



# Probabilistic Hierarchical Clustering



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- Algorithmic hierarchical clustering
  - Nontrivial to choose a good distance measure
  - Hard to handle missing attribute values
  - Optimization goal not clear: heuristic, local search
- Probabilistic hierarchical clustering
  - Use probabilistic models to measure distances between clusters
  - Generative model: Regard the set of data objects to be clustered as a sample of the underlying data generation mechanism to be analyzed
  - Easy to understand, same efficiency as algorithmic agglomerative clustering method, can handle partially observed data
- In practice, assume the generative models adopt common distribution functions, e.g., Gaussian distribution or Bernoulli distribution, governed by parameters

# Generative Model

- Given a set of 1-D points  $X = \{x_1, \dots, x_n\}$  for clustering analysis & assuming they are generated by a Gaussian distribution:

$$\mathcal{N}(\mu, \sigma^2) = \frac{1}{\sqrt{2\pi\sigma^2}} e^{-\frac{(x-\mu)^2}{2\sigma^2}}$$

- The probability that a point  $x_i \in X$  is generated by the model:

$$P(x_i|\mu, \sigma^2) = \frac{1}{\sqrt{2\pi\sigma^2}} e^{-\frac{(x_i-\mu)^2}{2\sigma^2}}$$

- The likelihood that  $X$  is generated by the model:

$$L(\mathcal{N}(\mu, \sigma^2) : X) = P(X|\mu, \sigma^2) = \prod_{i=1}^n \frac{1}{\sqrt{2\pi\sigma^2}} e^{-\frac{(x_i-\mu)^2}{2\sigma^2}}$$

- The task of learning the generative model: find the parameters  $\mu$  and  $\sigma^2$  such that

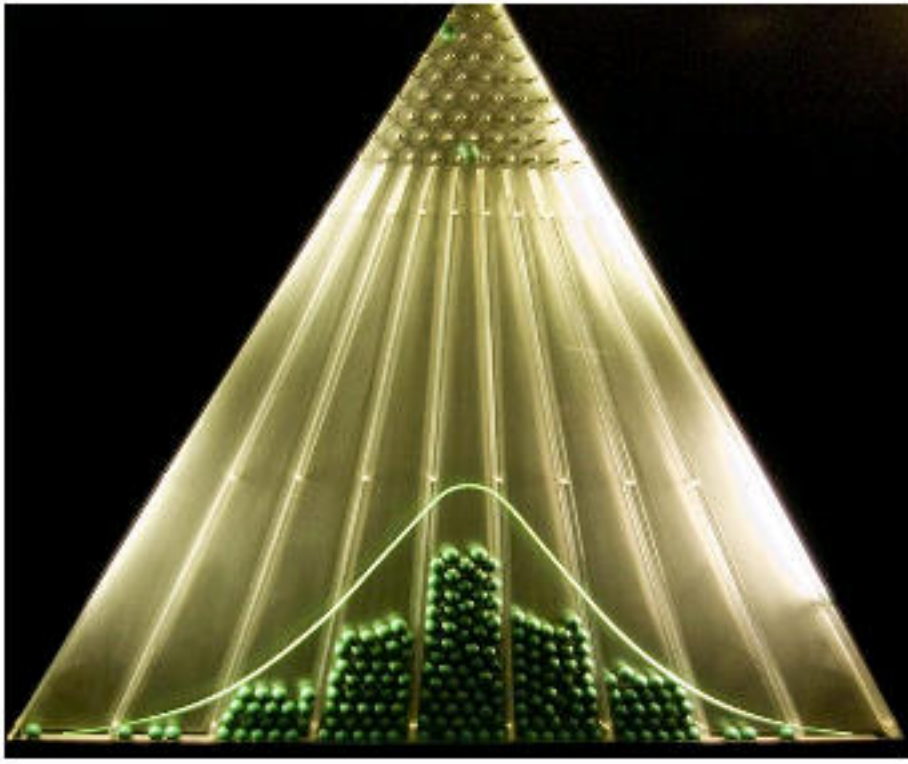
$$\mathcal{N}(\mu_0, \sigma_0^2) = \arg \max \{L(\mathcal{N}(\mu, \sigma^2) : X)\}$$

the maximum likelihood

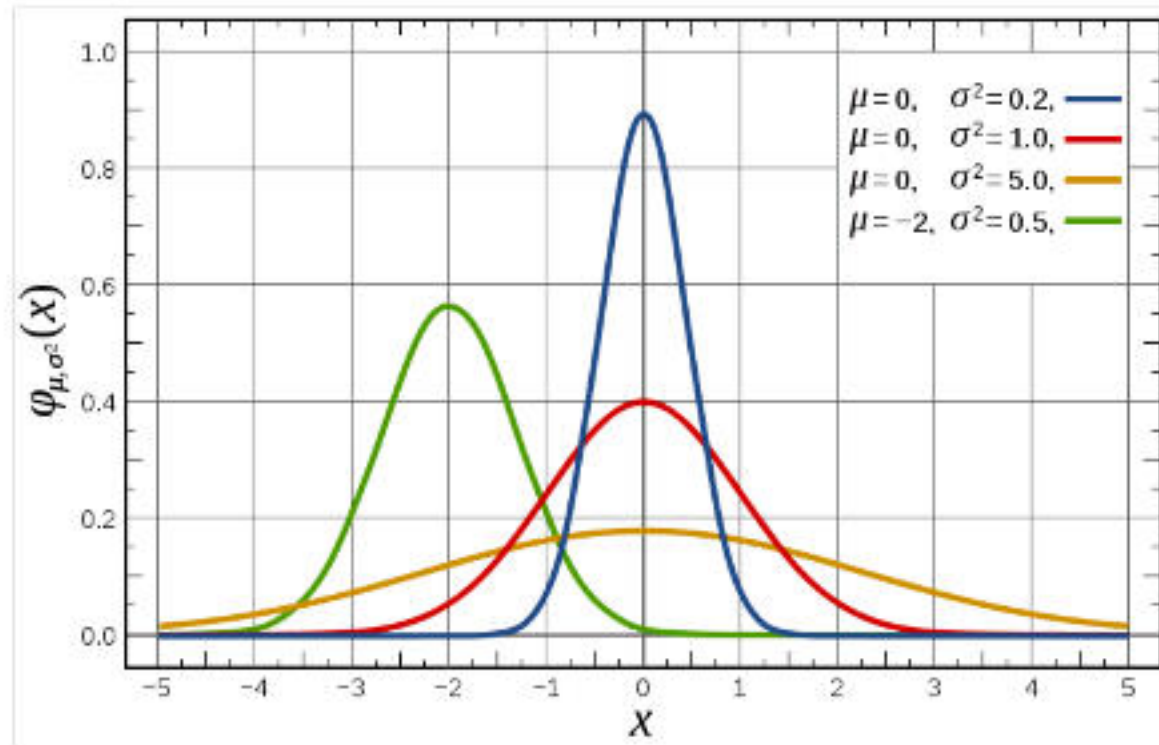
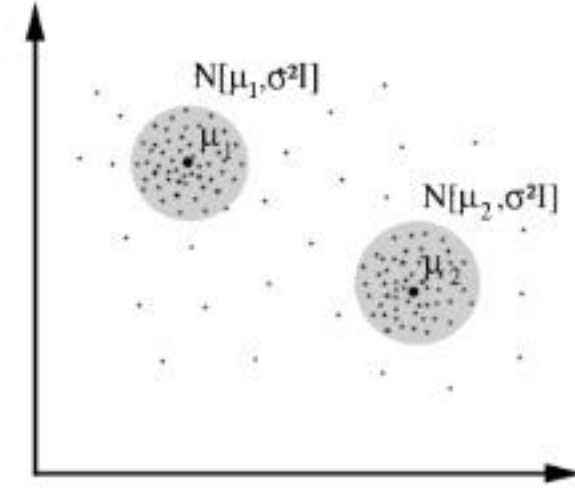




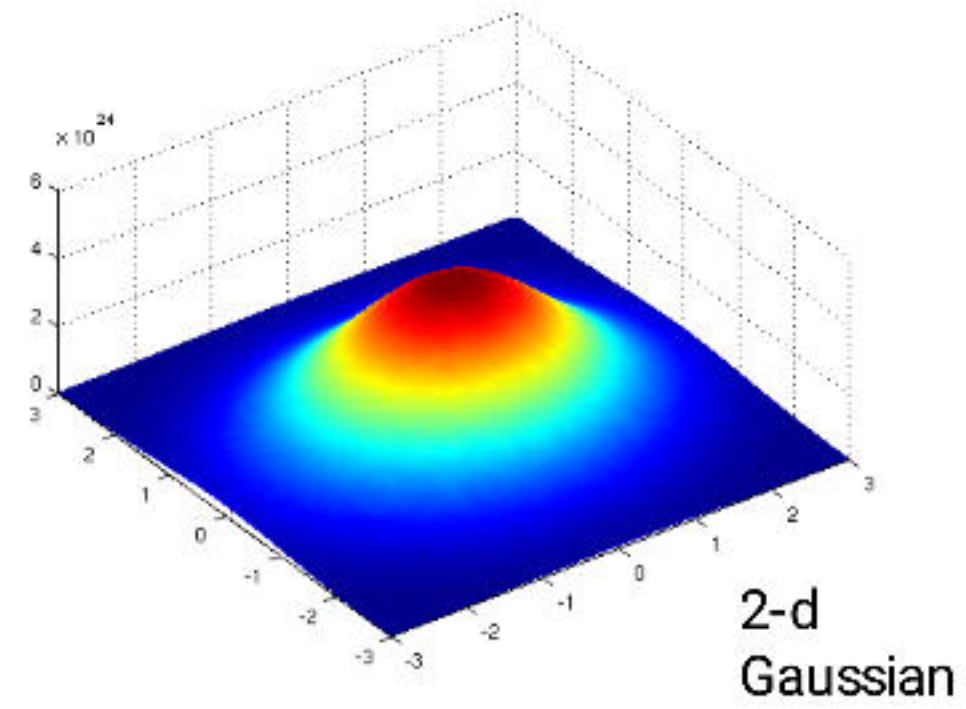
# Gaussian Distribution



Bean  
machine:  
drop ball  
with pins



1-d  
Gaussian



2-d  
Gaussian

From wikipedia and <http://home.dei.polimi.it>

# A Probabilistic Hierarchical Clustering Algorithm

- For a set of objects partitioned into  $m$  clusters  $C_1, \dots, C_m$ , the quality can be measured by,

$$Q(\{C_1, \dots, C_m\}) = \prod_{i=1}^m P(C_i)$$

where  $P()$  is the maximum likelihood

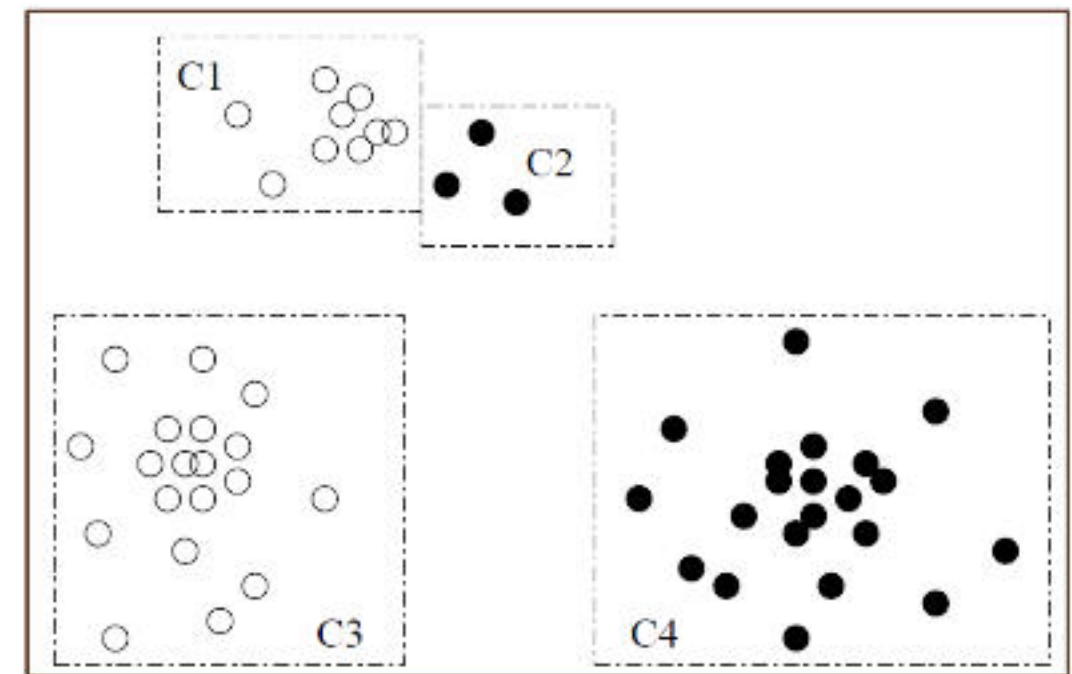
- If we merge two clusters  $C_{j_1}$  and  $C_{j_2}$  into a cluster  $C_{j_1} \cup C_{j_2}$ , the change in quality of the overall clustering is

$$\begin{aligned} & Q(\{C_1, \dots, C_m\} - \{C_{j_1}, C_{j_2}\} \cup \{C_{j_1} \cup C_{j_2}\}) - Q(\{C_1, \dots, C_m\}) \\ &= \frac{\prod_{i=1}^m P(C_i) \cdot P(C_{j_1} \cup C_{j_2})}{P(C_{j_1})P(C_{j_2})} - \prod_{i=1}^m P(C_i) \\ &= \prod_{i=1}^m P(C_i) \left( \frac{P(C_{j_1} \cup C_{j_2})}{P(C_{j_1})P(C_{j_2})} - 1 \right) \end{aligned}$$

- Distance between clusters  $C_1$  and  $C_2$ :

$$\text{dist}(C_i, C_j) = -\log \frac{P(C_1 \cup C_2)}{P(C_1)P(C_2)}$$

- If  $\text{dist}(C_i, C_j) < 0$ , merge  $C_i$  and  $C_j$





# Recommended Readings

- A. K. Jain and R. C. Dubes. Algorithms for Clustering Data. Prentice Hall, 1988
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- Jiawei Han, Micheline Kamber, and Jian Pei. Data Mining: Concepts and Techniques. Morgan Kaufmann, 3<sup>rd</sup> ed. , 2011 (Chap. 10)
- C. K. Reddy and B. Vinzamuri. A Survey of Partitional and Hierarchical Clustering Algorithms, in (Chap. 4) Aggarwal and Reddy (eds.), Data Clustering: Algorithms and Applications. CRC Press, 2014
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