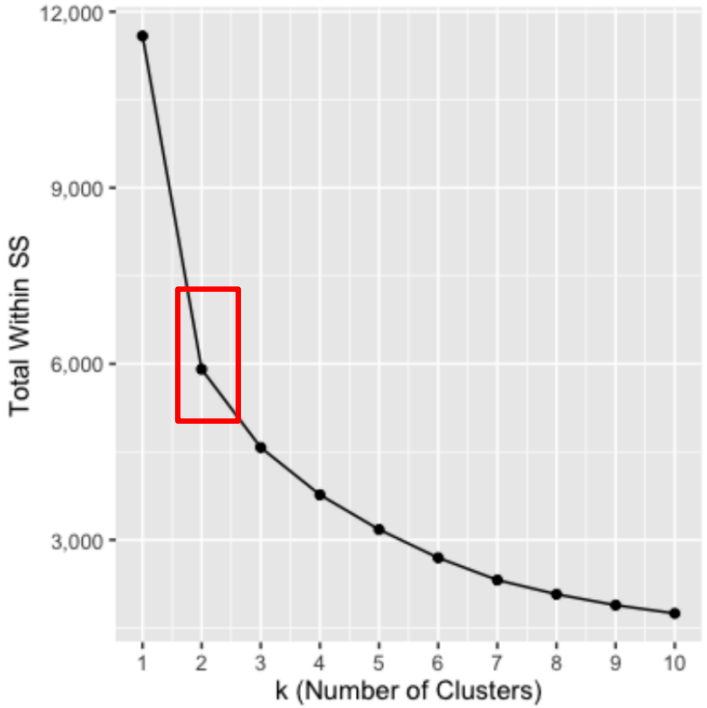


K-mean

- **Find best K**
  - The decision should be based upon how the business plans to use the results, and the level of granularity they want to see in the clusters.



Graph variance explained by number of clusters



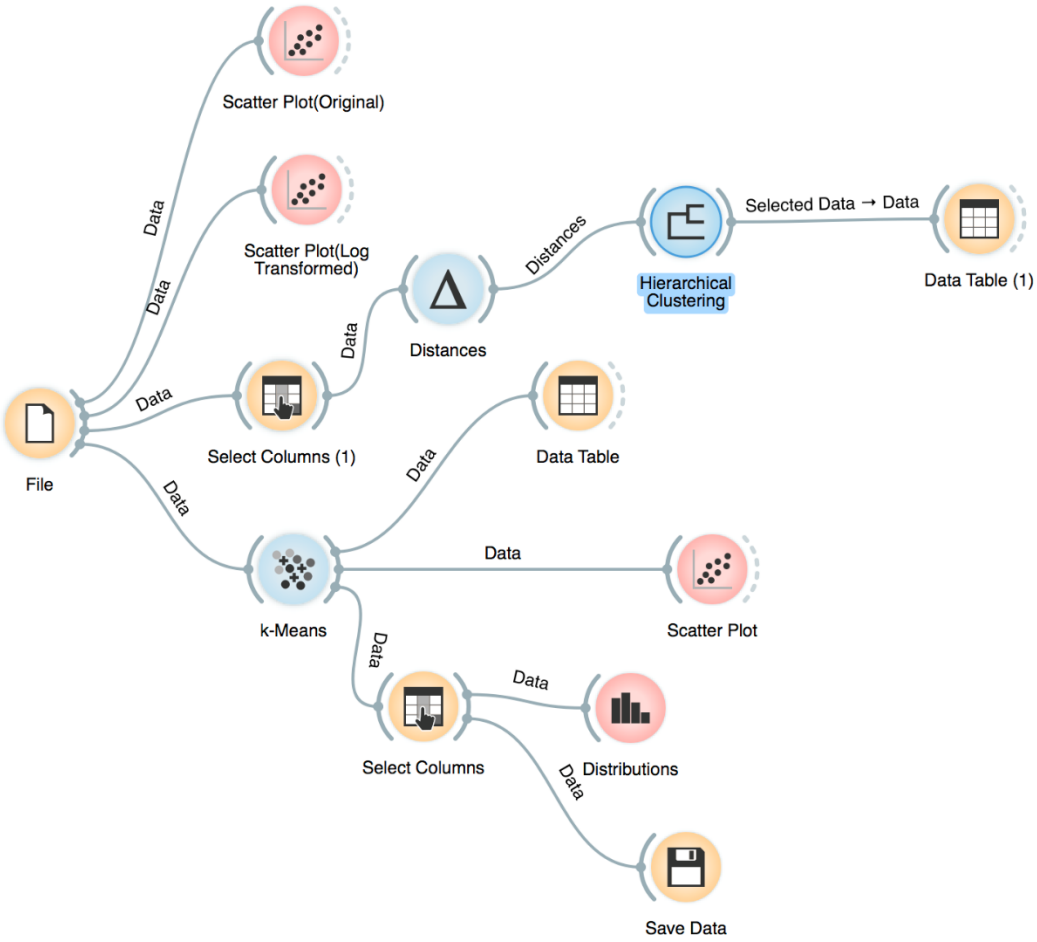
Graph within sums of squares by number of clusters

H-Clustering (Cont'd)

- **Do same procedure By H-clustering algorithm**
  - Time limit : 15min

H-Clustering

- **Schema**



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- https://docs.orange.biolab.si/3/visual-programming/widgets/unsupervised/hierarchicalclustering.html
- https://docs.orange.biolab.si/2/reference/rst/Orange.projection.som.html
- http://www.algorithmsinnature.org/
- http://www.kimberlycoffey.com/blog/2016/8/k-means-clustering-for-customer-segmentation

Thank you