Lecture 15: Unsupervised Learning: Clustering

Iain Styles

29 November 2019

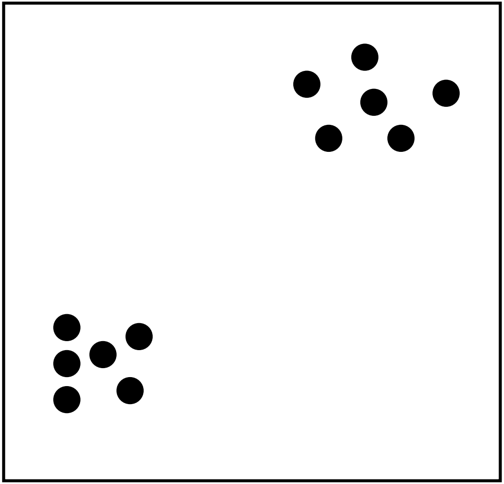
Learning Outcomes

By the end of this lecture you should

- Understand how to use the k-means algorithm in practice
- Understand the principles of hierarchical clustering
- Understand and apply the concept of linkage
- Be able to interpret a dendrogram

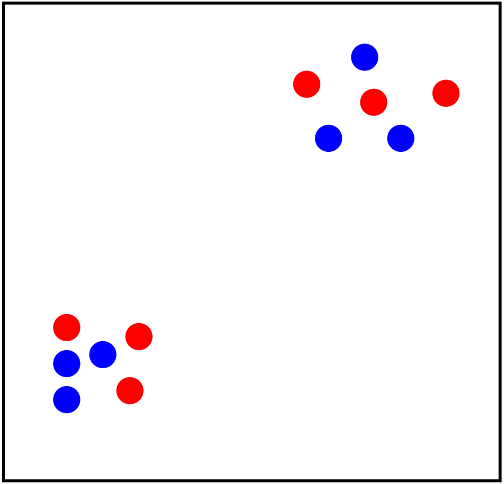
Recap: The k-means Algorithm

Initial data points



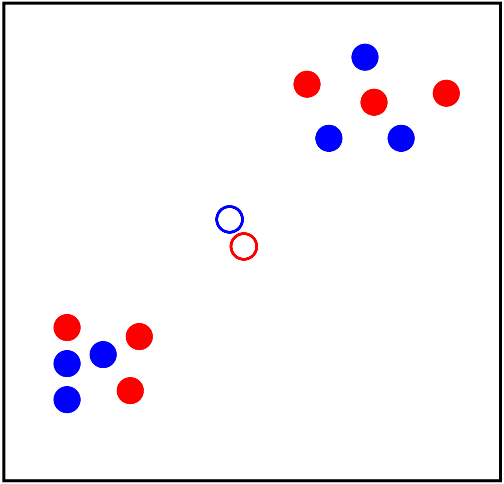
Recap: The k-means Algorithm

Randomly assign points to groups



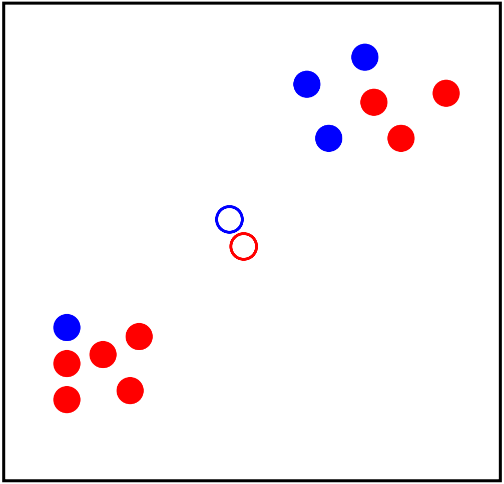
Recap: The k-means Algorithm

Compute group average



Recap: The k-means Algorithm

Re-assign points to groups



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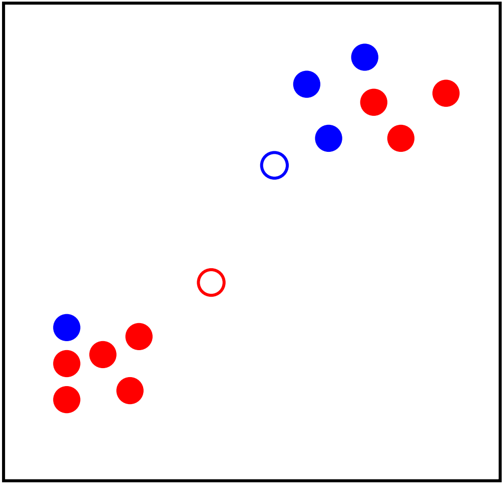

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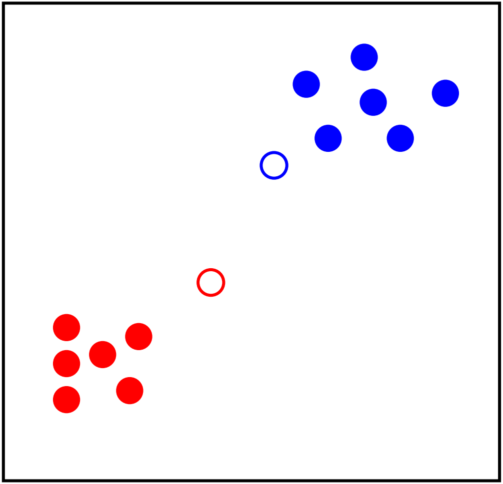

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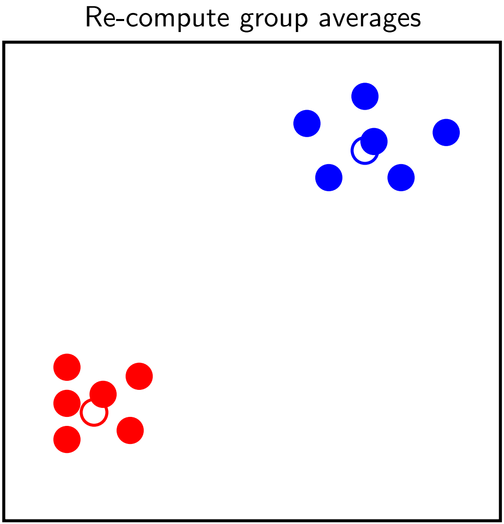

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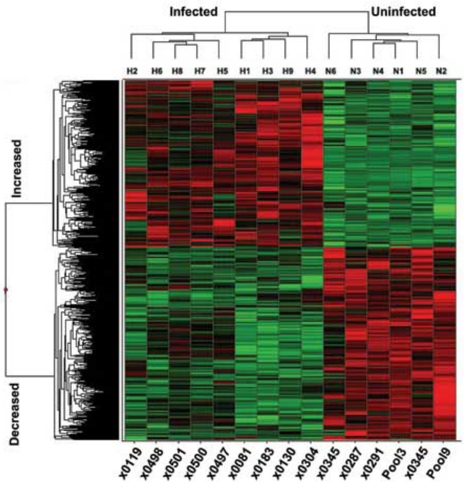
- Build hierarchy of relationships between data points
- All degrees of cluster can be extracted from this

Agglomerative Clustering

Very common in genomics



http://compbio.pbworks.com/w/page/16252903/MicroarrayClusteringMethodsandGeneOntology

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5) Go to 2) and continue grouping until all points are grouped

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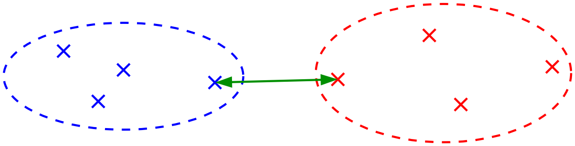

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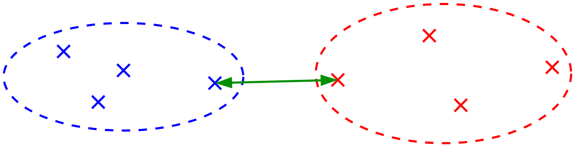
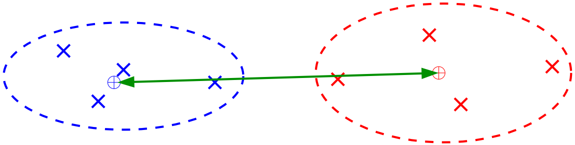


  - Average Linkage



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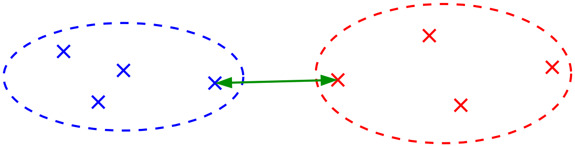

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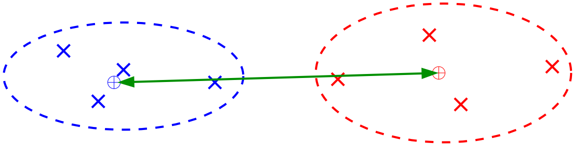
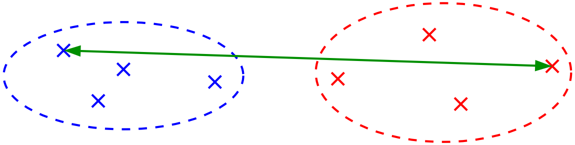


  - Complete Linkage



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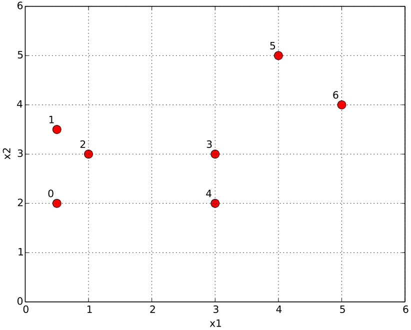

List of points 0,1,2,3,4,5,6

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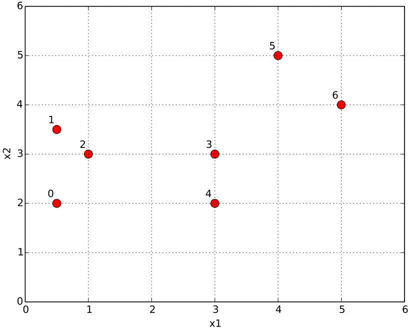

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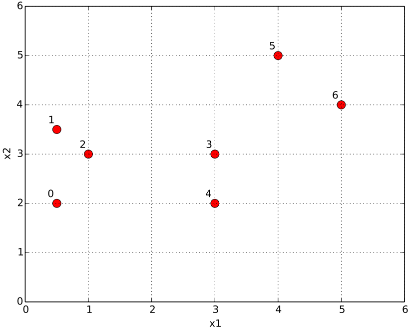

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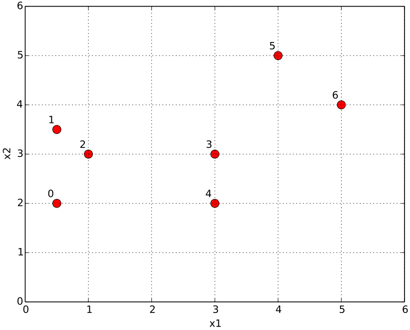

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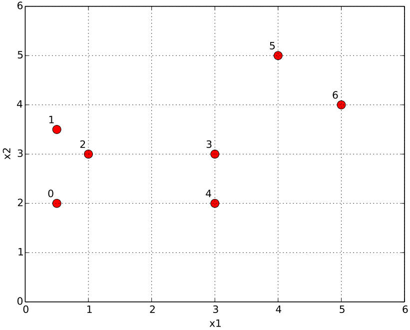

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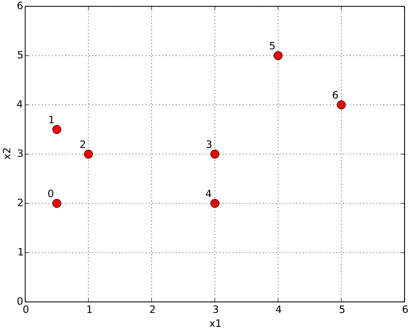

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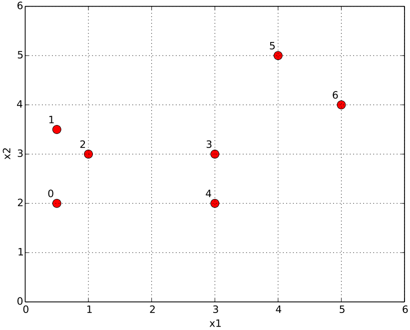

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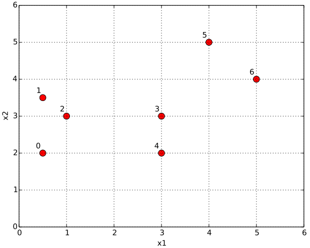

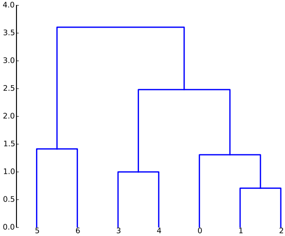

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- Clustering: which component generated the data point

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- Clustering is then formulated as
  1. Learn the parameters of the GMM which best describe the data.
  2. Determine from which component a data point is most likely to have been generated.

Learning Gaussian Mixture Models

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we interpret

- $A_k = p(k)$ as the prior probability of choosing a point from component k
- $\mathcal{N}(\mathbf{x}|\boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k) = p(\mathbf{x}|k)$ as the class-conditional likelihoods.

Learning Gaussian Mixture Models

- Finally, using Bayes' theorem we compute the posterior *responsibilities*

$$r_k(\mathbf{x}) = p(k|\mathbf{x}) \tag{5}$$

$$= \frac{p(k)p(\mathbf{x}|k)}{\sum_{k'=1}^{K} p(k')p(\mathbf{x}|k')} \tag{6}$$

$$= \frac{A_k \mathcal{N}(\mathbf{x}|\boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k)}{\sum_{k'=1}^{K} A_{k'} \mathcal{N}(\mathbf{x}|\boldsymbol{\mu}_{k'}, \boldsymbol{\Sigma}_{k'})} \tag{7}$$

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\begin{aligned}
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\end{aligned}
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- Probability that component k explains $\mathbf{x}$
- GMM gives *soft* cluster assignments

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