Unsupervised learning
Clustering

Statistical Learning Part II – LM Data Science + LM Mathematics
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Motivation (1/2)

- **Supervised methods** (learning with a teacher):
  - **Input**: predictor variables $X^T=(X_1, \ldots , X_p)$
  - **Output**: Y
  - Predictions based on the **training set** $(x_1,y_1), \ldots, (x_N,y_N)$ of previously solved cases
  - **Loss function** $L(y, \hat{y})$, such as $L(y, \hat{y}) = (y - \hat{y})^2$
  - Supposing (X,Y) random variables supervised learning is a **density estimation problem**:

Determining the properties of the conditional density Pr(Y|X)

E.g.: location parameters that minimize the expected error

$$\mu(x) = \underset{\theta}{\operatorname{argmin}}\, E_{Y|X} L(Y, \theta).$$

Motivation (2/2)

- **Unsupervised methods** (learning **without** a teacher):
  - **Input**: predictor variables $X^T=(X_1, \dots , X_p)$
  - **Output**: not available
  - **Goal**: infer the **properties of the joint probability Pr(X)** without the help of a supervisor/teacher
  - In **low dimensional problems (p<=3)** Pr(X) can be directly estimated and graphically represented
  - In **high dimensional problems** descriptive statistics methods are used to characterize Pr(X)
    - **Low dimensional manifolds** representing high data density may be identified by **PCA** or other **dimensionality reduction** methods
    - **Cluster analysis** attempts to find multiple convex regions of the X-space that contain **modes** of Pr(X)
  - No direct measure of success (as loss function)

Unsupervised learning methods

- Association rules
- Clustering analysis
  - K-means
  - K-medoids
  - Gaussian Mixture Models
  - Hierarchical clustering
- Self-organizing maps
- Principal components, curves and subspaces
  - Spectral clustering
- Matrix factorization
- Other methods

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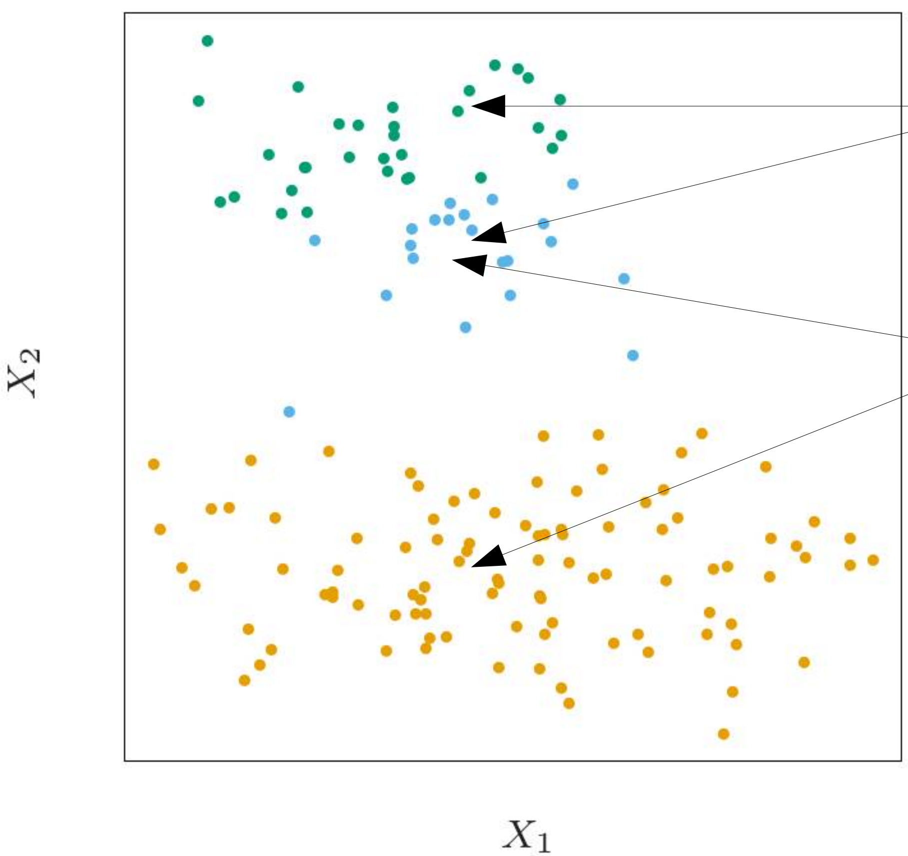
Cluster analysis

Goal

Grouping a collection of **objects** into **subsets** (**clusters**) such that objects **within** each clusters are **more closely related** to one another **than** objects assigned to **different** clusters



Not well separated
(similar properties)

Why?

Well separated
(different properties)

Measures of similarity/dissimilarity

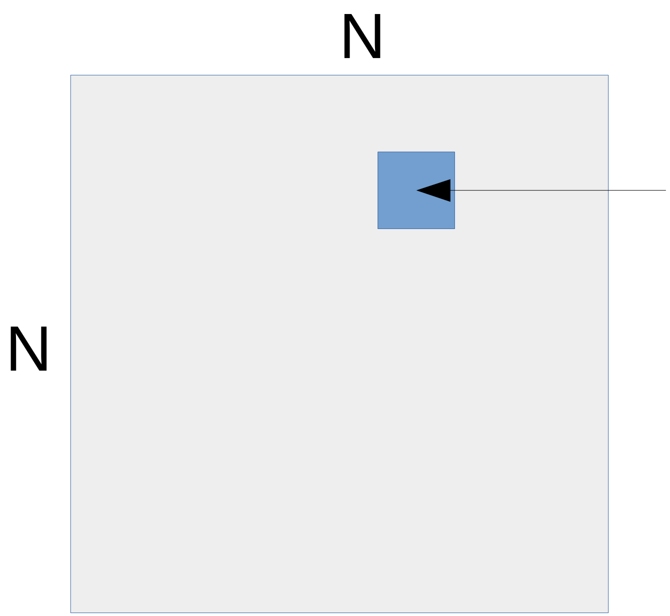
- Central to clustering analysis is the notion of **similarity/dissimilarity between individual objects**
- **Clustering methods** attempt to **group** the objects according to the definition of **similarity** supplied to it.

Similarity measure (clustering) ⟷ Loss function (supervised learning)

- **Examples of similarity/dissimilarity measures:**
  - Euclidean distance $$d(\mathbf{p},\mathbf{q}) = \sqrt{\sum_{i=1}^{n}(q_i - p_i)^2}$$
  - Manhattan distance $$d_1(\mathbf{p},\mathbf{q}) = \|\mathbf{p}-\mathbf{q}\|_1 = \sum_{i=1}^{n}|p_i - q_i|$$
  - Mahalanobis distance $$D_M(\vec{x}) = \sqrt{(\vec{x}-\vec{\mu})^T S^{-1}(\vec{x}-\vec{\mu})}$$
  - Correlation $$\rho_{X,Y} = \frac{E[(X-\mu_X)(Y-\mu_Y)]}{\sigma_X\sigma_Y}$$
  - Jaccard distance (categorical) $$J(A,B) = \frac{|A\cap B|}{|A\cup B|} = \frac{|A\cap B|}{|A|+|B|-|A\cap B|}$$

Proximity matrices

- Sometimes the data is represented directly in terms of proximity between pairs of objects (similarities or dissimilarities).
- N x N matrix



d_{ij} proximity between object i and object j

$d_{ii}=0$

- Dissimilarities are ***distances*** in the strict sense only if the triangle inequality $d_{ii'} \leq d_{ik} + d_{i'k}$, for all $k \in \{1, \ldots, N\}$ holds.

Dissimilarities based on attributes (1/2)

- Usually we have measurements x_{ij} i=1,…,N, on variables j=1,…,p (**attributes**).
- Then **pairwise dissimilarities** between **observations** can be expressed in terms of **attribute** values, that is

$$D(x_i, x_{i'}) = \sum_{j=1}^{p} d_j(x_{ij}, x_{i'j})$$

  where $d_j(x_{ij},x_{i'j})$ is the dissimilarity between values of the *j*-th attribute.
- Most common **d** function is the **squared distance**

$$d_j(x_{ij}, x_{i'j}) = (x_{ij} - x_{i'j})^2$$

Dissimilarities based on attributes (2/2)

- **Other choices** are possible depending on attribute types
  - **Quantitative variables**
    - Absolute difference $d(x_i, x_{i'}) = l(|x_i - x_{i'}|)$
    - Correlation $\rho(x_i, x_{i'}) = \dfrac{\sum_j (x_{ij} - \bar{x}_i)(x_{i'j} - \bar{x}_{i'})}{\sqrt{\sum_j (x_{ij} - \bar{x}_i)^2 \sum_j (x_{i'j} - \bar{x}_{i'})^2}}$
  - **Ordinal variables**
  - **Categorical variables**

Object dissimilarity (1/2)

- **Dissimilarities** of p **attributes** are then **combined** into a single overall measure of **dissimilarity $D(x_i,x_{i'})$ between objects**

- **Weighted average (convex combination):**

$$\boxed{D(x_i, x_{i'}) = \sum_{j=1}^{p} w_j \cdot d_j(x_{ij}, x_{i'j}); \quad \sum_{j=1}^{p} w_j = 1}$$

Weight of j-th attribute

- **Weight w_j** regulates the **relative influence** of **variable *j*** in determining the **overall dissimilarity** between objects

- All w_j=1 does **NOT** give all attributes equal influence

- The relative influence of the j-th variable is w_j * avg(d_j)

  where

$$\bar{d}_j = \frac{1}{N^2} \sum_{i=1}^{N} \sum_{i'=1}^{N} d_j(x_{ij}, x_{i'j})$$

Object dissimilarity (2/2)

- Hence, setting $w_j \sim 1/\mathrm{avg}(d_j)$ gives all attributes **equal influence** on the overall dissimilarity
- This is related to **data standardization** in supervised learning
- E.g., for squared error distance

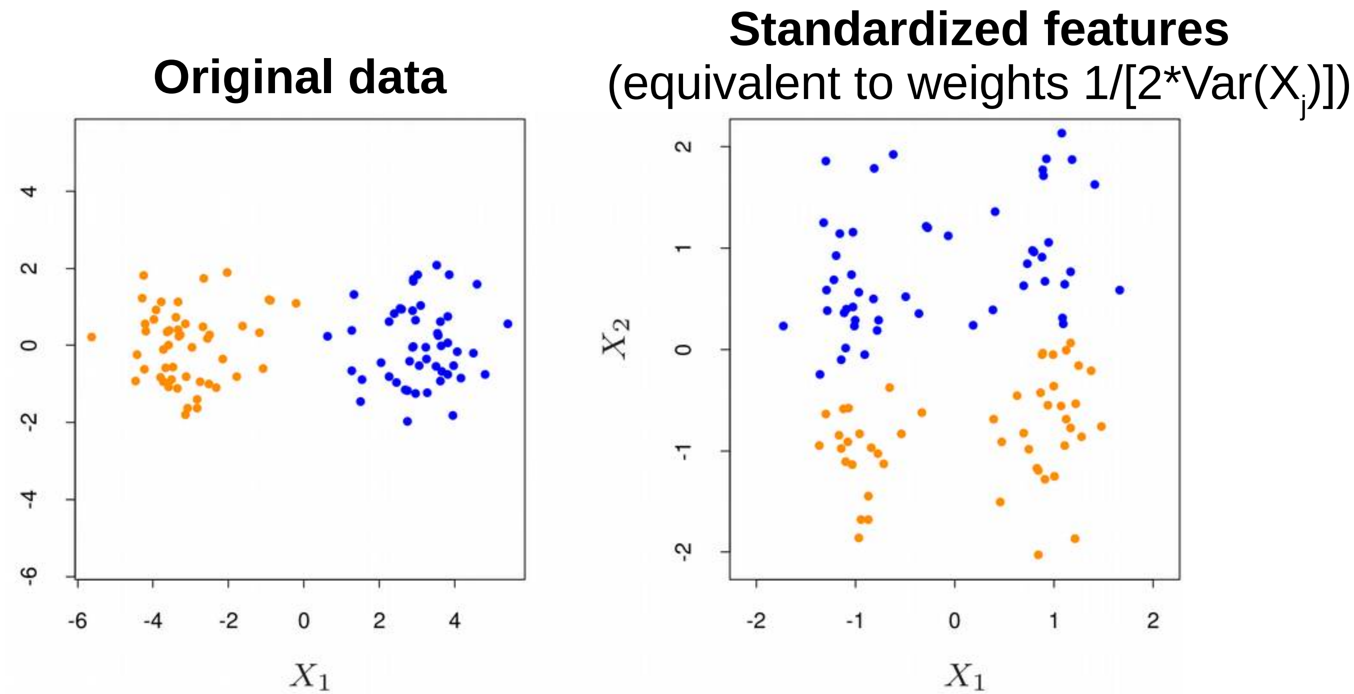
$$D_I(x_i, x_{i'}) = \sum_{j=1}^{p} w_j \cdot (x_{ij} - x_{i'j})^2$$

$$\bar{d}_j = \frac{1}{N^2} \sum_{i=1}^{N} \sum_{i'=1}^{N} (x_{ij} - x_{i'j})^2 = 2 \cdot \mathrm{var}_j$$

the **relative importance** of each attribute is **proportional** to its **variance** over the data

Attribute relative importance

- If the goal is **discovering natural grouping**, forcing equal influence among attributes can be **counterproductive.**
- **More relevant variables should have higher influence** in the object dissimilarity
- Giving all attributes equal influence tend to obscure the clusters to clustering algorithms



The choice of **appropriate dissimilarity measures** is often more **important** than the choice of the clustering algorithm

Clustering algorithms

Goal of clustering algorithms: to partition observations into groups such that pairwise dissimilarities between observations assigned to the same cluster tend to be smaller than those in different clusters

Algorithm types:

- Combinatorial
- Mixture modeling based
- Mode seekers

Combinatorial algorithms

- Most popular
- No probability model
- Pre-specified number of clusters K < N
- Each observation labeled by an integer *k* in {1,…,K}
- Assignments characterized by a many-to-one mapping (**encoder**):

$$k = C(i)$$

that assigns the i-th observation to the k-th cluster

Goal: seek the encoder $C^*(i)$ that minimizes a loss (or energy) function which depends on pairwise dissimilarities

$$W(C) = \frac{1}{2} \sum_{k=1}^{K} \sum_{C(i)=k} \sum_{C(i')=k} d(x_i, x_{i'})$$

Within cluster point scatter

- **Total point scatter**

$$T = \frac{1}{2}\sum_{i=1}^{N}\sum_{i'=1}^{N} d_{ii'} = \frac{1}{2}\sum_{k=1}^{K}\sum_{C(i)=k}\left(\sum_{C(i')=k} d_{ii'} + \sum_{C(i')\neq k} d_{ii'}\right)$$

- **Between-cluster point scatter**

$$B(C) = \frac{1}{2}\sum_{k=1}^{K}\sum_{C(i)=k}\sum_{C(i')\neq k} d_{ii'}$$

- **Relationships**

$$T = W(C) + B(C)$$

Minimizing W(C) is equivalent to maximizing B(C)

Complexity

- **Number of possible assignments** *(Jain ad Dubes, 1988)*

$$S(N,K) = \frac{1}{K!}\sum_{k=1}^{K}(-1)^{K-k}\binom{K}{k}k^N$$

- E.g., S(10,4)=34105, S(19,4)=10^{10}
- Heuristic strategies: iterative greedy descent
- Initial partition
- Iterative steps for reducing the loss
- Local optima

K-means

- **Squared error distance**

$$d(x_i, x_{i'}) = \sum_{j=1}^{p} (x_{ij} - x_{i'j})^2 = ||x_i - x_{i'}||^2$$

- **Within point scatter**

$$\begin{aligned} W(C) &= \frac{1}{2} \sum_{k=1}^{K} \sum_{C(i)=k} \sum_{C(i')=k} ||x_i - x_{i'}||^2 \\ &= \sum_{k=1}^{K} N_k \sum_{C(i)=k} ||x_i - \bar{x}_k||^2, \end{aligned}$$

Euclidean distance from the centroid (mean vector) of the k-th cluster

K-means algorithm

1) Given a cluster assignment C, the total cluster variance is minimized

$$\min_{C,\{m_k\}_1^K} \sum_{k=1}^{K} N_k \sum_{C(i)=k} ||x_i - m_k||^2$$

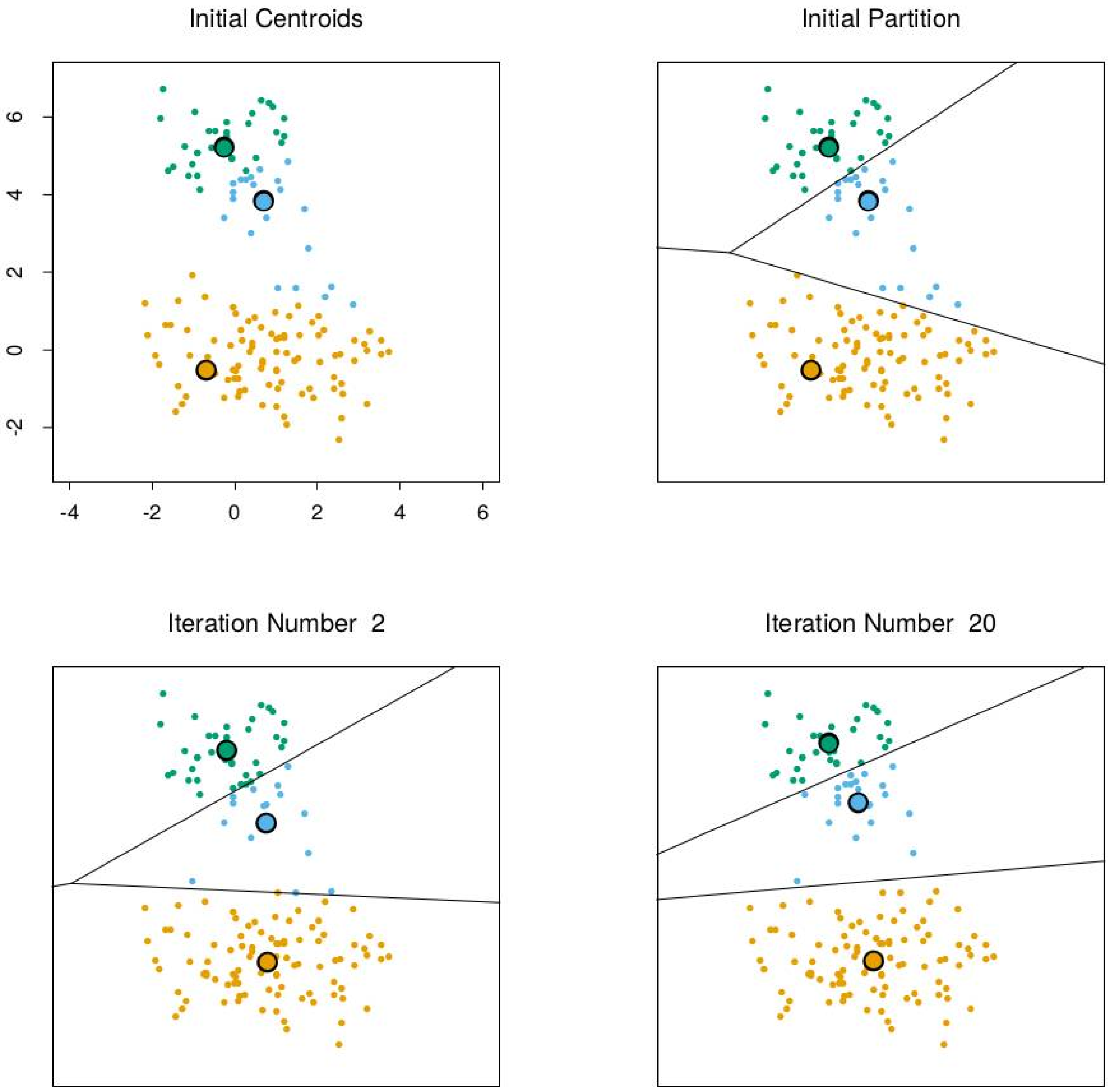
with respect to $\{m_1,\ldots,m_K\}$ yielding the means of the currently assigned clusters (i.e., computation of centroids from observations).

2)Given the current set of means $\{m_1,\ldots,m_K\}$ the total cluster variance is minimized by assigning each observation to the closest (current) cluster mean:

$$C(i) = \underset{1\le k\le K}{\operatorname{argmin}} ||x_i - m_k||^2$$

3) Itarate steps 1 and 2 until the assignments do not change.

Successive iterations of K-means



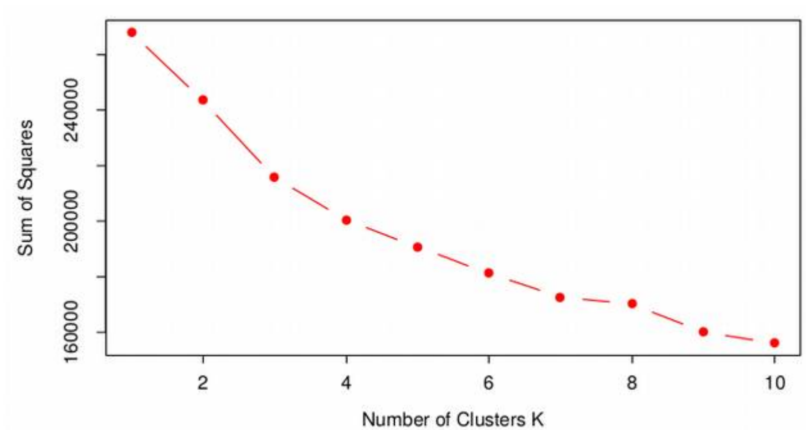
Exercise: Clustering of Human tumor microarray data

Description:

In The Elements of Statistical Learning
https://web.stanford.edu/~hastie/ElemStatLearn/
Page 5 abd Page 512

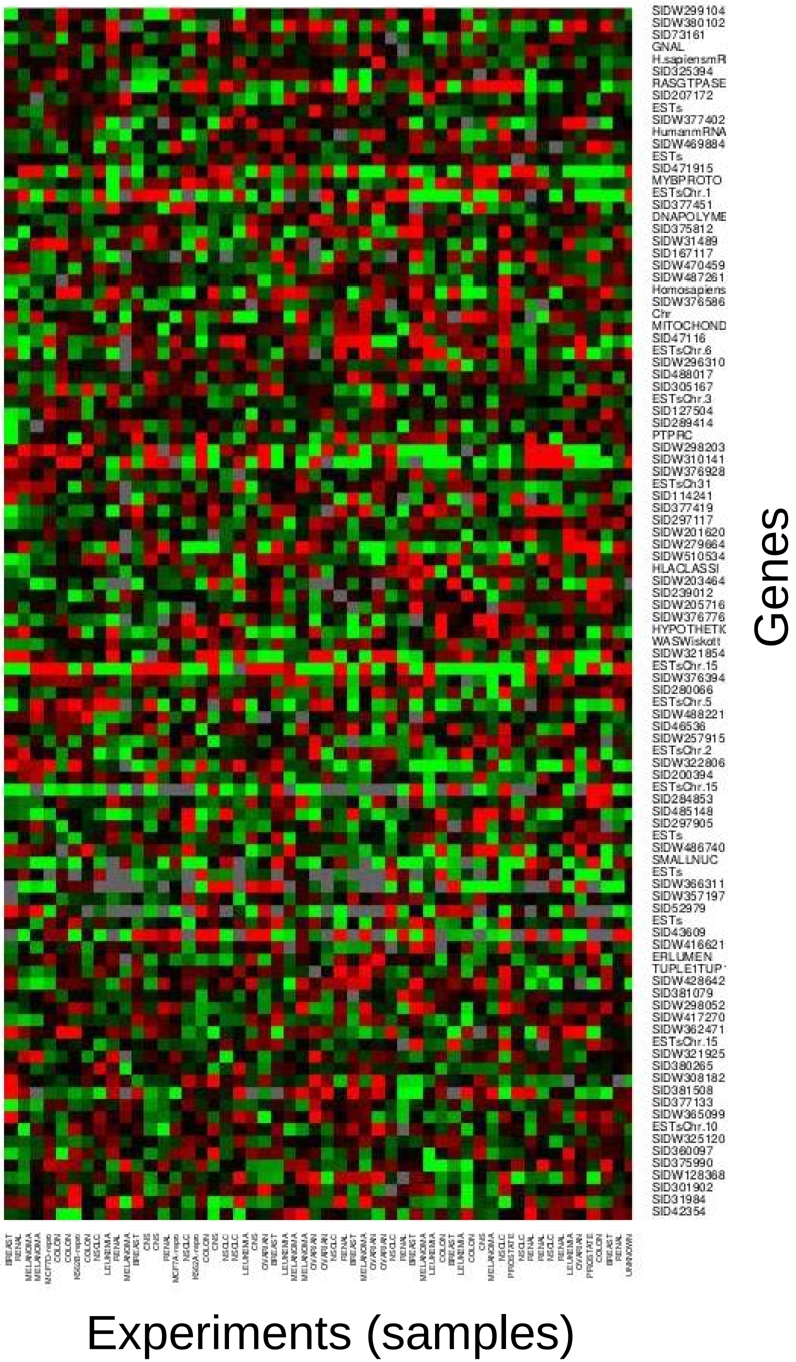
Description: See text of Exercise 5

Results:



Cluster	Breast	CNS	Colon	K562	Leukemia	MCF7
1	3	5	0	0	0	0
2	2	0	0	2	6	2
3	2	0	7	0	0	0

Cluster	Melanoma	NSCLC	Ovarian	Prostate	Renal	Unknown
1	1	7	6	2	9	1
2	7	2	0	0	0	0
3	0	0	0	0	0	0



References

[Hastie 2009] Trevor Hastie, Robert Tibshirani, Jerome Friedman. The Elements of Statistical Learning: Data Mining, Inference, and Prediction (second edition). Springer. 2009.