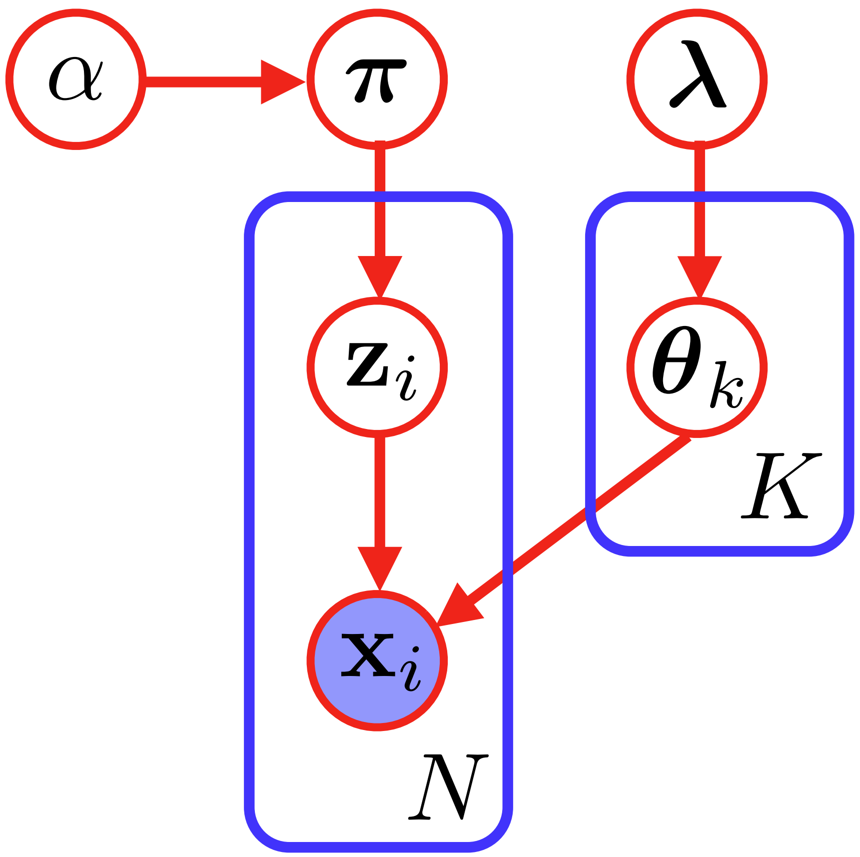
Clustering using Mixture Models

- The full posterior of the Gaussian Mixture Model is

$$p(X, Z, \boldsymbol{\mu}, \Sigma, \boldsymbol{\pi}) = \underbrace{p(X \mid Z, \boldsymbol{\mu}, \Sigma)}_{\text{data likelihood (Gaussian)}} \underbrace{p(Z \mid \boldsymbol{\pi})}_{\text{correspondence prob. (Multinomial)}} \underbrace{p(\boldsymbol{\pi} \mid \alpha)}_{\text{mixture prior (Dirichlet)}} \underbrace{p(\boldsymbol{\mu}, \Sigma \mid \boldsymbol{\lambda})}_{\text{parameter prior (Gauss-IW)}}$$



Given this model, we can create new samples:

1. Sample $\boldsymbol{\pi}, \boldsymbol{\theta}_k$ from priors
2. Sample corresp. $\mathbf{z}_i$
3. Sample data point $\mathbf{x}_i$

Repetition: MAP for Regression

In MLE, we searched for parameters $\mathbf{w}$, that maximize the data likelihood. Now, we assume a Gaussian ***prior***:

$$p(\mathbf{w} \mid \sigma_2) = \mathcal{N}(\mathbf{w}; \mathbf{0}, \sigma_2 I)$$

Using this, we can compute the ***posterior*** (Bayes):

$$\underbrace{p(\mathbf{w} \mid \mathbf{x}, \mathbf{t})}_{\text{Posterior}} \propto \underbrace{p(\mathbf{t} \mid \mathbf{w}, \mathbf{x})}_{\text{Likelihood}} \underbrace{p(\mathbf{w})}_{\text{Prior}}$$

"Maximum A-Posteriori Estimation (MAP)"

Generalization: The Bayesian Approach

This idea can be generalized:

- Given a data-dependent **likelihood** term
- Find an appropriate **prior** distribution
- Multiply both and obtain the (unnormalized) **posterior** from Bayes rule
- Main benefit: less overfitting

However:

- How should we define the prior?

Often used principle: **Conjugacy**

Conjugate Priors

A conjugate prior distribution allows to represent the posterior in the **same functional** (closed) form as the prior, e.g.:

$$\underbrace{\mathcal{N}(\mathbf{w}; \mathbf{0}, \sigma_2^2 I_M)}_{\text{Gaussian prior}}\underbrace{\mathcal{N}(\mathbf{t}; \Phi\mathbf{w}, \sigma_1^2 I_M)}_{\text{Gaussian likelihood}} = \underbrace{\mathcal{N}(\mathbf{w}; \boldsymbol{\mu}, \Sigma)}_{\text{Gaussian posterior}}$$

Common pairs of likelihood and conjugate priors are:

Likelihood	Conjugate Prior
Normal with known variance	Normal
Binomial	Beta
Multinomial	Dirichlet
Multivariate Normal	Normal-inverse Wishart

Multinomial

- Given K clusters and probabilities of these clusters $\pi_1, \ldots, \pi_K$ where $\sum_{k=1}^{K} \pi_k = 1$
- The probability that out of N samples m_k are in cluster k is:

$$p(m_1, \ldots, m_K \mid \boldsymbol{\pi}, N) = \binom{N}{m_1 \cdots m_K} \prod_{k=1}^{K} \mu_k^{m_k}$$

- This is called the **multinomial distribution**
- In our case:

$$p(Z \mid \boldsymbol{\pi}) = \prod_{n=1}^{N} \prod_{k=1}^{K} \mu_k^{z_{nk}} = \prod_{k=1}^{K} \mu_k^{m_k}$$

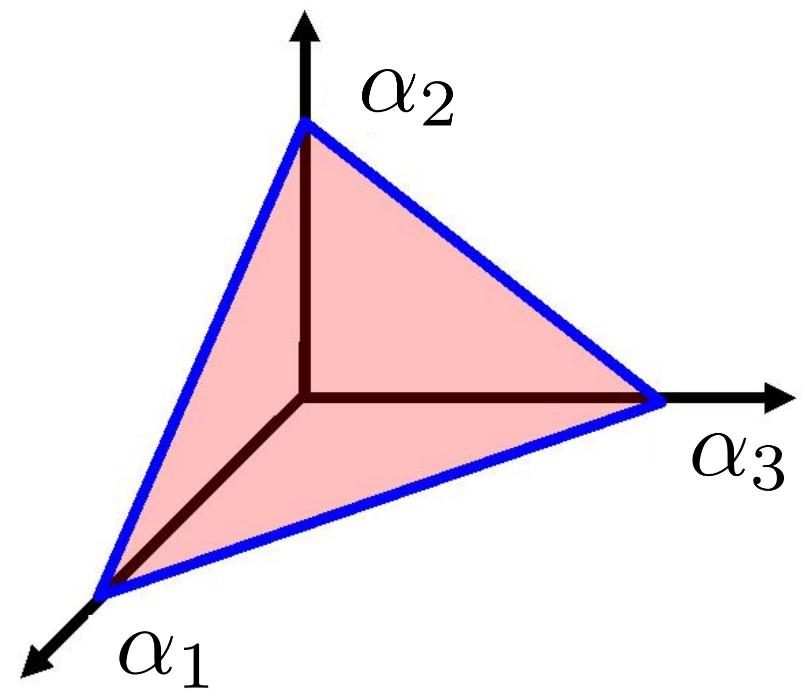
The Dirichlet Distribution

- The Dirichlet distribution is defined as:

$$\mathrm{Dir}(\boldsymbol{\mu} \mid \boldsymbol{\alpha}) = \frac{\Gamma(\alpha_0)}{\Gamma(\alpha_1)\cdots\Gamma(\alpha_K)} \prod_{k=1}^{K} \mu_k^{\alpha_k - 1} \qquad \alpha_0 = \sum_{k=1}^{K} \alpha_k$$

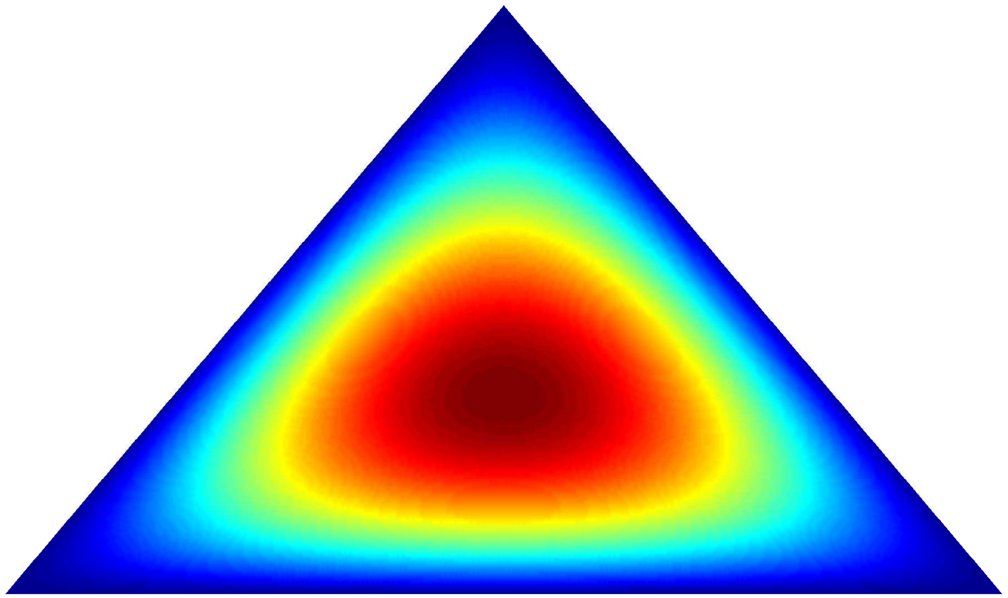
$$0 \leq \mu_k \leq 1 \qquad \sum_{k=1}^{K} \mu_k = 1$$

- It is the conjugate prior for the multinomial distribution
- There, the parameter $\boldsymbol{\alpha}$ can be interpreted as the effective number of observations for every state

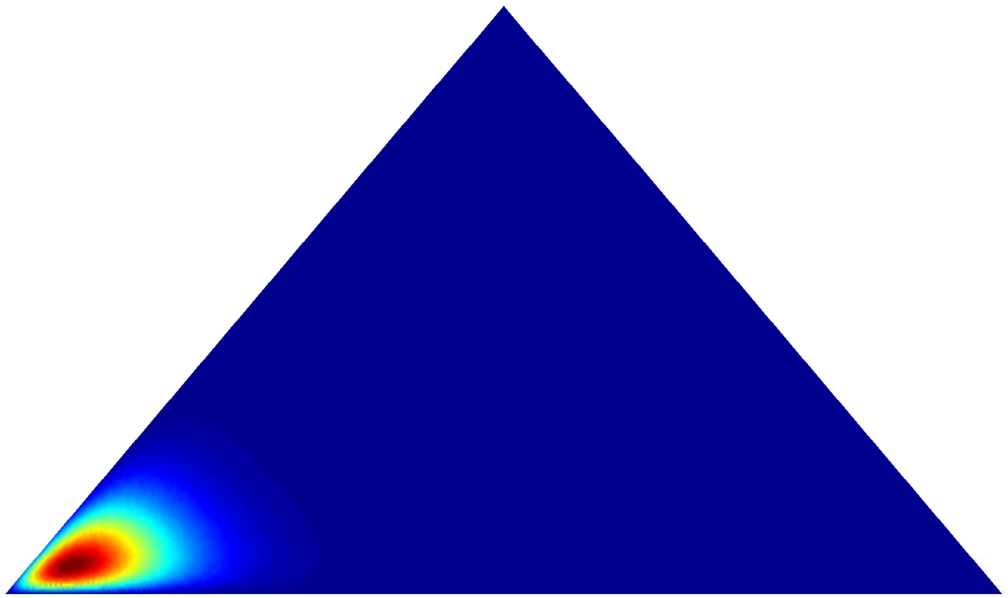


The simplex for K=3

Some Examples

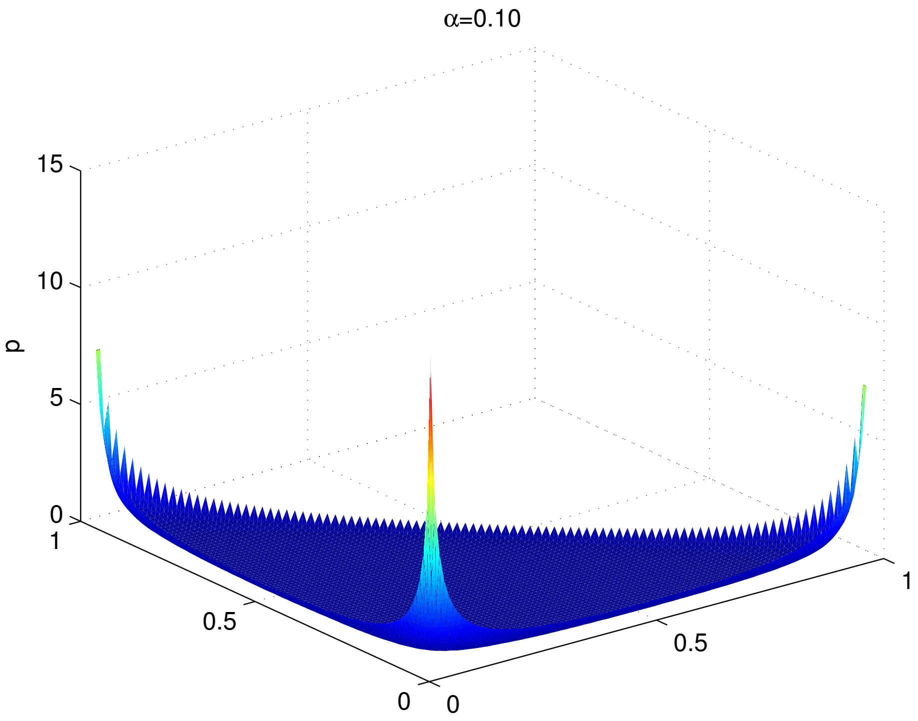


$\alpha = (2, 2, 2)$



$\alpha = (20, 2, 2)$

- α_0 controls the strength of the distribution ("peakedness")
- α_k control the location of the peak



$\alpha = (0.1, 0.1, 0.1)$

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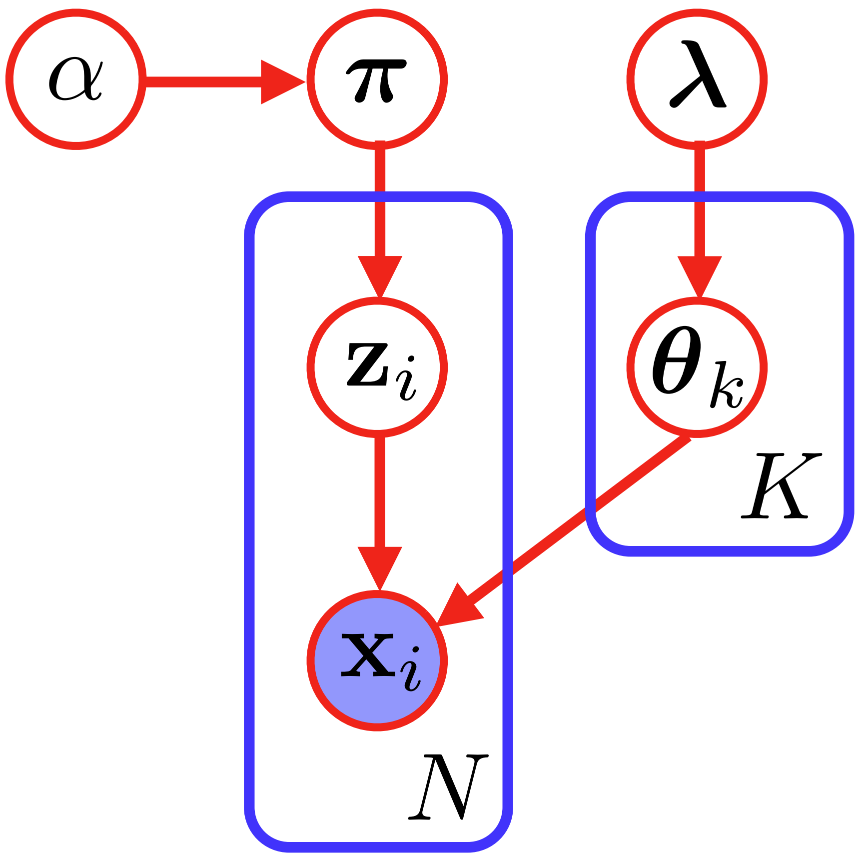

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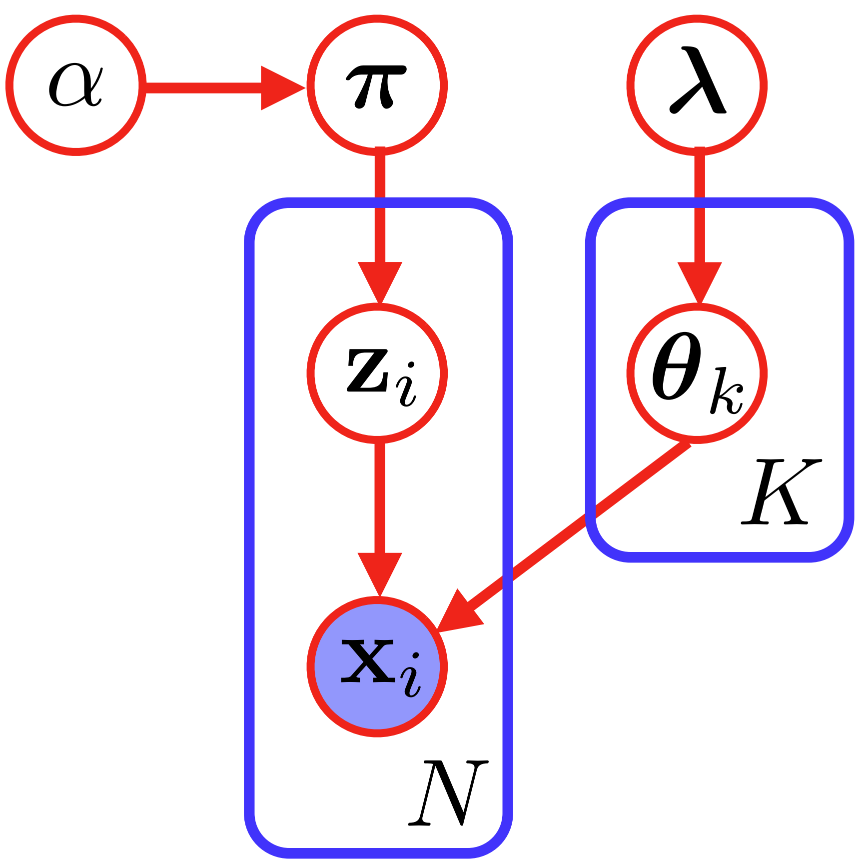

$$\boldsymbol{\pi} \sim \mathrm{Dir}(\frac{\alpha}{K}, \ldots, \frac{\alpha}{K})$$

$$\mathbf{z}_i \sim \mathrm{Mult}(\boldsymbol{\pi})$$

$$\boldsymbol{\theta}_k \sim \mathrm{NIW}(\boldsymbol{\lambda})$$

$$\mathbf{x}_i \sim \mathcal{N}(\boldsymbol{\theta}_{\mathbf{z}_i})$$

Clustering using Mixture Models

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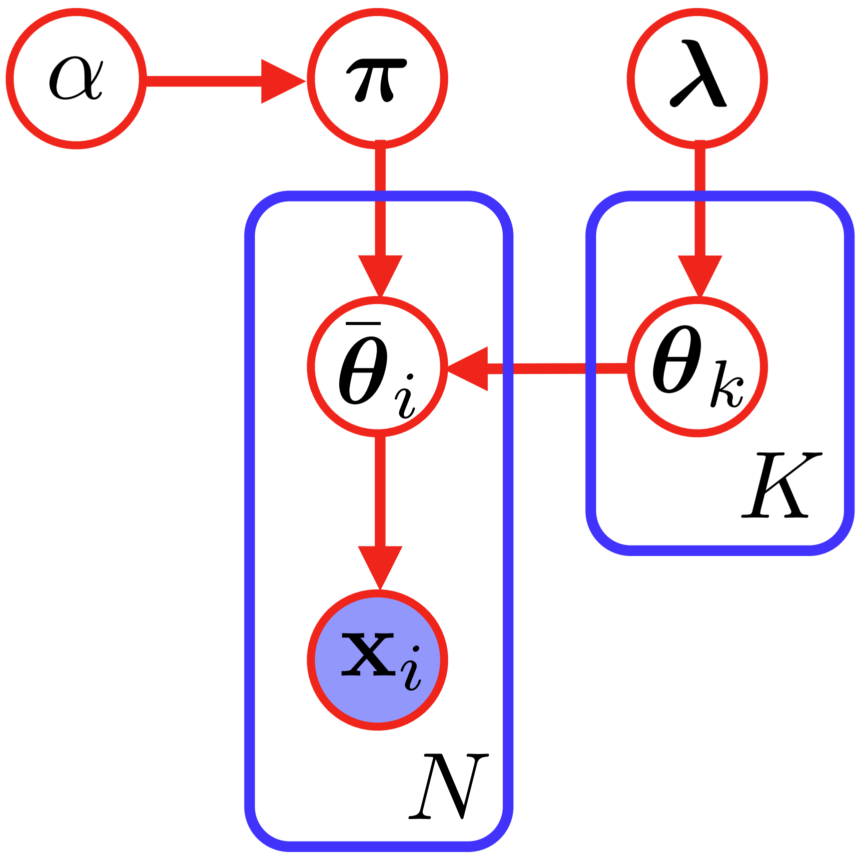
An equivalent formulation of this model is this:

1. Sample $\boldsymbol{\pi}, \boldsymbol{\theta}_k$ from priors
2. Sample params $\bar{\boldsymbol{\theta}}_i$ from a discrete dist. G
3. Sample data point $\mathbf{x}_i$

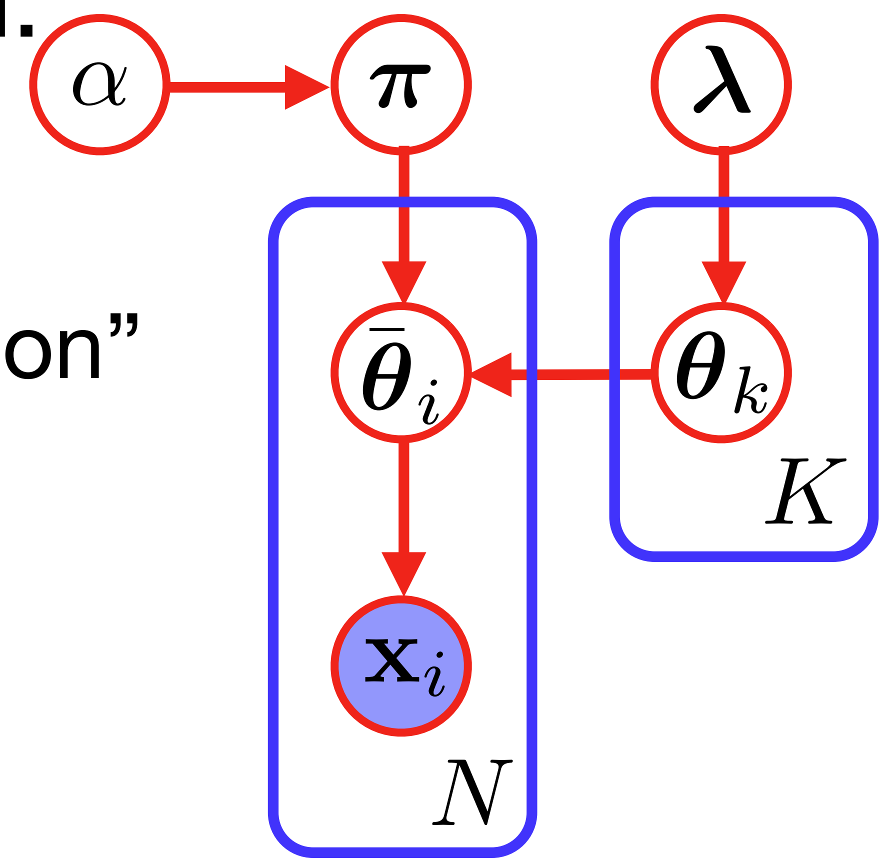


Clustering using Mixture Models

What is the difference in that model?

- there is one parameter $\bar{\boldsymbol{\theta}}_i$ for each observation $\mathbf{x}_i$
- intuitively: we first sample the location of the cluster and then the data that corresponds to it

In general, we use the notation:



$$\boldsymbol{\pi} \sim \mathrm{Dir}(\frac{\alpha}{K}\mathbf{1})$$

$$\boldsymbol{\theta}_k \sim \mathrm{H}(\boldsymbol{\lambda})$$ “Base distribution”

$$\bar{\boldsymbol{\theta}}_i \sim \mathrm{G}(\boldsymbol{\pi}, \boldsymbol{\theta}_k)$$ where

$$G(\boldsymbol{\pi}, \boldsymbol{\theta}_k) = \sum_{k=1}^{K} \pi_k \delta(\boldsymbol{\theta}_k, \bar{\boldsymbol{\theta}}_i)$$

However: We need to know K

The Dirichlet Process

- So far, we assumed that K is known
- To extend that to infinity, we use a trick:

Definition: A Dirichlet process (DP) is a distribution over probability measures G, i.e. $G(\boldsymbol{\theta}) \geq 0$ and $\int G(\boldsymbol{\theta}) d\boldsymbol{\theta} = 1$. If for any partition $(T_1, \dots, T_K)$ it holds:

$$(G(T_1), \dots, G(T_K)) \sim \mathrm{Dir}(\alpha H(T_1), \dots, \alpha H(T_K))$$

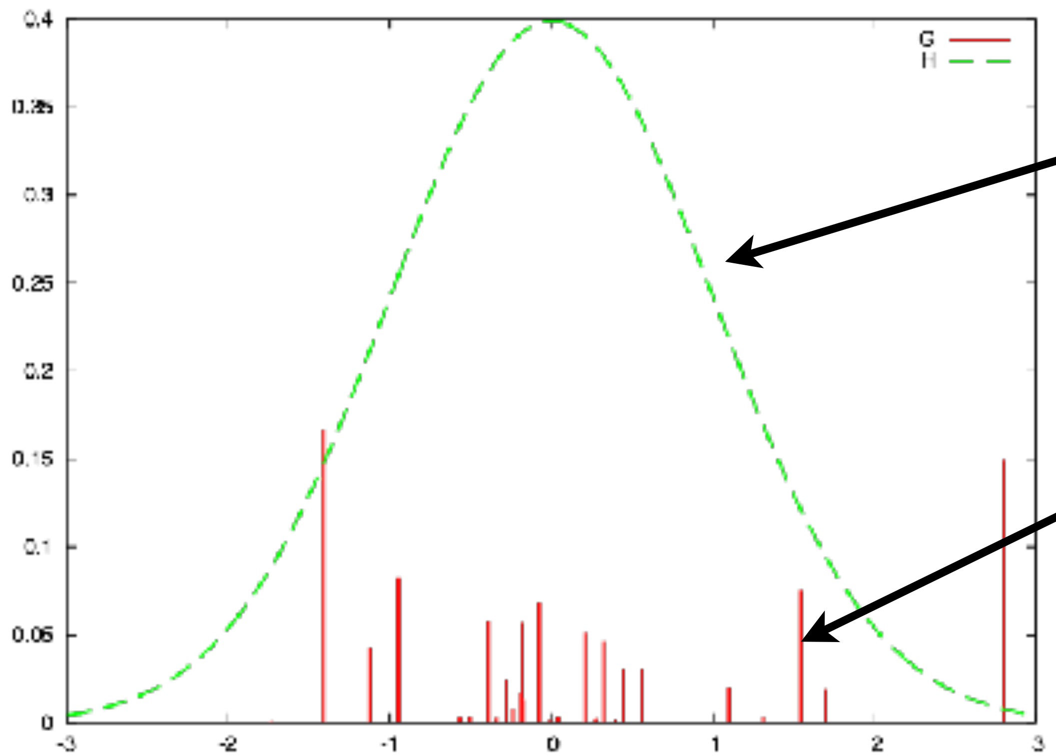
then G is sampled from a Dirichlet process.

Notation: $G \sim \mathrm{DP}(\alpha, H)$

where α is the **concentration parameter**
and H is the **base measure**

Intuitive Interpretation

- Every sample from a Dirichlet distribution is a vector of K positive values that sum up to 1, i.e. the sample itself is a finite distribution
- Accordingly, a sample from a Dirichlet process is an infinite (but still discrete!) distribution



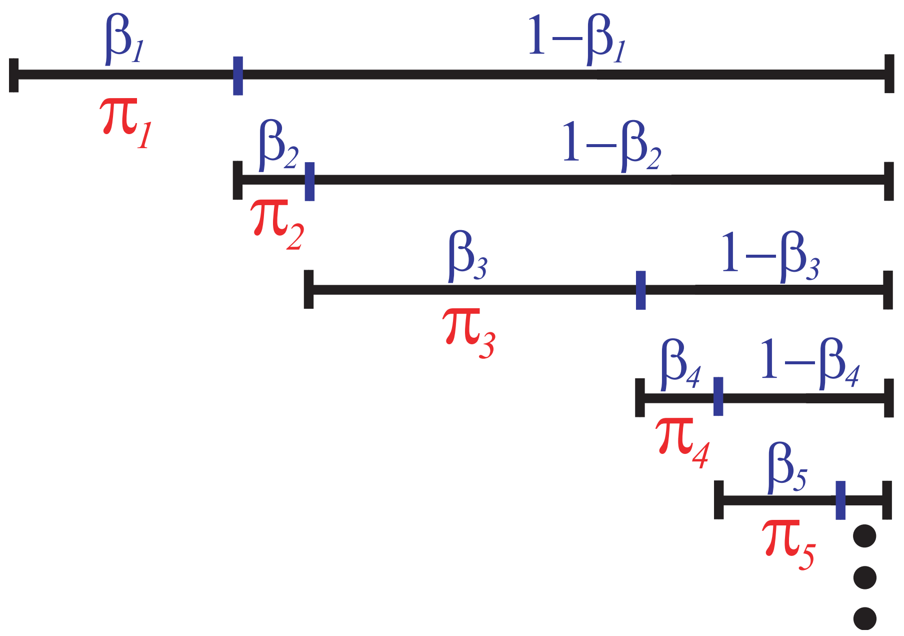
Base distribution (here Gaussian)

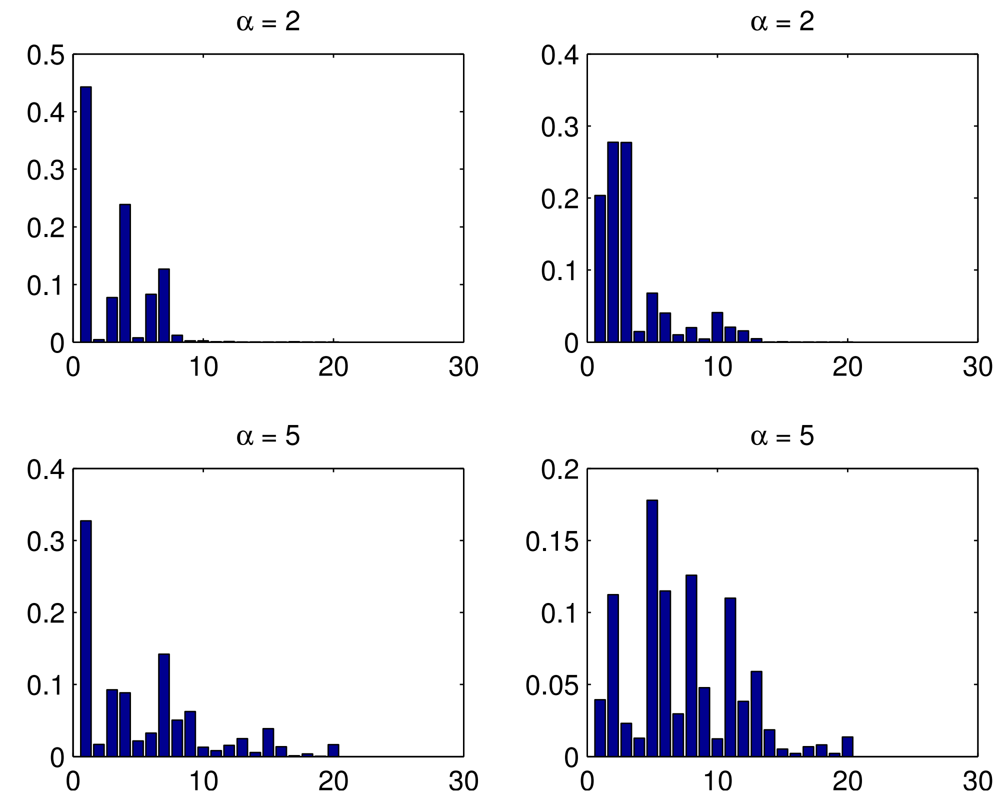
Infinitely many samples (sum up to 1)

Construction of a Dirichlet Process

- The Dirichlet process is only defined **implicitly**, i.e. we can test whether a given probability measure is sampled from a DP, but we can not yet construct one.
- A DP can be constructed using the “stick-breaking” analogy:
  - imagine a stick of length 1
  - we select a random number β between 0 and 1 from a Beta-distribution
  - we break the stick at $\pi = \beta$ * length-of-stick
  - we repeat this infinitely often

The Stick-Breaking Construction





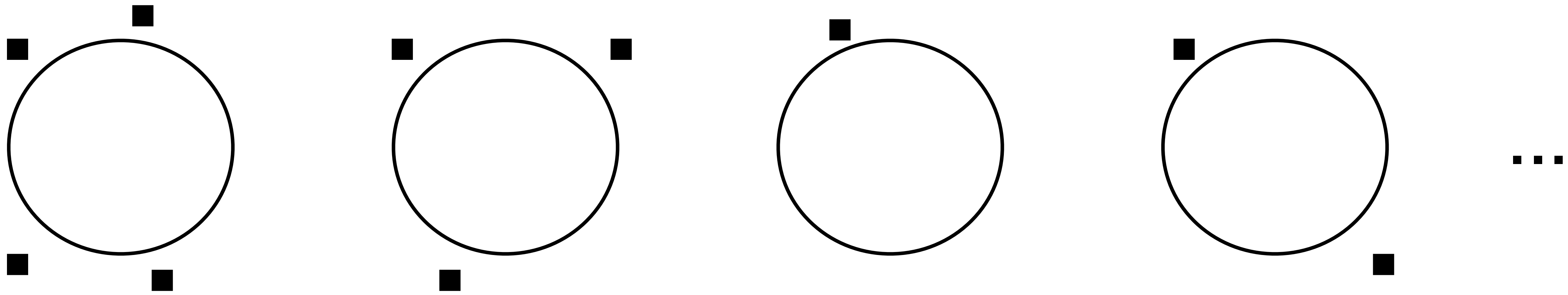
- formally, we have

$$\beta_k \sim \mathrm{Beta}(1, \alpha) \qquad \pi_k = \beta_k \prod_{l=1}^{k-1}(1-\beta_l) = \beta_k(1 - \sum_{l=1}^{k-1}\pi_l)$$

- now we define

$$G(\boldsymbol{\theta}) = \sum_{k=1}^{\infty} \pi_k \delta(\boldsymbol{\theta}_k, \boldsymbol{\theta}) \qquad \boldsymbol{\theta}_k \sim H \qquad \text{then:} \quad G \sim \mathrm{DP}(\alpha, H)$$

The Chinese Restaurant Process



- Consider a restaurant with infinitely many tables
- Everytime a new customer comes in, he sits at an **occupied table** with probability **proportional to the number of people** sitting at that table, but he may choose to sit on a **new** table with **decreasing** probability as more customers enter the room.

The Chinese Restaurant Process

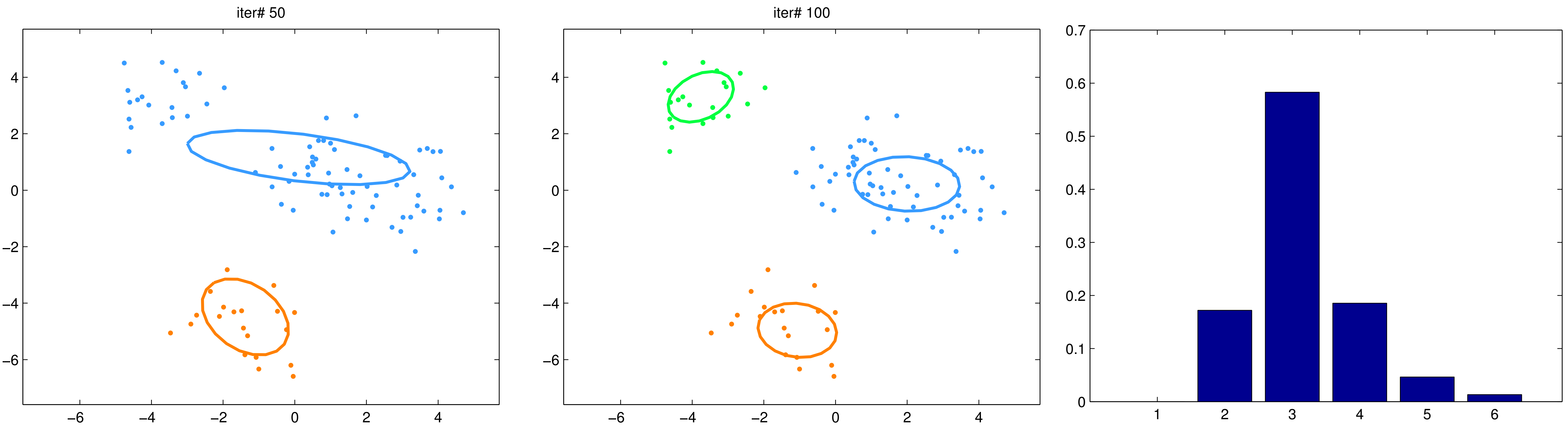
- It can be shown that the probability for a new customer is

$$p(\bar{\boldsymbol{\theta}}_{N+1} = \boldsymbol{\theta} \mid \bar{\boldsymbol{\theta}}_{1:N}, \alpha, H) = \frac{1}{\alpha + N} \left(\alpha H(\boldsymbol{\theta}) + \sum_{k=1}^{K} N_k \delta(\bar{\boldsymbol{\theta}}_k, \boldsymbol{\theta}) \right)$$

- This means that currently occupied tables are more likely to get new customers (**rich get richer**)
- The number of occupied tables grows logarithmically with the number of customers

The DP for Mixture Modeling

- Using the stick-breaking construction, we see that we can extend the mixture model clustering to the situation where K goes to infinity
- The algorithm can be implemented using Gibbs sampling



Questions

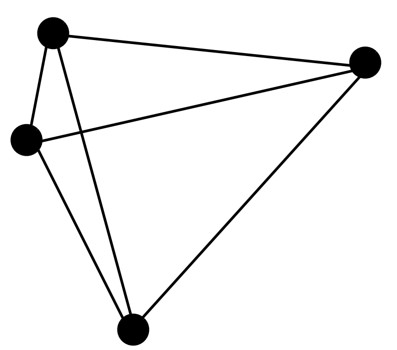
- What if the clusters can not be approximated well by Gaussians?

- Can we formulate an algorithm that only relies on pairwise similarities?

One example for such an algorithm is Spectral Clustering

Spectral Clustering

- Consider an undirected graph that connects all data points
- The edge weights are the similarities (“closeness”)
- We define the weighted degree d_i of a node as the sum of all outgoing edges



$$W = \begin{array}{|c|c|c|c|}\hline & & & \\ \hline & & & \\ \hline & & & \\ \hline & & & \\ \hline \end{array}$$

$$d_i = \sum_{j=1}^{N} w_{ij}$$

$$D = \begin{array}{|c|c|c|c|}\hline d_1 & & & \\ \hline & d_2 & & \\ \hline & & d_3 & \\ \hline & & & d_4 \\ \hline \end{array}$$

Spectral Clustering

- The Graph Laplacian is defined as:

$$L = D - W$$

- This matrix has the following properties:
  - the 1 vector is eigenvector with eigenvalue 0

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Spectral Clustering

- The Graph Laplacian is defined as:

$$L = D - W$$

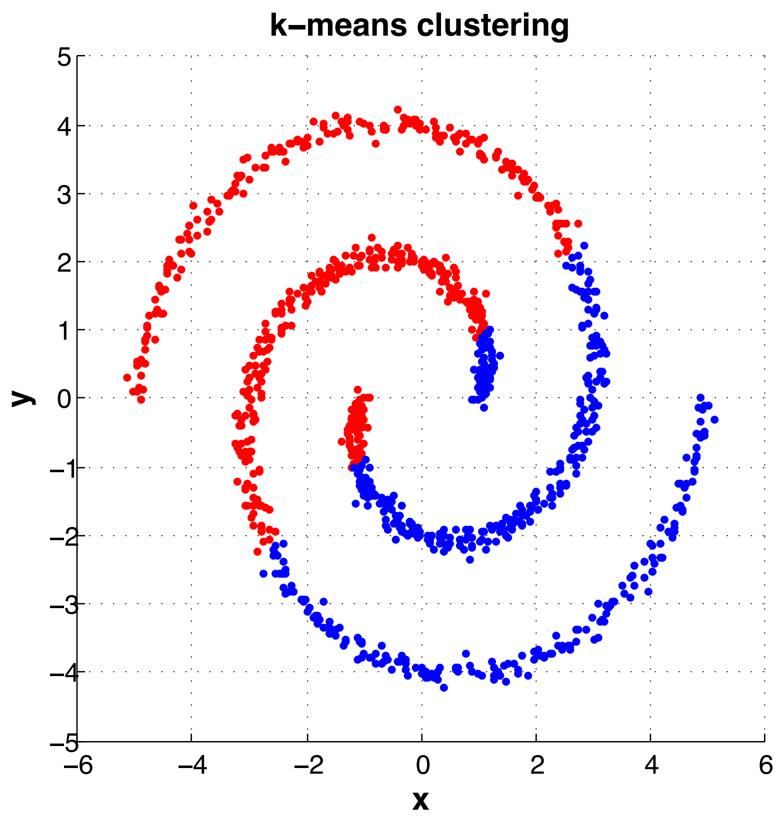
- This matrix has the following properties:
  - the 1 vector is eigenvector with eigenvector 0
  - the matrix is symmetric and positive semi-definite
- With these properties we can show:

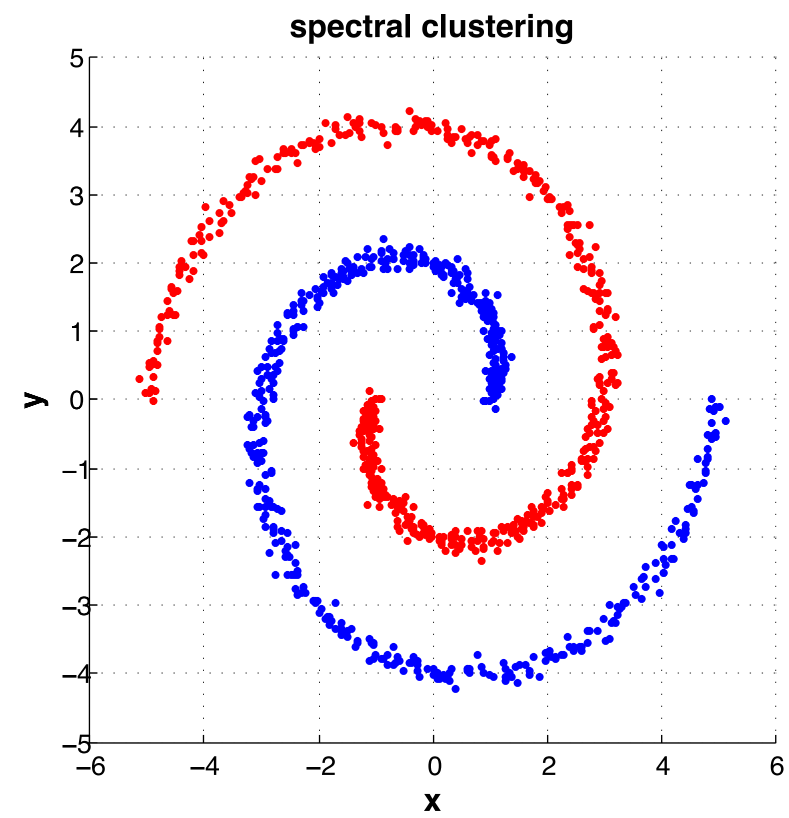
Theorem: The set of eigenvectors of L with eigenvalue 0 is spanned by the indicator vectors $\mathbf{1}_{A_1}, \ldots, \mathbf{1}_{A_K}$, where A_k are the K connected components of the graph.

The Algorithm

- Input: Similarity matrix W
- Compute L = D - W
- Compute the eigenvectors that correspond to the K smallest eigenvalues
- Stack these vectors as columns in a matrix U
- Treat each row of U as a K-dim data point
- Cluster the N rows with K-means clustering
- The indices of the rows that correspond to the resulting clusters are those of the original data points.

An Example



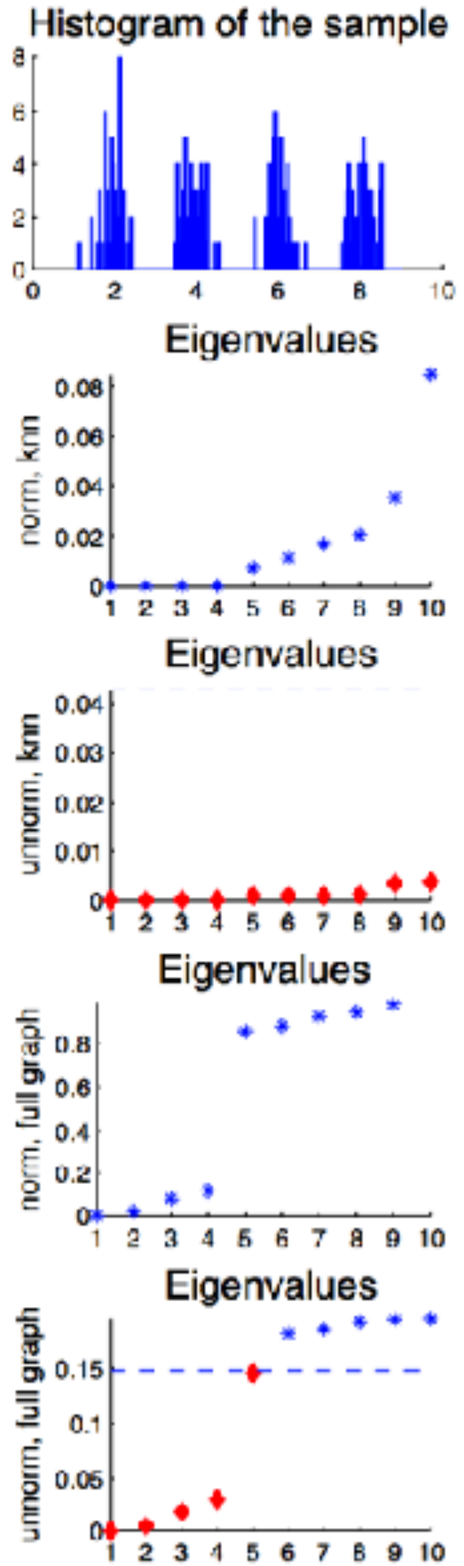


- Spectral clustering can handle complex problems such as this one
- The complexity of the algorithm is $O(N^3)$, because it has to solve an eigenvector problem
- But there are efficient variants of the algorithm

Further Remarks

- To account for nodes that are highly connected, we can use a normalized version of the graph Laplacian
- Two different methods exist:
  - $L_{rw} = D^{-1}L = I - D^{-1}W$
  - $L_{sym} = D^{-\frac{1}{2}}LD^{-\frac{1}{2}} = I - D^{-\frac{1}{2}}WD^{-\frac{1}{2}}$
- These have similar eigenspaces than the original Laplacian L
- Clustering results tend to be better than with the unnormalized Laplacian
- The number of clusters K can be found using the "eigen-gap heuristic"

Eigen-Gap Heuristic



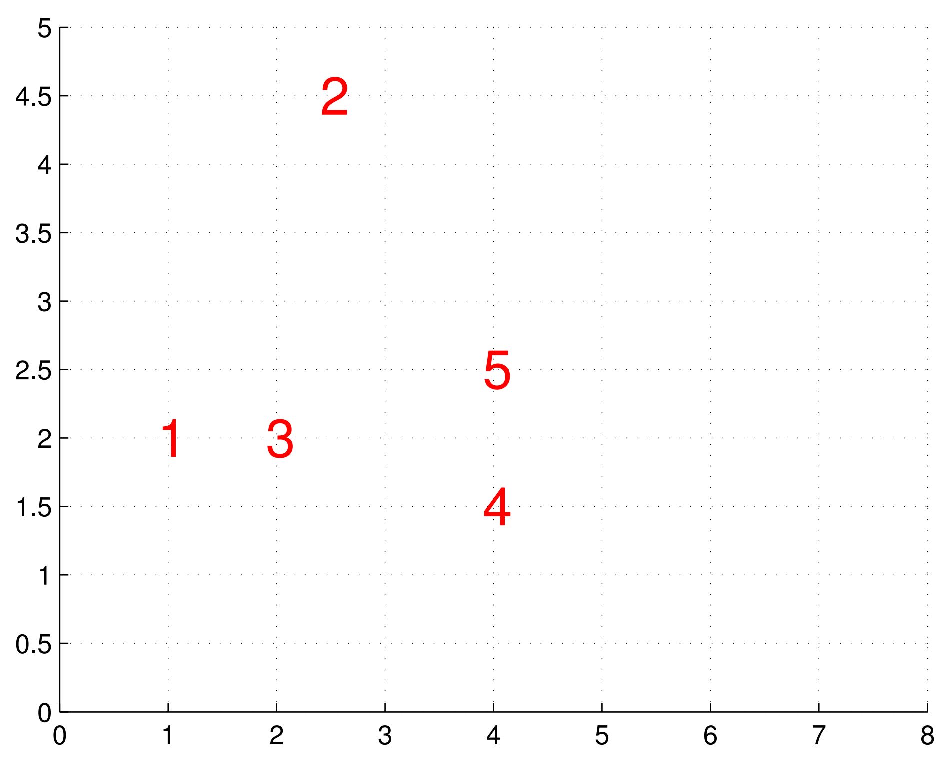
- Compute all eigen values of the graph Laplacian
- Sort them in increasing order
- Usually, there is a big “jump” between two consecutive eigen values
- The corresponding number K is a good choice for the estimated number of clusters

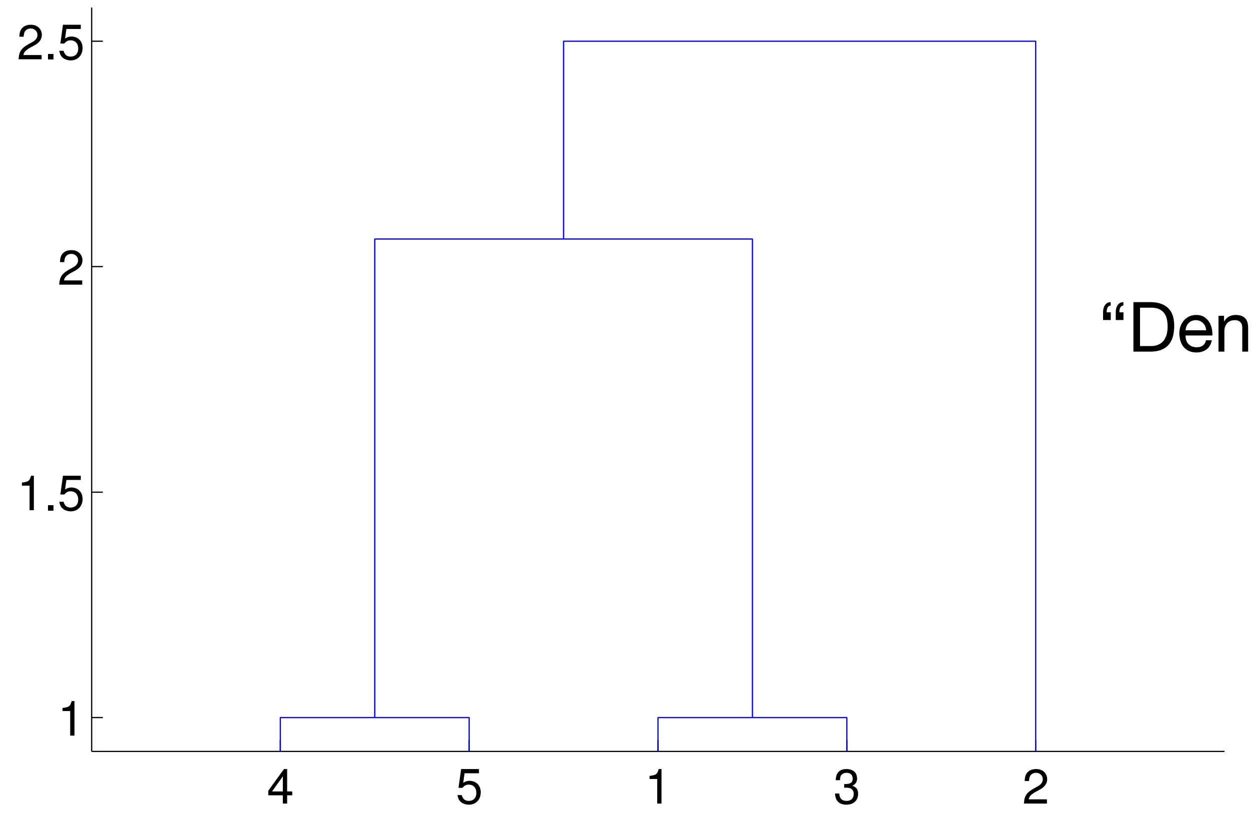
Hierarchical Clustering

- Often, we want to have nested clusters instead of a “flat” clustering
- Two possible methods:
  - “bottom-up” or agglomerative clustering
  - “top-down” or divisive clustering
- Both methods take a dissimilarity matrix as input
- Bottom-up grows merges points to clusters
- Top-down splits clusters into sub-clusters
- Both are heuristics, there is no clear objective function
- They always produce a clustering (also for noise)

Agglomerative Clustering

- Start with N clusters, each contains exactly one data point
- At each step, merge the two most similar groups
- Repeat until there is a single group





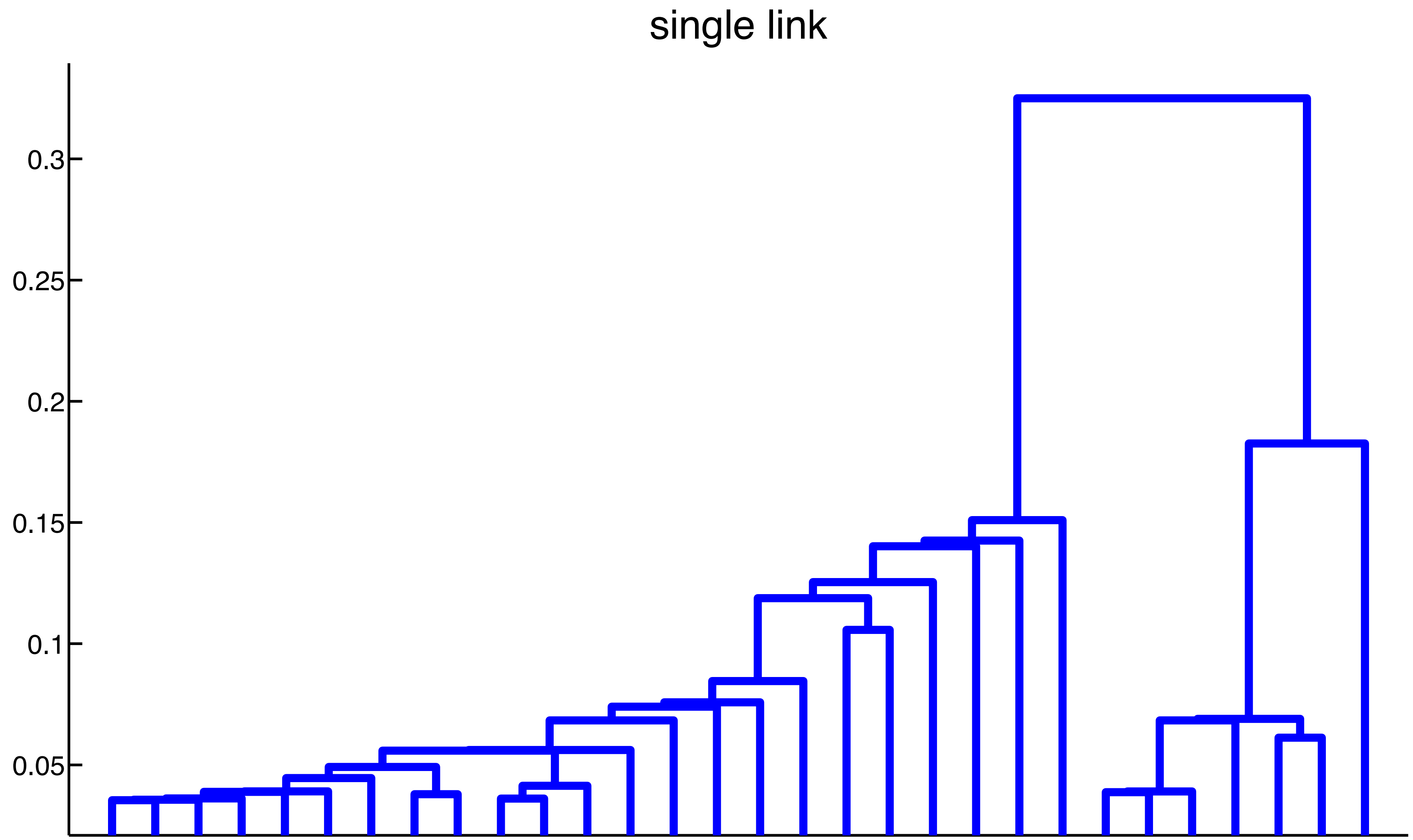
"Dendrogram"

Linkage

- In agglomerative clustering, it is important to define a distance measure between two clusters
- There are three different methods:
  - Single linkage: considers the two closest elements from both clusters and uses their distance
  - Complete linkage: considers the two farthest elements from both clusters
  - Average linkage: uses the average distance between pairs of points from both clusters
- Depending on the application, one linkage should be preferred over the other

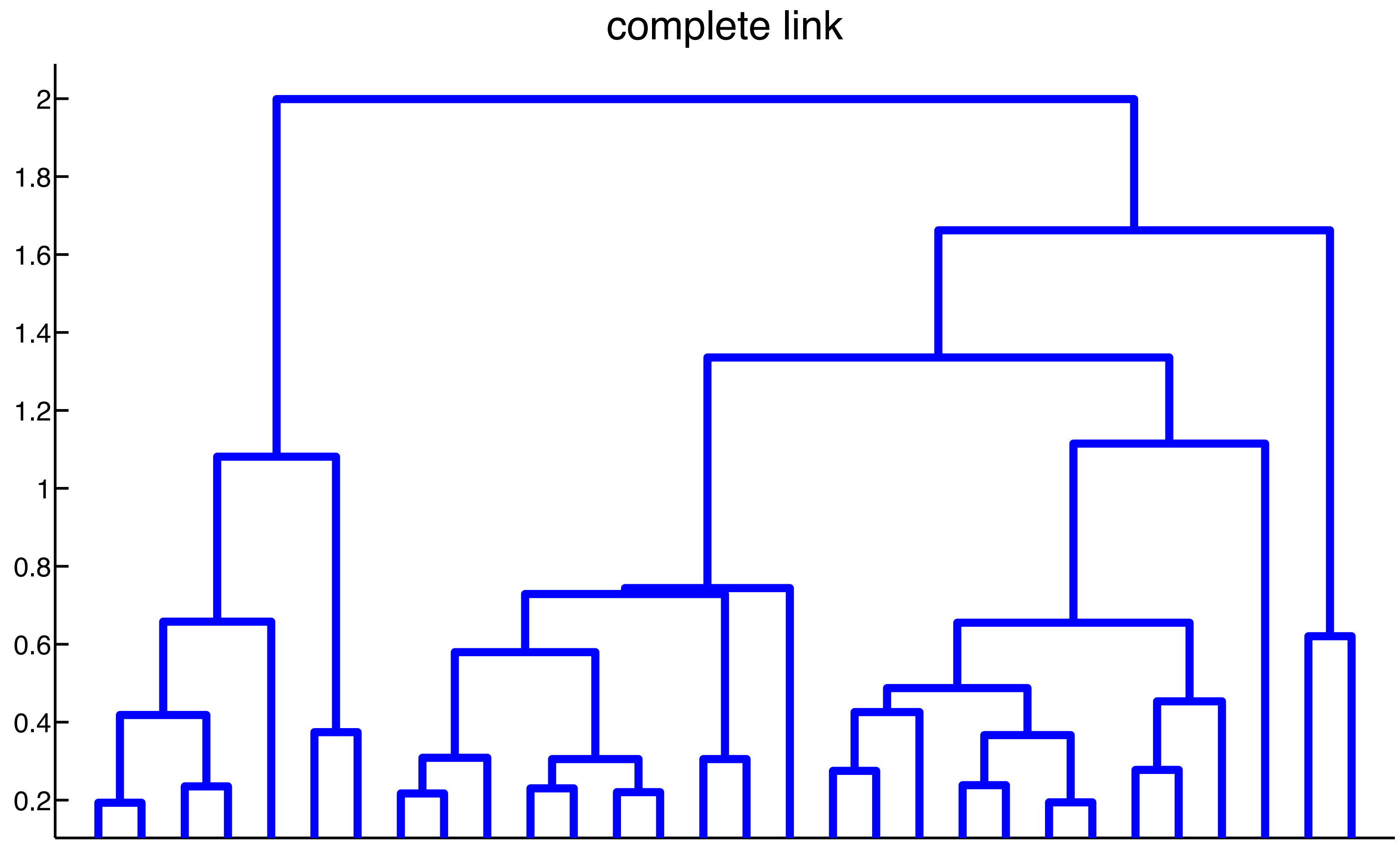
Single Linkage

- The distance is based on $d_{SL}(G,H) = \min_{i \in G, i' \in H} d_{i,i'}$
- The resulting dendrogram is a minimum spanning tree, i.e. it minimizes the sum of the edge weights
- Thus: we can compute the clustering in $O(N^2)$ time



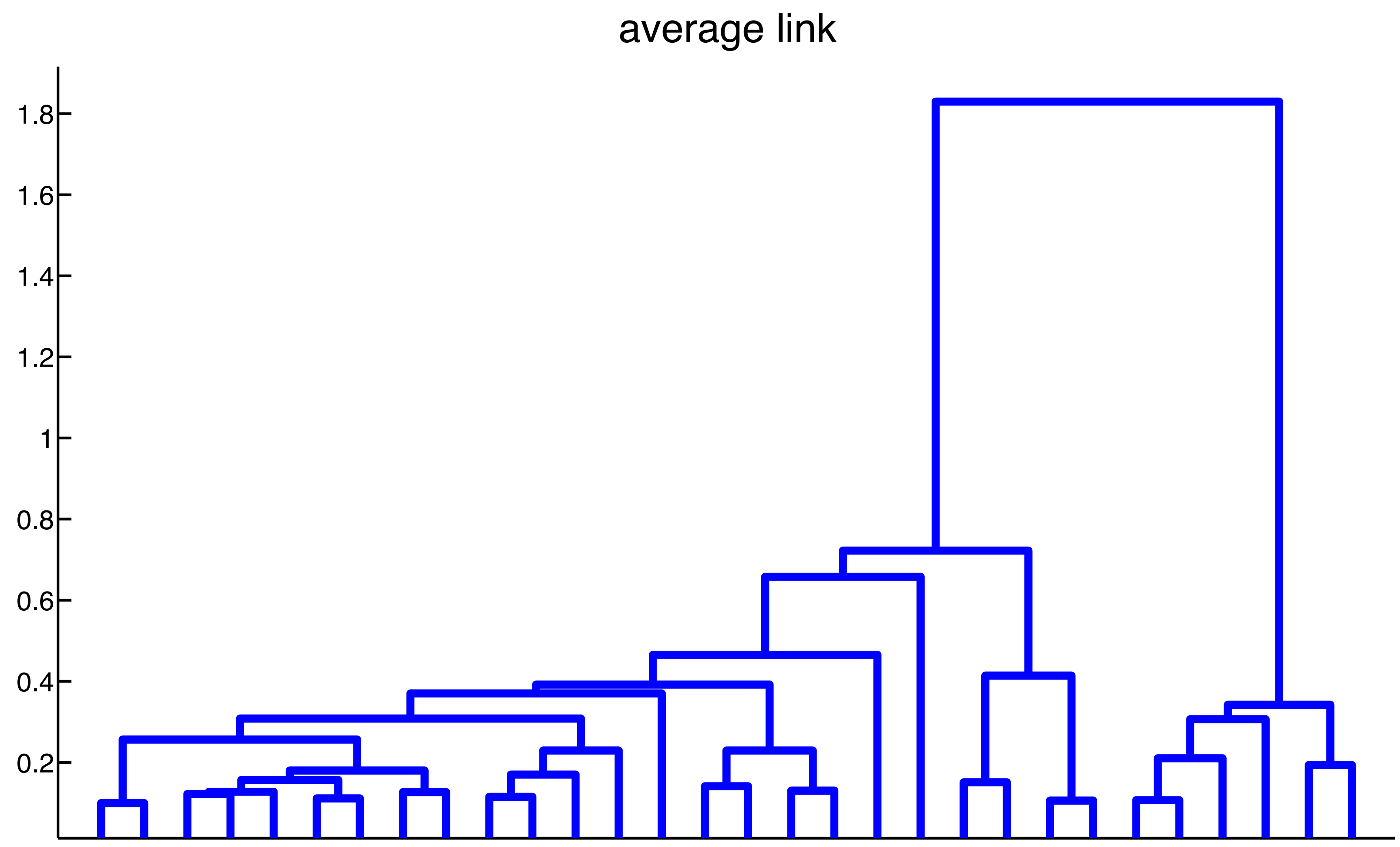
Complete Linkage

- The distance is based on $d_{CL}(G,H) = \max_{i \in G, i' \in H} d_{i,i'}$
- Complete linkage fulfills the **compactness property**, i.e. all points in a group should be similar to each other
- Tends to produce clusters with smaller diameter



Average Linkage

- The distance is based on $d_{avg}(G,H) = \frac{1}{n_G n_H} \sum_{i \in G} \sum_{i' \in H} d_{i,i'}$
- Is a good compromise between single and complete linkage
- However: sensitive to changes on the meas. scale



Divisive Clustering

- Start with all data in a single cluster
- Recursively divide each cluster into two child clusters
- Problem: optimal split is hard to find
- Idea: use the cluster with the largest diameter and use K-means with $K = 2$
- Or: use minimum-spanning tree and cut links with the largest dissimilarity
- In general two advantages:
    - Can be faster
    - More globally informed (not myopic as bottom-up)

Choosing the Number of Clusters

- As in general, choosing the number of clusters is hard
- When a dendrogram is available, a gap can be detected in the lengths of the links
- This represents the dissimilarity between merged groups
- However: in real data this can be hard to detect
- There are Bayesian techniques to address this problem (Bayesian hierarchical clustering)

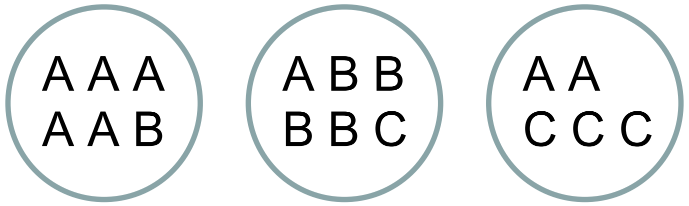
Evaluation of Clustering Algorithms

- Clustering is unsupervised: evaluation of the output is hard, because no ground truth is given
- Intuitively, points in a cluster should be similar and points in different clusters dissimilar
- However, better methods use external information, such as labels or a reference clustering
- Then we can compare clusterings with the labels using different metrics, e.g.
  - purity
  - mutual information

Purity

- Define N_{ij} the number of objects in cluster i that are in class j
- Define $N_i = \sum_{j=1}^{C} N_{ij}$ number of objects in cluster i
- $p_{ij} = \dfrac{N_{ij}}{N_i}$ $\quad p_i = \max_j p_{ij}$ "Purity"
- overall purity

$$\sum_i \frac{N_i}{N} p_i$$



Purity = 0.71

- Purity ranges from 0 (bad) to 1 (good)
- But: a clustering with each object in its own cluster has a purity of 1

Mutual Information

- Let U and V be two clusterings
- Define the probability that a randomly chosen point belongs to cluster u_i in U and to v_j in V

$$p_{UV}(i,j) = \frac{|u_i \cap v_j|}{N}$$

- Also: The prob. that a point is in u_i $\quad p_U(i) = \frac{|u_i|}{N}$

$$\mathbb{I}(U,V) = \sum_{i=1}^{R} \sum_{j=1}^{C} p_{UV}(i,j) \log \frac{p_{UV}(i,j)}{p_U(i) p_V(j)}$$

- This can be normalized to account for many small clusters with low entropy

Summary

- Several Clustering methods exist:
  - K-means clustering and Expectation-Maximization, both based on Gaussian Mixture Models
  - K-means uses hard assignments, whereas EM uses soft assignments and estimates also the covariances
  - The Dirichlet Process is a non-parametric model to perform clustering without specifying K
  - Spectral clustering uses the graph Laplacian and performs an eigenvector analysis
- Major Problem:
  - most clustering algorithms require the number of clusters to be given