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 $X = \{x_1, \ldots, x_n\}$ 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:

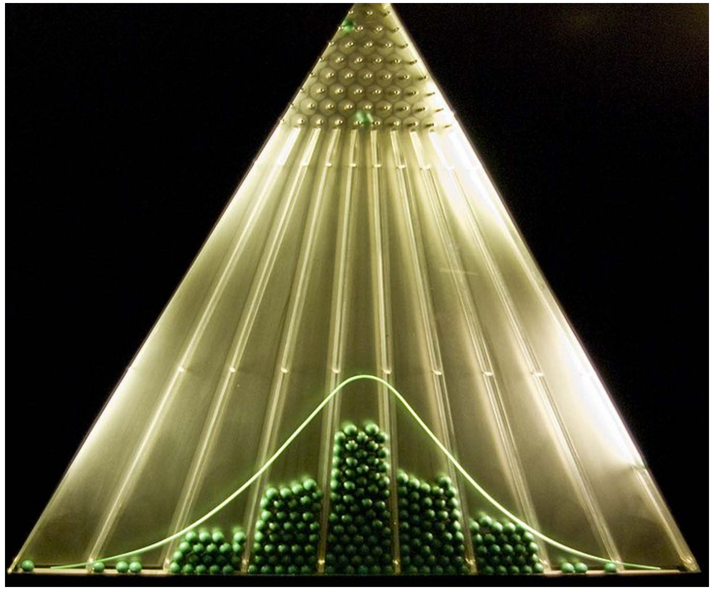
$$L(\mathcal{N}(\mu, \sigma^2) : X) = P(X|\mu, \sigma^2) = \prod_{i=1}^{n} \frac{1}{\sqrt{2\pi\sigma^2}} e^{-\frac{(x_i-\mu)^2}{2\sigma^2}}$$

- The task of learning the generative model: find the parameters μ and σ^2 such that

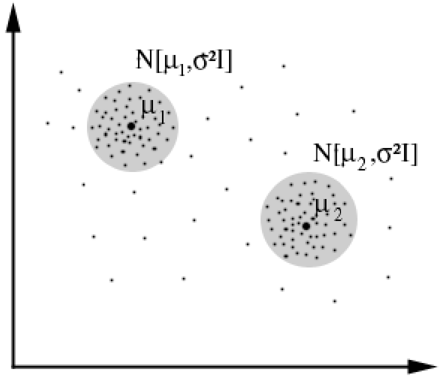
the maximum likelihood

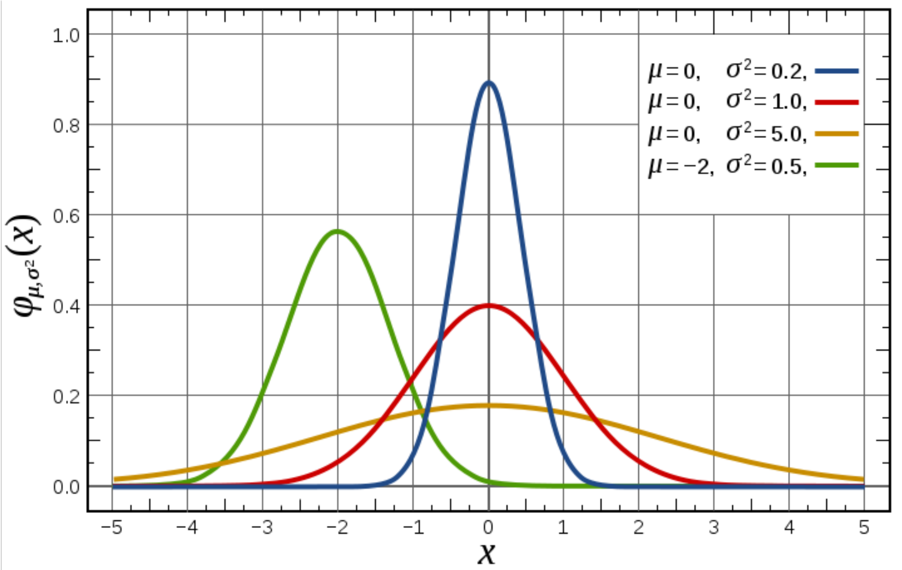
$$\mathcal{N}(\mu_0, \sigma_0^2) = \arg\max\{L(\mathcal{N}(\mu, \sigma^2) : X)\}$$

Gaussian Distribution

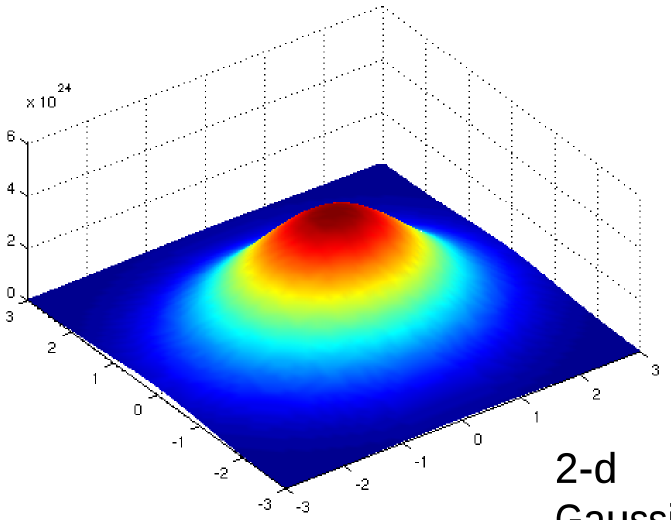


Bean machine: drop ball with pins





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,

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

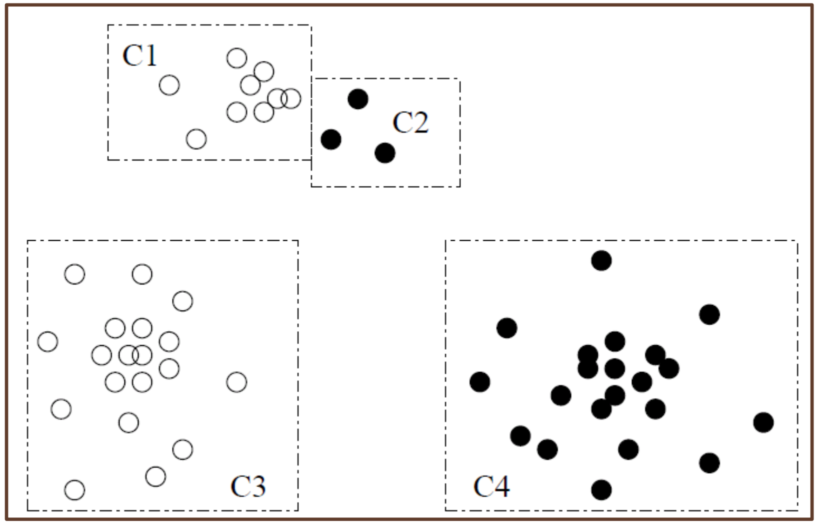
  where *P*() is the maximum likelihood

- If we merge two clusters C_{j1} and C_{j2} into a cluster $C_{j1} \cup C_{j2}$, the change in quality of the overall clustering is

$$Q((\{C_1, \dots, C_m\} - \{C_{j_1}, C_{j_2}\}) \cup \{C_{j_1} \cup C_{j_2}\}) - Q(\{C_1, \dots, C_m\})$$

$$= \frac{\prod_{i=1}^{m} P(C_i) \cdot P(C_{j_1} \cup C_{j_2})}{P(C_{j_1}) P(C_{j_2})} - \prod_{i=1}^{m} P(C_i)$$

$$= \prod_{i=1}^{m} P(C_i) \left(\frac{P(C_{j_1} \cup C_{j_2})}{P(C_{j_1}) P(C_{j_2})} - 1 \right)$$



- Distance between clusters C_1 and C_2:

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

- If $dist(C_i, C_j) < 0$, merge C_i and C_j

Recommended Readings

- A. K. Jain and R. C. Dubes. Algorithms for Clustering Data. Prentice Hall, 1988
- L. Kaufman and P. J. Rousseeuw. Finding Groups in Data: An Introduction to Cluster Analysis. John Wiley & Sons, 1990
- T. Zhang, R. Ramakrishnan, and M. Livny. BIRCH: An Efficient Data Clustering Method for Very Large Databases. SIGMOD'96
- S. Guha, R. Rastogi, and K. Shim. Cure: An Efficient Clustering Algorithm for Large Databases. SIGMOD’98
- G. Karypis, E.-H. Han, and V. Kumar. CHAMELEON: A Hierarchical Clustering Algorithm Using Dynamic Modeling. *COMPUTER*, 32(8): 68-75, 1999.
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- 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
- M. J. Zaki and W. Meira, Jr.. Data Mining and Analysis: Fundamental Concepts and Algorithms. Cambridge Univ. Press, 2014