Machine Learning: from Theory to Practice

Unsupervised Learning

Dimension Reduction and Clustering

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Outline

Outline

Motivation

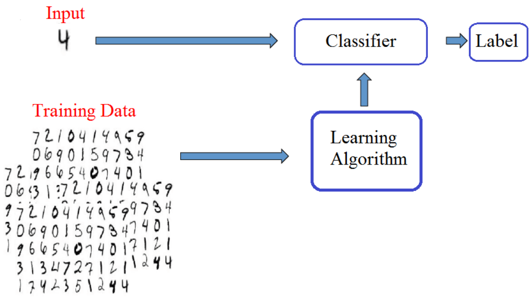
- **Marketing:** finding groups of customers with similar behavior given a large database of customer data containing their properties and past buying records;
- **Biology:** classification of plants and animals given their features;
- **Libraries:** book ordering;
- **Insurance:** identifying groups of motor insurance policy holders with a high average claim cost; identifying frauds;
- **City-planning:** identifying groups of houses according to their house type, value and geographical location;
- **Internet:** document classification; clustering weblog data to discover groups of similar access patterns.

Marketing

- **Data:** Base of customer data containing their properties and past buying records
- **Goal:** Use the customers *similarities* to find groups.
- **Two directions:**
  - **Clustering:** propose an explicit *grouping* of the customers
  - **Visualization:** propose a representation of the customers so that the groups are *visibles*

Outline

Machine Learning



A definition by Tom Mitchell (`http://www.cs.cmu.edu/~tom/`)

A computer program is said to learn from experience E with respect to some class of tasks T and performance measure P, if its performance at tasks in T, as measured by P, improves with experience E.

Supervised Learning

Experience, Task and Performance measure

- Training data : $\mathcal{D} = \{(\mathbf{X}_1, Y_1), \ldots, (\mathbf{X}_n, Y_n)\}$ (i.i.d. $\sim \mathbf{P}$)
- Predictor: $f : \mathcal{X} \to \mathcal{Y}$ measurable
- Cost/Loss function : $\ell(f(\mathbf{X}), Y)$ measure how well $f(\mathbf{X})$ “predicts" Y
- Risk:

$$\mathcal{R}(f) = \mathbb{E}\left[\ell(Y, f(\mathbf{X}))\right] = \mathbb{E}_X\left[\mathbb{E}_{Y|\mathbf{X}}\left[\ell(Y, f(\mathbf{X}))\right]\right]$$

- Often $\ell(f(\mathbf{X}), Y) = \|f(\mathbf{X}) - Y\|^2$ or $\ell(f(\mathbf{X}), Y) = \mathbf{1}_{Y \neq f(\mathbf{X})}$

Goal

- Learn a rule to construct a classifier $\widehat{f} \in \mathcal{F}$ from the training data $\mathcal{D}_n$ s.t. the risk $\mathcal{R}(\widehat{f})$ is small on average or with high probability with respect to $\mathcal{D}_n$.

Unsupervised Learning

Experience, Task and Performance measure

- Training data : $\mathcal{D} = \{\mathbf{X}_1, \dots, \mathbf{X}_n\}$ (i.i.d. $\sim \mathbf{P}$)
- Task: ???
- Performance measure: ???

- No obvious task definition!

Tasks for today

- **Dimension reduction:** construct a map of the data in a low dimensional space without distorting it too much.
- **Clustering (or unsupervised classification):** construct a grouping of the data in homogeneous classes.

Dimension Reduction

- Training data : $\mathcal{D} = \{\mathbf{X}_1, \ldots, \mathbf{X}_n\} \in \mathcal{X}^n$ (i.i.d. $\sim \mathbf{P}$)
- Space $\mathcal{X}$ of possibly high dimension.

Dimension Reduction Map

- Construct a map Φ from the space $\mathcal{X}$ into a space $\mathcal{X}'$ of smaller dimension:

$$\begin{aligned} \Phi : \quad & \mathcal{X} \to \mathcal{X}' \\ & \mathbf{X} \mapsto \Phi(\mathbf{X}) \end{aligned}$$

- Map can be defined only on the dataset.

Motivations

- Visualization of the data
- Dimension reduction before further processing

Dimension Reduction

- Need to control the distortion between $\mathcal{D}$ and $\Phi(\mathcal{D}) = \{\Phi(\mathbf{X}_1), \dots, \Phi(\mathbf{X}_n)\}$

Distortion(s)

- Reconstruction error:
  - Construct $\widetilde{\Phi}$ from $\mathcal{X}'$ to $\mathcal{X}$
  - Control the error between $\mathbf{X}$ and its reconstruction $\widetilde{\Phi}(\Phi(\mathbf{X}))$
- Distance preservation:
  - Measure the distance between $\mathbf{X}_i$ and $\mathbf{X}_j$ and the distance between $\Phi(\mathbf{X}_i)$ and $\Phi(\mathbf{X}_j)$
  - Control the difference between those two distances

- Leads to different constructions....

Clustering

- Training data : $\mathcal{D} = \{\mathbf{X}_1, \ldots, \mathbf{X}_n\} \in \mathcal{X}^n$ (i.i.d. $\sim \mathbf{P}$)
- Latent groups?

Clustering

- Construct a map f from $\mathcal{D}$ to $\{1, \ldots, K\}$ where K is a number of classes to be fixed:

$$f : \quad \mathbf{X}_i \mapsto k_i$$

- Similar to classification except:
  - no ground truth (no given labels)
  - label only elements of the dataset!

Motivations

- Interpretation of the groups
- Use of the groups in further processing

Clustering

- Need to define the quality of the cluster.
- No obvious measure!

Clustering quality

- Inner homogeneity: samples in the same group should be similar.
- Outer inhomogeneity: samples in two different groups should be different.

- Several possible definitions of similar and different.
- Often based on the distance between the samples.
- Example based on the euclidean distance:
  - Inner homogeneity = intra class variance,
  - Outer inhomogeneity = inter class variance.
- **Beware:** choice of the number of cluster K often complex!

Outline

Dimension Reduction

- Training data : $\mathcal{D} = \{\mathbf{X}_1, \dots, \mathbf{X}_n\} \in \mathcal{X}^n \quad$ (i.i.d. $\sim \mathbf{P}$)
- Space $\mathcal{X}$ of possibly high dimension.

Dimension Reduction Map

- Construct a map Φ from the space $\mathcal{X}$ into a space $\mathcal{X}'$ of smaller dimension:

$$\begin{aligned} \Phi : \quad & \mathcal{X} \to \mathcal{X}' \\ & \mathbf{X} \mapsto \Phi(\mathbf{X}) \end{aligned}$$

Criterion

- Reconstruction error
- Distance preservation

Outline

Reconstruction Error Approach

Goal

- Construct a map Φ from the space $\mathcal{X}$ into a space $\mathcal{X}'$ of smaller dimension:
$$\begin{aligned}\Phi: \quad & \mathcal{X} \to \mathcal{X}' \\ & \mathbf{X} \mapsto \Phi(\mathbf{X})\end{aligned}$$
- Construct $\widetilde{\Phi}$ from $\mathcal{X}'$ to $\mathcal{X}$
- Control the error between $\mathbf{X}$ and its reconstruction $\widetilde{\Phi}(\Phi(\mathbf{X}))$

- Canonical example for $\mathbf{X} \in \mathbb{R}^d$: find Φ and $\widetilde{\Phi}$ in a parametric family that minimize
$$\frac{1}{n}\sum_{i=1}^{n} \|\mathbf{X}_i - \widetilde{\Phi}(\Phi(\mathbf{X}_i))\|^2$$

Principal Component Analysis

- $\mathcal{X} \in \mathbb{R}^d$ and $\mathcal{X}' = \mathbb{R}^{d'}$
- Affine model $\mathbf{X} \sim m + \sum_{l=1}^{d'} \mathbf{X}'^{(l)} V^{(l)}$ with $(V^{(l)})$ an orthonormal family.
- Equivalent to:
$$\Phi(\mathbf{X}) = V^t(\mathbf{X} - m) \quad \text{and} \quad \widetilde{\Phi}(\mathbf{X}') = m + V\mathbf{X}'$$
- Reconstruction error criterion:
$$\frac{1}{n}\sum_{i=1}^{n} \|\mathbf{X}_i - (m + VV^t(\mathbf{X}_i - m)\|^2$$
- **Explicit solution:** m is the empirical mean and V is any orthonormal basis of the space spanned by the d' first eigenvectors (the one with largest eigenvalues) of the empirical covariance matrix $\frac{1}{n}\sum_{i=1}^{n}(\mathbf{X}_i - m)(\mathbf{X}_i - m)^t$.

Principal Component Analysis

PCA Algorithm

- Compute the empirical mean $m = \frac{1}{n} \sum_{i=1}^{n} \mathbf{X}_i$
- Compute the empirical covariance matrix $\frac{1}{n} \sum_{i=1}^{n} (\mathbf{X}_i - m)(\mathbf{X}_i - m)^t$.
- Compute the d' first eigenvectors of this matrix: $V^{(1)}, \ldots, V^{(d')}$
- Set $\Phi(\mathbf{X}) = V^t(\mathbf{X} - m)$

- Complexity: $O(n(1 + d^2) + d' d^2)$
- Interpretation:
  - $\Phi(\mathbf{X}) = V^t(\mathbf{X} - m)$: coordinates in the restricted space.
  - $V^{(i)}$: influence of each original coordinates in the ith new one.
- **Scaling:** This method is not invariant to a scaling of the variables! It is custom to normalize the variables (at least within groups) before applying PCA.

Multiple Factor Analysis

- PCA assumes $\mathcal{X} = \mathbb{R}^d$!
- How to deal with categorical values?
- MFA = PCA with clever coding strategy for categorical values.

Categorical value code for a single variable

- Classical redundant dummy coding:
$$\mathbf{X} \in \{1, \dots, V\} \mapsto P(\mathbf{X}) = (\mathbf{1}_{\mathbf{X}=1}, \dots, \mathbf{1}_{\mathbf{X}=V})^t$$
- Compute the mean (i.e. the empirical proportion) $\overline{P} = \frac{1}{n} P(\mathbf{X})$
- *Renormalize* $P(\mathbf{X})$ by $1/\sqrt{(V-1)\overline{P}}$:
$$P(\mathbf{X}) \mapsto P^r(\mathbf{X})$$
$$(\mathbf{1}_{\mathbf{X}=1}, \dots \mathbf{1}_{\mathbf{X}=V}) \mapsto \left(\frac{\mathbf{1}_{\mathbf{X}=1}}{\sqrt{(V-1)\overline{P}_1}}, \dots, \frac{\mathbf{1}_{\mathbf{X}=V}}{\sqrt{(V-1)\overline{P}_V}} \right)$$

- χ^2 type distance!

Multiple Factor Analysis

- PCA becomes the minimization of

$$\frac{1}{n}\sum_{i=1}^{n}\|P^r(\mathbf{X}_i)-(m+VV^t(P^r(\mathbf{X}_i)-m))\|^2$$

$$=\frac{1}{n}\sum_{i=1}^{n}\sum_{v=1}^{V}\frac{\left|\mathbf{1}_{\mathbf{X}_i=v}-(m'+\sum_{l=1}^{d'}V^{(l)t}(P(\mathbf{X}_i)-m')V^{(l,v)})\right|^2}{(V-1)\overline{P}_v}$$

- Interpretation:
  - $m'=\overline{P}$
  - $\Phi(\mathbf{X})=V^t(P^r\mathbf{X}-m)$: coordinates in the restricted space.
  - $V^{(l)}$ can be interpreted s as a probability profile.
- Complexity: $O(n(1+V^2)+d'V^2)$
- Link with Correspondence Analysis (CA)

Multiple Factor Analysis

MFA Algorithm

- Redundant dummy coding of each categorical variable.
- Renormalization of each block of dummy variable.
- Classical PCA algorithm on the resulting variables

- Interpretation as a reconstruction error with a rescaled/χ^2 metric.
- Interpretation:
  - $\Phi(\mathbf{X}) = V^t(P^r(\mathbf{X}) - m)$: coordinates in the restricted space.
  - $V^{(l)}$: influence of each modality/variable in the ith new coordinates.
- **Scaling:** This method is not invariant to a scaling of the continuous variables! It is custom to normalize the variables (at least within groups) before applying PCA.

Non Linear PCA

PCA Model

- PCA: Linear model assumption

$$\mathbf{X} \simeq m + \sum_{l=1}^{d'} \mathbf{X}'^{,(l)} V^{(l)} = m + V\mathbf{X}'$$

- with
  - $V^{(l)}$ orthonormal
  - $\mathbf{X}'^{,(l)}$ without constrains.

- Two directions of extension:
  - Other constrains on V (or the coordinates in the restricted space): ICA, NMF, Dictionary approach
  - PCA on a non linear image of $\mathbf{X}$: kernel-PCA
- Much more complex algorithm!

Non Linear PCA

ICA (Independent Component Analysis)

- Linear model assumption
- with
$$\mathbf{X} \simeq m + \sum_{l=1}^{d'} \mathbf{X}'^{,(l)} V^{(l)} = m + V\mathbf{X}'$$
  - $V^{(l)}$ without constrains.
  - $\mathbf{X}'^{,(l)}$ independent

NMF (Non Negative Matrix Factorization)

- (Linear) Model assumption
- with
$$\mathbf{X} \simeq m + \sum_{l=1}^{d'} \mathbf{X}'^{,(l)} V^{(l)} = m + V\mathbf{X}'$$
  - $V^{(l)}$ non negative
  - $\mathbf{X}'^{,(l)}$ non negative.

Non Linear PCA

Dictionary

- (Linear) Model assumption

$$\mathbf{X} \simeq m \sum_{l=1}^{d'} \mathbf{X}'^{,(l)} V^{(l)} = m + V\mathbf{X}'$$

- with
  - $V^{(l)}$ without constrains
  - $\mathbf{X}'$ sparse (with a lot of 0)

kernel PCA

- Linear model assumption

$$\Psi(\mathbf{X} - m) \simeq \sum_{l=1}^{d'} \mathbf{X}'^{,(l)} V^{(l)} = V\mathbf{X}'$$

- with
  - $V^{(l)}$ orthonormal
  - $\mathbf{X}'_l$ without constrains.

Link with SVD

- Linear model assumption:

$$\mathbf{X} \simeq m + \sum_{l=1}^{d'} \mathbf{X}'^{,(l)} V^{(l)} = m + V\mathbf{X}'$$

- Vector rewriting

$$\mathbf{X}^t \simeq m^t + \mathbf{X}'^t V^t$$

Matrix Rewriting and Low Rank Factorization

- Matrix rewriting

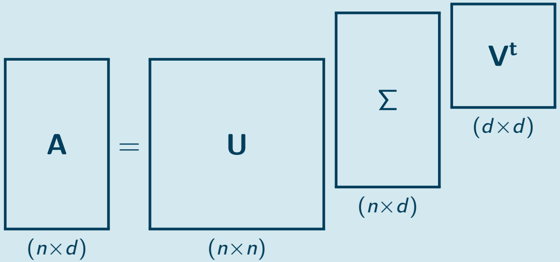
$$\underset{(n \times d)}{\boxed{\begin{array}{c} \mathbf{X}_1^t - m^t \\ \vdots \\ \vdots \\ \mathbf{X}_n^t - m^t \end{array}}} \simeq \underset{(n \times d')}{\boxed{\begin{array}{c} \mathbf{X}_1'^t \\ \vdots \\ \vdots \\ \mathbf{X}_n'^t \end{array}}} \; \underset{(d' \times d)}{\boxed{\quad \mathbf{V}^{\mathbf{t}} \quad}}$$

- Low rank matrix factorization! (Truncated SVD solution...)

SVD

SVD Decomposition

- Any matrix $n \times d$ matrix A can de decomposed as

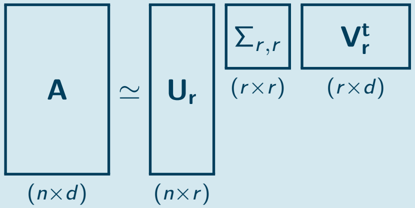


with U and V two orthononormal matrices and Σ a *diagonal* matrix with decreasing values.

SVD

Low Rank Approximation

- The best low rank approximation or rank r is obtained by restriction of the matrices to the first r dimensions:



for both the operator norm and the Frobenius norm!

- PCA: Frobenius norm, $d' = r$ and

$$\begin{pmatrix} \mathbf{X}_1^t - m^t \\ \vdots \\ \vdots \\ \mathbf{X}_n^t - m^t \end{pmatrix} \leftrightarrow A, \quad \begin{pmatrix} \mathbf{X}_1'^t \\ \vdots \\ \vdots \\ \mathbf{X}_n'^t \end{pmatrix} \leftrightarrow \mathbf{U_r}\Sigma_{r,r}, \quad \mathbf{V^t} \leftrightarrow \mathbf{V_r^t}$$

Outline

Pairwise Distance

- Different point of view!
- Focus on pairwise distance $d(\mathbf{X}_i, \mathbf{X}_j)$.

Distance Preservation

- Construct a map Φ from the space $\mathcal{X}$ into a space $\mathcal{X}'$ of smaller dimension:

$$\begin{aligned} \Phi: \quad & \mathcal{X} \to \mathcal{X}' \\ & \mathbf{X} \mapsto \Phi(\mathbf{X}) = \mathbf{X}' \end{aligned}$$

- such that

$$d(\mathbf{X}_i, \mathbf{X}_j) \sim d'(\mathbf{X}'_i, \mathbf{X}'_j)$$

- Most natural criterion:

$$\frac{1}{n^2} \sum_{i=1}^{n} \sum_{j=1}^{n} \left| d(\mathbf{X}_i, \mathbf{X}_j) - d'(\mathbf{X}'_i, \mathbf{X}'_j) \right|^2$$

- Φ often defined only on $\mathbf{D}$...

Random Projection

Random Projection Heuristic

- Draw at random d' unit vector (direction) U_i.
- Use $\mathbf{X}' = U^t(\mathbf{X} - m)$ with $m = \frac{1}{n} \sum_{i=1}^{n} \mathbf{X}_i$

- **Property:** If $\mathbf{X}$ lives in a space of dimension d'', then, as soon as, $d' \sim d'' \log(d'')$,

$$\|\mathbf{X}_i - \mathbf{X}_j\|^2 \sim \frac{d}{d'} \|\mathbf{X}'_i - \mathbf{X}'_j\|^2$$

- Do not really use the data!

Locally Linear Embedding

LLE Heuristic

- For each point $\mathbf{X}_i$, define a neighborhood $\mathcal{N}_i$ (either by a distance or a number of points).
- Compute some weights $W_{i,j}$ such that
$$W_{i,j} = 0 \quad \text{if } \mathbf{X}_j \notin \mathcal{N}_i$$
$$\mathbf{X}_i \sim \sum_j W_{i,j} \mathbf{X}_j$$
- Find some $\mathbf{X}'_i$ in a space $\mathcal{X}'$ of smaller dimension such that
$$\mathbf{X}'_i \sim \sum_j W_{i,j} \mathbf{X}'_j$$

- LLE: use a least square metric for the fits.

MultiDimensional Scaling

MDS Heuristic

- If $d(x, y) = \|x - y\|^2$, one can compute a Gram matrix
$$(\mathbf{X}_i - m)^t(\mathbf{X}_j - m)$$
for $m = \frac{1}{n}\sum_{i=1}^n \mathbf{X}_i$
- Match the *scalar* products:
$$\frac{1}{n^2}\sum_{i=1}^n\sum_{j=1}^n \left|(\mathbf{X}_i - m)^t(\mathbf{X}_j - m) - \mathbf{X}_i'^t\mathbf{X}_j'\right|^2$$
- Linear method: $\mathbf{X}' = U^t(\mathbf{X} - m)$ with U orthonormal

- **Beware:** $\mathbf{X}$ is unknown!

MultiDimensional Scaling

- Resulting criterion: minimization in $U^t(\mathbf{X}_i - m)$ of
$$\frac{1}{n^2}\sum_{i=1}^{n}\sum_{j=1}^{n}\left|(\mathbf{X}_i - m)^t(\mathbf{X}_j - m) - (\mathbf{X}_i - m)^t UU^t(\mathbf{X}_j - m)\right|^2$$
without knowing explicitly $\mathbf{X}$...
- Explicit solution obtained through the eigendecomposition of the know Gram matrix $(\mathbf{X}_i - m)^t(\mathbf{X}_j - m)$ by keeping only the d' largest eigenvalues.
- In this case, MDS yields the same result than the PCA (but with different inputs, distance between observation vs correlations)!

MultiDimensional Scaling

- **Explanation:** Same SVD problem up to a transposition:
  - MDS
$$\overline{\mathbf{X}}_{(n)}^t \overline{\mathbf{X}}_{(n)} \sim \overline{\mathbf{X}}_{(n)}^t U U^t \overline{\mathbf{X}}_{(n)}$$
  - PCA
$$\overline{\mathbf{X}}_{(n)} \overline{\mathbf{X}}_{(n)}^t \sim U^t \overline{\mathbf{X}}_{(n)} \overline{\mathbf{X}}_{(n)}^t U$$
- Complexity: ACP $O(d'd^2)$ vs MDS $O(d'n^2)$...

MDS

- Apply this algorithm even if $d(x,y) \neq \|x-y\|^2$!

- **True distance minimization:** Simple gradient descent can be used (can be stuck in local minima).

ISOMAP

- MDS: equivalent to PCA (but more expensive) if $d(x,y) = \|x-y\|^2$!
- ISOMAP: use a *localized* distance instead to limit the influence of very far point.

ISOMAP

- For each point $\mathbf{X}_i$, define a neighborhood $\mathcal{N}_i$ (either by a distance or a number of points) and let
$$d_0(\mathbf{X}_i,\mathbf{X}_j) = \begin{cases} +\infty & \text{if } \mathbf{X}_j \notin \mathcal{N}_i \\ \|\mathbf{X}_i - \mathbf{X}_j\|^2 & \text{otherwise} \end{cases}$$
- Compute the shortest path distance for each pair.
- Use the MDS algorithm with this distance

Graph based

Graph heuristic

- Construct a graph with weighted edges $w_{i,j}$ measuring the *proximity* of $\mathbf{X}_i$ and $\mathbf{X}_j$ ($w_{i,j}$ large if close and 0 if there is no information).
- Find the points $\mathbf{X}'_i \in \mathbb{R}^{d'}$ minimizing
$$\frac{1}{n}\frac{1}{n}\sum_{i=1}^{n}\sum_{j=1}^{n} w_{i,j}\|\mathbf{X}'_i - \mathbf{X}'_j\|^2$$

- Need of a constraint on the size of $\mathbf{X}'_i$...
- Explicit solution through linear algebra: d' eigenvectors with smallest eigenvalues of the Laplacian of the graph $D - W$, where D is a diagonal matrix with $D_{i,i} = \sum_j w_{i,j}$.
- Variation on the definition of the Laplacian...

t-Stochastic Neighbor Embedding

SNE heuristic

- From $\mathbf{X}_i \in \mathcal{X}$, construct a set of conditional probability:
$$P_{j|i} = \frac{e^{-\|\mathbf{X}_i - \mathbf{X}_j\|^2/2\sigma_i^2}}{\sum_{k\neq i} e^{-\|\mathbf{X}_i - \mathbf{X}_j\|^2/2\sigma_i^2}} \qquad P_{i|i} = 0$$
- Find $\mathbf{X}'_i$ in $\mathbb{R}^{d'}$ such that the set of conditional probability:
$$Q_{j|i} = \frac{e^{-\|\mathbf{X}'_i - \mathbf{X}'_j\|^2/2\sigma_i^2}}{\sum_{k\neq i} e^{-\|\mathbf{X}'_i - \mathbf{X}'_j\|^2/2\sigma_i^2}} \qquad Q_{i|i} = 0$$
is close from P.

- **t-SNE:** use a Student-t term $(1 + \|\mathbf{X}'_i - \mathbf{X}'_j\|^2)^{-1}$ for $\mathbf{X}'_i$
- Minimize the Kullback-Leibler divergence $(\sum_{i,j} P_{j|i} \log \frac{P_{j|i}}{Q_{j|i}})$ by a simple gradient descent (can be stuck in local minima).
- Parameters σ_i such that $H(P_i) = -\sum_{j=1}^n P_{j|i} \log P_{j|i} = \text{cst}$.

Outline

Clustering

- Training data : $\mathcal{D} = \{\mathbf{X}_1, \ldots, \mathbf{X}_n\} \in \mathcal{X}^n$ (i.i.d. $\sim \mathbf{P}$)
- Latent groups?

Clustering

- Construct a map f from $\mathcal{D}$ to $\{1, \ldots, K\}$ where K is a number of classes to be fixed:

$$f: \quad \mathbf{X}_i \mapsto k_i$$

Motivations

- Interpretation of the groups
- Use of the groups in further processing

- Several strategies possible!
- Can use dimension reduction as a preprocessing.

Partition based

Partition Heuristic

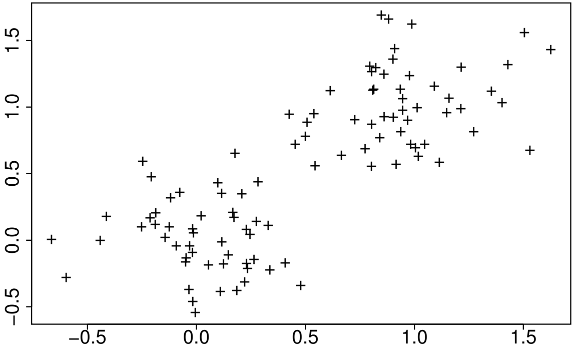
- Clustering is defined by a partition in K classes...
- that minimizes a homogeneity criterion.

K- Means

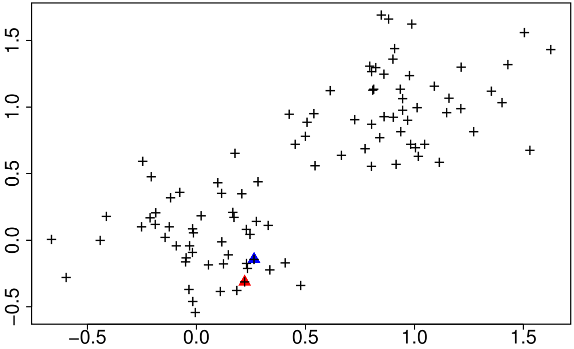
- Cluster k defined by a *center* μ_k.
- Each sample is associated to the closest center.
- Centers defined as the minimizer of $\sum_{i=1}^{n} \min_k \|\mathbf{X}_i - \mu_k\|^2$

- Iterative scheme (Loyd):
    - Start by a (pseudo) random choice for the centers μ_k
    - Assign each samples to its nearby center
    - Replace the center of a cluster by the mean on its assigned samples.
    - Repeat the last two steps until convergence.

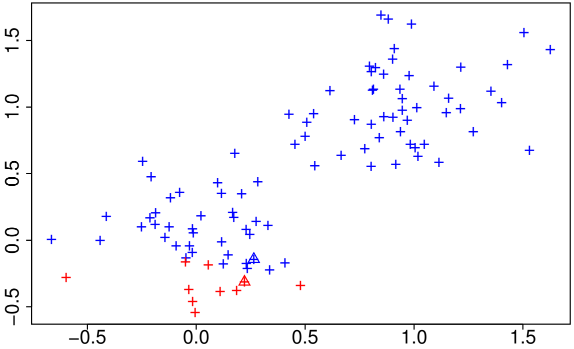
Partition based



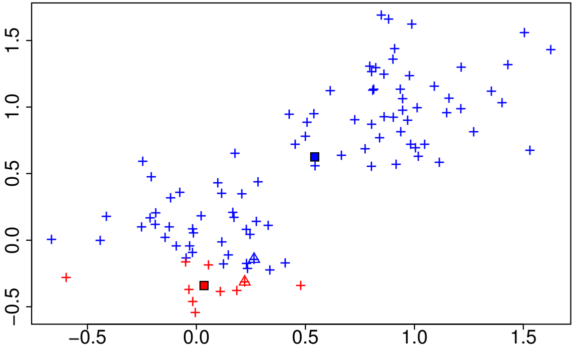
Partition based



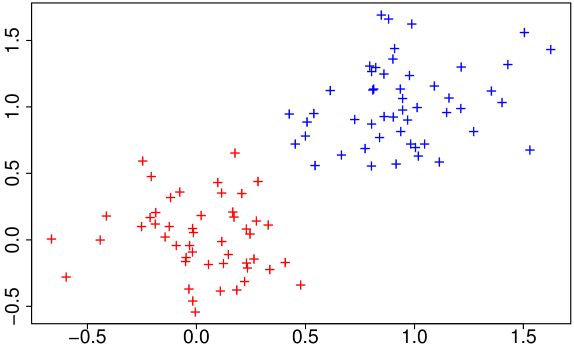
Partition based



Partition based



Partition based



Partition based

- Other schemes:
  - McQueen: modify the mean each time a sample is assigned to a new cluster.
  - Hartigan: modify the mean by removing the considered sample, assign it to the nearby center and recompute the new mean after assignment.
- A good initialization is crucial!
  - Initialize by samples.
  - k-Mean++: try to take them as separated as possible.
  - No guarantee to converge to a global optimum: repeat and keep the best result!
- Complexity : $O(n \times K \times T)$ where T is the number of step in the algorithm.

Partition based

- k-Medoid: use a sample as a center
  - PAM: for a given cluster, use the sample that minimizes the intra distance (sum of the squared distance to the other points)
  - Approximate medoid: for a given cluster, assign the point that is the closest to the mean.
- Complexity:
  - PAM: $O(n^2 \times T)$ in the worst case!
  - Approximate medoid: $O(n \times K \times T)$ where T is the number of step in the algorithm.
- **Remark:** Any distance can be used...

Model Based

Model Heuristic

- Use a generative model of the data:
$$\mathbb{P}\left\{\mathbf{X}\right\} = \sum_{k=1}^{K} \pi_k \mathbb{P}_{\theta_k}\left\{\mathbf{X}|k\right\}$$
where π_k are proportions and $\mathbb{P}_\theta\left\{\mathbf{X}|k\right\}$ are parametric probability models.
- Estimate those parameters (often by a ML principle).
- Assign each observations to the class maximizing the a posteriori probability (obtained by Bayes formula)
$$\frac{\widehat{\pi_k}\mathbb{P}_{\widehat{\theta_k}}\left\{\mathbf{X}|k\right\}}{\sum_{k'=1}^{K}\widehat{\pi_{k'}}\mathbb{P}_{\widehat{\theta_{k'}}}\left\{\mathbf{X}|k'\right\}}$$

- Link with Generative model in supervised classification!

Model Based

- Large choice of parametric models.

Gaussian Mixture Model

- Use
$$\mathbb{P}_{\theta_k}\left\{\mathbf{X}|k\right\} \sim \mathcal{N}(\mu_k, \Sigma_k)$$
with $\mathcal{N}(\mu, \Sigma)$ the Gaussian law of mean μ and covariance matrix Σ.

- Efficient optimization algorithm available (EM)
- Often some constrain on the covariance matrices: identical, with a similar structure...
- Strong connection with K-means when the covariance matrices are assumed to be the same multiple of the identity.

Model Based

Probabilistic latent semantic analysis (PLSA)

- Couples words/documents (w, d)
- Model:

$$\mathbb{P}\left\{(w,d)\right\} = \mathbb{P}\left\{d\right\} \sum_{k=1}^{K} \mathbb{P}\left\{k|d\right\} \mathbb{P}_{\theta_k}\left\{w|k\right\}$$

  with k the (hidden) topic, $\mathbb{P}\left\{k|d\right\}$ a topic probability and $\mathbb{P}\left\{w|k\right\}$ a multinomial law for a given topic.
- Clustering according to

$$\mathbb{P}\left\{k|(w,d)\right\} = \frac{\widehat{\mathbb{P}\left\{k|d\right\}}\mathbb{P}_{\widehat{\theta_k}}\left\{w|k\right\}}{\sum_{k'} \widehat{\mathbb{P}\left\{k'|d\right\}}\mathbb{P}_{\widehat{\theta_{k'}}}\left\{w|k'\right\}}$$

- Same idea than GMM!
- Bayesian variant called LDA.

Model Based

- Framework based on density estimation principle.
- Assign a probability of membership.
- Lots of theoretical studies...
- Model selection principle can be used to select K the number of class:
    - AIC / BIC /MDL penalization
    - Cross Validation is also possible!
- Complexity: $O(n \times K \times T)$

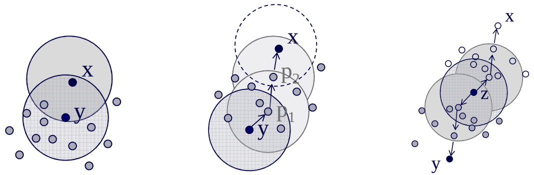
Density based

Density heuristic

- Cluster are connected dense zone separated by low density zone.
- Not all points belong to a cluster.

- Basic bricks:
  - Estimate the density.
  - Find points with high densities.
  - Gather those points according to the density
- Density estimation:
  - Classical kernel density estimate...
- Gathering:
  - Link points of high density and use the resulted component.
  - Move them toward top of density *hill* by following the gradient and gather all the points arriving at the same *summit*.

Density based



- Examples:
  - DBSCAN: link point of high densities using a very simple kernel.
  - PdfCLuster: find connected zone of high density.
  - Mean-shift: move points toward top of density *hill* following an evolving kernel density estimate.
- Complexity: $O(n^2 \times T)$ in the worst case.
- Can be reduced to $O(n \log(n) T)$ if samples can be encoded in a tree structure (n-body problem type approximation).

Agglomerative Clustering

Agglomerative Clustering Heuristic

- Start with very small clusters (a sample by cluster?)
- Sequential merging of the most similar clusters...
- according to some *greedy* criterion Δ.

- Generates a hierarchy of clustering instead of a single one.
- Need to select the number of cluster afterwards.
- Several choice for the merging criterion...
- Examples:
    - Minimum Linkage: merge the closest cluster in term of the usual distance
    - Ward Indice: merge the two clusters yielding the less inner inertia loss (k-means criterion)

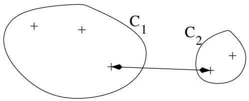
Agglomerative Clustering

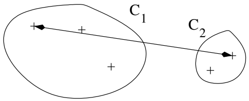
Algorithm

- Start with $(\mathcal{C}_i^{(0)}) = (\{\mathbf{X}_i\})$ the collection of all singletons.
- At step s, we have $n - s$ clusters $(\mathcal{C}_i^{(s)})$:
  - Find the two clusters the most similar according to a criterion Δ:
  $$(i, i') = \operatorname*{argmin}_{(j,j')} \Delta(\mathcal{C}_j^{(s)}, \mathcal{C}_{j'}^{(s)})$$
  - Merge $\mathcal{C}_i^{(s)}$ and $\mathcal{C}_{i'}^{(s)}$ into $\mathcal{C}_i^{(s+1)}$
  - Keep the $n - s - 2$ other clusters $\mathcal{C}_{i''}^{(s+1)} = \mathcal{C}_{i''}^{(s)}$
- Repeat until there is only one cluster.

- Complexity: $O(n^3)$ if no restriction on the merging possibilities.
- Can be reduced to $O(n^2)$ if only a bounded number of merging is possible for a given cluster.

Agglomerative Clustering





Merging criterion based on the distance between points

- Minimum linkage:

$$\Delta(\mathcal{C}_i, \mathcal{C}_j) = \min_{\mathbf{X}_i \in \mathcal{C}_i} \min_{\mathbf{X}_{\in} \mathcal{C}_j} d(\mathbf{X}_i, \mathbf{X}_j)$$

- Maximum linkage:

$$\Delta(\mathcal{C}_i, \mathcal{C}_j) = \max_{\mathbf{X}_i \in \mathcal{C}_i} \max_{\mathbf{X}_{\in} \mathcal{C}_j} d(\mathbf{X}_i, \mathbf{X}_j)$$

- Average linkage:

$$\Delta(\mathcal{C}_i, \mathcal{C}_j) = \frac{1}{|\mathcal{C}_i||\mathcal{C}_j|} \sum_{\mathbf{X}_i \in \mathcal{C}_i} \sum_{\mathbf{X}_{\in} \mathcal{C}_j} d(\mathbf{X}_i, \mathbf{X}_j)$$

- Clustering based on the proximity...

Agglomerative Clustering

Merging criterion based on the inertia (distance to the mean)

- Ward Indice:

$$\Delta(\mathcal{C}_i, \mathcal{C}_j) = \sum_{\mathbf{X}_i \in \mathcal{C}_i} \left(d^2(\mathbf{X}_i, \mu_{\mathcal{C}_i \cup \mathcal{C}_j}) - d^2(\mathbf{X}_i, \mu_{\mathcal{C}_i}) \right) + \sum_{\mathbf{X}_j \in \mathcal{C}_j} \left(d^2(\mathbf{X}_j, \mu_{\mathcal{C}_i \cup \mathcal{C}_j}) - d^2(\mathbf{X}_j, \mu_{\mathcal{C}_j}) \right)$$

- If d is the euclidian distance:

$$\Delta(\mathcal{C}_i, \mathcal{C}_j) = \frac{2|\mathcal{C}_i||\mathcal{C}_j|}{|\mathcal{C}_i| + |\mathcal{C}_j|} d^2(\mu_{\mathcal{C}_i}, \mu_{\mathcal{C}_j})$$

- Same criterion than in the k-means algorithm but greedy optimization.

Grid based

Grid heuristic

- Split the space in pieces
- Group those of high density according to their proximity

- Similar to density based estimate (with partition based initial clustering)
- Space splitting can be fixed or adaptive to the data.
- Examples:
  - STING (Statistical Information Grid): Hierarchical tree construction plus DBSCAN type algorithm
  - AMR (Adaptive Mesh Refinement): Adaptive tree refinement plus k-means type assignment from high density leaves.
  - CLIQUE: Tensorial grid and 1D detection.
- Linked to Divisive clustering (DIANA)

Others

Graph based

- Spectral clustering: dimension reduction + k-means
- Message passing:
- Max Flow / Min Flow:

- Evolutionary algorithm,
- ...

Scalability

Large dataset issue

- When n is large, a $O(n^{\alpha} \log n)$ with $\alpha > 1$ is not acceptable!
- How to deal with such a situation?

- **Beware:** Computing all the pairwise distance requires $O(n^2)$ operations!

Ideas

- Sampling
- Online processing
- Simplification
- Parallelization

Sampling

Sampling heuristic

- Use only a subsample to construct the clustering.
- Assign the other points to the constructed clusters afterwards.

- Requires a clustering method that can assign new points (partition, model...)
- Often repetition and choice of the best clustering
- Example:
  - CLARA: K-medoid with sampling and repetition

Online

Online heuristic

- Modify the current clusters according to the value of a single observation.

- Requires compactly described clusters.
- Examples:
  - Add to an existing cluster (and modify it) if it is close enough and create a new cluster otherwise (k-means without reassignment)
  - Stochastic descent gradient (GMM)
- May leads to far from optimal clustering.
- Often used in a sequential way:
  - Several passes
  - Two step algorithm:
    - Generate a large number n' of clusters using the online algorithm (with $n' \ll n$)
    - Cluster the clusters with a more accurate algorithm.

Simplification

Simplification heuristic

- Simplify the algorithm to be more efficient at the cost of some precision.

- Algorithm dependent!
- Examples:
    - Replace groups of observation (preliminary cluster) by the (approximate) statistics.
    - Approximate the distances by cheaper ones.
    - Use n-body type techniques.

Parallelization

Parallelization heuristic

- Split the computation on several computers.

- Algorithm dependent!
- Examples:
  - Distance computation in k-means, parameter gradient in model based clustering
  - Grid density estimation, Space splitting strategies
- Classical batch sampling not easy to perform as partitions are not easily merged...