Unsupervised Learning: Clustering

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Outline

Clustering

Goal

Automatically discover clusters in the data

- Points within the same cluster should be similar (close)
- Points within two different clusters should be dissimilar (distant)

- Model-based clustering:
  - assume that the data was generated by a model
  - try to recover the original model from the data
- Model-free clustering:
  - no assumption on the mechanism producing data
  - vector quantization
  - cluster should be *homogeneous* and *different from one another*
  - data-driven loss function to minimize

Model-based clustering: choice of distance

- Data often in $\mathbb{R}^p$ (or projected to)
- Distance sometimes natural, sometimes not
- Often: need to *normalize* first
- Default choice: Euclidian distance $d(x, x') = \sqrt{\sum_{j=1}^{p} (x_j - x'_j)^2}$
- Other possible norms: L^1, L^∞, etc.
- Mahalanobis distance: $d(x, x') = \sqrt{(x - x')^T \Sigma^{-1} (x - x')}$
- Categorical data: typically χ^2 distance

Ressources

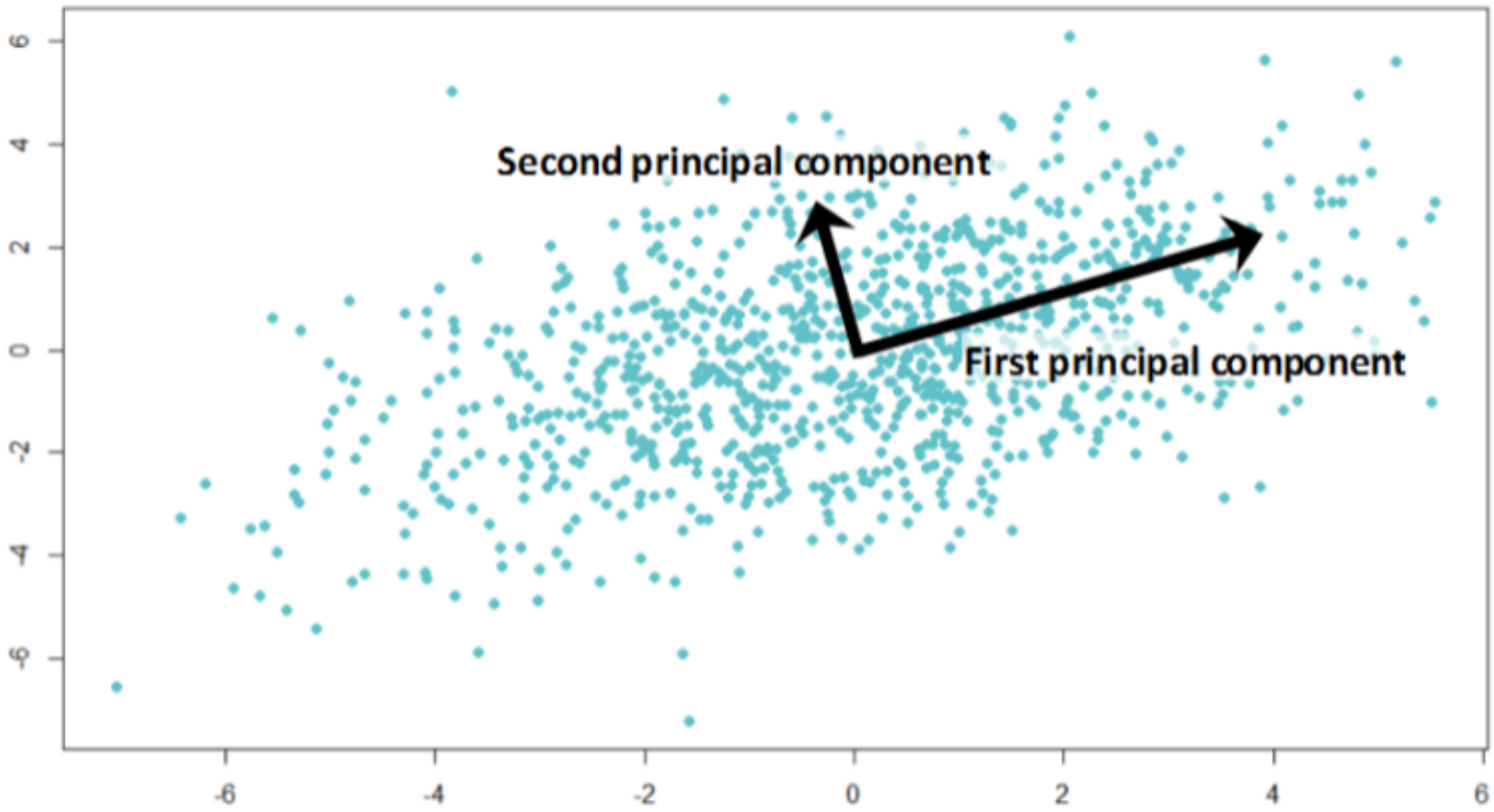
- The Elements of Statistical Learning, *T. Hastie, R. Friedman, J. Tibshirani*, Springer
- Data Mining , *S. Tufféry*, Technip
- WikiStat *P. Besse et al.* `http://wikistat.fr/`
- Interesting overview at `http://scikit-learn.org/stable/modules/clustering.html`
- Interesting demos on `https://www.toptal.com/machine-learning/clustering-algorithms`

Outline

Principal Component Analysis

- Observation $X_1, \ldots, X_n$ in $\mathbb{R}^p$, *centered*
- PCA = Dimension reduction tool (for visual clustering)
- Idea: project onto a subspace $R^d \subset \mathbb{R}^p$ so as to save as much variance as possible
- Big Picture: orthogonal linear transformation such that the first component has highest variance, then the second, etc.
- First component: $w_1 = \mathrm{argmax}_{\|w\|=1} \sum_i (x_i \cdot w)^2$ is the eigenvector of $X^T X$ corresponding to the highest eigenvalue.
- Similar reasonning for the next components in the orthogonal of w_1.

PCA: visualization



Src: [https://techannouncer.com/

global-pca-unit-market-2017-adelte-airmak-industries-amss-ltd-cavotec-airport-division-ciat-effeti/]

PCA algorithm

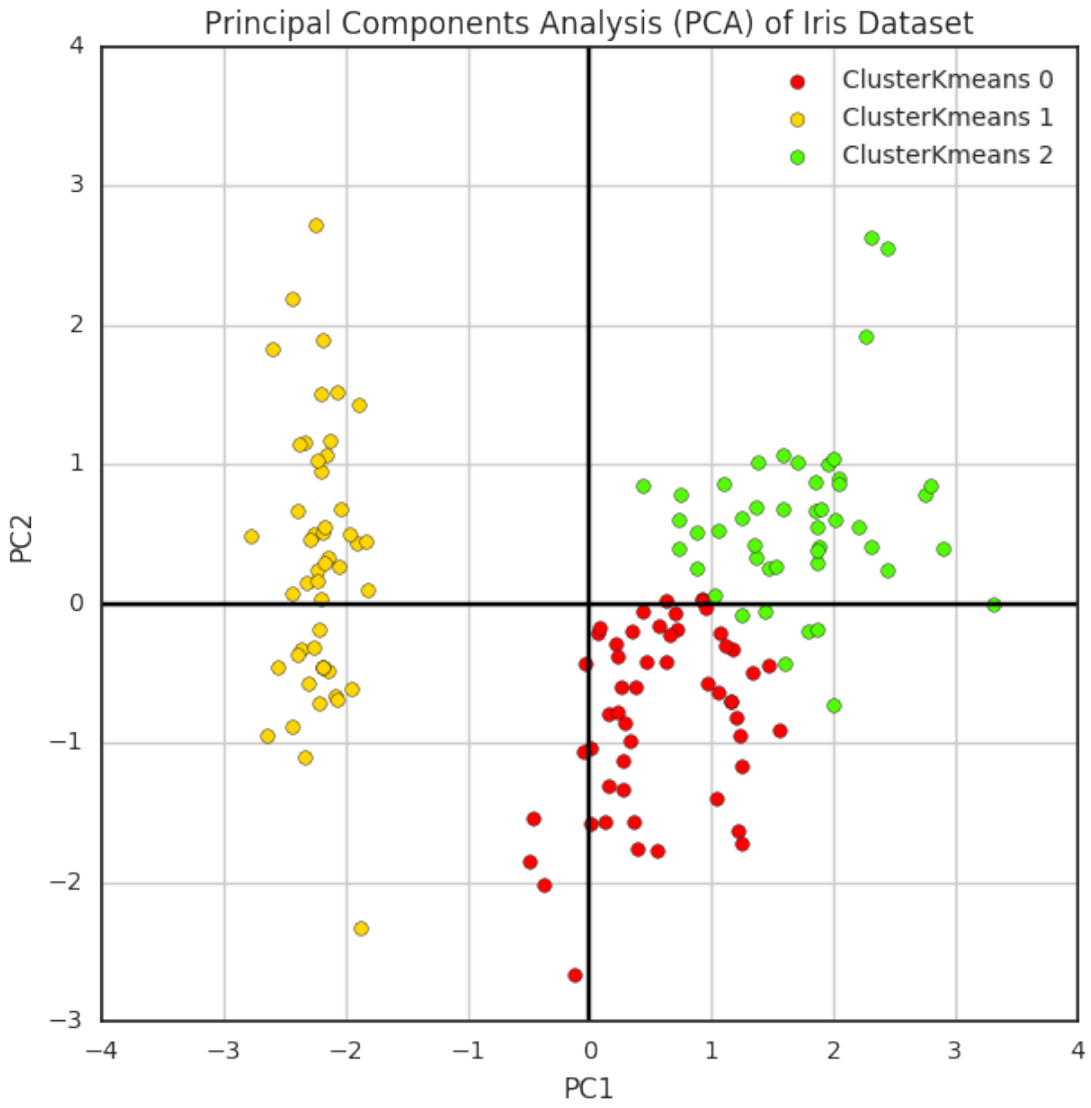
PCA

- Center all variables
- Compute the $p \times p$ empirical covariance matrix $X^T X$.
- Compute the components W_d = the d first eigenvectors of $X^T X$ in decreasing order of the eigenvalues
- Return the projection of X onto the d first components $T_d = X\, W_d$.

Then:

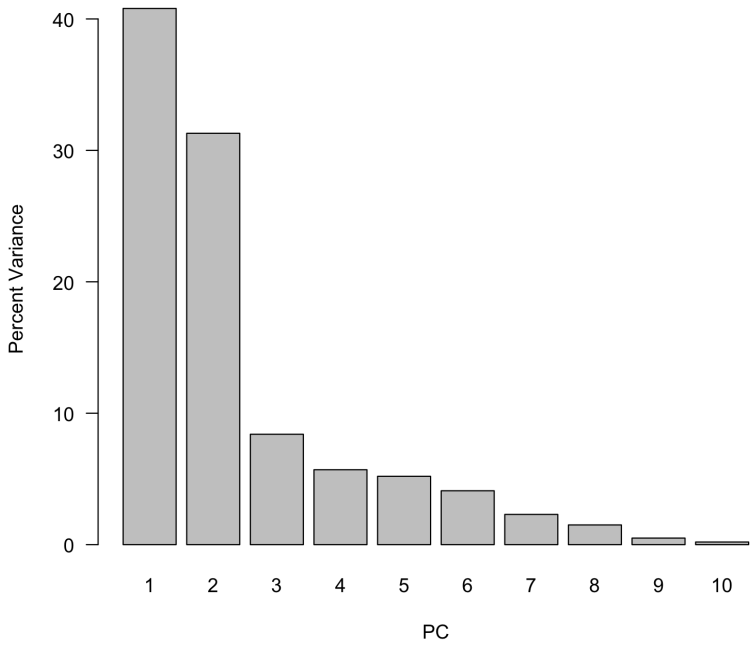
- either visualize clusters (2d or 3d plots)
- or use another clustering algorithm on the lower-dimensionnal data T_d (*dimension reduction*)

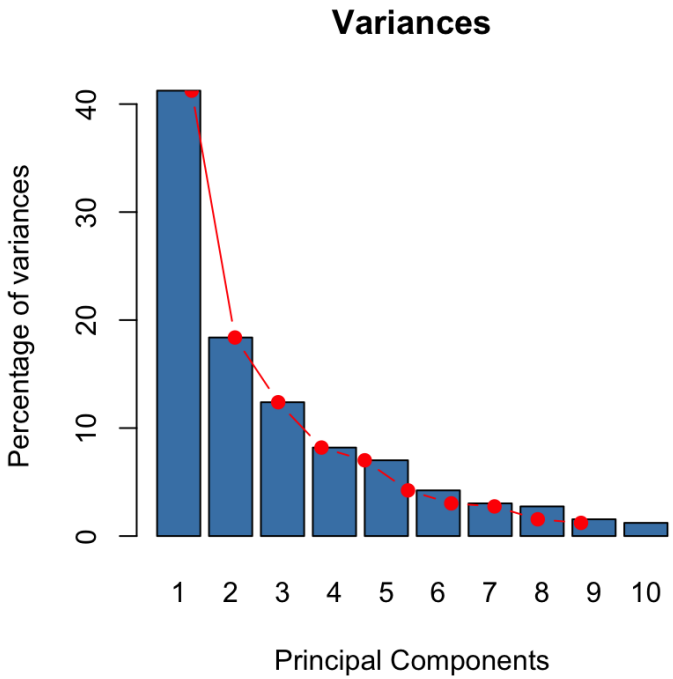
Example: IRIS



[Src: https://www.kaggle.com/bburns/iris-exploration-pca-k-means-and-gmm-clustering]

PCA scree plot





Src: `http://strata.uga.edu/8370/lecturenotes/principalComponents.html` and

`http://www.sthda.com/english/wiki/print.php?id=207`

Independent Component Analysis (ICA)

- similar idea, but search for *independent* (instead of uncorrelated) components
- computationally more demanding, but iterative (entropy-based) algorithm exists
- often used for blind source separation
- see also Non-negative Matrix Factorization (NMF)
- for visualization, see also t-SNE: *t*-distributed Stochastic Neighbor Embedding

Commands

scikitlearn:

```
class sklearn.decomposition.PCA(n_components=None,
copy=True, whiten=False, svd_solver=?auto?, tol=0.0,
iterated_power=?auto?, random_state=None)
```

ICA: `sklearn.decomposition.FastICA`

R: package stats

```
prcomp() et princomp() [fonction de base, package stats],
PCA() [package FactoMineR],
dudi.pca() [package ade4],
epPCA() [package ExPosition]
```

ICA: `ica`

Outline

Model-based approach: Gaussian Mixtures

- Observations $X_1, \ldots, X_n$ in $\mathbb{R}^p$
- K cluster centers: $\mu_1, \ldots, \mu_K$
- Cluster k has probability p_k
- Points in cluster k have law $\mathcal{N}(\mu_k, \Sigma)$

- Given a sample $(X_1, \ldots, X_n)$, how to estimate the cluster centers $(\mu_k)_k$ and how to identify the clusters?

Expectation-Maximization Algorithm

- Likelihood: the parameter $\theta = (p, \mu)$ has likelihood

$$L(\theta) \propto \sum_{z_1,\ldots,z_n \in \{1,\ldots,K\}^n} \prod_{i=1}^{n} p_{z_i} e^{-\frac{1}{2}(X_i - \mu_{z_i})^T \Sigma^{-1} (X_i - \mu_{z_i})}$$

$\implies$ non-convex, very hard to maximize

- *Approximate* iterative optimization

Expectation-Maximization Algorithm

Given an estimate $\theta^j = (p^j, \mu^j)$, compute

- *membership weights*

$$w_{i,k}^j = P_{\theta^j}(z_i = k|X_i) = \frac{p_k^j \, e^{-\frac{1}{2}(X_i-\mu_{z_i})^T \Sigma^{-1}(X_i-\mu_{z_i})}}{\sum_{\ell=1}^K p_\ell^j \, e^{-\frac{1}{2}(X_i-\mu_{z_i})^T \Sigma^{-1}(X_i-\mu_{z_i})}}$$

- updated cluster weights:

$$p_k^{j+1} = \frac{\sum_{i=1}^n w_{i,k}^j}{n}$$

- updated cluster means:

$$\mu_k^{j+1} = \frac{\sum_{i=1}^n w_{i,k}^j \, X_i}{\sum_{i=1}^n w_{i,k}^j}$$

Convergence of the Expectation-Maximization Algorithm

Theorem

The likelihood increases over the iterations:

$$L\left(\theta^{j+1}\right) \geq L\left(\theta^{j}\right)$$

Good: converges
Bad: can be a local optimum

EM Algorithm

- randomly initialize θ_0
- compute EM iterations until convergence:
  - *membership weights* $(w_{i,k}^{j})_{i,k}$
  - *updated cluster weights* $(p_k^{j+1})_k$
  - *updated cluster means* $(\mu_k^{j+1})_k$
- start again (a few times) to look for a better local optimum

Commands

scikitlearn:

```
class sklearn.mixture.GaussianMixture(n_components=1,
covariance_type=?full?, tol=0.001, reg_covar=1e-06,
max_iter=100, n_init=1, init_params=?kmeans?,
weights_init=None, means_init=None, precisions_init=None,
random_state=None, warm_start=False, verbose=0,
verbose_interval=10)
```

R:

```
MClust() [package MASS],
GuassianMixtures() [package sBIC]
```

Outline

Model-free clustering

- Observations $X_1, \ldots, X_n$ in $\mathbb{R}^p$;
- Objective function: for candidate cluster centers $\mu = (\mu_1, \ldots, \mu_K)$ and cluster assignations $z = (z_1, \ldots, z_n)$:

$$L(\mu, z) = \sum_{k=1}^{K} \sum_{i:z_i=k} \|X_i - \mu_k\|^2 = \sum_{i=1}^{n} \sum_{k=1}^{K} \mathbb{1}\{z_i = k\} \|X_i - \mu_k\|^2$$

- If $S_k = \{i : z_i = k\}$,

$$L(\mu, z) = \sum_{k=1}^{K} |S_k| \, \mathbb{V}ar[S_k]$$

- Minimizing L is equivalent to minimizing pairwise deviations in the clusters:

$$\mathrm{argmin}_{\mu,z} L(\mu, z) = \mathrm{argmin}_{\mu,z} \sum_{k=1}^{K} \frac{1}{|S_k|} \sum_{i,j \in S_k} \|X_i - X_j\|^2$$

Lloyd's algorithm

- For a fixed μ, optimizing in z is easy: $z_i = \mathrm{argmin}_k \|X_i - \mu_k\|$
- For a fixed z, optimizing in μ is easy: $\mu_k =$ mean of cluster k
- BUT optimizing in (μ, z) is NP-hard!

k-means

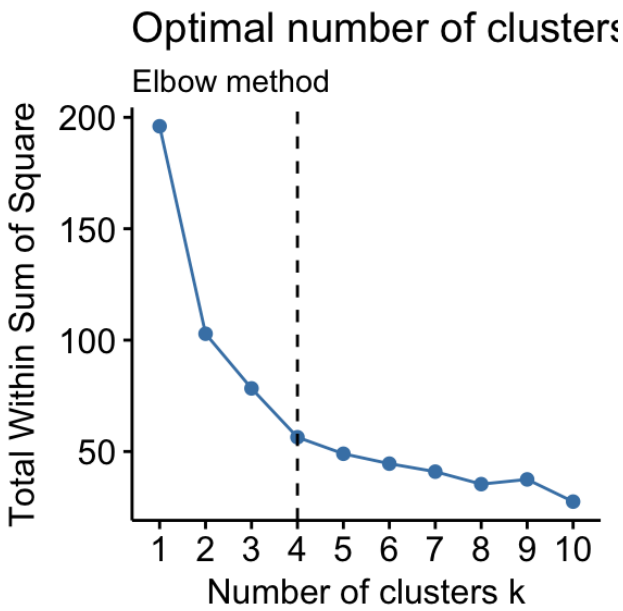
- randomly initialize $\theta_0 = (\mu_1^0, \ldots, \mu_K^0)$
- compute Lloyd's iterations until convergence:
  - *membership variables* $z_i^j = \mathrm{argmin}_k \{\|X_i - \mu_k^j\|$
  - *update cluster weights* $N_k^j = \sum_{i=1}^{n} \mathbb{1}\{z_i^j = k\}$
  - *update cluster means* $\mu_k^{j+1} = \dfrac{\sum_{i:z_i^j=k} X_i}{N_k^j}$
- start again (a few times) to look for a better local optimum

Comments on k-means

- k-means is a "hard" version of EM for mixtures! (when variances tends to 0)
- Complexity: linear in n and k (fast)
- Requires only a dissimilarity measure (not necessarily a distance)
- Quality of solution found depends on (random) initialization
- Not robust to outliers

- Problem: how to choose k?

  [Src: `http://www.sthda.com/english/articles/29-cluster-validation-essentials/`]



Improved Initialization: k-means++

[Arthur, D.; Vassilvitskii, S. (2007). "k-means++: the advantages of careful seeding" (PDF). Proceedings of the eighteenth annual ACM-SIAM symposium on Discrete algorithms.]

Idea: enforce distant cluster centers from the start

k-means++

- Choose first center μ_1 uniformly at random
- For $k = 2$ to K, repeat:
  - compute $D_i = \min_{\ell \leq k-1} \|X_i - \mu_\ell\|$ (distance to closest center)
  - choose $\mu_k = X_i$ with probability proportional to D_i^2
- Run k-means with initial centers $\theta_0 = (\mu_1, \ldots, \mu_K)$

- theoretical guarantee of $O(\log k)$ approximation from the start
- still linear complexity
- often a dramatic improvement in practice

k-medoids: robustness vs computation time

k-medoids

- randomly initialize θ_0 with K points from the dataset
- iterate until convergence:
  - *membership variables* $z_i^j = \mathrm{argmin}_k \{\|X_i - \mu_k^j\|$
  - *update cluster medoids* $\mu_k^{j+1} = \mathrm{argmin}_{X_i \in S_k} \sum_{\ell \in S_k} \|X_\ell - X_i\|$
- start again (a few times) to look for a better local optimum

- k-medoids is similar to k-means, with $\|\cdot\|$ instead of $\|\cdot\|^2$
  $\rightsquigarrow$ Robust to outliers (cf median versus mean)
- BUT computation time is quadratic in n

Commands

scikitlearn:

```
class sklearn.cluster.KMeans(
n_clusters=8, init=?k-means++?, n_init=10, max_iter=300,
tol=0.0001, precompute_distances='auto', verbose=0,
random_state=None, copy_x=True, n_jobs=1, algorithm='auto'
```

R: package stats

```
kmeans(x, centers, iter.max = 10, nstart = 1,
algorithm = c("Hartigan-Wong", "Lloyd", "Forgy",
"MacQueen"), trace=FALSE)
```

Variants to be found in various packages: `ClusterR`, `kmed`, etc.

Outline

Agglomerative clustering

- greedy bottom-up algorithm
- requires a distance (dissimilarity) between observations $\|x - x'\|$
- choice of *distance between clusters:*
  - complete linkage: $d(A, B) = \max\left\{\|x - x'\| : x \in A,\, x' \in B\right\}$
  - single linkage: $d(A, B) = \min\left\{\|x - x'\| : x \in A,\, x' \in B\right\}$
  - average linkage distance: $d(A, B) = \dfrac{1}{|A|\,|B|} \sum_{x \in A} \sum_{x' \in B} \|x - x'\|$
  - Ward distance for Euclidian mean: $d(A, B) = \dfrac{|A|\,|B|}{n\big(|A| + |B|\big)} \left\|\bar{A} - \bar{B}\right\|$
  - sum of intra-cluster variance
  - etc.

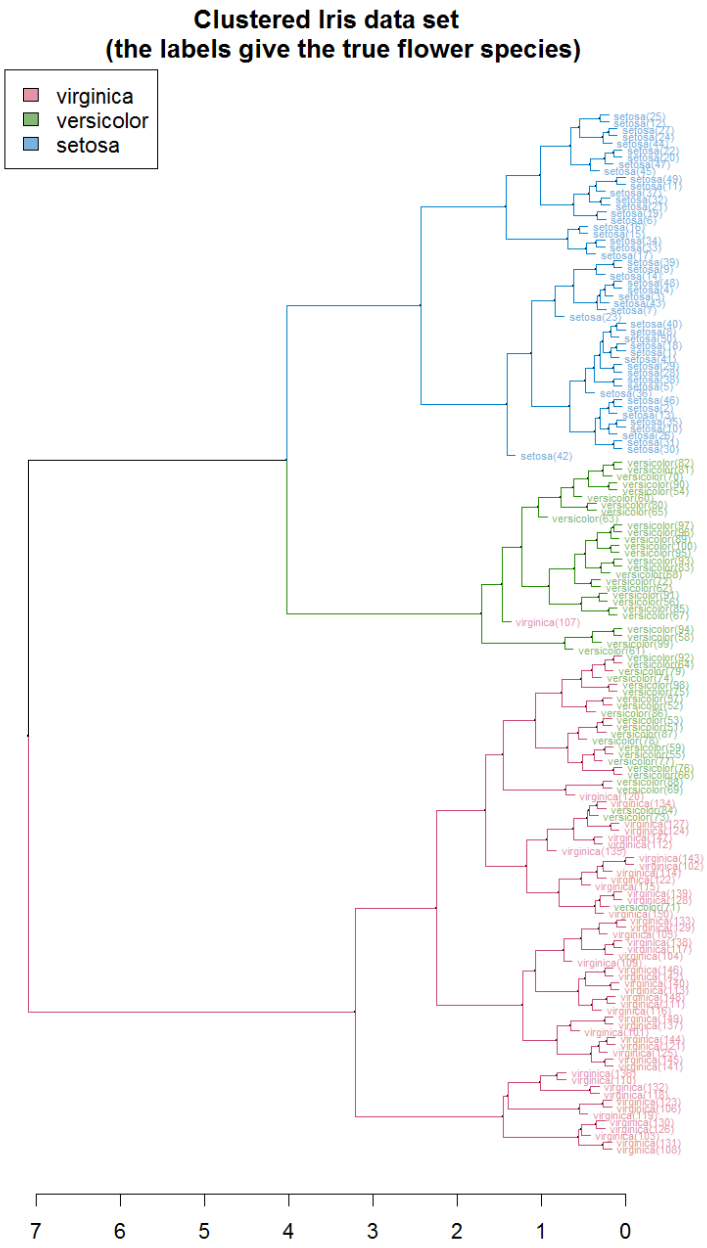
HCA algorithm

HCA

- Initialization: all observations are clusters $\{X_1\}, \ldots, \{X_n\}$
- As long as there are at least two clusters:
  - add a link between two clusters with smallest distance
  - merge them for the next iterations
- Return the *dendrogram* = hierarchy of clusters

Property of Ward for Euclidean distance: interclass variance decreases with the number of classes.

Dendrogram



Author: Talgalili

https://commons.wikimedia.org/wiki/File:Iris_dendrogram.png

Pros and Cons

- No need to specify the number of clusters in advance
- A relevant choice can be deduced from the observation of the dendrogram (and practical needs)
- Computational complexity in $O\left(n^2\right)$
- Does not find an optimal solution

Commands

scikitlearn:

```
class sklearn.cluster.AgglomerativeClustering(n_clusters=2,
affinity=?euclidean?, memory=None, connectivity=None,
compute_full_tree=?auto?, linkage=?ward?,
pooling_func=<function mean>)
```

R:

```
hclust(d, method = "complete", members = NULL)
```

Outline

Affinity Propagation

- Message-passing algorithm
- affinity function $s(x, x')$, for example $s(x, x') = -\|x - x'\|^2$
- $s(x, x) =$ input preference: the lower, the higher the chances to be an exemplar
- responsibility matrix R: $r(i, k) =$ how well-suited X_k can serve as an exemplar for X_i (wrt other candidate exemplars)
- availability matrix A: $a(i, k) =$ how appropriate it is for X_i to pick X_k as an exemplar, taking into account other points' preferences for X_k as an exemplar

Affinity Propagation

Affinity Propagation

- Initialize R and A with 0
- Repeat until convergence:
  - update responsibilities:
    $r(i,k) \leftarrow s(i,k) - \max_{k' \neq k} \left\{ a(i,k') + s(i,k') \right\}$
  - update availabilities:
    $$a(i,k) \leftarrow \min \left\{ 0, r(k,k) + \sum_{i' \notin \{i,k\}} \max(0, r(i',k)) \right\} \text{ for } i \neq k$$
    $$\text{and } a(k,k) \leftarrow \sum_{i' \neq k} \max\left(0, r(i',k)\right)$$
- Pick exemplars as maximizers of $r(i,i) + a(i,i)$

Affinity Propagation: pros/cons

- No need to specify the number of clusters
- ... but a parameter plays the same role
- quadratic time complexity
- some improvement over k-means in some cases

Commands

scikitlearn:

```
class sklearn.cluster.AffinityPropagation(damping=0.5,
max_iter=200, convergence_iter=15, copy=True,
preference=None, affinity=?euclidean?, verbose=False)
```

R: package APCluster

```
apcluster(s, x, p=NA, q=NA, maxits=1000,
convits=100, lam=0.9, includeSim=FALSE, details=FALSE,
nonoise=FALSE, seed=NA)
```

Spectral Clustering

- Similarity matrix $S_{i,j}$, for example $S_{i,j} = -\|X_i - X_j\|^2$
- Idea: use standard clustering method on eigenvectors of the (normalized) Laplacian matrix

$$L = Id - D^{-1/2}\, S\, D^{-1/2}$$

  where D is diagonal with $D_{i,i} = \sum_j S_{i,j}$
- Intuition: if S is diagonal by blocks, the eigenvectors are the indicators of the blocks (up to a multiplication by $D^{1/2}$)
- Other Laplacian matrices are also considered:

$$L = D - S \qquad \text{or} \qquad L = Id - D^{-1} S$$

Commands

scikitlearn:

```
class sklearn.cluster.SpectralClustering(n_clusters=8,
eigen_solver=None, random_state=None, n_init=10, gamma=1.0,
affinity=?rbf?, n_neighbors=10, eigen_tol=0.0,
assign_labels=?kmeans?, degree=3, coef0=1,
kernel_params=None, n_jobs=1)
```

R: package kernlab

```
specc(x, data = NULL, na.action = na.omit, ...)
```

DBscan

- DBscan = density-based spatial clustering of applications with noise
- parameters: radius ϵ and minimal cluster size *minSize*

DBscan

Repeat as long as at least one point has not been visited:

- pick an unvisited point X_i at random
- if it has less than *minSize* ϵ-neighbors, mark it as an outlier
- otherwise, form the cluster of all points that can be reached by jumps of at most ϵ starting from X_i

DBscan: comments

- simple and fast
- no need to specify number of clusters
- Problem: sensitive to the choice of parameters
- choosing the right parameters ϵ and *minSize* properly is hard
  $\rightsquigarrow$ for instance, choose ϵ and *minSize* such that the proportion of outliers is at most 10% (say)
- unable to handle clusters with very different densities

Commands

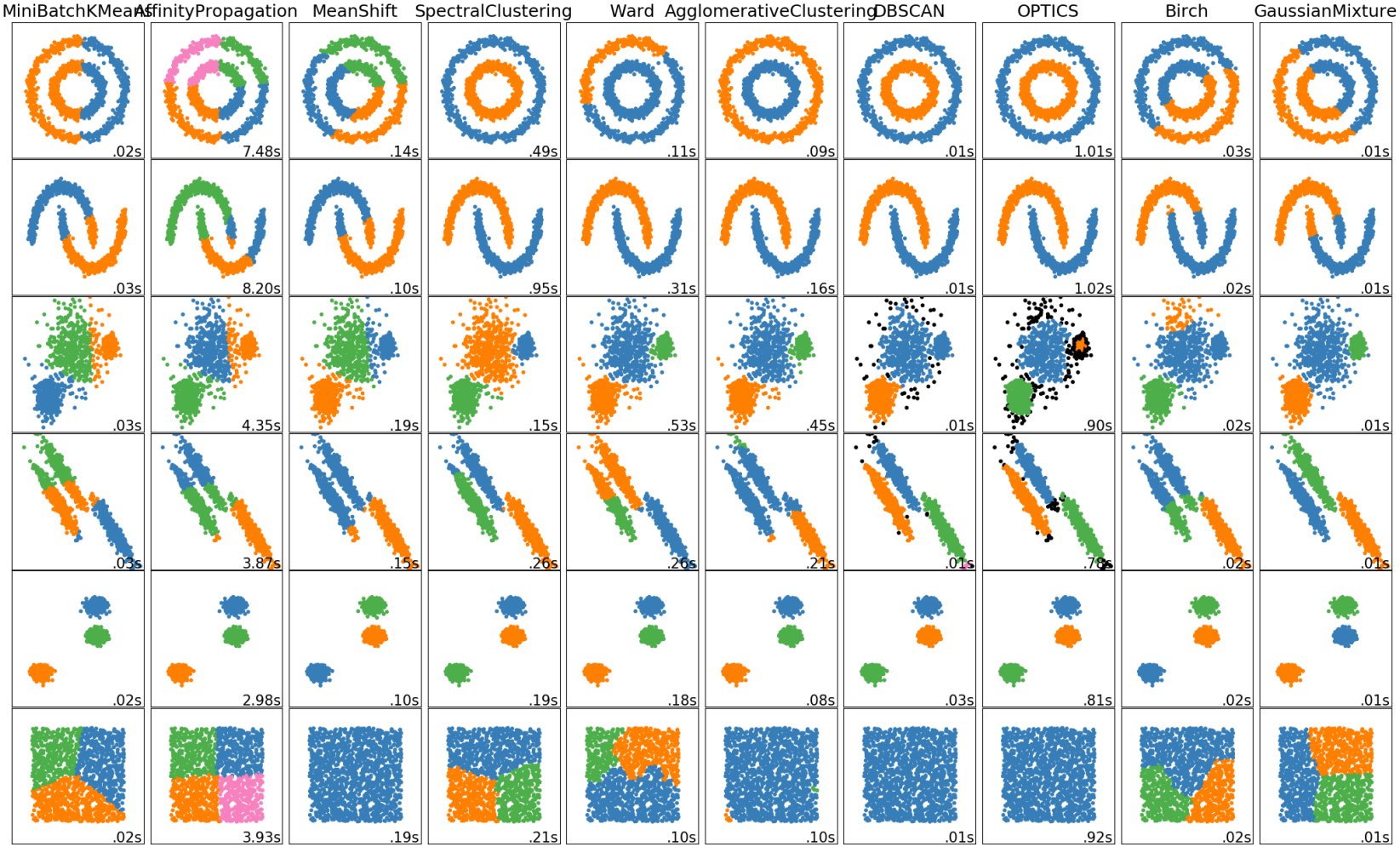
scikitlearn:

```
class sklearn.cluster.DBSCAN(eps=0.5, min_samples=5,
metric='euclidean', metric_params=None, algorithm='auto',
leaf_size=30, p=None, n_jobs=1)
```

R: package dbscan

```
dbscan(x, eps, minPts = 5, weights = NULL,
borderPoints = TRUE, ...)
```

Which algorithm to choose?



Src: [http://scikit-learn.org/stable/auto_examples/cluster/plot_cluster_comparison.html]

Clustering time series

Features:

- mean
- trend
- auto-correlation coefficients
- inter-series correlation
- etc.

$\Longrightarrow$ it depends on the nature of the problem and on the goal of the clustering!