Clustering: Models and Algorithms

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2019-02-28

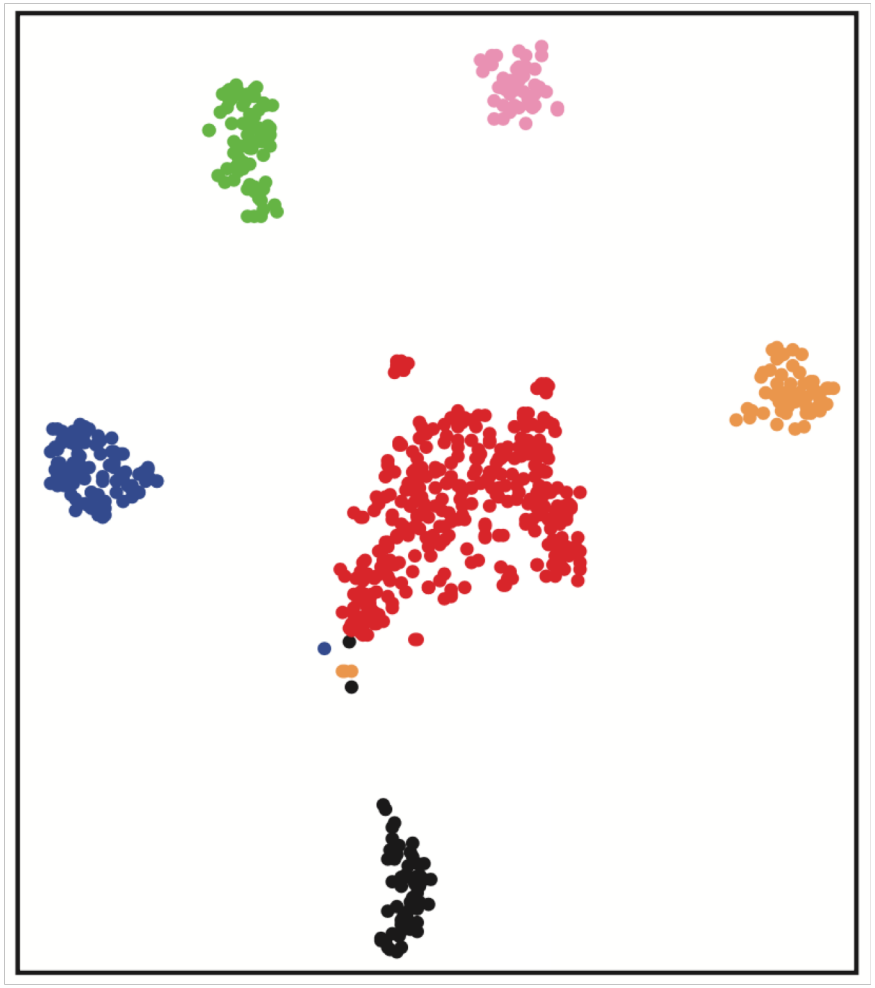
Outline

- Clustering
  - K-mean clustering, hierarchical clustering
- Adaptive learning (online learning)
  - CL, FSCL, RPCL
- Gaussian Mixture Models (GMM)
- Expectation-Maximization (EM) for maximum likelihood

What is clustering?

例子：不同类型的癌细胞会各自聚在一起

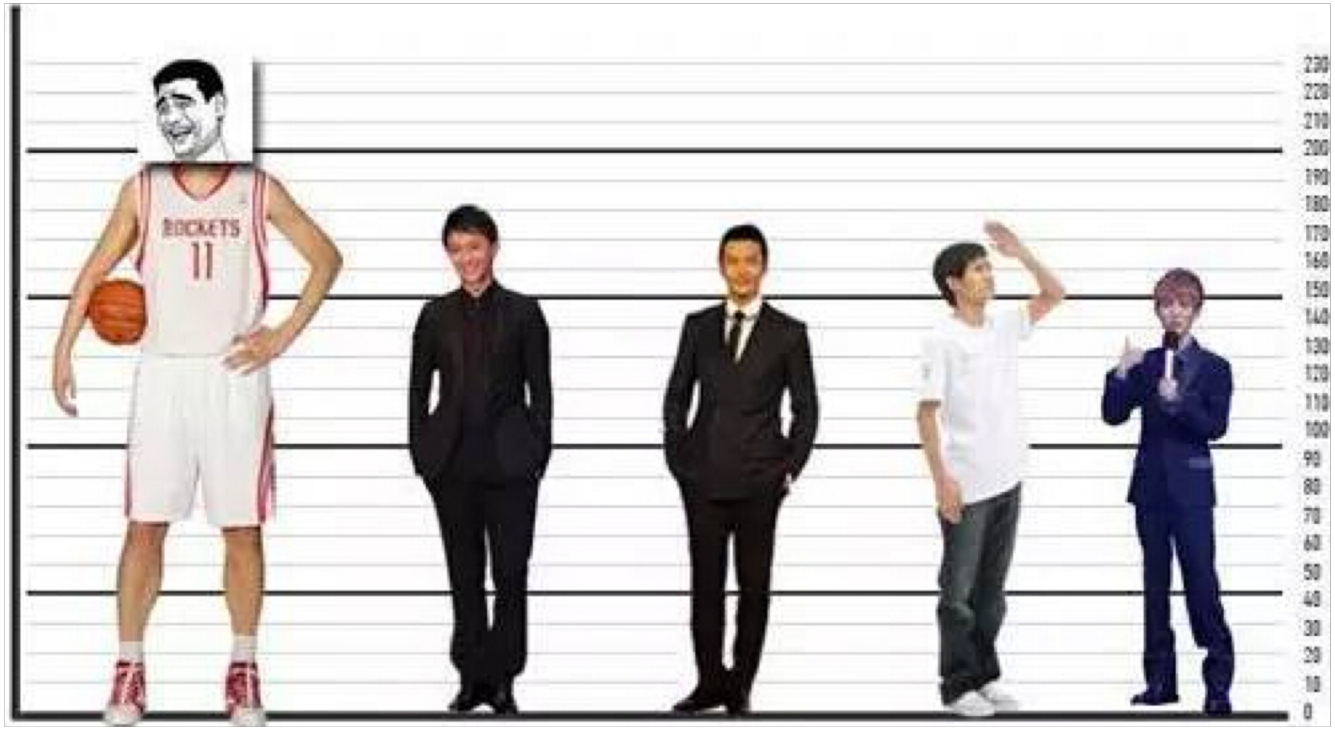
物以类聚



Six malignant tumors (melanoma)

How to represent a cluster

- 例如：将每个人的身高记下来

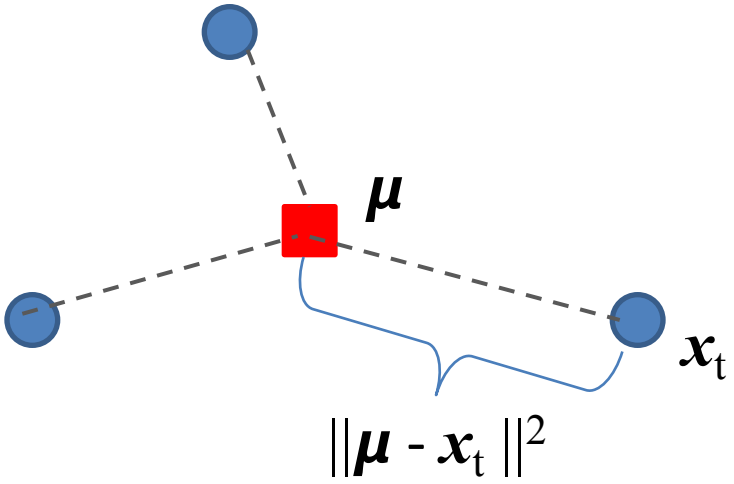


但是，如果只能记一个身高数值…

平均值　　总误差最小

How to define error?

Square distance:



$$\|\boldsymbol{\mu} - \boldsymbol{x}_1\|^2 + \|\boldsymbol{\mu} - \boldsymbol{x}_2\|^2 + \|\boldsymbol{\mu} - \boldsymbol{x}_3\|^2$$

可以证明：当$\boldsymbol{\mu}$是所有数据点的均值时，平方距离和最小

Matrix derivatives

$$\left[\frac{\partial \mathbf{x}}{\partial y}\right]_i = \frac{\partial x_i}{\partial y} \qquad \left[\frac{\partial x}{\partial \mathbf{y}}\right]_i = \frac{\partial x}{\partial y_i} \qquad \left[\frac{\partial \mathbf{x}}{\partial \mathbf{y}}\right]_{ij} = \frac{\partial x_i}{\partial y_j}$$

$$\frac{\partial \mathbf{x}^T\mathbf{a}}{\partial \mathbf{x}} = \frac{\partial \mathbf{a}^T\mathbf{x}}{\partial \mathbf{x}} = \mathbf{a} \tag{69}$$

$$\frac{\partial \mathbf{a}^T\mathbf{X}\mathbf{b}}{\partial \mathbf{X}} = \mathbf{a}\mathbf{b}^T \tag{70}$$

$$\frac{\partial \mathbf{a}^T\mathbf{X}^T\mathbf{b}}{\partial \mathbf{X}} = \mathbf{b}\mathbf{a}^T \tag{71}$$

$$\frac{\partial \mathbf{a}^T\mathbf{X}\mathbf{a}}{\partial \mathbf{X}} = \frac{\partial \mathbf{a}^T\mathbf{X}^T\mathbf{a}}{\partial \mathbf{X}} = \mathbf{a}\mathbf{a}^T \tag{72}$$

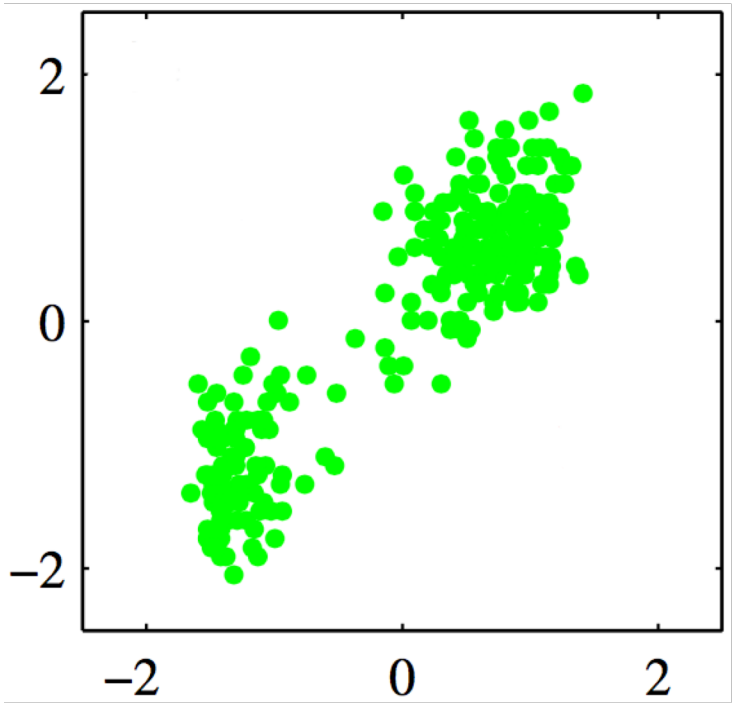
$$\frac{\partial \det(\mathbf{X})}{\partial \mathbf{X}} = \det(\mathbf{X})(\mathbf{X}^{-1})^T \tag{49}$$

$$\frac{\partial \mathbf{Y}^{-1}}{\partial x} = -\mathbf{Y}^{-1}\frac{\partial \mathbf{Y}}{\partial x}\mathbf{Y}^{-1} \tag{59}$$

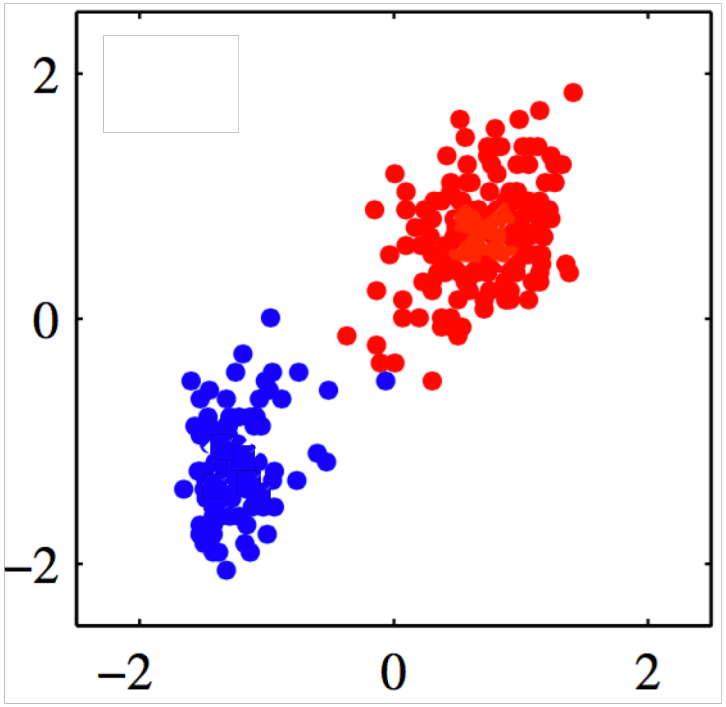
http://www2.imm.dtu.dk/pubdb/views/edoc_download.php/3274/pdf/imm3274.pdf

Clustering the data

We have the following data:



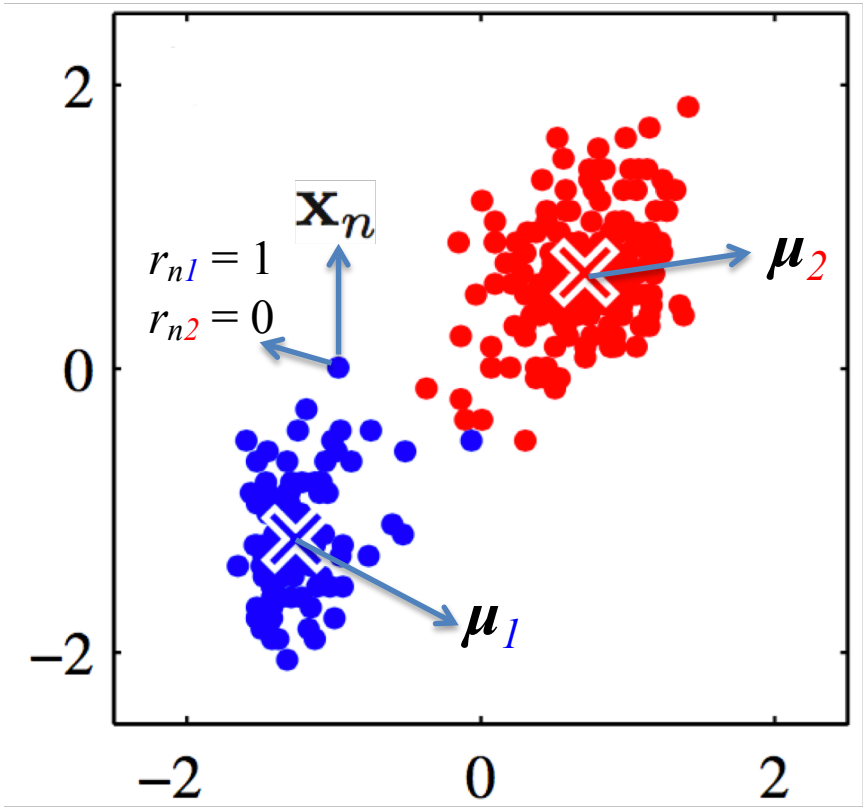
We want to cluster the data into two clusters (red and blue)



How?

Minimize the sum of square distances J

minimize $$J = \sum_{n=1}^{N} \sum_{k=1}^{K} r_{nk} \|\mathbf{x}_n - \boldsymbol{\mu}_k\|^2$$



$r_{nk} = 1$ if and only if data point $\mathbf{x}_n$ is assigned to cluster k;
otherwise $r_{nk} = 0$.

$k = 1, 2$; K = 2 clusters

$n = 1, \ldots, N$;
N: the total number of points.

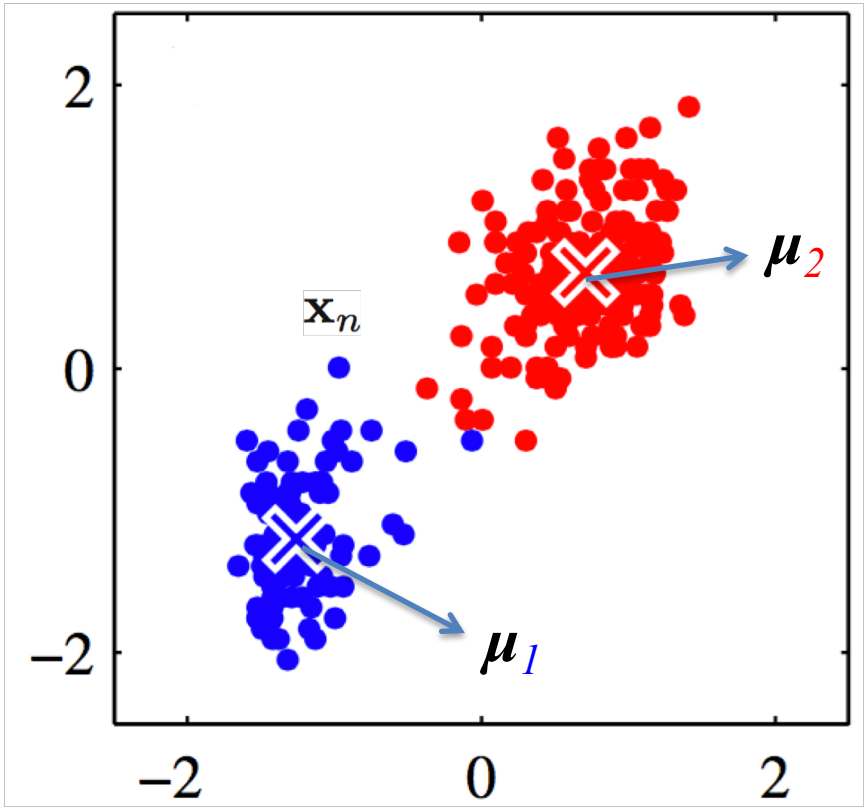
We need to calculate $\{ r_{nk} \}$ and $\{ \boldsymbol{\mu}_k \}$.

If we know r_{n1} , r_{n2} for all n=1,…,N

Since the points have been assigned to cluster 1 or cluster 2, we calculate

$\boldsymbol{\mu}_1$ = mean of the points in cluster 1

$\boldsymbol{\mu}_2$ = mean of the points in cluster 2



Or formally

$$\boldsymbol{\mu}_k = \frac{\sum_n r_{nk}\mathbf{x}_n}{\sum_n r_{nk}}$$

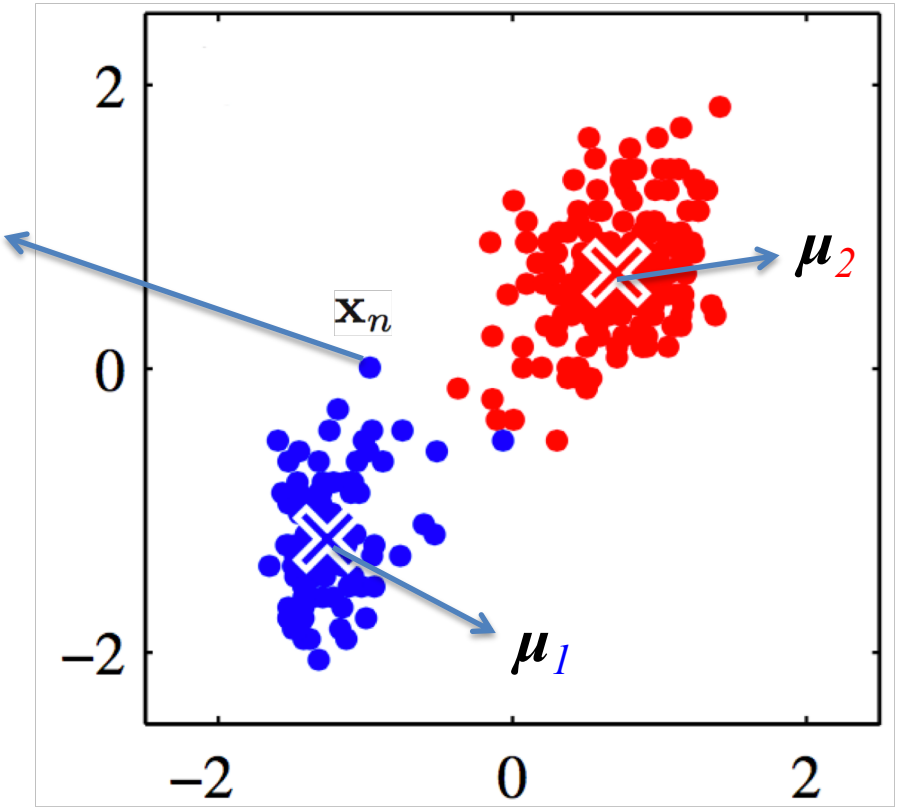
We call it the **M Step.**

If we know $\boldsymbol{\mu}_1, \boldsymbol{\mu}_2$

We should assign point $\mathbf{x}_n$ to cluster 1, because

$$\| \mathbf{x}_n - \boldsymbol{\mu}_1 \|^2 < \| \mathbf{x}_n - \boldsymbol{\mu}_2 \|^2$$

Then, $r_{n1} = 1$
$r_{n2} = 0$

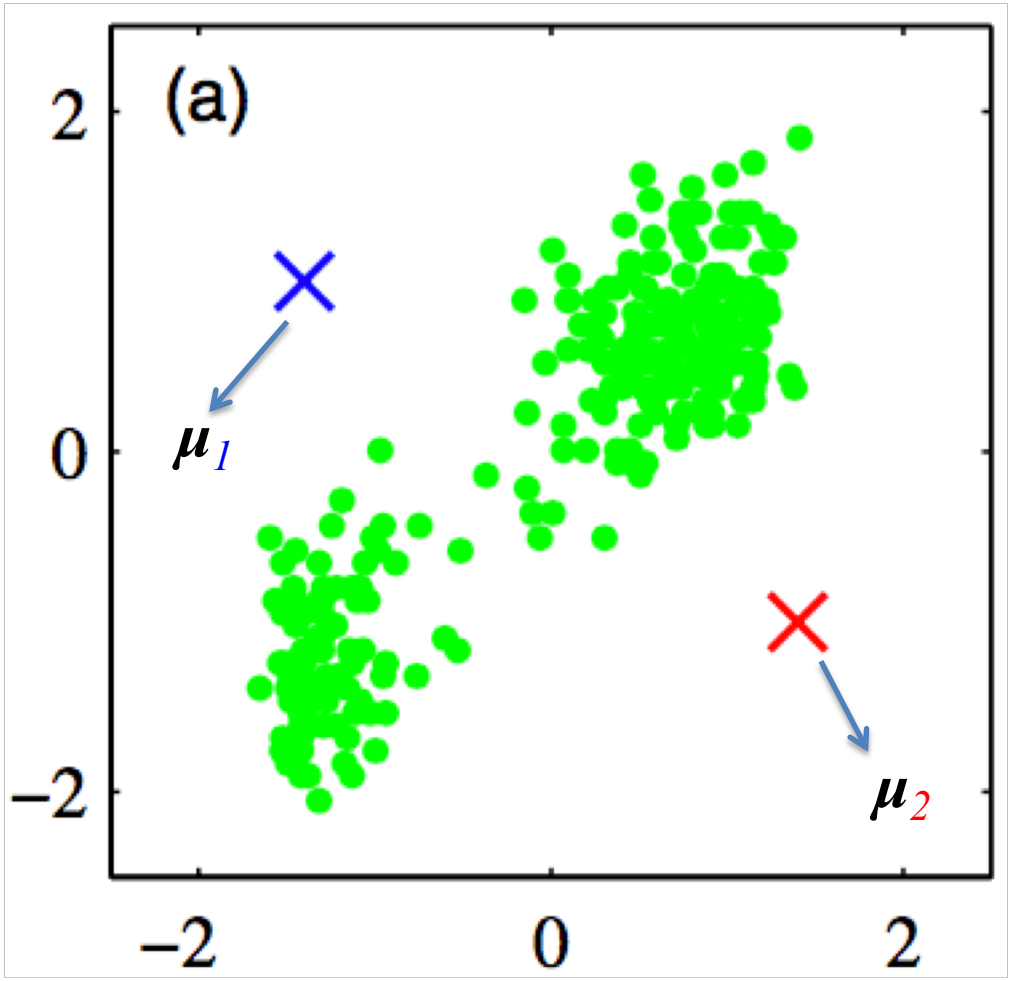


Or formally

$$r_{nk} = \begin{cases} 1 & \text{if } k = \arg\min_j \|\mathbf{x}_n - \boldsymbol{\mu}_j\|^2 \\ 0 & \text{otherwise.} \end{cases}$$

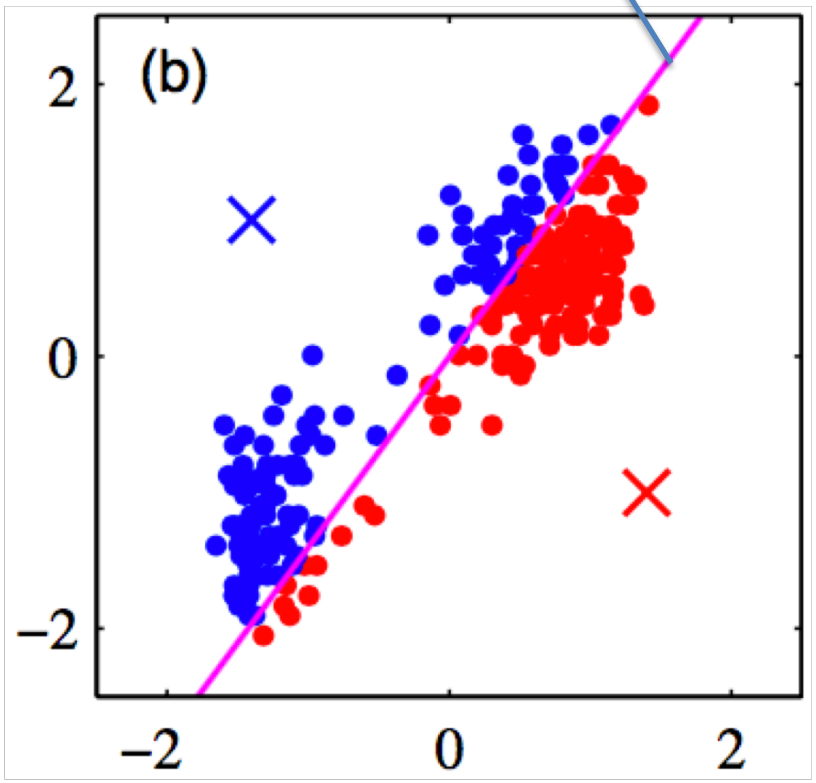
We call it the **E Step**

Initialization



Given $\boldsymbol{\mu}_1, \boldsymbol{\mu}_2$, calculate r_{n1}, r_{n2} for all n=1,…,N

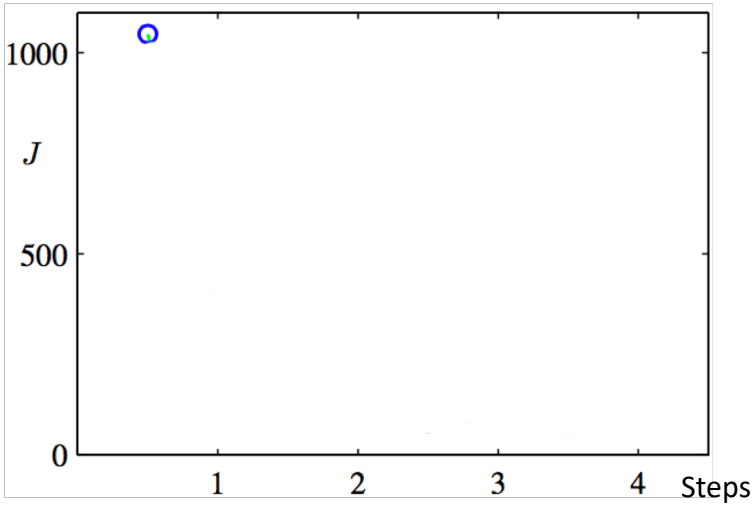
Equal distance line



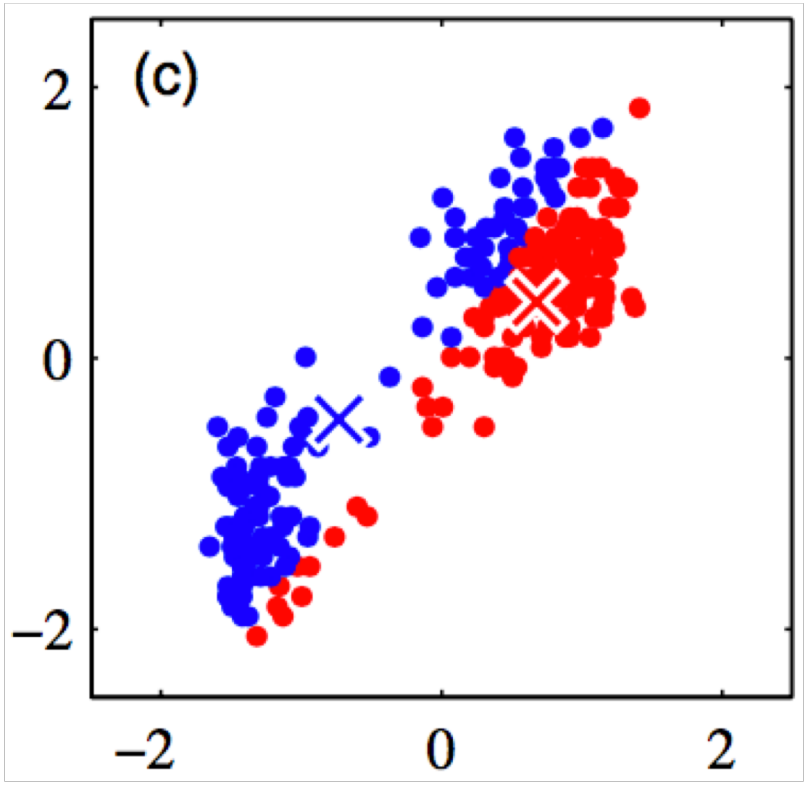
E Step

Assign the points to the nearest cluster:

$$r_{nk} = \begin{cases} 1 & \text{if } k = \arg\min_j \|\mathbf{x}_n - \boldsymbol{\mu}_j\|^2 \\ 0 & \text{otherwise.} \end{cases}$$



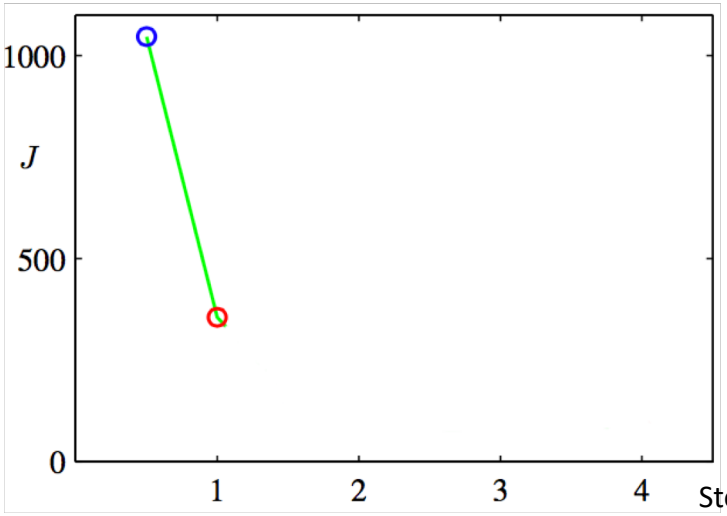
Given r_{n1}, r_{n2}, calculate $\boldsymbol{\mu}_1, \boldsymbol{\mu}_2$



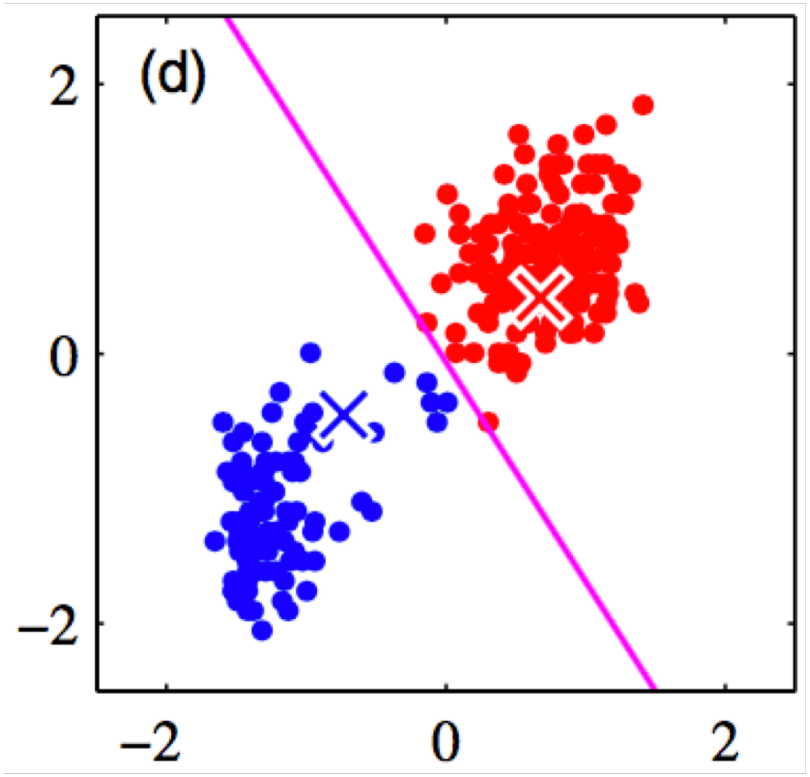
M Step

Calculate the means of the points in each cluster:

$$\boldsymbol{\mu}_k = \frac{\sum_n r_{nk}\mathbf{x}_n}{\sum_n r_{nk}}$$



Given $\boldsymbol{\mu}_1, \boldsymbol{\mu}_2$, calculate r_{n1}, r_{n2} for all n=1,…,N



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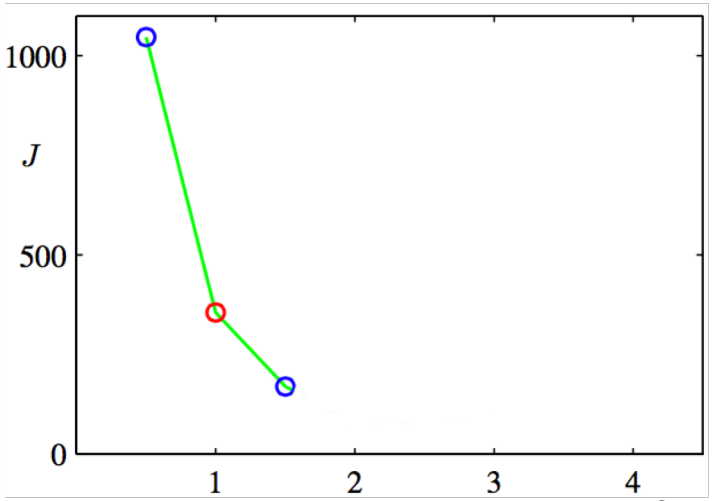
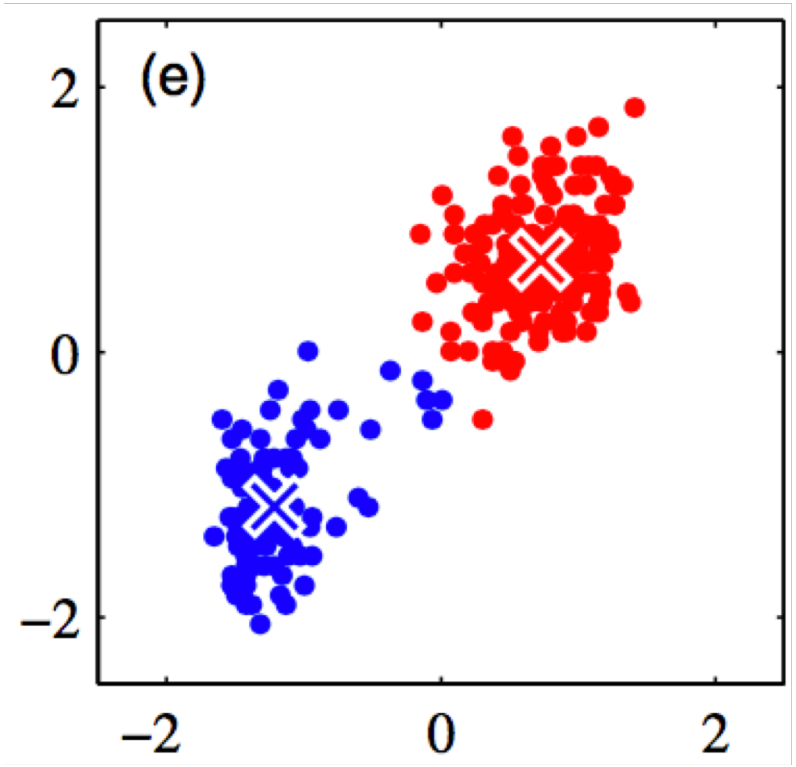


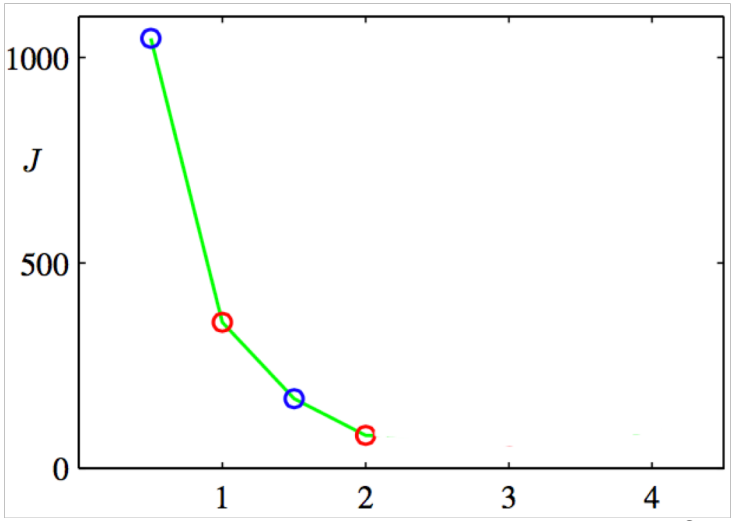
Given r_{n1}, r_{n2}, calculate $\boldsymbol{\mu}_1, \boldsymbol{\mu}_2$

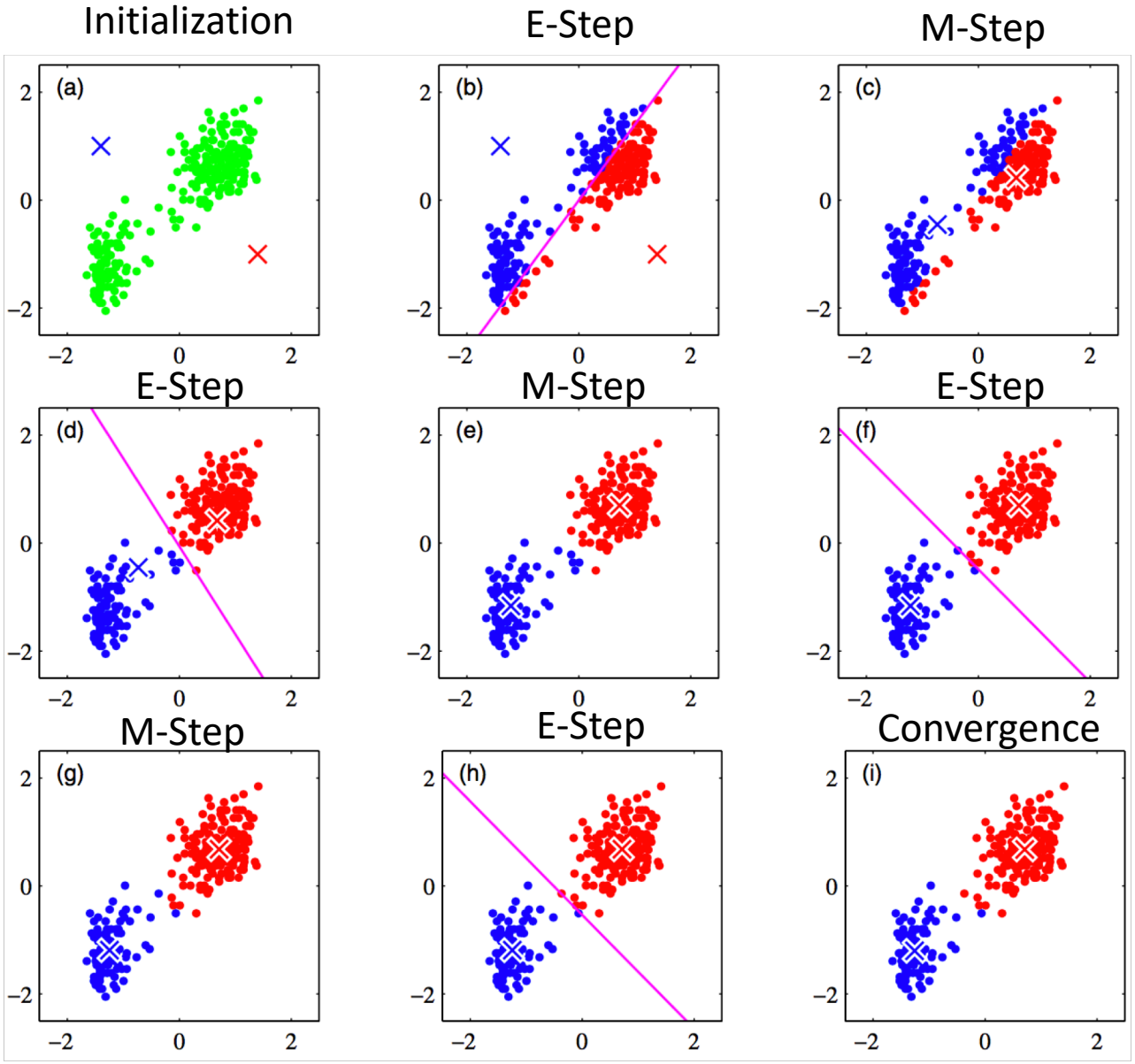


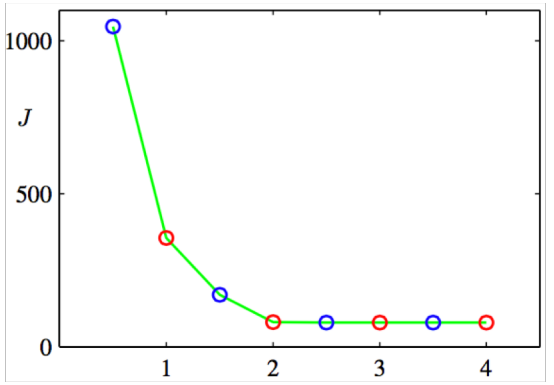
M Step

Calculate the means of the points in each cluster:

$$\boldsymbol{\mu}_k = \frac{\sum_n r_{nk}\mathbf{x}_n}{\sum_n r_{nk}}$$







If J does not change, or $\{ \boldsymbol{\mu}_1, \boldsymbol{\mu}_2 \}$ do not change, then the algorithm converges.

K均值法小结

- 初始化均值点$\boldsymbol{\mu}_1,\ldots,\boldsymbol{\mu}_k$
- 迭代如下
  - 把每个数据点按照就近原则分配给相应的$\boldsymbol{\mu}_i$
  - 把$\boldsymbol{\mu}_i$更新为所分配的数据点的均值
- 迭代停止，如果聚类分配不变

Initialize $\boldsymbol{m}_i, i = 1, \ldots, k$, for example, to k random $\boldsymbol{x}^t$

Repeat

For all $\boldsymbol{x}^t \in \mathcal{X}$

$$b_i^t \leftarrow \begin{cases} 1 & \text{if } \|\boldsymbol{x}^t - \boldsymbol{m}_i\| = \min_j \|\boldsymbol{x}^t - \boldsymbol{m}_j\| \\ 0 & \text{otherwise} \end{cases}$$

For all $\boldsymbol{m}_i, i = 1, \ldots, k$

$$\boldsymbol{m}_i \leftarrow \sum_t b_i^t \boldsymbol{x}^t / \sum_t b_i^t$$

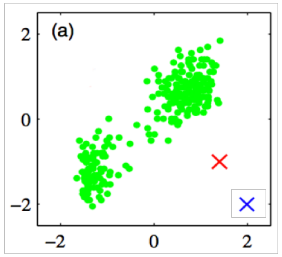
Until $\boldsymbol{m}_i$ converge

Basic ingredients

- Model or structure
- Objective function
- Algorithm
- Convergence

Questions for K-mean algorithm

- Does it find the global optimum of J?
  - No, the nearest local optimum, depending on initialization



- If Euclidean distance is not good for some data, do we have other choices?

- Can we assign each data point to the clusters probabilistically?

- If K (the total number of clusters) is unknown, can we estimate it from the data?

Outline

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  - K-mean clustering, **hierarchical clustering**
- Adaptive learning (online learning)
  - CL, FSCL, RPCL
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Hierarchical Clustering

- *k*-means clustering requires
  - *k*
  - Positions of initial centers
  - A distance measure between points (*e.g.* Euclidean distance)
- Hierarchical clustering requires a measure of distance between *groups* of data points

Adapted from Blei, D. *Hierarchial Cluster* [PwerPoint slides]. www.cs.princeton.edu/courses/archive/spr08/cos424/slides/clustering-2.pdf

Hierarchical Clustering

- Agglomerative clustering
- A very simple procedure:
  - Assign each data point into its own group
  - Repeat: look for the two closest groups and merge them into one group
  - Stop when all the data points are merged into a single cluster

Adapted from Blei, D. *Hierarchial Cluster* [PwerPoint slides]. www.cs.princeton.edu/courses/archive/spr08/cos424/slides/clustering-2.pdf

Distance Measure

- Distance between data points *a* and *b*:
  - $d(a, b)$
- Group A and B
  - Single-linkage

$$d(A, B) = \min_{a \in A, b \in B} d(a, b)$$

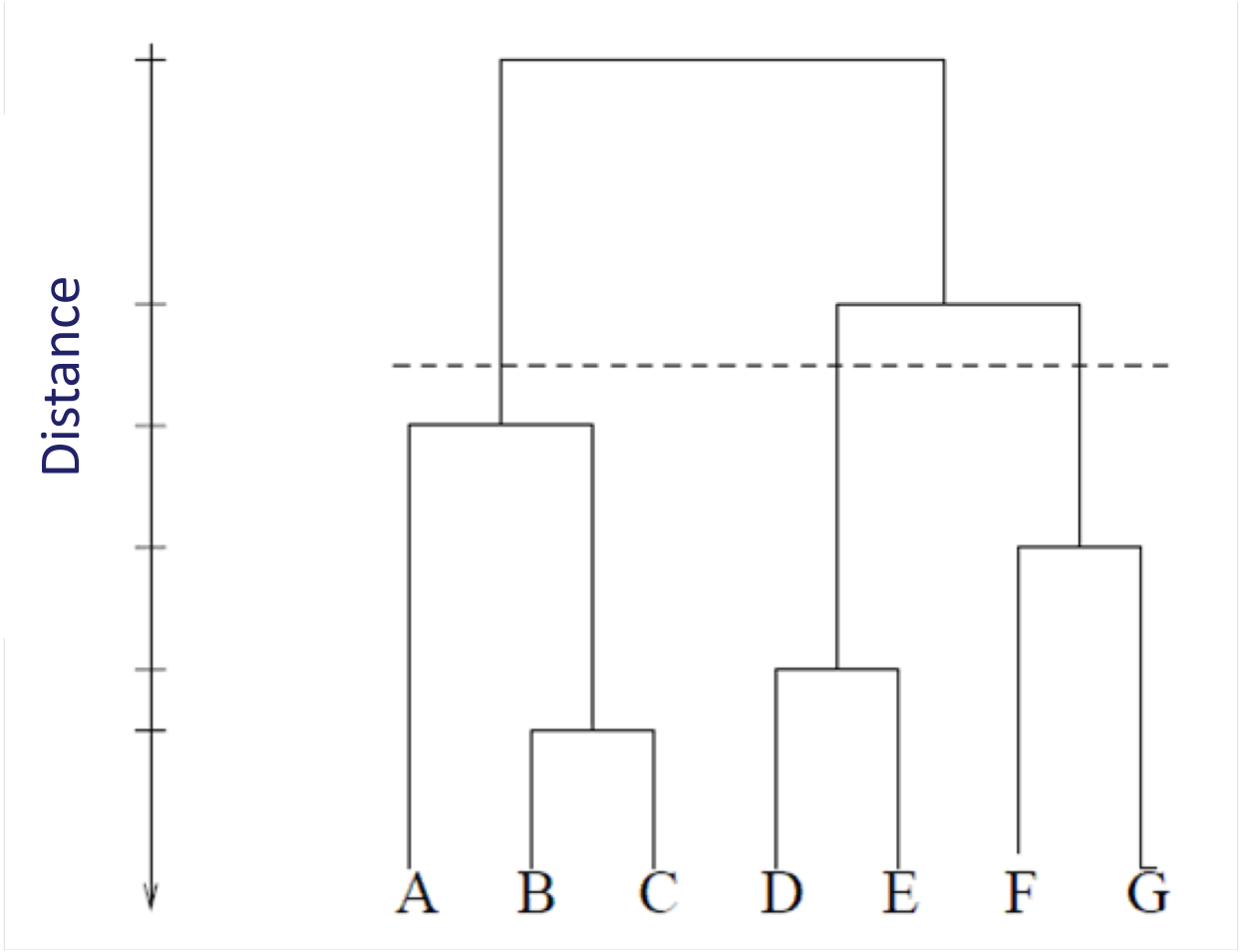
  - Complete-linkage

$$d(A, B) = \max_{a \in A, b \in B} d(a, b)$$

  - Average-linkage

$$d(A, B) = \frac{\sum_{a \in A, b \in B} d(a, b)}{|A| \cdot |B|}$$

Dendrogram



Jain, A. K., Murty, M. N., Flynn, P. J. (1999) "Data Clustering: A Review". ACM Computing Surveys (CSUR), 31(3), p.264-323, 1999.

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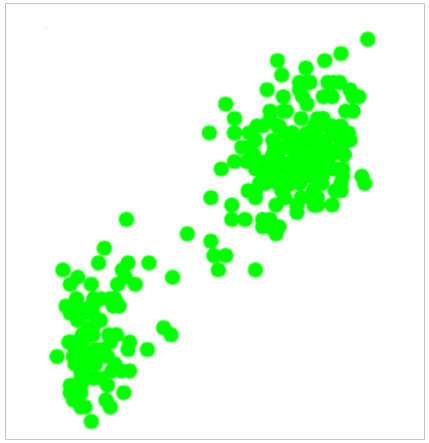
From batch to adaptive

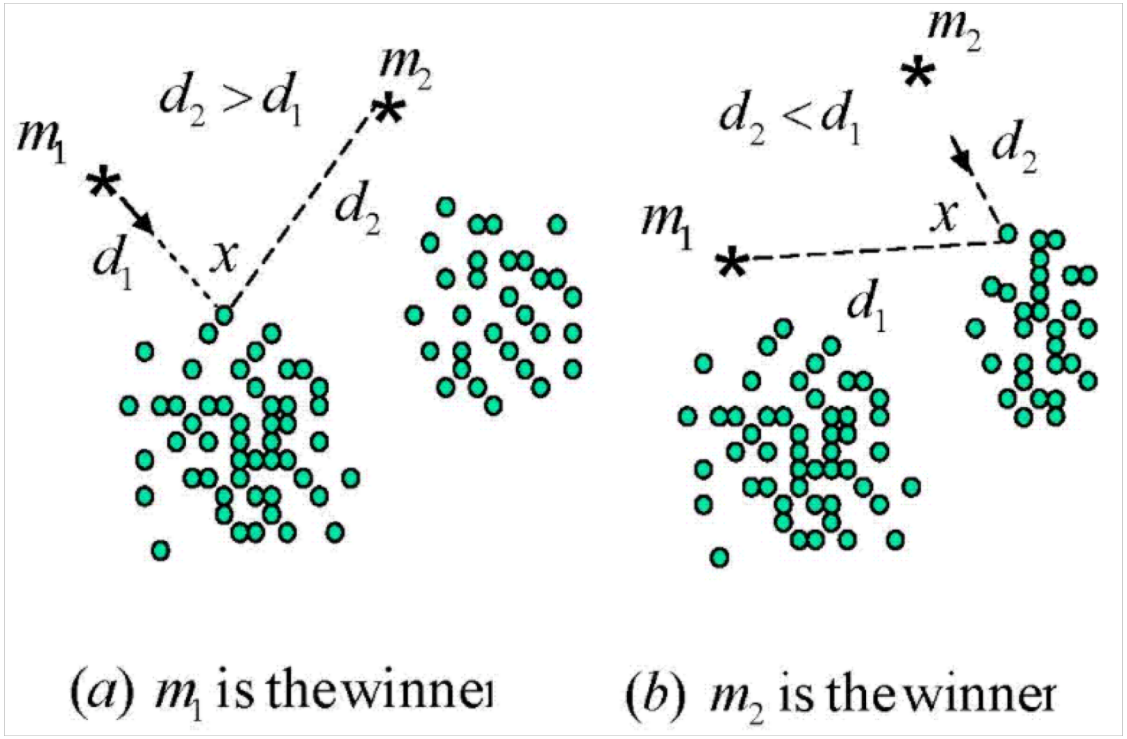
- Given a batch of data points



- Data points come one by one:

Competitive learning

- Data points come one by one:



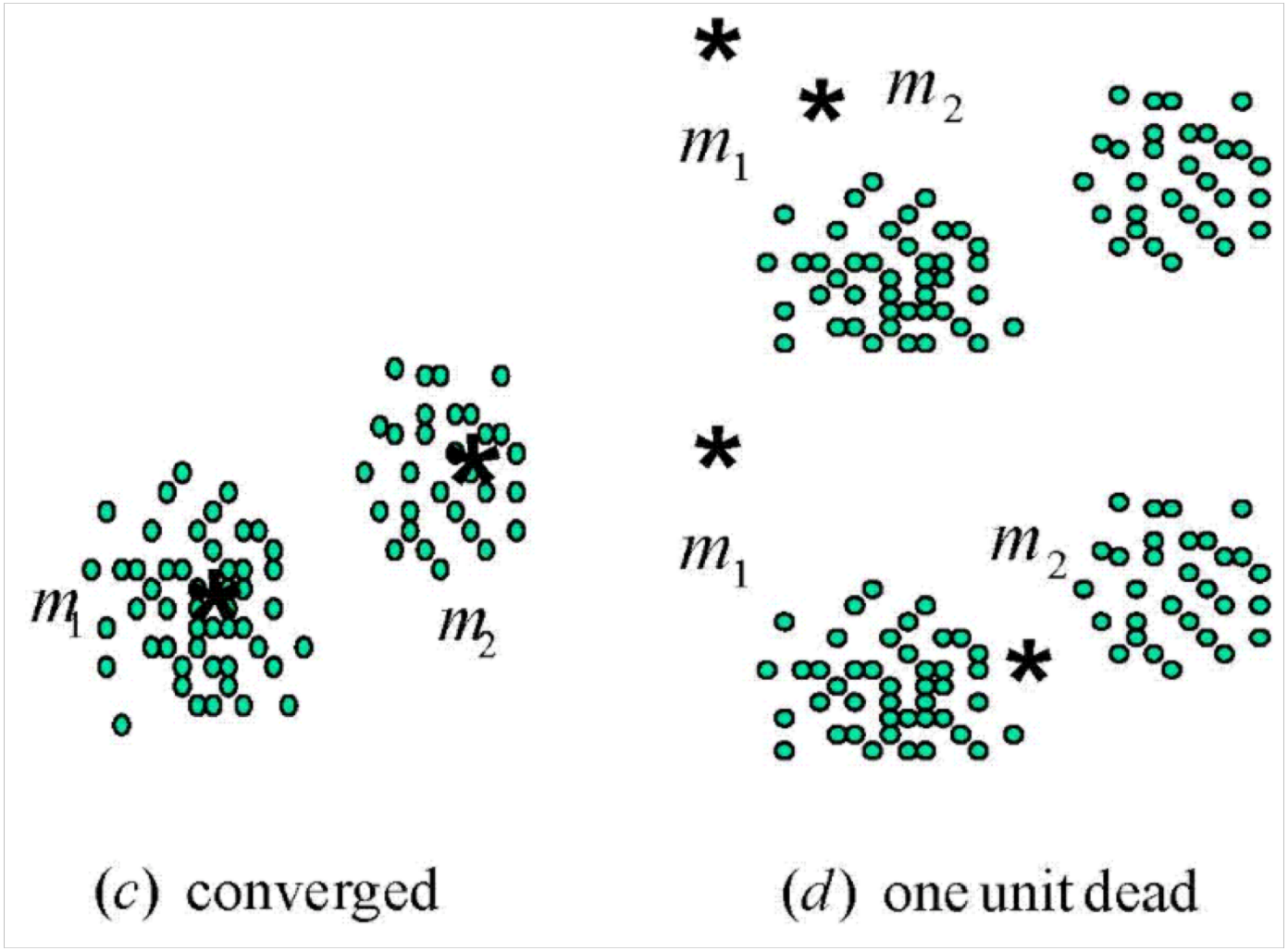
$$\varepsilon_t(\theta_j) = \|x_t - m_j\|^2$$

$$p_{j,t} = \begin{cases} 1, & \text{if } j = c, \\ 0, & \text{otherwise;} \end{cases}$$

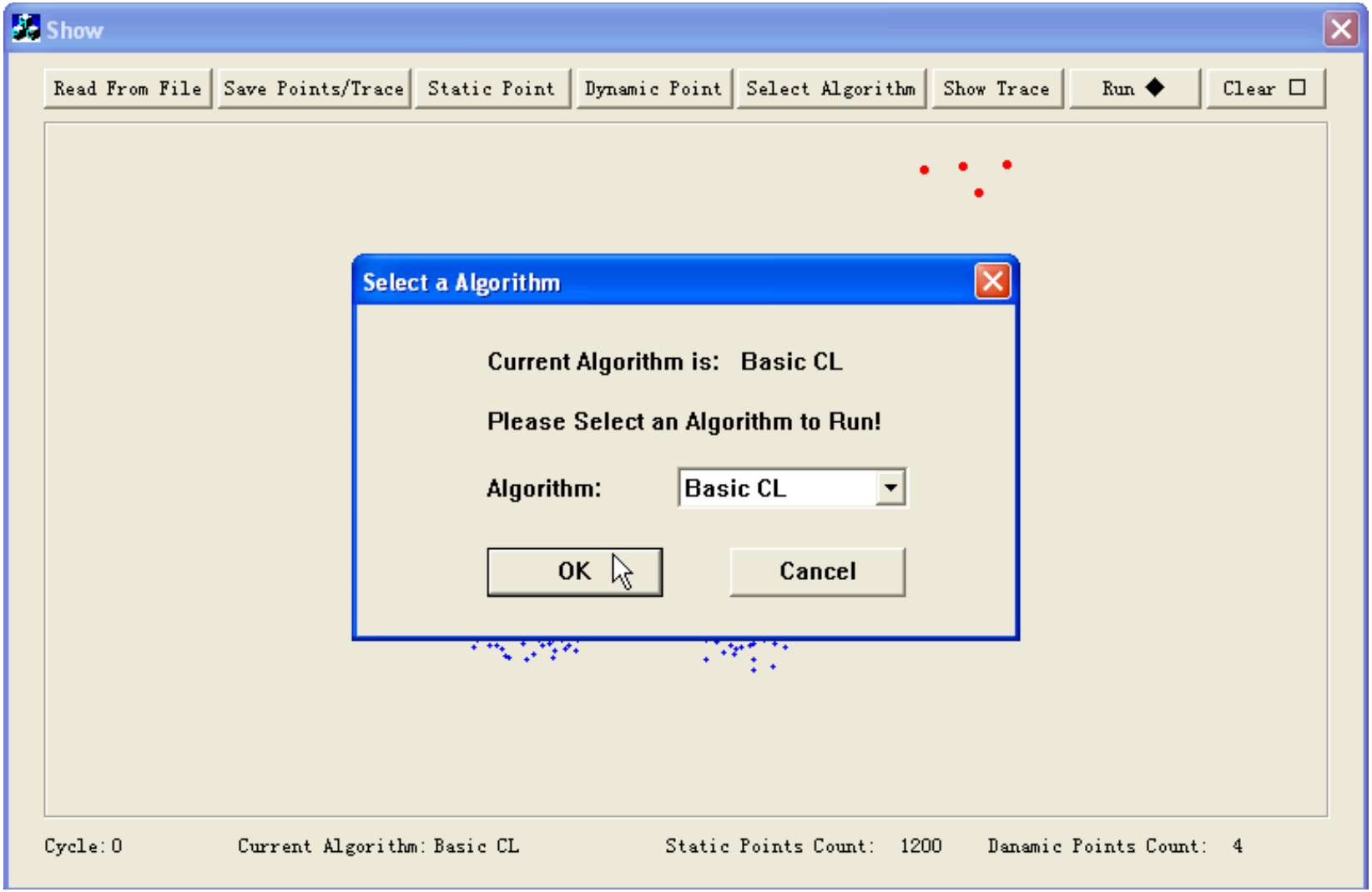
$$c = arg\ min_j \varepsilon_t(\theta_j).$$

$$m_j^{new} = m_j^{old} + \eta p_{j,t}(x_t - m_j^{old}).$$

When starting with “bad initializations”



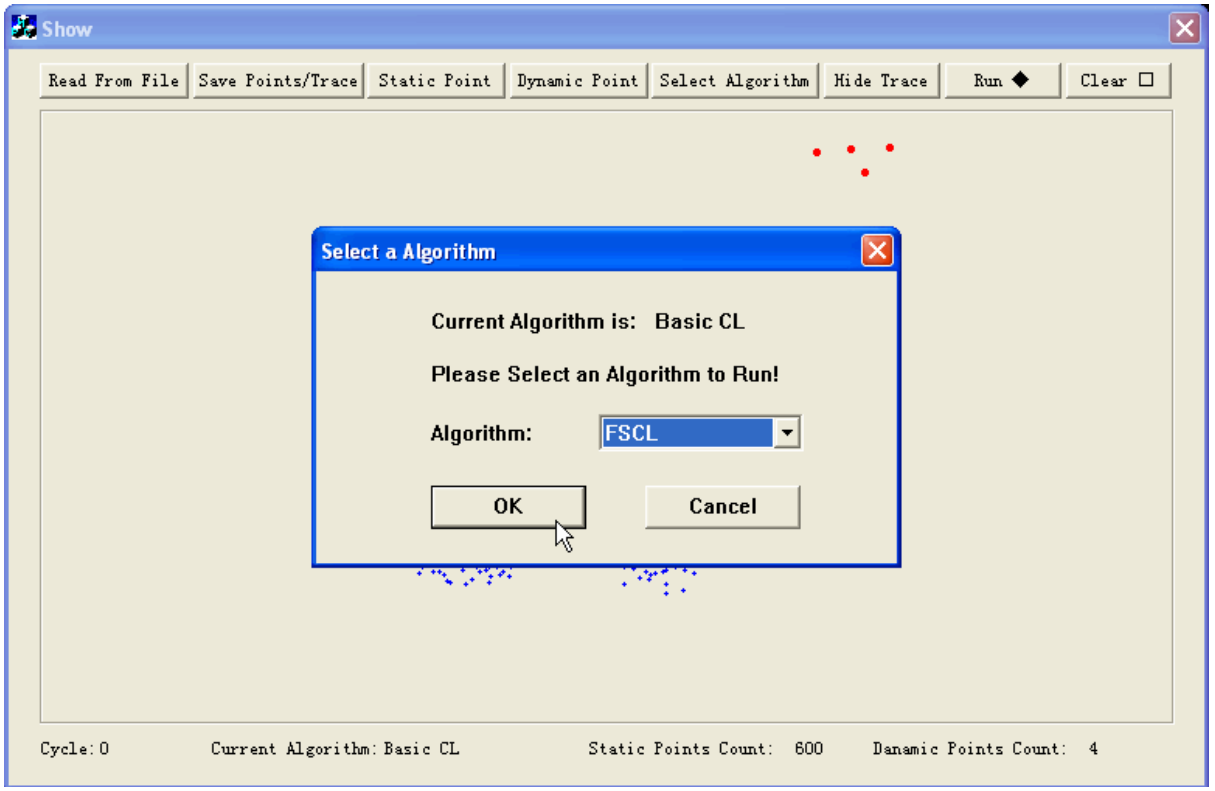
A four-cluster case



frequency sensitive competitive learning (FSCL) [Ahalt et al., 1990]

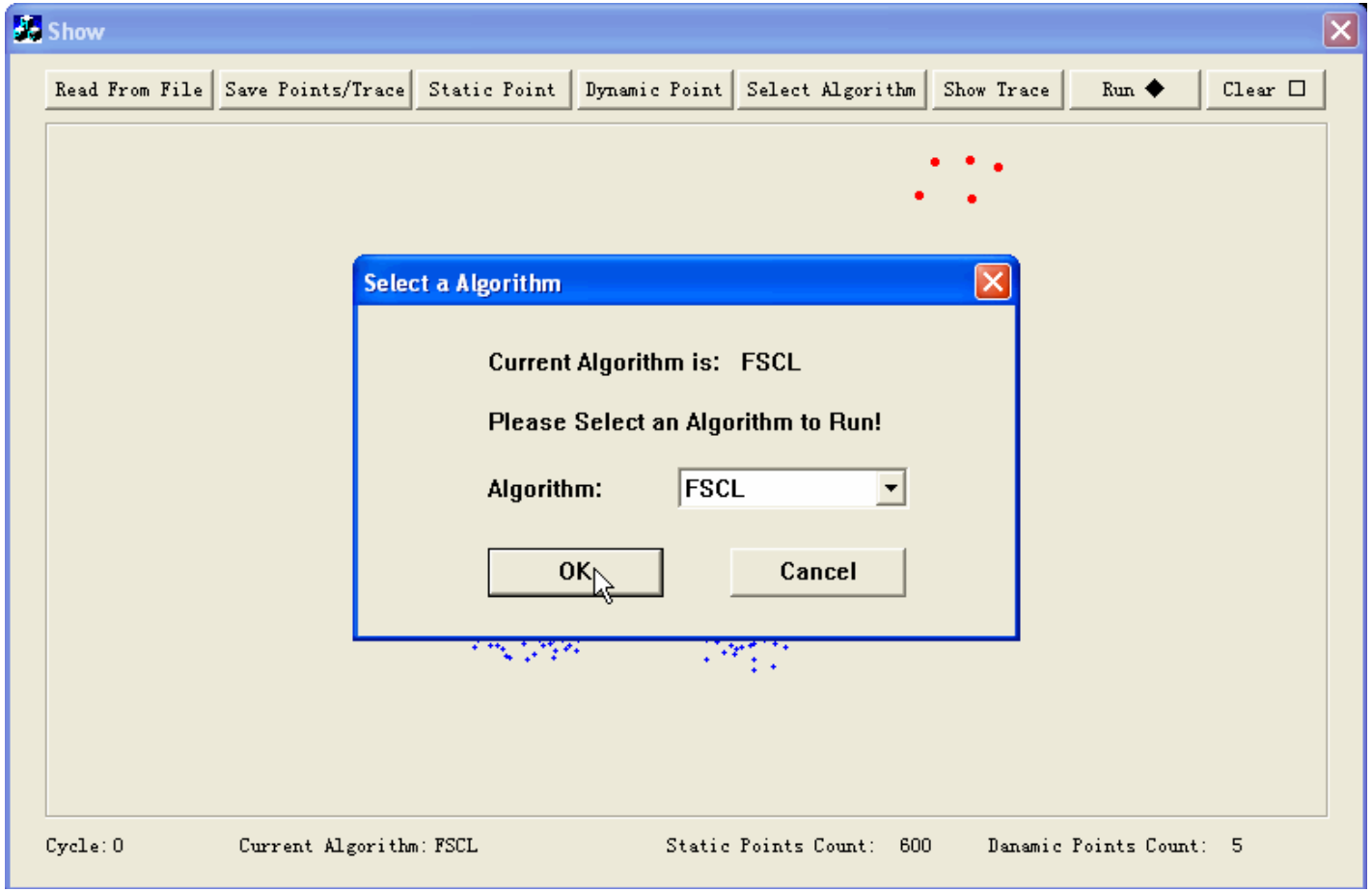
The idea is to penalize the frequent winners:

$$\varepsilon_t(\theta_j) = \alpha_j \|x_t - m_j\|^2$$



FSCL is not good when there are extra centers

When k is pre-assigned to 5. the frequency sensitive mechanism also brings the extra one into data to disturb the correct locations of others



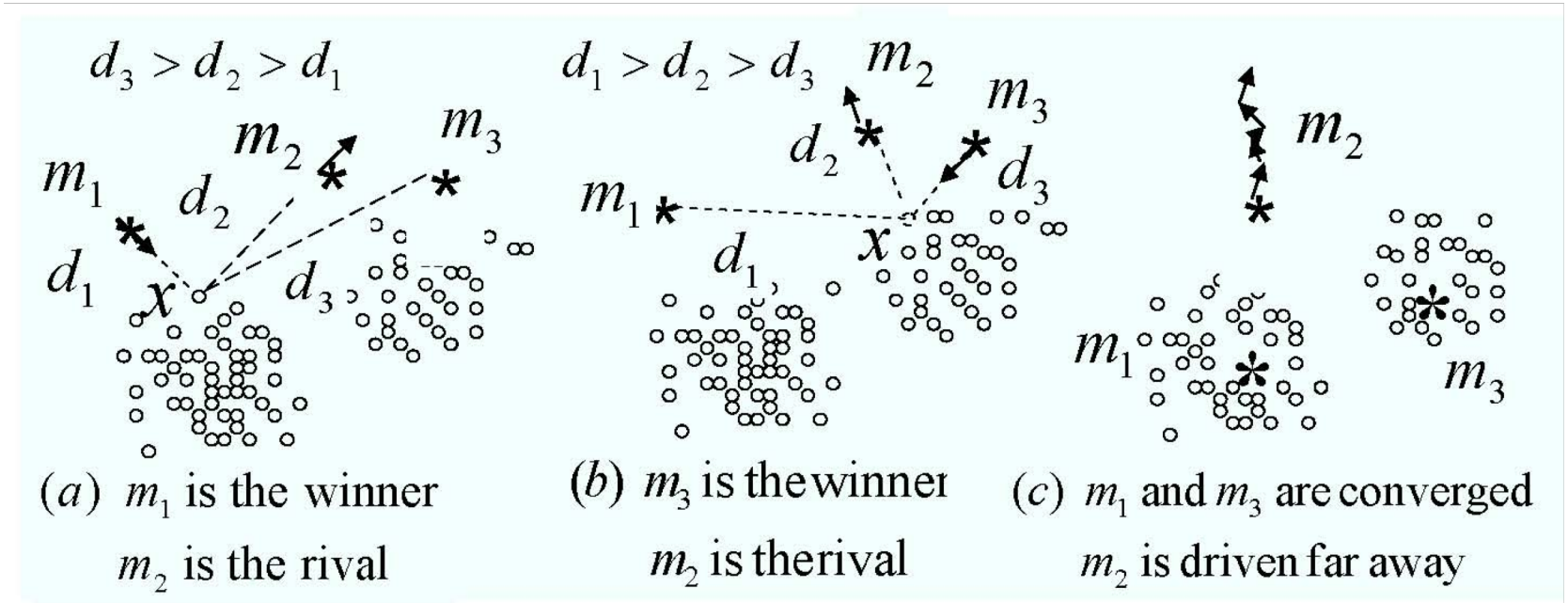
Rival penalized competitive learning (RPCL)

(Xu, Krzyzak, & Oja, 1992 , 1993)

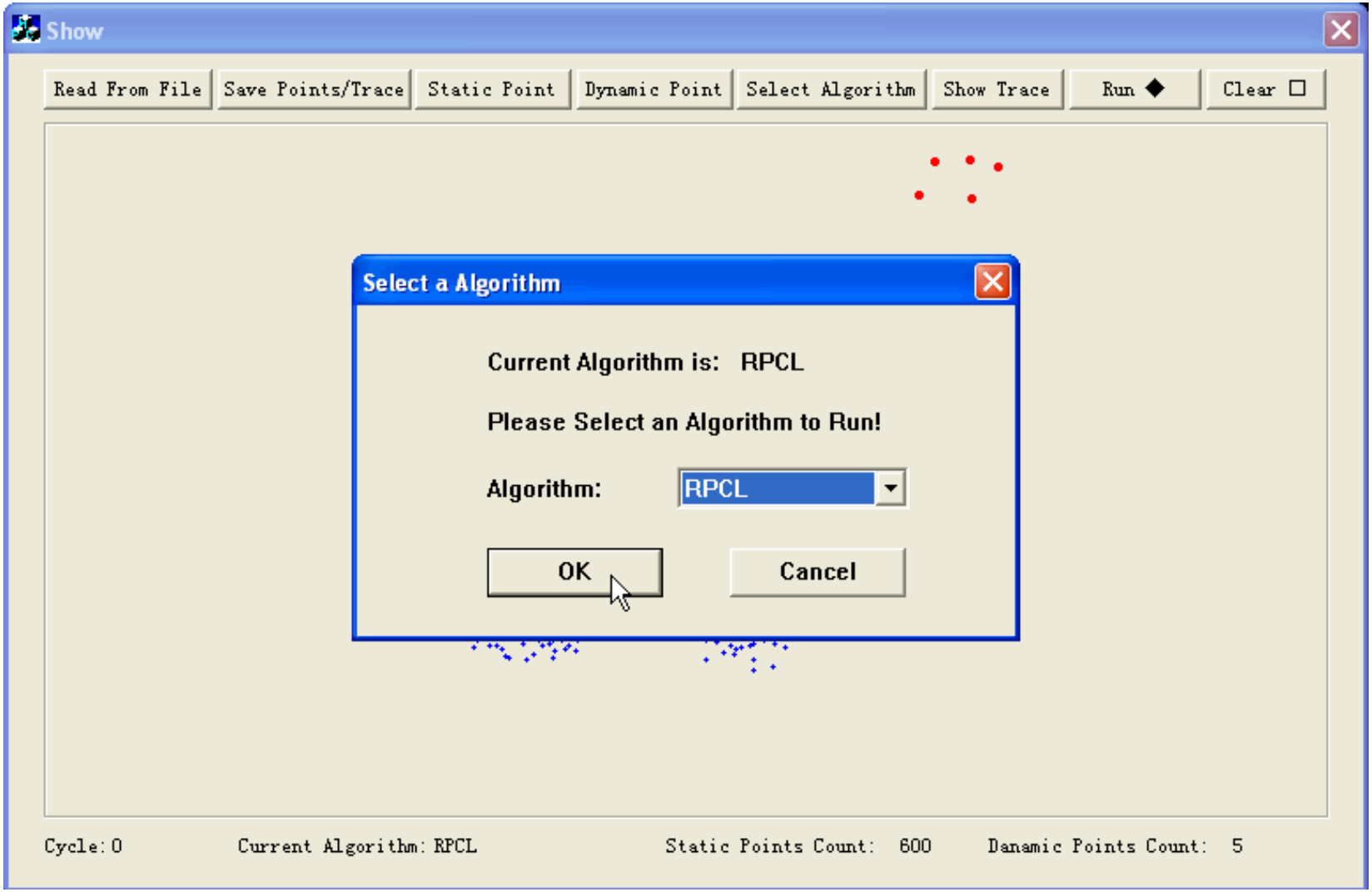
The RPCL differs from FSCL by implementing $p_{j,t}$ as follows:

$$p_{j,t} = \begin{cases} 1, & \text{if } j = c, \\ -\gamma, & \text{if } j = r, \\ 0, & \text{otherwise,} \end{cases} \quad \begin{cases} c = arg\ min_j \varepsilon_t(\theta_j), \\ r = arg\ min_{j \neq c} \varepsilon_t(\theta_j), \end{cases}$$

where γ approximately takes a number between 0.05 and 0.1 for controlling the penalizing strength.



Rival penalized mechanism makes extra agents driven far away.



Thank you!