Practical introduction to machine learning

Part 2 : Unsupervised learning

Rémi Flamary - CMAP, École Polytechnique

Master Data Science, Institut Polytechnique de Paris

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Overview of MAP654I

1. Data and Machine Learning problems

- Data properties and visualization
- Pre-processing
- Finding your Machine Learning problem

2. Unsupervised learning

- Clustering
- Density estimation and generative modeling
- Dictionary learning and collaborative filtering
- Dimensionality reduction and manifold learning

3. Supervised learning

- Bayesian decision and Nearest neighbors
- Linear models nonlinear methods for regression and classification
- Trees, forest and ensemble methods

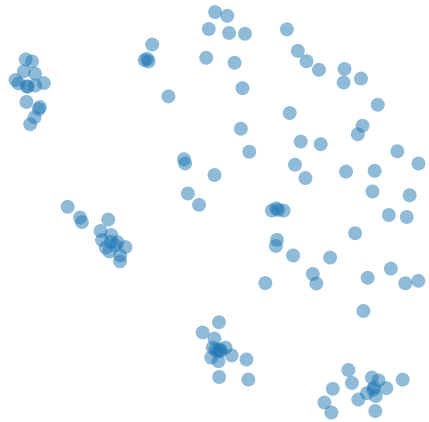
4. Validation and interpretation

- Performance measures
- Models and parameter selection (validation)
- Interpretation of the methods

Overview for the current part

Unsupervised dataset

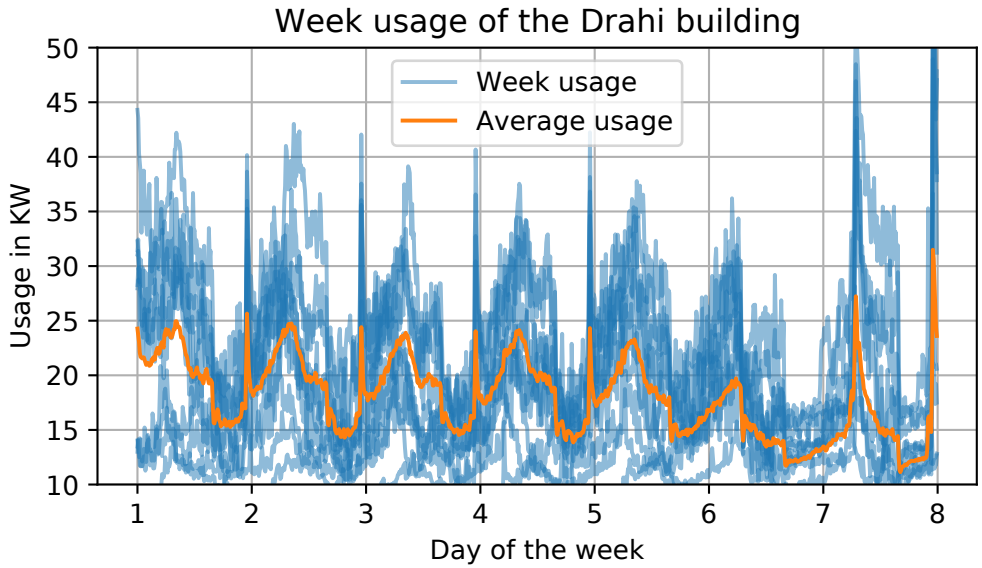
$$\mathbf{X} = \begin{bmatrix} \mathbf{x}_1^\top \\ \mathbf{x}_2^\top \\ \vdots \\ \mathbf{x}_i^\top \\ \vdots \\ \mathbf{x}_n^\top \end{bmatrix} = \begin{bmatrix} x_{11} & x_{12} & \dots & x_{1j} & \dots & x_{1d} \\ x_{21} & x_{22} & \dots & x_{2j} & \dots & x_{2d} \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\ x_{i1} & x_{i2} & \dots & x_{ij} & \dots & x_{id} \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\ x_{n1} & x_{n2} & \dots & x_{nj} & \dots & x_{nd} \end{bmatrix}$$



Unsupervised learning

- The dataset contains the samples $\{\mathbf{x}_i\}_{i=1}^n$ with n samples of size d.
- d and n define the dimensionality of the learning problem.
- Data stored as a matrix $\mathbf{X} \in \mathbb{R}^{n \times d}$ with $\mathbf{X} = [\mathbf{x}_1, \dots, \mathbf{x}_n]^\top$ containing the transposed training samples as lines (features are in columns).
- Note: in the course we use 1-based indexing as standard in math but in python 0-based indexing is used.

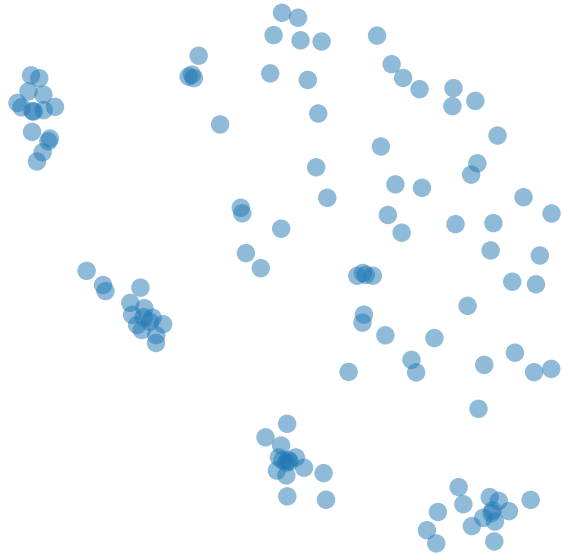
Example of real life dataset



Electrical usage of the Drahi X-Novation Center

- Demonstrator of Energy4Climate of IP Paris.
- Recording of the electrical usage of the building during 1.5 years.
- Can be completed by weather measurement (linked to energy usage).
- Data will be used on samples of energy usage during 1 week.
- Note that some pre-processing of the data is necessary before getting the unsupervised of supervised datasets.

Unsupervised learning, data description/exploration



Different problems (many methods can solve several of them)

- **Clustering**
  Group in clusters the similar samples.
- **Probability density estimation**
  Estimate from finite samples a probability distribution.
- **Generative modeling**
  Learn model that can generate data similar to the samples.
- **Dimensionality reduction**
  Reduce the dimensionality of the data for visualization or interpretation/modeling.

Scikit-learn estimator for unsupervised learning

Scikit-learn object API

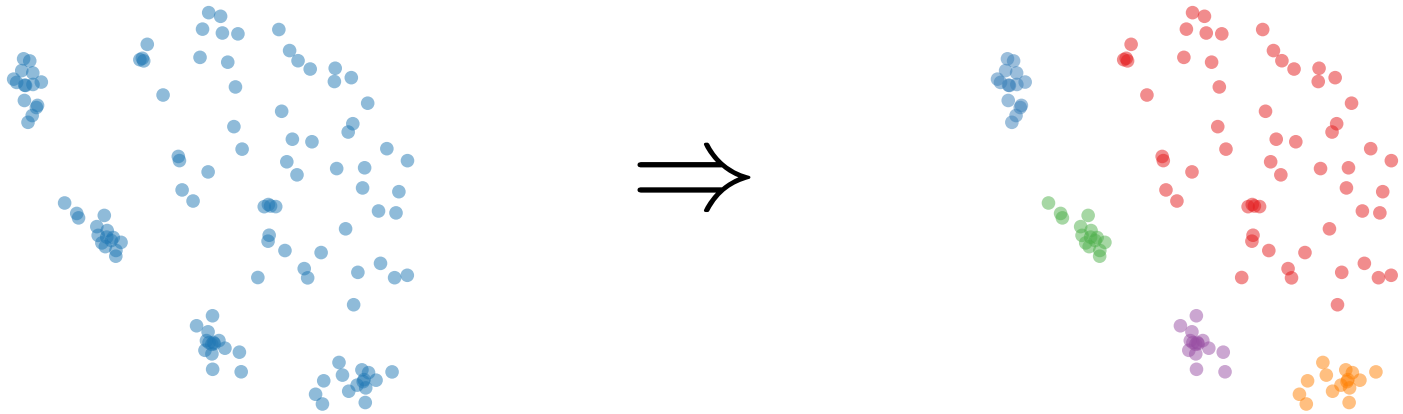
- Scikit-learn and its API became in recent years a standard for ML in Python.
- The estimator is usually used in 2 steps:
  1. Creation of the estimator :
     ```
     est = Estimator(param='parameter value',param2=10)
     ```
  2. Fitting of the estimator to the data:
     ```
     est.fit(X)
     ```
- After the fitting step, new attributes from the algorithms have been added to the object.

Using the estimator in unsupervised learning

- **Clustering**
  Predict the clusters with `est.predict(X)` or `est.fit_predict(X)`
- **Probability density estimation**
  Compute the log-probability of samples with `est.score_samples(X)`.
- **Generative modeling**
  Generate new samples with `est.sample(n_samples)`.
- **Dimensionality reduction/ Dictionary learning**
  Transform the data (in low dimension) with `est.transform(X)`, sometimes an inverse transform is available with `est.inverse_transform(X)`.

Section

Clustering



Objective

$$\{\mathbf{x}_i\}_{i=1}^n \quad \Rightarrow \quad \{\hat{y}_i\}_{i=1}^n$$

- Organize training examples in groups: Find the labels $\hat{y}_i \in \mathcal{Y} = \{1, \ldots, K\}$.
- Optional : find a clustering function $\hat{f}(\mathbf{x}) \in \mathcal{Y}$ that can cluster new samples.

Parameters

- K number of classes.
- Similarity measure between samples.
- Minimal distance between clusters.

Methods

- K-means.
- Gaussian mixtures.
- Spectral clustering.
- Hierarchical clustering.

Main clustering approaches

Connectivity-based (Hierachical)

- Use pairwise relation between samples/cluster to agglomerate/divide clusters to create a hierarchical tree.
- The tree contains the whole clustering between n to 1 cluster and select with parameter (distance threshold or number of cluster K)

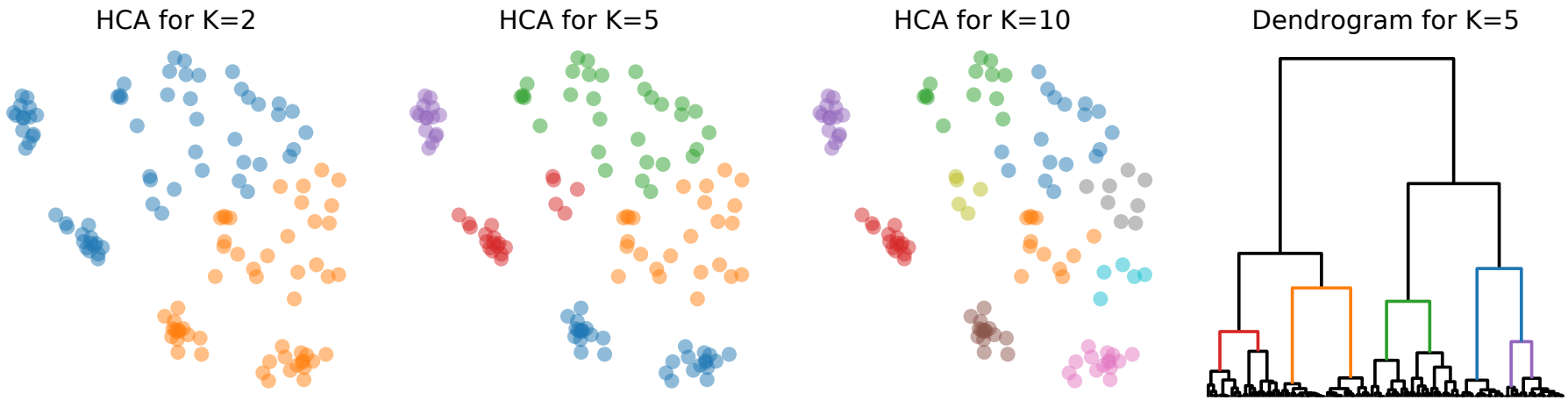
Centroid Based (K-means)

- Express the dataset as a list of K cluster centroids that represent the diversity of the data (each sample is associated to centroid).
- Minimize the average distance of all samples to their closest centroid (intra cluster variance).

Density based (DBSCAN)

- Local density estimation for each sample using a neighborhood in a ball around the sample.
- Two samples belong to the same cluster if they are close enough and are in a high density area.

Hierarchical Clustering Analysis (HCA)



Principle (Tutorial [Nielsen, 2016])

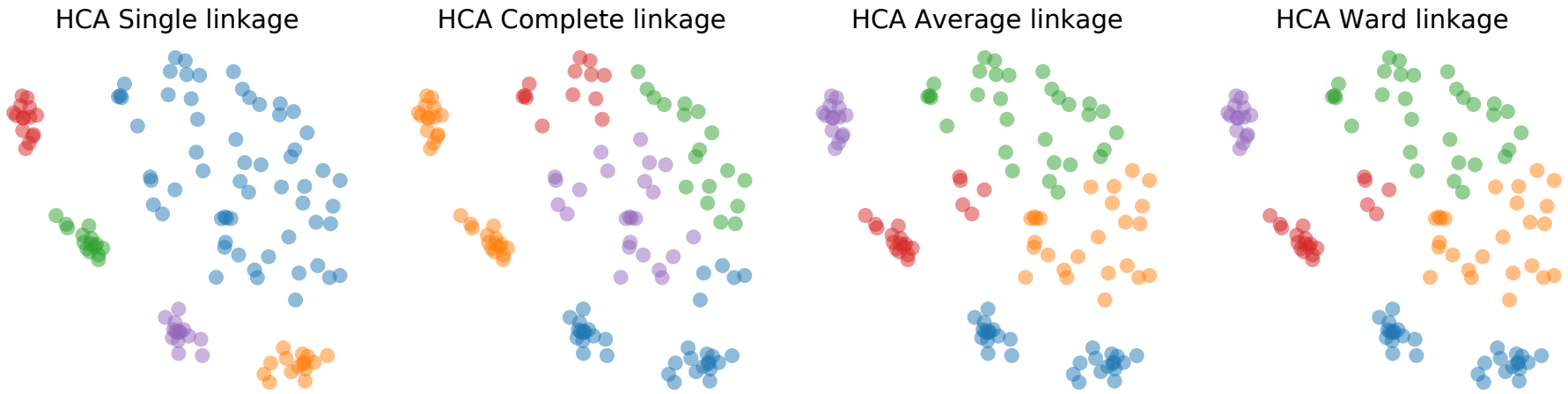
- HCA is an approach that find clusters recursively through **Agglomeration** (or sometime division).
- The **linkage function** $\Delta(\mathcal{C}_i, \mathcal{C}_j)$ is a measure of "distance" between two clusters.
- Final clustering with a fixed K nb. of clusters or a threshold on $\Delta(\mathcal{C}_i, \mathcal{C}_j)$.
- The tree visualization of the agglomeration steps is called the dendrogram.

Agglomerative HCA algorithm

1: Init. clusters $\{\mathcal{C}_i\}_i$ with n Clusters $\mathcal{C}_i$ (one per sample).
2: **while** $|\{\mathcal{C}_i\}_i| > 1$ **do**
3: Find the pair $\mathcal{C}_i, \mathcal{C}_j$ minimizing $\Delta(\mathcal{C}_i, \mathcal{C}_j)$ among all pairs.
4: Merge $\mathcal{C}_i$ and $\mathcal{C}_j$.
5: **end while**

- Algorithm is $O(n^3)$ in general but $O(n^2)$ possible for single and complete linkage.

HCA Linkage functions and implementation



Most common Linkage functions

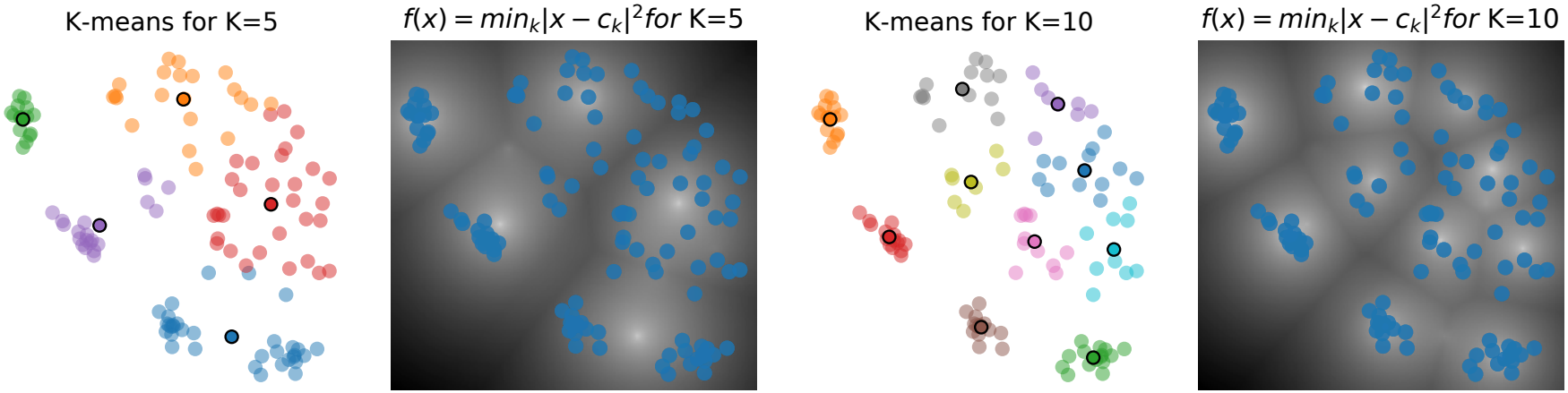
- **Single** [Sibson, 1973]
  $\Delta(\mathcal{C}_i, \mathcal{C}_j) = \min_{\mathbf{x}\in\mathcal{C}_i, \mathbf{x}'\in\mathcal{C}_j} d(\mathbf{x}, \mathbf{x}')$
- **Complete** [Defays, 1977]
  $\Delta(\mathcal{C}_i, \mathcal{C}_j) = \max_{\mathbf{x}\in\mathcal{C}_i, \mathbf{x}'\in\mathcal{C}_j} d(\mathbf{x}, \mathbf{x}')$
- **Average** [Sokal, 1958]
  $\Delta(\mathcal{C}_i, \mathcal{C}_j) = \frac{1}{|\mathcal{C}_i||\mathcal{C}_j|} \sum_{\mathbf{x}\in\mathcal{C}_i, \mathbf{x}'\in\mathcal{C}_j} d(\mathbf{x}, \mathbf{x}')$
- **Ward** [Ward Jr, 1963] ($\bar{\mathcal{C}} = \frac{1}{|\mathcal{C}|} \sum_{\mathbf{x}\in\mathcal{C}} \mathbf{x}$)
  $\Delta(\mathcal{C}_i, \mathcal{C}_j) = \frac{|\mathcal{C}_i||\mathcal{C}_j|}{|\mathcal{C}_i|+|\mathcal{C}_j|} \|\bar{\mathcal{C}}_i - \bar{\mathcal{C}}_j\|^2$

Python code

```
1  from sklearn.cluster import
       AgglomerativeClustering
2
3  # HCA with K=2
4  clf = AgglomerativeClustering(
       n_clusters=2)
5  # fit the model
6  clf.fit(X)
7  # predict the cluster labels
8  yc = clf.predict(X)
9  # get the structure of the tree
10 children = clf.children_
11 # can be used for visualization with
12 # scipy.cluster.hierarchy.dendrogram
```

Also see `scipy.cluster.hierarchy`.

K-means clustering



Principle [Steinhaus et al., 1956, MacQueen et al., 1967]

Find K clusters $\mathbf{c}_k \in \mathbb{R}^d$ that optimize:

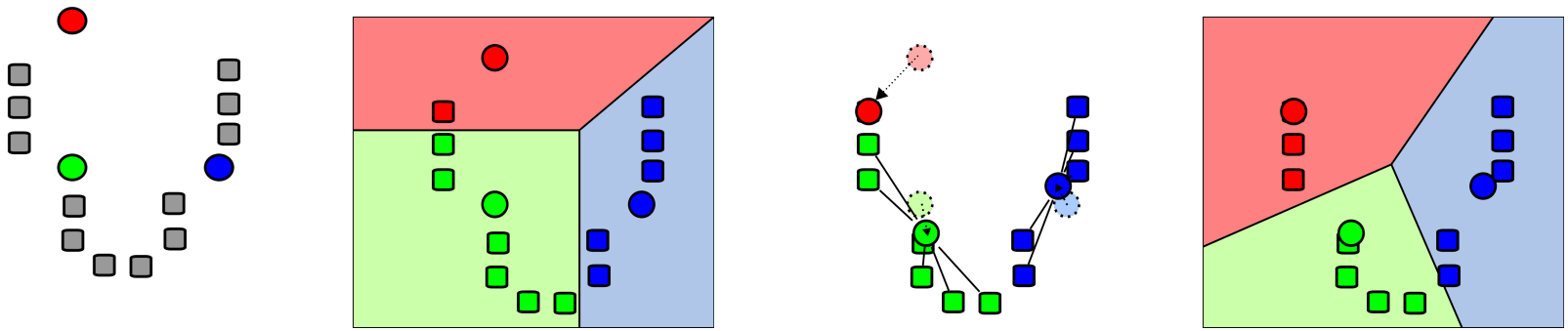
$$\min_{\mathbf{c}_k, \forall k} \quad \sum_{i=1}^{n} \min_k \left\| \mathbf{x}_i - \mathbf{c}_k \right\|^2 \tag{1}$$

- Minimize the sum of squared distance between $\mathbf{x}_i$ and its closest cluster $\mathbf{c}_k$.
- Can be seen as the minimization *w.r.t.* $\mathbf{c}_k$ of the expectation on the data of function $f(\mathbf{x}) = \min_k \left\| \mathbf{x}_i - \mathbf{c}_k \right\|^2$.
- The optimization problem can be reformulated with $\mathbf{A} \in \{0,1\}^{n \times K}$ a cluster assignment binary matrix ($A_{i,k} = 1$ means that $\mathbf{x}_i$ is in cluster k) as

$$\min_{\mathbf{c}_k \in \mathbb{R}^d, \forall k, \mathbf{A} \in \{0,1\}^{n \times K}, \mathbf{A}\mathbf{1}_K = \mathbf{1}_n} \quad \sum_{i=1,k=1}^{n,K} A_{i,k} \left\| \mathbf{x}_i - \mathbf{c}_k \right\|^2 \tag{2}$$

Kmeans algorithm

Init. Step 1 Step 2 Step 3



K-means Algorithm

1: Init. clusters $\{\mathbf{c}_k\}_k$.
2: **while** Not converged **do**
3: Update $\mathbf{A}$ by assigning each sample to its closest cluster.
4: Update $\mathbf{c}_k$ as the mean of the samples in the cluster.
5: **end while**

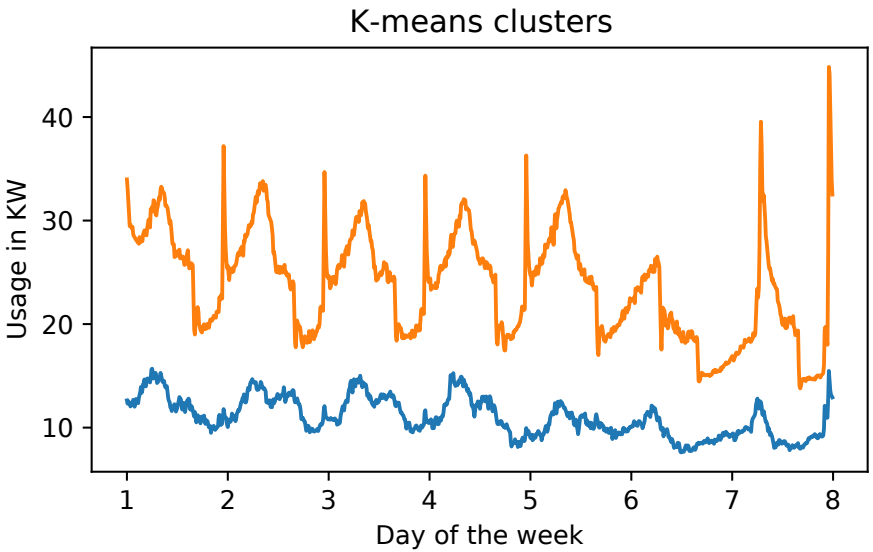
- This is a Block Coordinate Descent (BCD) algorithm on the problem 2.

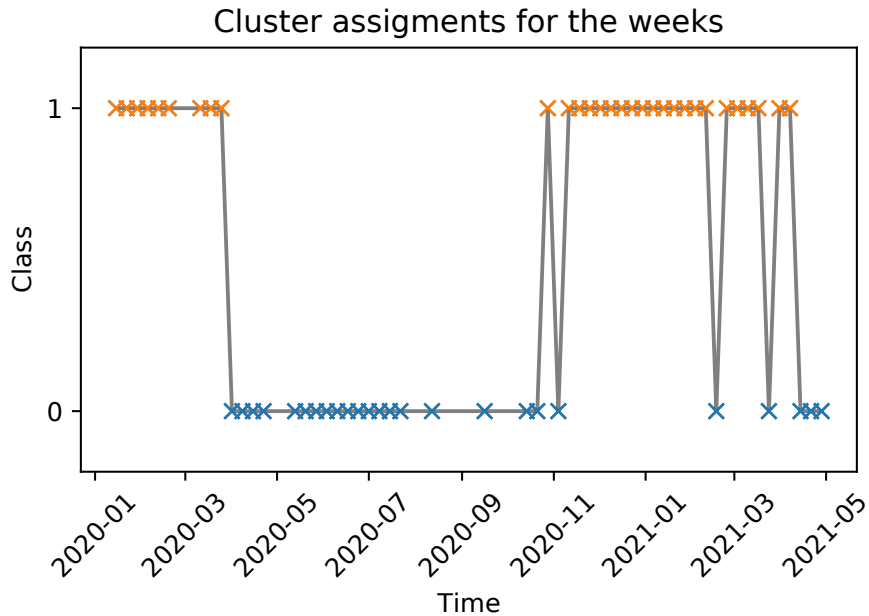
Python code

```
1  from sklearn.cluster import KMeans
2
3  # K-means with K=2
4  clf = KMeans(2)
5
6  # fit the model et predict classes
7  y = clf.fit_predict(X)
8
9  # distance from samples to clusters
10 dist = clf.transform(X)
11
12 # get the centroids
13 C = clf.cluster_centers_
```

Images from Wikipedia

K-means on energy usage dataset





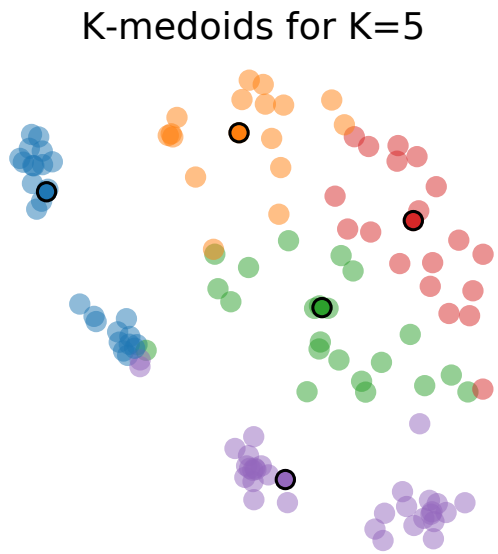
Application

- Run K-means with $K = 2$ on the $n = 55$ samples of size $d = 1008$.
- Left : plot cluster centroids $\mathbf{c}_k$ as signals of week usage.
- Right : plot clusters assignments as a function of date of the monday of the week.
- Cluster 1 with more energy usage than cluster 0.
- Seasonal clustering along the year (1 for winter, 0 for summer).

K-means variants

K-medoids [Maranzana, 1963]

$$\min_{\mathbf{c}_k \in \{\mathbf{x}_1, \ldots, \mathbf{x}_n\}, \forall k} \quad \sum_{i=1}^{n} \min_{k} \|\mathbf{x}_i - \mathbf{c}_k\|^2 \qquad (3)$$

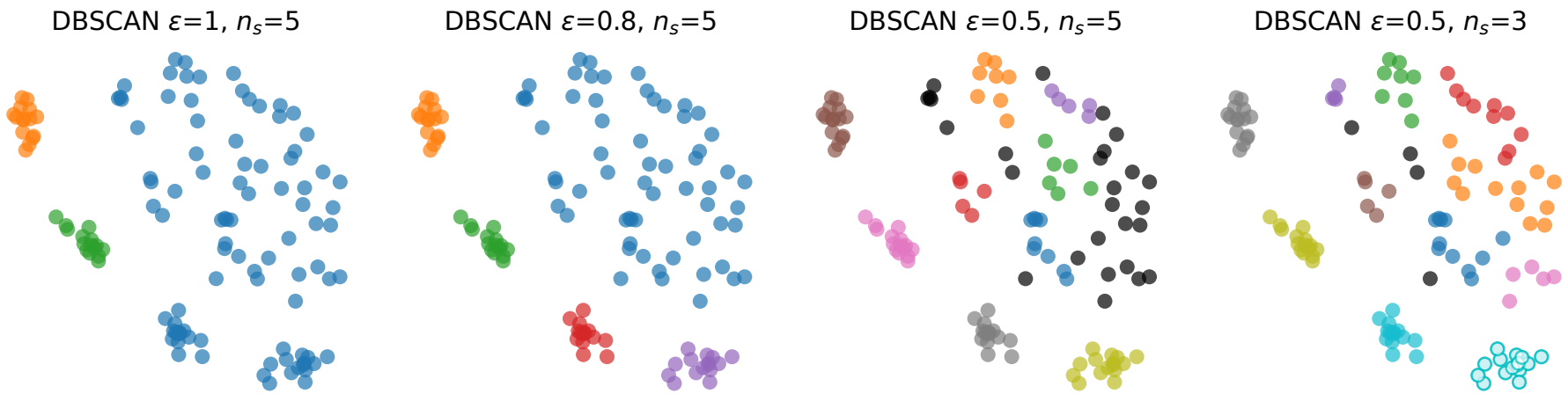


- Similar to K-means but the clusters have to be selected among the data points.
- Can be solved using BCD (as K-means) or the well known Partitioning Around Medoids (PAM) algorithm [Kaufman and Rousseeuw, 1990].

K-means and extensions

- Initialization of the clusters is important. In Scikit-learn, K-means++ initialization is used by default [Arthur and Vassilvitskii, 2006].
- Large scale dataset K-means solver with Stochastic Gradient Descent [Bottou and Bengio, 1995] or Minibatch-Kmeans [Sculley, 2010] (sklearn.cluster.MiniBatchKMeans).
- K-median [Bradley et al., 1997] allows clustering robust to outlier by changing the norm (L1 instead of L2).

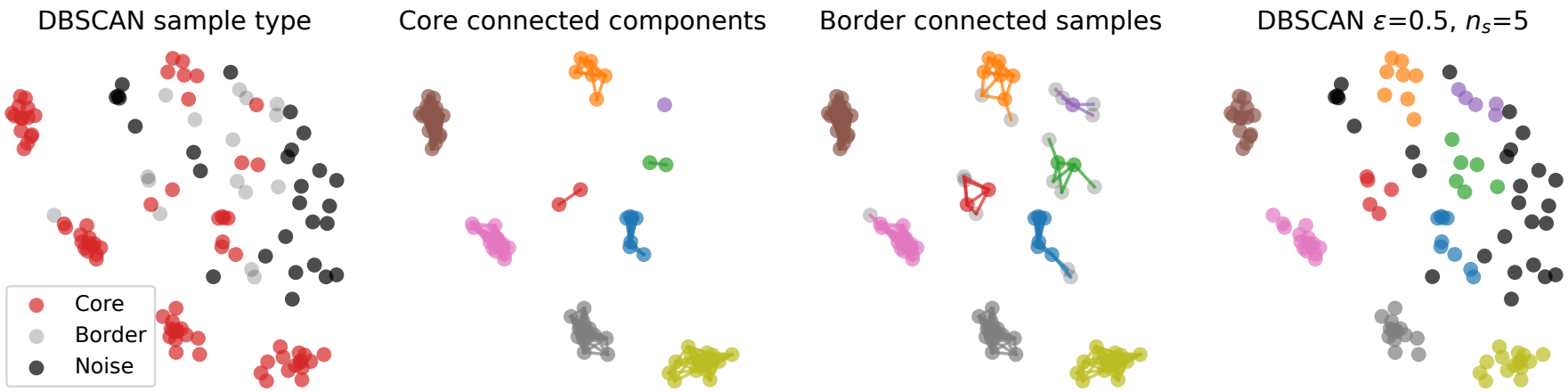
DBSCAN



Density-based spatial clustering of applications with noise (DBSCAN) [Ester et al., 1996, Schubert et al., 2017]

- Density estimation method that group into clusters samples that are in high density area and detect noise in low density area (black samples above).
- Local density around a sample is estimated using the number of neighbors in the ϵ ball $N_\epsilon(\mathbf{x}) = |\{\mathbf{x}_j | D(\mathbf{x}_i, \mathbf{x}) \leq \epsilon\}|$.
- Parameters are ϵ (size of the ball) around and n_s minimum number of sample in neighborhood for detecting dense areas.
- Clustering uses different type of samples:
  - Core samples have high density : $N_\epsilon(\mathbf{x}) > n_s$.
  - Border (connected) samples : $N(\mathbf{x})_\epsilon \leq n_s$ but $\exists \mathbf{x}_c$ core sample s.t. $D(\mathbf{x}, \mathbf{x}_c) \leq \epsilon$.
  - Noise sample : $N(\mathbf{x})_\epsilon \leq n_s$ and $D(\mathbf{x}, \mathbf{x}_c) > \epsilon$, $\forall \mathbf{x}_c$ core samples.

DBSCAN Algorithm



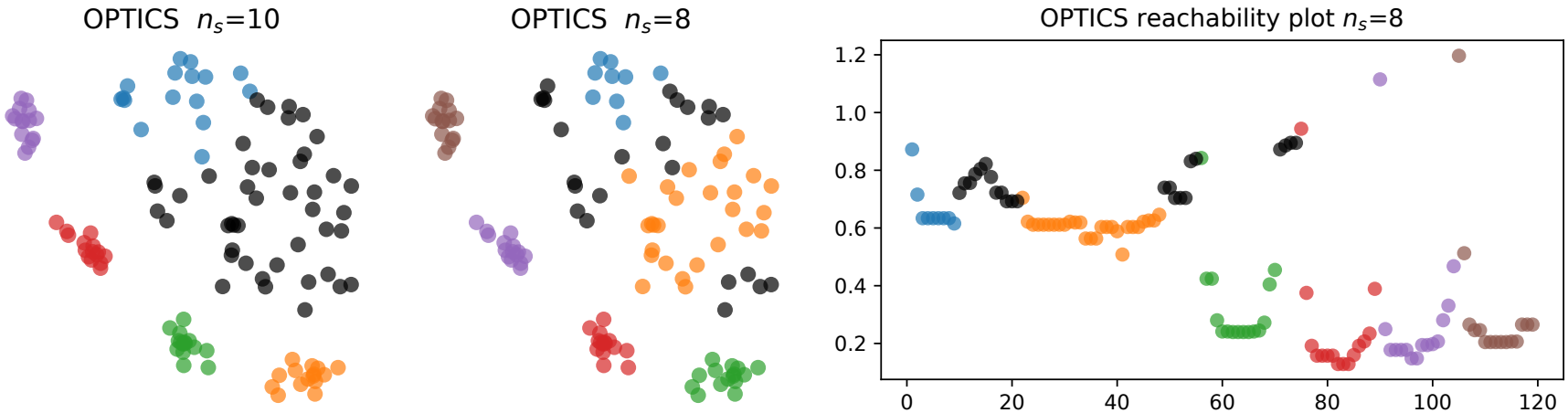
Algorithm (simplified) [Ester et al., 1996]

1. Compute the neighborhood $N_\epsilon(\mathbf{x}_i)$ of all samples and find core samples.
2. Find the connected components of the core samples (ignore all other samples).
3. Go through the non-core sample and label them to a cluster if in the ϵ neighborhood of a core sample or to noise if not.

- In practice DBSCAN goes through the dataset sample by sample. Clustering for border samples connected to more than 1 cluster depends on the order.
- DBSCAN is a celebrated method[1], and is used a lot in practical applications.
- Scikit-learn estimator : `sklearn.cluster.DBSCAN(eps=0.5,min_samples=5)` .

[1] Test of time award ACM SIGKDD 2014

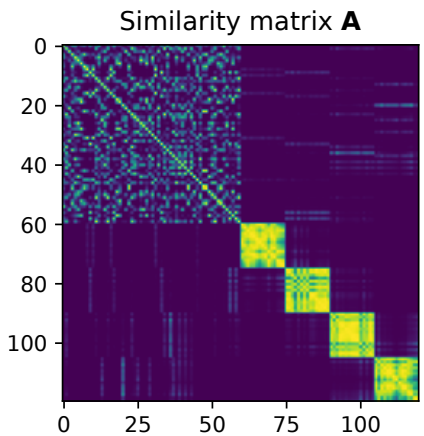
OPTICS

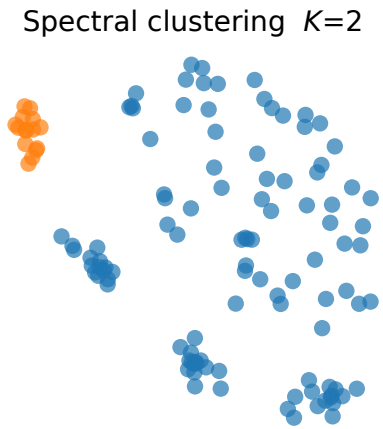


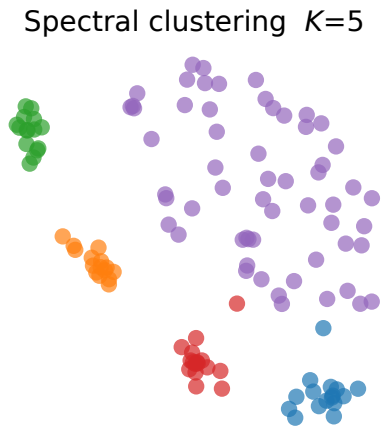
Ordering points to identify the clustering structure (OPTICS) [Ankerst et al., 1999]

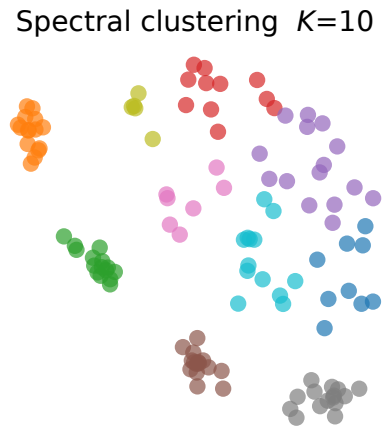
- Local density estimation similar to DBSCAN but done with ordering of the samples.
- Use the reachability of samples (distance to core samples) to order (and go through) samples in a reachability plot.
- Perform clustering from the reachability plot by searching for valleys or thresholding (similar to DBSCAN).
- Scikit-learn estimator : `sklearn.cluster.OPTICS(min_samples=5, max_eps=np.inf)` .

Spectral clustering









Principle (Tutorial [Von Luxburg, 2007], [Shi and Malik, 2000])

1. Represent pairwise relationship between samples with a similarity matrix $\mathbf{A}$ (kernel or binary) an compute its Laplacian or normalized Laplacian:

$$\mathbf{L} = \mathbf{D} - \mathbf{A}, \quad \text{or} \quad \mathbf{L}_n = \mathbf{I} - \mathbf{D}^{-\frac{1}{2}}\mathbf{A}\mathbf{D}^{-\frac{1}{2}}$$

   with $\mathbf{D} = \text{diag}(\mathbf{A}\mathbf{1}_n)$
2. Perform eigen-decomposition of this matrix and keep the Kth largest eigenvectors.
3. Perform clustering (usually K-means) on the $n \times K$ matrix of eigenvectors.

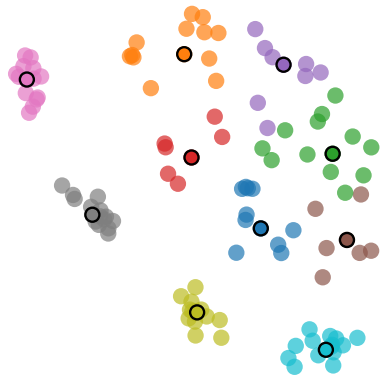
- Strongly related to nonlinear dimensionality reduction (DR + clustering).
- Allows for highly nonlinear separation between clusters.
- Scikit-learn estimator : `sklearn.cluster.SpectralClustering(n_clusters=5)` .

Other Clustering approaches

Affinity propagation [Frey and Dueck, 2007]

- Use message passing between samples to estimate a clustering based on selection of "examplars" (similar to K-medoids).
- Scikit-learn : `sklearn.cluster.AffinityPropagation()` .

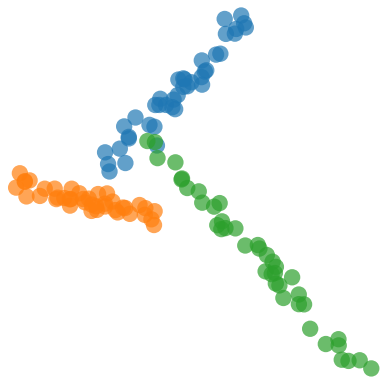
Affinity propagation



Subspace clustering [Parsons et al., 2004]

- Clusters in high dimension are defined by affine subspaces.
- Estimate optimal subspaces for each clusters and assign labels *w.r.t.* the distance to the subspaces.

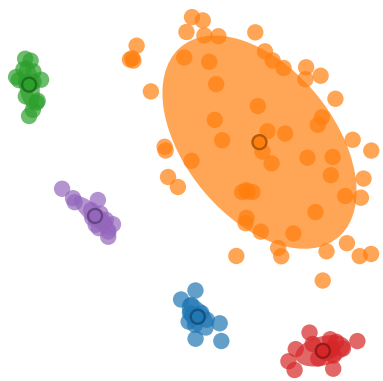
Subspace clustering



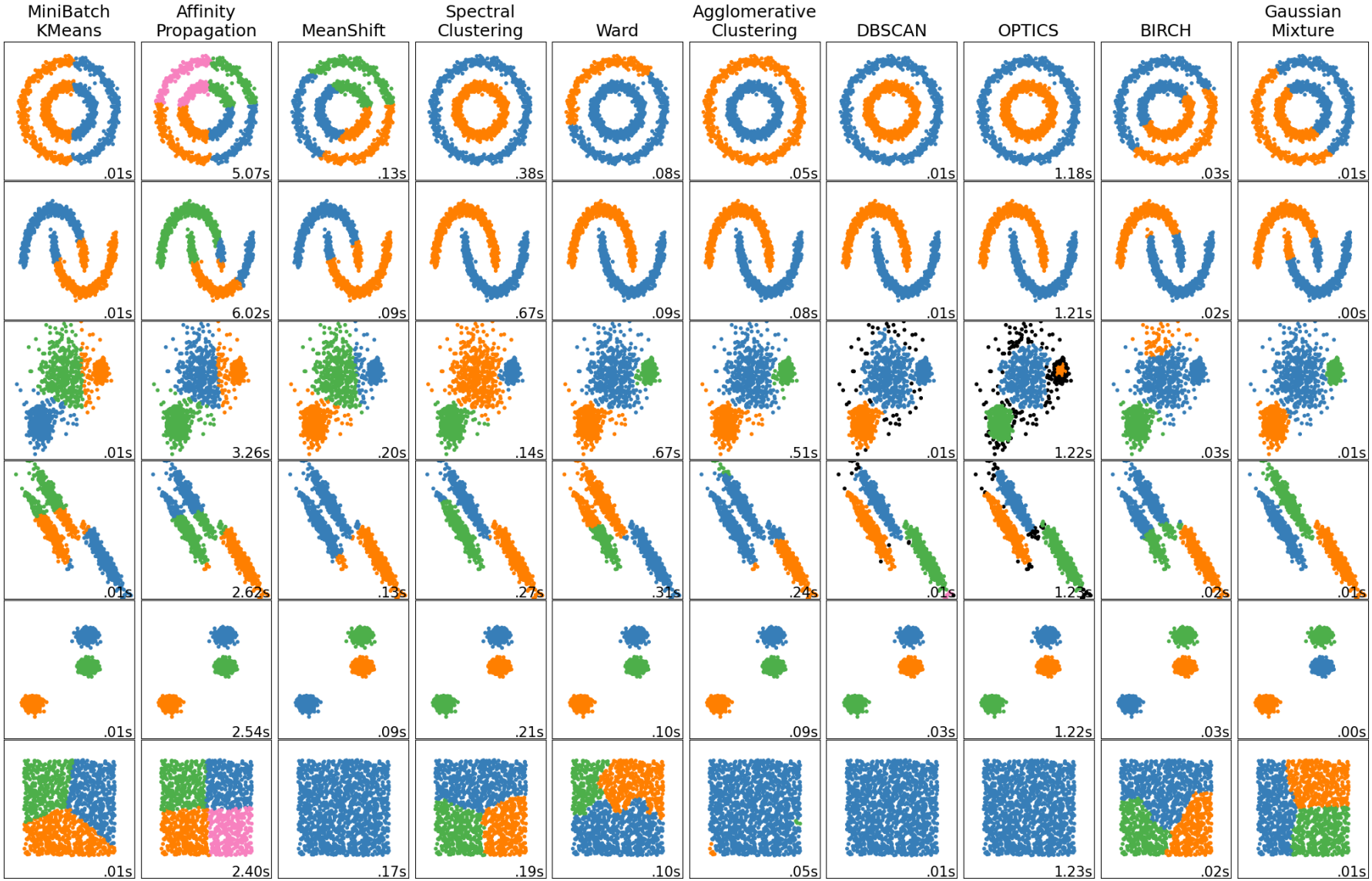
Mixture models [McLachlan et al., 2019]

- Density estimation based on a mixture of distributions.
- Clustering done by computing the probability of each samples to be generated by one of the distribution in the mixture.
- See Gaussian Mixture Models (GMM) in the next part.

GMM clustering

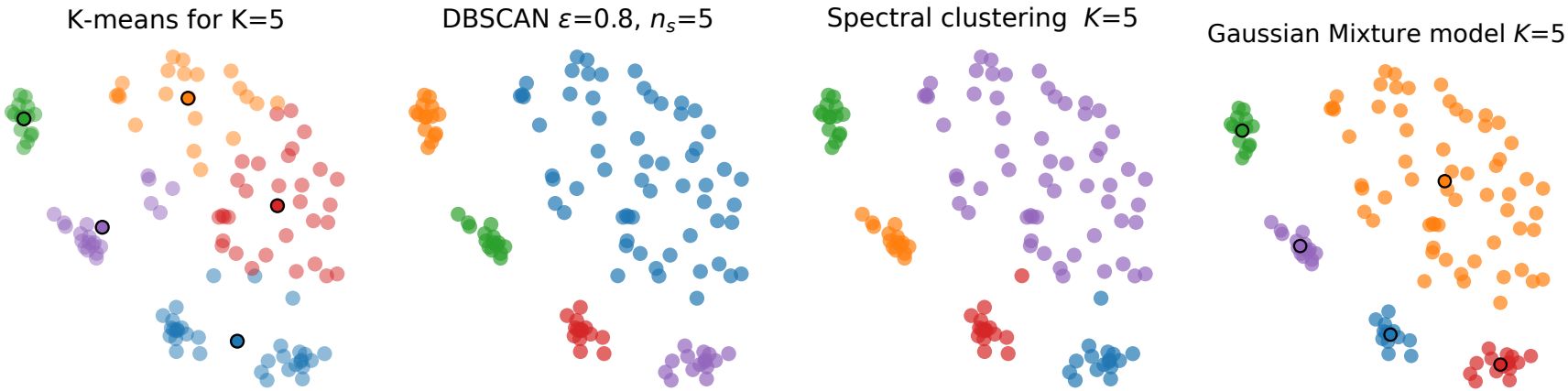


Comparison of clustering methods



https://scikit-learn.org/stable/auto_examples/cluster/plot_cluster_comparison.html

Clustering, in practice

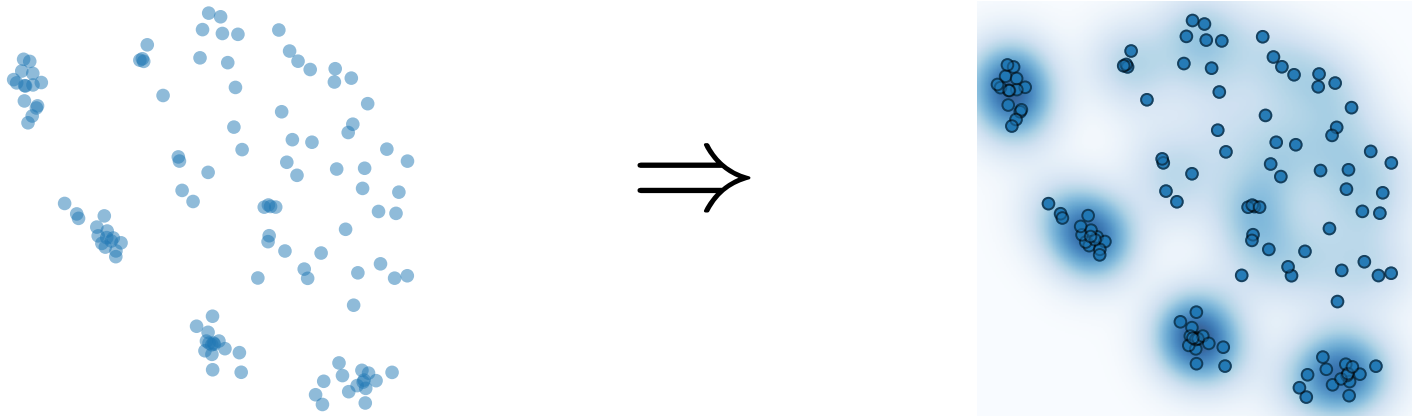


Which method to use ?

- First step: know you data (expert knowledge or visualization).
- Standard approaches are K-means when the number of cluster is known and DBSCAN when unknown.
- K-means and GMM works well on data with "blobs" and can handle different densities in the clusters (also they have interpretable clusters).
- DBSCAN and OPTICS can handle non-linearly separated clusters and the presence of noise/outliers in the data.
- Subspace clustering can handle data in different subspaces and Spectral clustering in nonlinear manifolds.

Section

Probability density estimation



Objective

$$\{\mathbf{x}_i\}_{i=1}^n \quad \Rightarrow \quad \hat{p}$$

- Estimate a probability density $\hat{p}(\mathbf{x})$ from the IID samples in the data.
- Probability density : $\hat{p}(\mathbf{x}) \geq 0, \ \forall \mathbf{x}$ and $\int \hat{p}(\mathbf{x}) d\mathbf{x} = 1$.
- Optional : generate new data with $\hat{p}(\mathbf{x})$, detect outliers in the data.

Parameters

- Type of distribution (Histogram, Gaussian, . . .).
- Parameters of the law (μ, Σ)

Methods

- Histogram (1D/2D).
- Parzen/kernel density estimation.
- Gaussian mixture.

Maximum Likelihood Estimator (MLE)

Principle

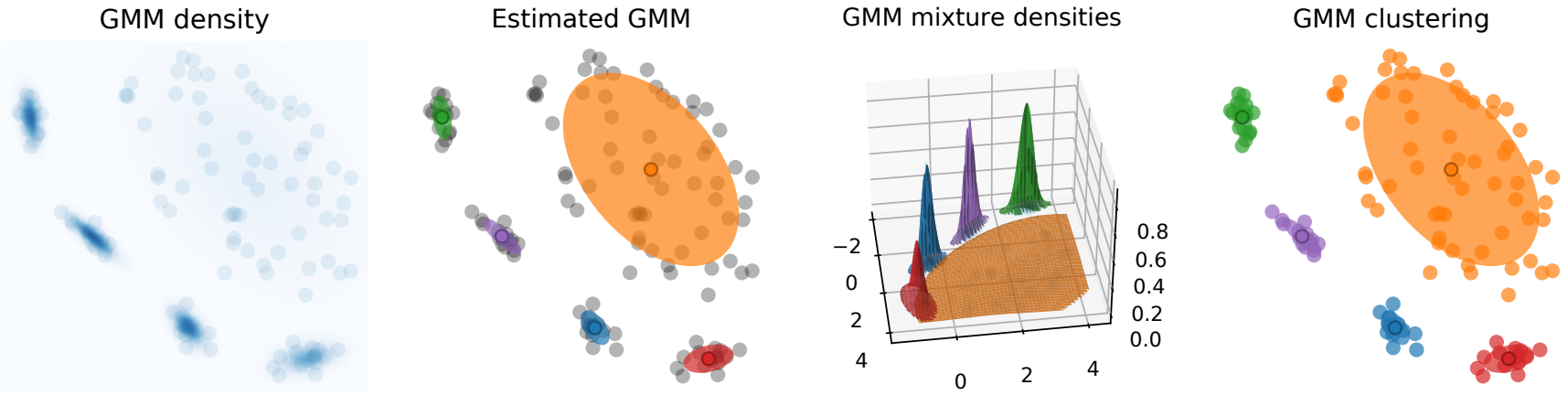
$$\max_{\boldsymbol{\theta}} \quad L(\boldsymbol{\theta}; \{\mathbf{x}_i\}_i)$$

- Let $p(\mathbf{x}|\boldsymbol{\theta})$ be a probability density distribution parametrized by $\boldsymbol{\theta}$.
- MLE consist in finding the optimal parameter $\boldsymbol{\theta}$ that maximizes the likelihood for a given empirical sample $\{\mathbf{x}_i\}_i$.
- For Independent and Identically Distributed (IID) samples the likelihood can be expressed as
$$L(\boldsymbol{\theta}; \{\mathbf{x}_i\}_i) = \prod_{i=1}^{n} p(\mathbf{x}_i|\boldsymbol{\theta})$$
- In practice the log-likelihood $l(\boldsymbol{\theta}; \{\mathbf{x}_i\}_i) = \log(L(\boldsymbol{\theta}; \{\mathbf{x}_i\}_i))$ that transforms the product as a sum is often optimized with the same solution.

Example of MLE : Multivariate Gaussian (Normal) distribution

- The density is parametrized by $\boldsymbol{\theta} = \{\boldsymbol{\mu}, \boldsymbol{\Sigma}\}$ and can expressed as
$$p(\mathbf{x}|\boldsymbol{\theta}) = p_{\mathcal{N}}(\mathbf{x}|\boldsymbol{\mu}, \boldsymbol{\Sigma}) = \left((2\pi)^d |\boldsymbol{\Sigma}|\right)^{-\frac{1}{2}} \exp\left(-\frac{1}{2}(\mathbf{x}-\boldsymbol{\mu})^{\mathrm{T}} \boldsymbol{\Sigma}^{-1} (\mathbf{x}-\boldsymbol{\mu})\right)$$
- The MLE estimated on the samples $\{\mathbf{x}_i\}_i$ is
$$\hat{\boldsymbol{\mu}} = \frac{1}{n}\sum_{i=1}^{n} \mathbf{x}_i, \qquad \hat{\boldsymbol{\Sigma}} = \frac{1}{n}\sum_{i=1}^{n} (\mathbf{x}_i - \boldsymbol{\mu})(\mathbf{x}_i - \boldsymbol{\mu})^{\top}$$

Gaussian Mixture Models (GMM)



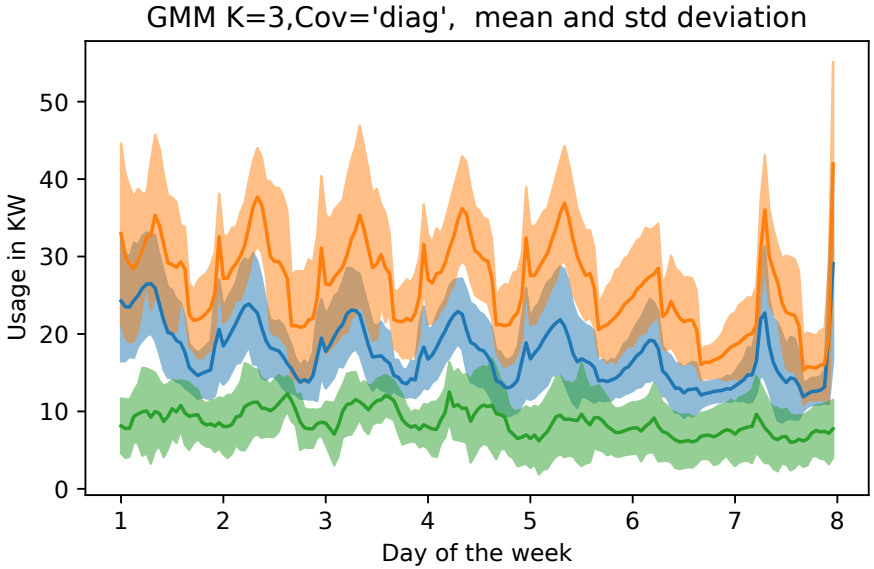
Principle [Dempster et al., 1977, Yu et al., 2011]

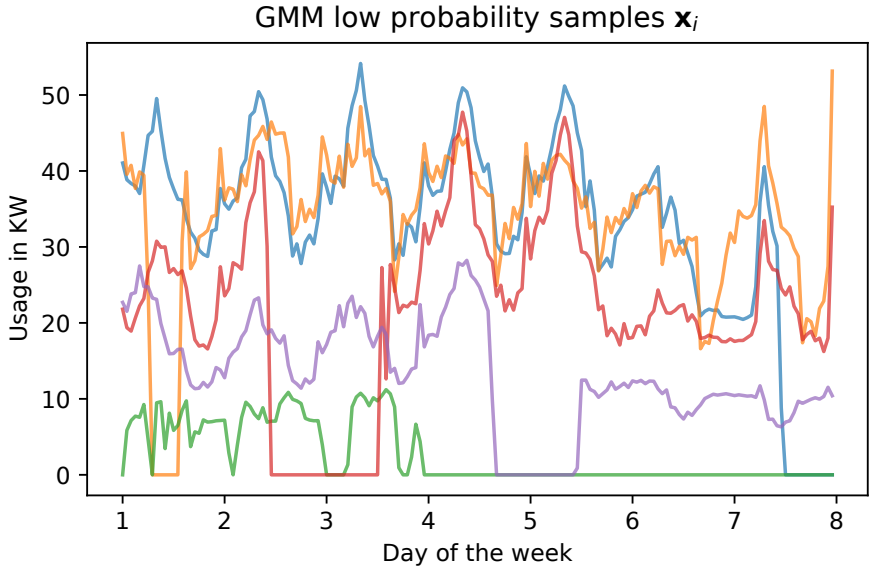
- Model the prob. distribution of the data as a sum of K Gaussian distributions :

$$p_{GMM}(\mathbf{x}|\boldsymbol{\theta}) = \sum_{k=1}^{K} \phi_k p_{\mathcal{N}}(\mathbf{x}|\boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k) \tag{4}$$

- Estimate $\boldsymbol{\theta} = \{\boldsymbol{\phi}, \boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k, \forall k\}$ by maximizing the likelihood on the data.
- Optimization performed using the Expectation Maximization that consists in maximizing at each iteration a lower bound of the likelihood.
- The algorithm updates iteratively the probability that each component k generated each sample $\mathbf{x}_i$ and the parameters $\boldsymbol{\theta}$.
- Covariances can be full, diagonal, or low rank [Houdard et al., 2018].
- Scikit-learn implementation : sklearn.mixture.GaussianMixture

GMM on energy usage data





Application

- GMM with $K = 3$ on week energy usage data with diagonal covariances (because data in high dimension).
- Plot left shows the mean and standard deviation of each component in the mixture.
- Each component correspond to a low/medium/high energy consumption.
- Plot right the 5 samples with lowest probability score to detect outliers in the dataset (week usage with missing data in this case).

```
from sklearn.mixture import
      GaussianMixture
# create and fit the model
clf = GaussianMixture(3)
clf.fit(X)

# predict cluster class
yc = clf.predict(X)
# compute proba of samples
p = np.exp(clf.score_samples(x))
# generate new samples
Xg = clf.sample(100)
# Get estimated parameters
phi = clf.weights_
mus = clf.means_
Sigmas = clf.covariances_
```

Maximum A Posteriori estimator (MAP)

Principle

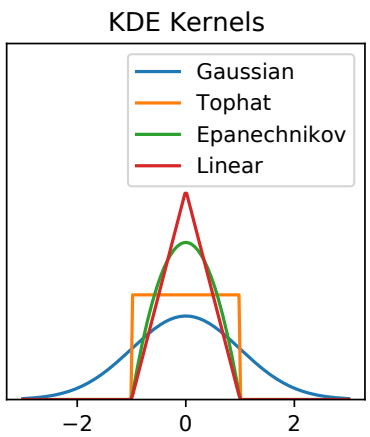
$$\max_{\boldsymbol{\theta}} \quad q(\boldsymbol{\theta}) L(\boldsymbol{\theta}; \{\mathbf{x}_i\}_i)$$

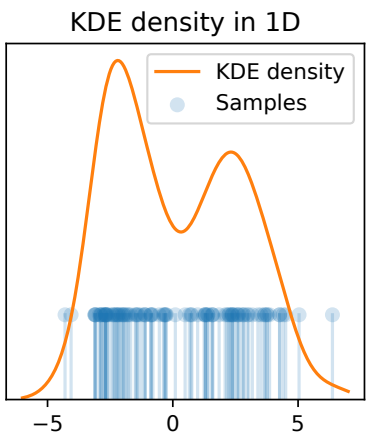
- $q(\boldsymbol{\theta})$ defines a prior distribution about the distribution parameter in addition to the likelihood $L(\boldsymbol{\theta}; \{\mathbf{x}_i\}_i)$ on the data.
- When the prior q is non informative (uniform), we recover the MLE, for simple priors (gaussian) we recover regularized estimators.
- The optimization problem can be solved with numerical optimization : EM algorithm, variational inference or Monte Carlo method.

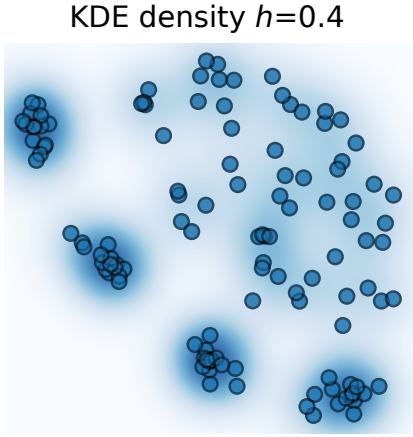
Example: Variational Gaussian Mixture Models [Blei and Jordan, 2006]

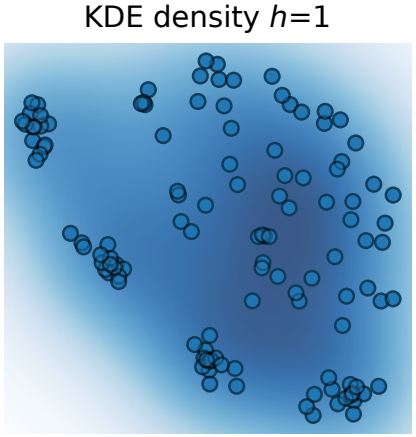
- Principle : Use a sparsity promoting prior on the weight ϕ of the components that can be of infinite size (Dirichlet process).
- The final number of components is controlled by the `weight_concentration_prior` parameter (less components for small values).
- In practice it allows to find automatically the number of components K.
- Scikit-learn implementation : BayesianGaussianMixture()

Kernel Density Estimation (KDE)







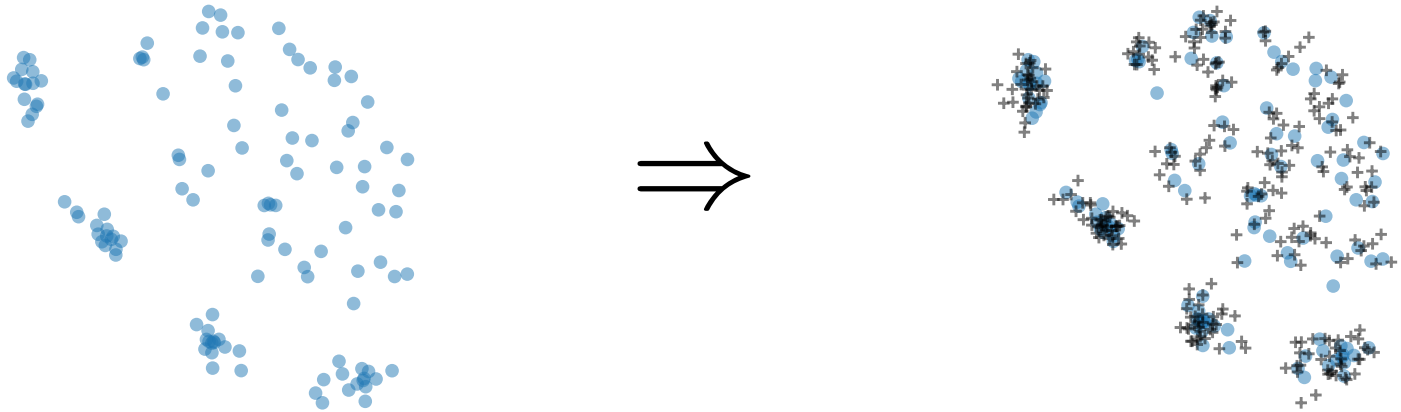


Principle [Rosenblatt, 1956, Parzen, 1962]

$$\hat{p}_h(\mathbf{x}) = \frac{1}{n}\sum_{i=1}^{n} k_h(\mathbf{x}, \mathbf{x}_i)$$

- $\{\mathbf{x}_i\}_{i=1,\dots,n}$ are supposed to be IID and the kernel function $k_h(\mathbf{x}, \mathbf{x}_i)$ is positive and of the form $k_h(\mathbf{x}, \mathbf{x}_i) = \tilde{k}(\frac{\mathbf{x}-\mathbf{x}_i}{h})$ where $h > 0$ is a bandwidth parameter.
- Can be seen as a convolution between the empirical distribution $\frac{1}{n}\sum_i \delta_{\mathbf{x}_i}$ and the centered kernel $k(\mathbf{x}, \mathbf{0})$, *i.e.* a low pass smoothing of the distribution.
- Common kernels (positive, symmetric and normalized $\int k(\mathbf{x}, \mathbf{0})d\mathbf{x} = 1$) are :
  - Gaussian kernel : $\tilde{k}(\mathbf{x}, \mathbf{x}') = \left((2\pi)^d d\right)^{-\frac{1}{2}} \exp\left(-\frac{1}{2}\|\mathbf{x} - \mathbf{x}'\|^2\right)$.
  - [Epanechnikov, 1969] : $\tilde{k}(x, x') = \frac{3}{4}\max(1 - |x - x'|^2, 0)$ in 1D.
  - Tophat (Rectangular) and Linear (Triangular) kernels.
- Scikit-learn implementation : sklearn.neighbors.KernelDensity

Generative modeling



Objective

$$\{\mathbf{x}_i\}_{i=1}^n \quad \Rightarrow \quad \hat{g} \text{ such that } p(\hat{g}(\mathbf{z})) \approx p(\mathbf{x}) \text{ with } \mathbf{z} \sim \mathcal{N}$$

- Estimate a mapping function $\hat{g}(\mathbf{z}) \in \mathbb{R}^d$ that generates similar samples to $\{\mathbf{x}_i\}_{i=1}^n$.
- Latent variable $\mathbf{z}$ follows a known Normal or Uniform distribution.
- Optional : recover an estimation of $\hat{p}(\mathbf{x})$ using the change of variable formula.

Parameters

- Type of distribution for $\mathbf{z}$ (Gaussian, uniform, ...).
- Type of function for g.

Methods

- PCA (Gaussian data), KDE, GMM.
- Gen. Adversarial Networks (GAN).
- Variational Auto-Encoders (VAE).
- Diffusion models.

Generative modeling by divergence minimization

Generator function

- $g : \mathbb{R}^p \to \mathbb{R}^d$ is a continuous function and μ_z a distribution on $\mathbb{R}^p$.
- g can be used to generate samples in $\mathbb{R}^d$ from samples $\mathbf{z} \sim \mu_z$ in $\mathbb{R}^p$.
- Notation : $g\#\mu_z$ is the distribution of the random variable $g(\mathbf{z})$ with $\mathbf{z} \sim \mu_z$.

Minimizing the divergence betwen distributions

$$\min_g \quad D(\mu_d, g\#\mu_z)$$

- Learn a generator g that minimize the divergence D between the generated data with samples $\mathbf{z} \sim \mu_z$ and the empirical data distribution $\mu_d = \frac{1}{n}\sum_i \delta_{\mathbf{x}_i}$.
- Different divergences that can be used:
  - Jensen-Shannon (JS) : Classical GAN [Goodfellow et al., 2014].
  - Wasserstein (Optimal Transport) [Arjovsky et al., 2017]
  - Maximum mean Discrepancy (MMD) [Li et al., 2015, Dziugaite et al., 2015].
  - f-divergences [Nowozin et al., 2016].
- Problem above can often be reformulated as a minimax between two functions hence the name adversarial.
- Not provided by Scikit-learn, see implementations in Pytorch or tensorflow.

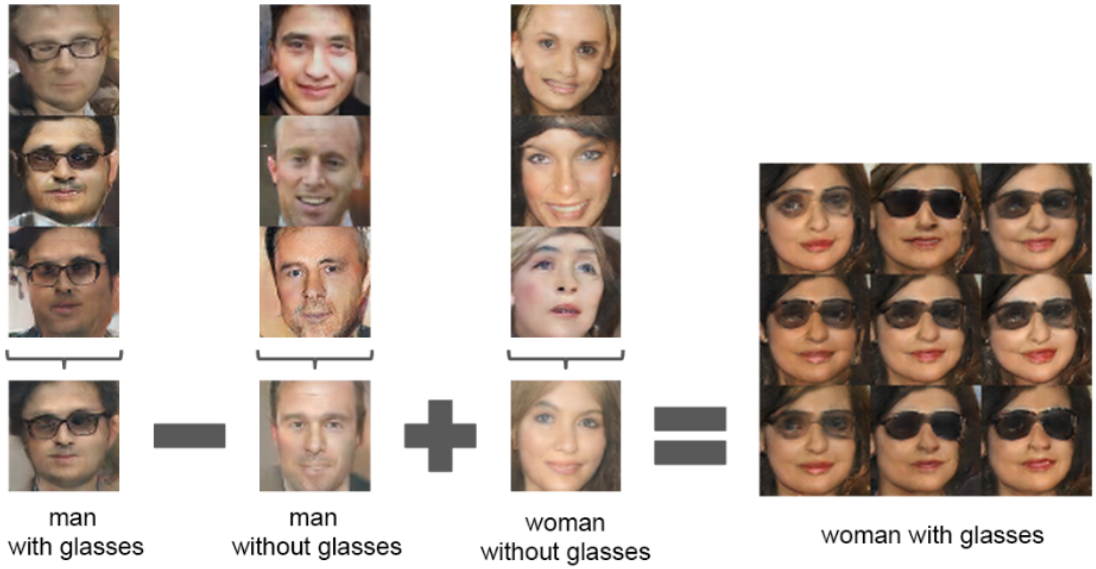
Generative adversarial learning (GAN)

Generative Adversarial Networks (GAN) [Goodfellow et al., 2014]

$$\min_g \max_h \quad E_{\mathbf{x}\sim\mu_d}[\log h(\mathbf{x})] + E_{\mathbf{z}\sim\mathcal{N}(0,\mathbf{I})}[\log(1 - h(g(\mathbf{z})))]$$

- h is a classifier trying to discriminate real data and data simulated by g.
- Data generated with g from IID random samples ($g(\mathbf{z})$ with $\mathbf{z} \sim N(0, \sigma^2)$).
- Both the generator g and classifier h compete (are adversaries).
- Generator space has semantic meaning [Radford et al., 2015].

Generative adversarial learning (GAN)



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Normalizing Flows

Change of variable

- Let $g : \mathbb{R}^d \to \mathbb{R}^d$ be an invertible (bijective) function and $f = g^{-1}$ with $f(g(\mathbf{z})) = \mathbf{z}$ and $\mu_z = \mathcal{N}$ is the normal distribution.
- The **change of variable** formula gives us the density of $g\#\mu_z$, *i.e.* of $g(\mathbf{z})$ when $\mathbf{z} \sim \mu_z$ as a function of the density $p_z(\mathbf{z})$ of μ_z:

$$p_x(\mathbf{x}) = p_z(f(\mathbf{x}))|\text{det}(Df(\mathbf{x}))|$$

where $Df(\mathbf{x}) = \frac{\partial f(\mathbf{x})}{\partial \mathbf{x}}$ is the Jacobian of the function f.

Principle of normalizing flows (Tutorial [Kobyzev et al., 2020])

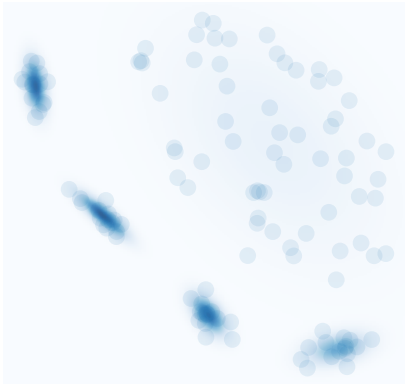
- g is called the generator function and $f = g^{-1}$ is the normalizing function.
- Density estimation and generator estimation can be done by maximum the log-likelihood on the IID dataset $\{\mathbf{x}_i\}_i$:

$$\max_f \quad \sum_{i=1}^{n} \log(p_z(f(\mathbf{x}_i))) + \log|\text{det}(Df(\mathbf{x}_i)|)$$

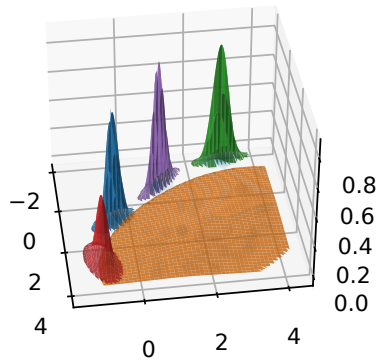
- The functions g have to be easy to apply, invert, and compute the determinant of its jacobian, they are formulated as neural networks:
  - Linear flows [Tomczak and Welling, 2017].
  - Planar or radial flows [Berg et al., 2018], [Rezende and Mohamed, 2015]
  - Coupling or autoregressive flows [Dinh et al., 2016, Kingma et al., 2016].

Probabiliy Density Estimation and generative modeling

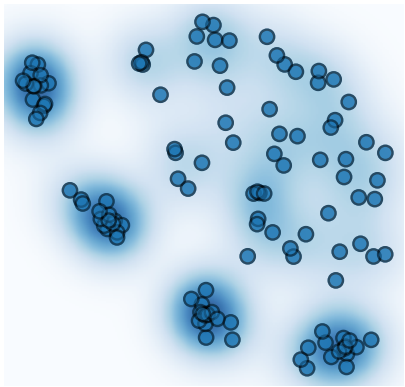
GMM density



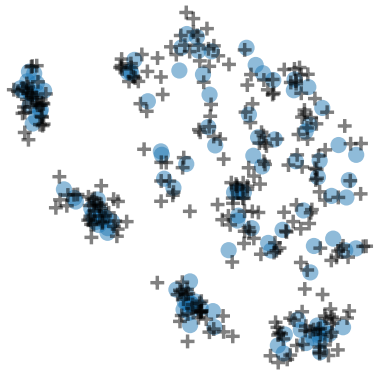
GMM mixture densities



KDE density h=0.4



KDE generated

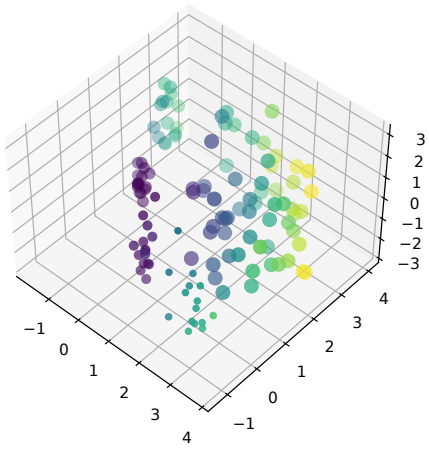


Why and when?

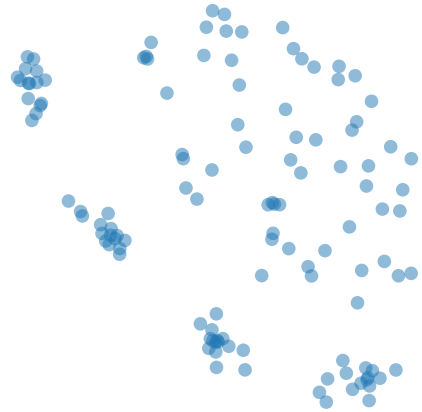
- Density estimation is hard (non-convex, large number of parameters).
- But it's the most informative modeling of unsupervised data.
- Density can be used for data generation, interpretation, outlier detection.
- When density is not necessary, generative modeling can be easier to estimate.
- Generative modeling can be used for other ML tasks (regularization for instance) but usually requires deep learning, harder to interpret.

Section

Dimensionality reduction



$\Rightarrow$



Objective

$$\{\mathbf{x}_i\}_{i=1}^n \quad \Rightarrow \quad \{\tilde{\mathbf{x}}_i \in \mathbb{R}^p\}_{i=1}^n \text{ with } p \ll d$$

- Project the data into a low dimensional space of size $p \ll d$.
- Preserve the information in the data (class, subspace, manifold).
- Optional : Learning a projection function $\hat{m} : \mathbb{R}^d \to \mathbb{R}^p$ for new data.

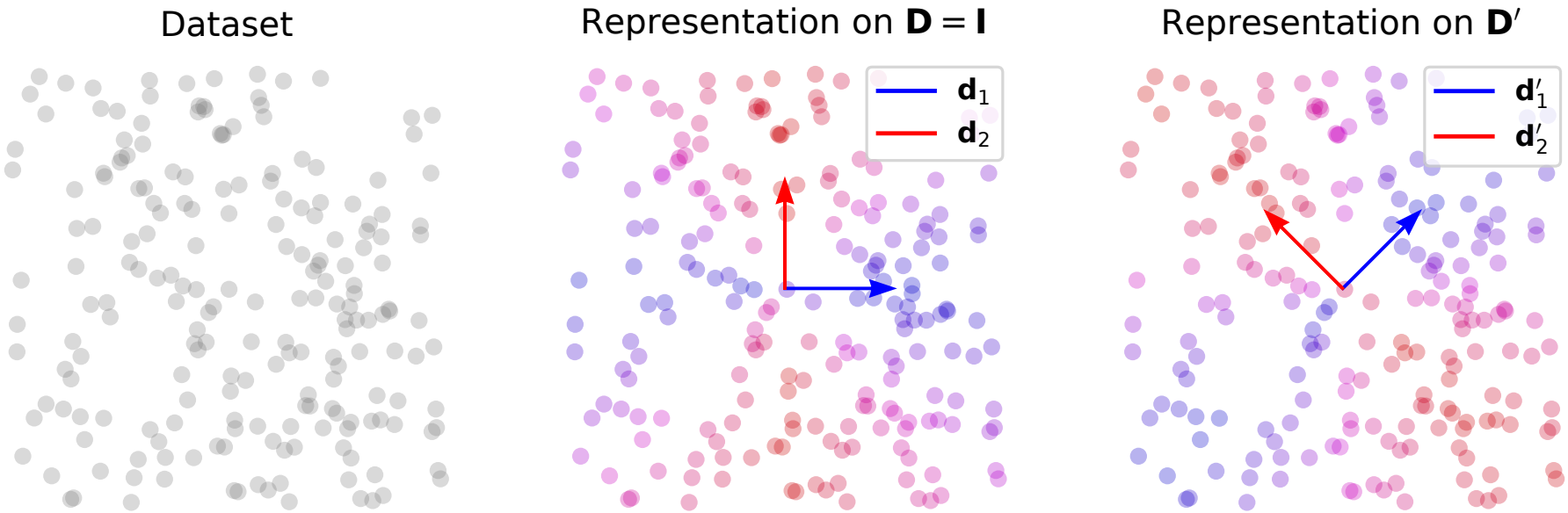
Parameters

- Type of projection (linear, nonlinear).
- Assumptions about the data (subspace, manifold).
- Similarity between samples.

Methods

- Feature selection.
- Principal Component Analysis (PCA).
- Dictionary learning, ICA.
- Non-linear dimensionality reduction (MDS, tSNE, Auto-Encoder)

Linear model for the data



Linear model

We suppose that $\mathbf{x} \in \mathbb{R}^d$ can be represented as a weighted sum of basis vectors:

$$\mathbf{x} \approx \mathbf{D}\mathbf{a} = \sum_{j=1}^{p} a_j \mathbf{d}_j \tag{5}$$

- $\mathbf{D} = [\mathbf{d}_1, \ldots, \mathbf{d}_p] \in \mathbb{R}^{d \times p}$ is the dictionary and the $\mathbf{d}_k$ are the basis vectors.
- $\mathbf{a} \in \mathbb{R}^p$ is the representation of the sample $\mathbf{x}$ on the dictionary $\mathbf{D}$.
- When $p < d$ the equality might not stand depending on $\mathbf{D}$ and the samples can be approximated in a smaller dimensionality.

Linear unmixing and dictionary learning

Linear unmixing

$$\hat{\mathbf{a}} = \arg\min_{\mathbf{a}} \quad L(\mathbf{x}, \mathbf{D}\mathbf{a}) \tag{6}$$

- L is a measure of divergence (usually quadratic $L(\mathbf{x}, \mathbf{x}') = \|\mathbf{x} - \mathbf{x}'\|^2$).
- Linear unmixing is a projection onto the linear subspace defined by $\mathbf{D}$.
- $\hat{\mathbf{a}}$ is the representation of sample $\mathbf{x}$ on dictionary $\mathbf{D}$ and the samples can be reconstructed by $\hat{\mathbf{x}} = \mathbf{D}\hat{\mathbf{a}}$.
- When $\mathbf{D}$ is orthonormal ($\mathbf{D}^\top \mathbf{D} = \mathbf{I}_p$), the solution of the problem with quadratic divergence is $\hat{a} = \mathbf{D}^\top \mathbf{x}$.

Dictionary Learning (DL)

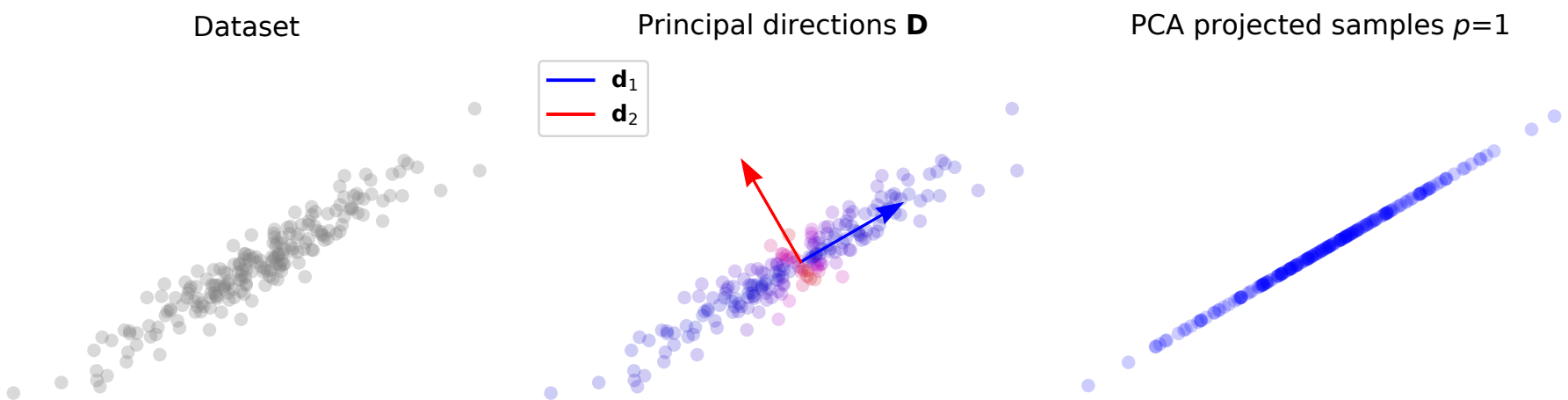
$$\hat{\mathbf{D}}, \hat{\mathbf{A}} = \arg\min_{\mathbf{D}, \mathbf{A}} \quad \sum_{i=1}^{n} L(\mathbf{x}_i, \mathbf{D}\mathbf{a}_i) \tag{7}$$

- Estimate simultaneously a dictionary $\hat{\mathbf{D}}$ and the representations $\hat{\mathbf{A}} = [\mathbf{a}_1, \ldots, \mathbf{a}_n]^T \in \mathbb{R}^{n \times p}$ on the dataset.
- DL is often called matrix factorization because the objective is to model the dataset $\mathbf{X}$ as a factorization:

$$\mathbf{X} \approx \hat{\mathbf{A}}\hat{\mathbf{D}}^\top$$

- Most linear dimensionality reduction methods also add constraints on $\mathbf{D}$ or $\mathbf{A}$

Principal Component Analysis (PCA)



Principle [Pearson, 1901]

$$\min_{\mathbf{D},\mathbf{D}^\top\mathbf{D}=\mathbf{I}_p} \sum_{i=1}^{n} \|\mathbf{x}_i^c - \mathbf{D}\mathbf{D}^\top\mathbf{x}_i^c\|^2 \quad \equiv \quad \max_{\mathbf{D},\mathbf{D}^\top\mathbf{D}=\mathbf{I}_p} \sum_{i=1}^{n} \|\mathbf{D}^\top\mathbf{x}_i^c\|^2 \tag{8}$$

- Find a linear subspace of dimensionality p defined by $\mathbf{D}$ that minimize the reconstruction error of the centered data $\mathbf{X}^c$ (0 means in the columns of $\mathbf{X}^c$).
- Equivalent to maximizing the variance of the projected samples $\hat{\mathbf{a}}_i = \mathbf{D}^\top\mathbf{x}_i^c$.
- DL problem (7) with orthonormality constraints on $\mathbf{D}$ and $\hat{\mathbf{a}}_i = \mathbf{D}^\top\mathbf{x}_i^c$.
- Principal directions are the columns $\mathbf{d}_k$ or $\mathbf{D}$.
- Scikit-learn implementation : sklearn.decomposition.PCA.

Principal Component Analysis in practice

PCA Algorithm

1. Center the data and compute the covariance $\hat{\mathbf{\Sigma}} = \frac{1}{n}\mathbf{X}^{c\top}\mathbf{X}^{c} = \frac{1}{n}\sum_i \mathbf{x}_i^c(\mathbf{x}_i^c)^\top$.
2. Perform eigendecomposition $\{\mathbf{v}_j, \lambda_j\}$ of the covariance matrix $\hat{\mathbf{\Sigma}}$ and sort the eigenvalues by decreasing order.
3. The optimal dictionary (projection matrix) is:

$$\hat{\mathbf{D}} = [\mathbf{v}_1, \ldots, \mathbf{v}_p]$$

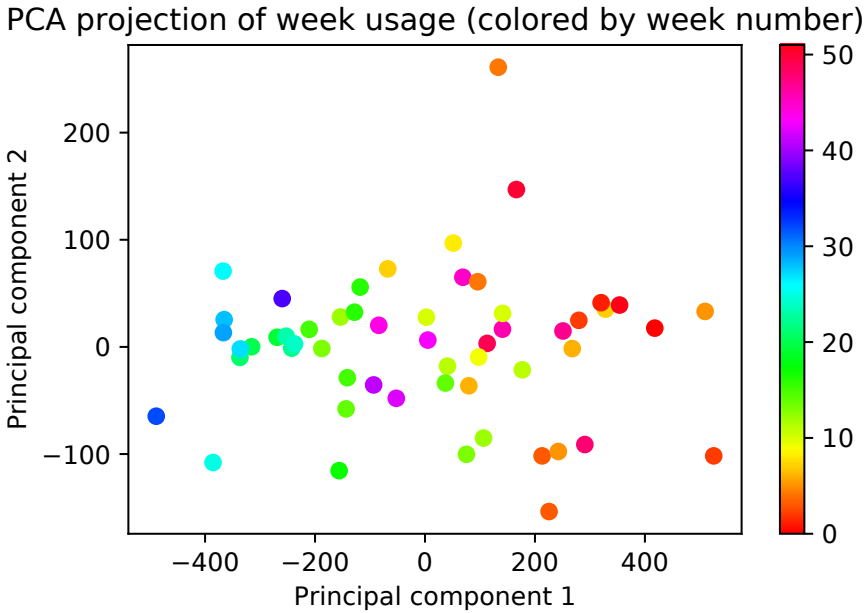
where $\{\mathbf{v}_1, \ldots, \mathbf{v}_p\}$ are the eigenvectors associated to the p largest eigenvalues.

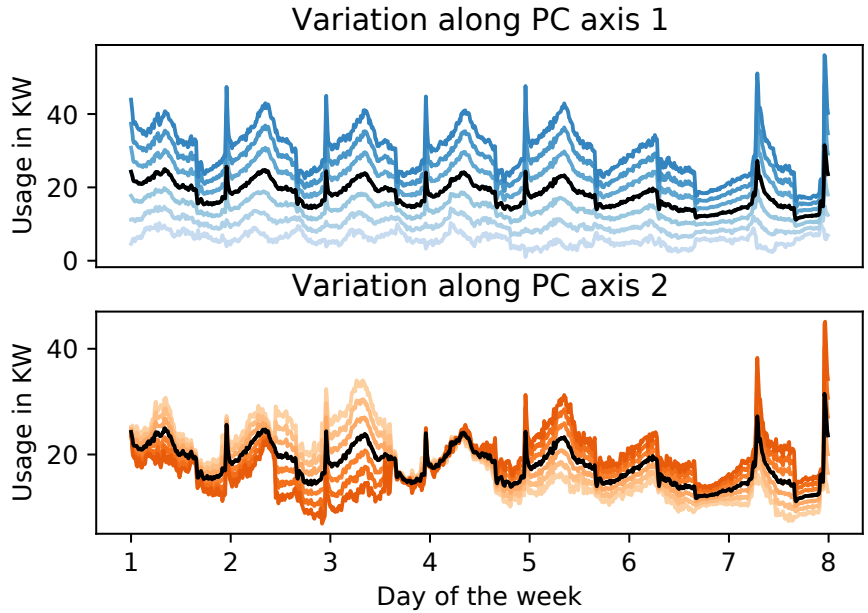
One can also use the equivalent Singular Value Decomposition of $\mathbf{X}^c$ (Scikit-learn).

PCA in practice

- PCA can be used for denoising data : additive random IID noise located in low variance subspaces.
- Selection of p can be used by plotting the sorted eigenvalues (searching for an elbow or ratio of explained variance) of with probabilistic modeling [Tipping and Bishop, 1999, Minka, 2000]
- Sparse PCA promotes sparsity on $\mathbf{d}_k$ for feature selection [Zou et al., 2006] .
- Warning : PCA focuses on correlation, *i.e.* linear relationship between features and can miss more complex relationships.

PCA on energy usage data





Application

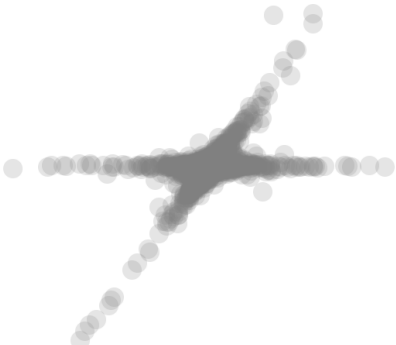
- Run PCA with $p = 2$.
- Plot plot projection in 2D colored by week number for interpretability.
- Summer/Winter dynamic along axis 1.
- Part of the week usage variation along axis 2.

Python Code

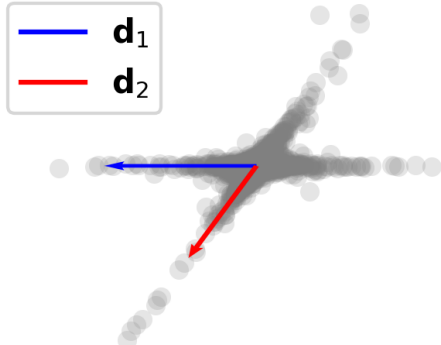
```
from sklearn.decomposition import PCA

# PCA with p=2
clf = PCA(2)
# fit the model and project in 2D
Xp = clf.fit_transform(X)
# Get the projections/axis P
D = clf.components_.T
```

Independent Component Analysis

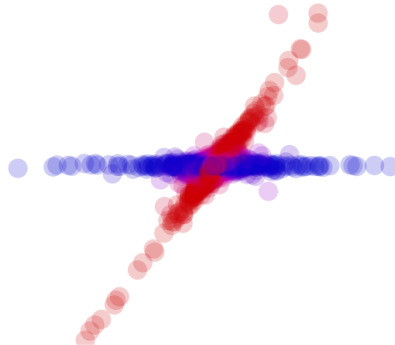
Dataset in 2D



ICA Dictionary



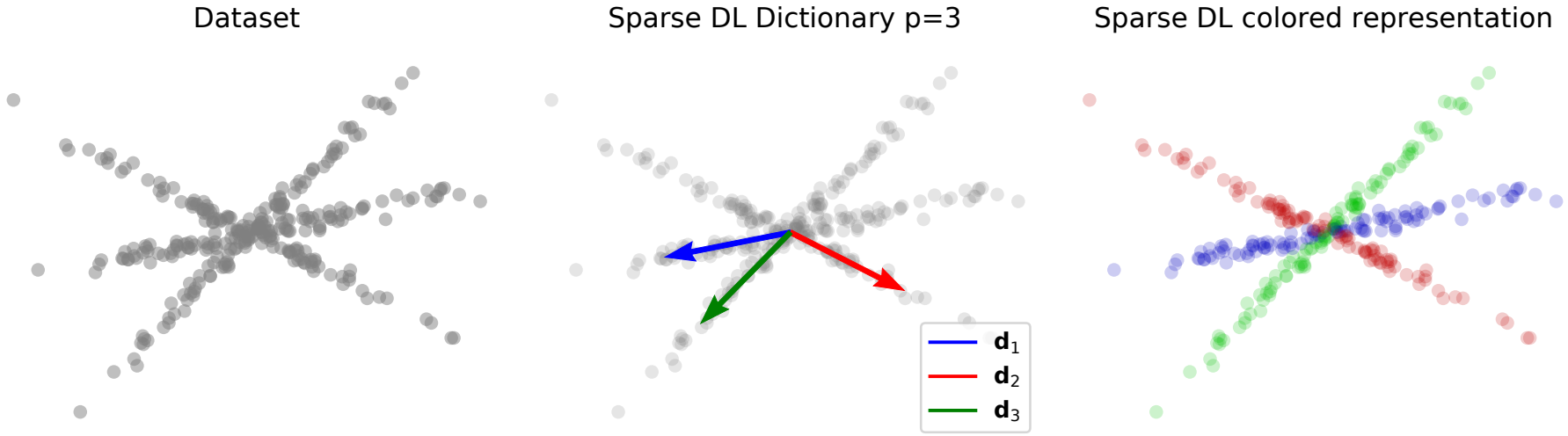
ICA Colored representation



Principle [Herault and Jutten, 1986]

- Find a decomposition of the samples $\hat{\mathbf{a}} = \mathbf{D}^\top \mathbf{x}$ that is independent (columns of $\mathbf{A}$ are independent, not necessarily orthogonal as in PCA).
- Linear model but not expressed as the general optimization problem (7).
- Works particularly well on non Gaussian data (or else PCA is optimal).
- Efficient algorithm : FastICA [Hyvärinen and Oja, 2000].
- Applied with success to several source separation problems (biomedical data).
- Scikit-learn implementation : sklearn.decomposition.FastICA.

Sparse Dictionary Learning



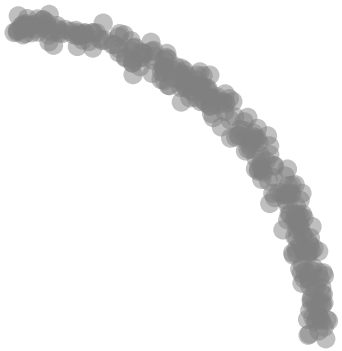
Principle

$$\min_{\mathbf{A}\in\mathbb{R}^{n\times p},\mathbf{D}\in\mathbb{R}^{d\times p},\|\mathbf{d}_k\|=1,\forall k} \sum_{i=1}^{n} \|\mathbf{x}_i - \mathbf{D}\mathbf{a}_i\|^2 + \lambda\|\mathbf{a}_i\|_1 \tag{9}$$

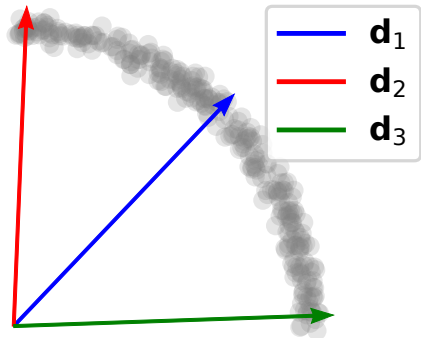
- Constraints on the norm of $\mathbf{d}_i$ ensure normalized basis (not orthogonal).
- Sparsity promoting L_1 regularization (see Lasso in next course) on the representations $\mathbf{a}_i$ promotes samples in linear subspaces of the span of $\mathbf{D}$.
- Similar to Sparse PCA but sparsity on $\mathbf{a}_i$ instead of the dictionary $\mathbf{d}_k$.
- Can be solved efficiently with stochastic optimization [Mairal et al., 2009].
- Scikit-learn implementation : sklearn.decomposition.DictionaryLearning.

Non-negative Matrix Factorization (NMF)

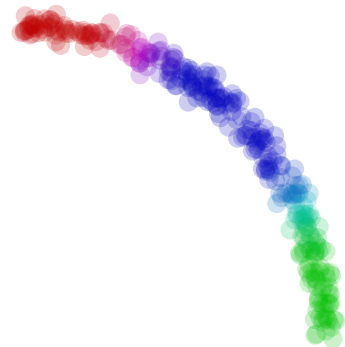
Dataset



NMF Dictionary p=3



NMF colored representation

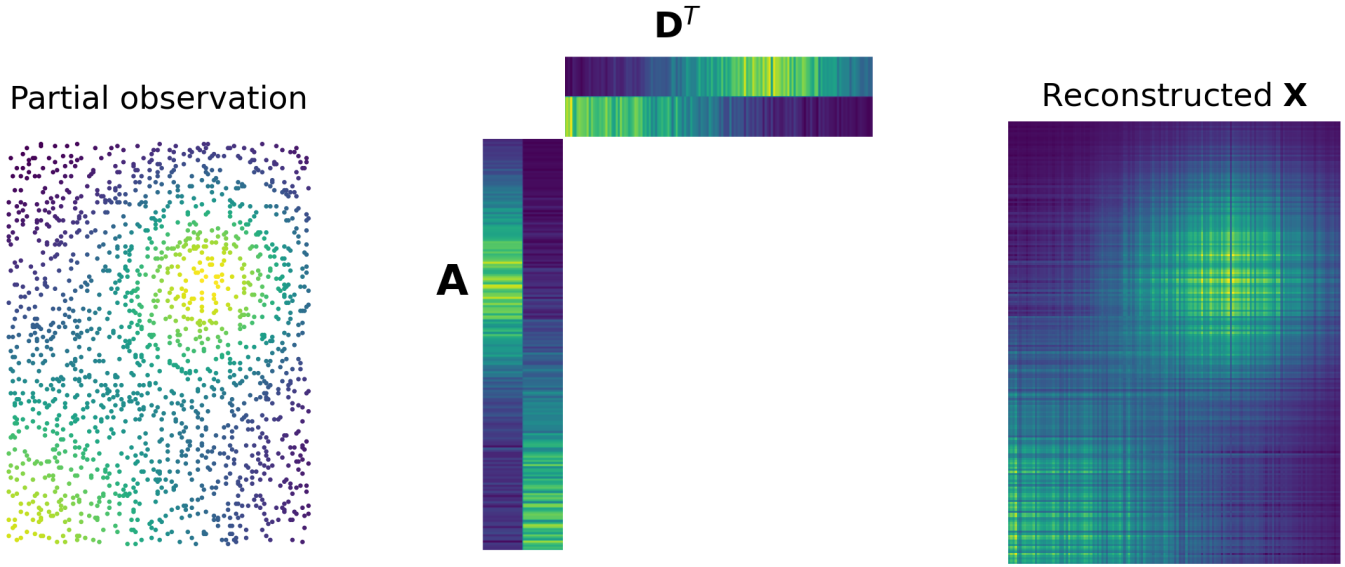


Principle [Lee and Seung, 2000]

$$\min_{\mathbf{A}\in\mathbb{R}_+^{n\times p},\mathbf{D}\in\mathbb{R}_+^{d\times p},\|\mathbf{d}_k\|=1,\forall k} \sum_{i=1}^{n} L(\mathbf{x}_i, \mathbf{D}\mathbf{a}_i) \tag{10}$$

- For positive data (for instance power densities) it makes sens to have both dictionary elements $\mathbf{d}_j$ and representations $\mathbf{a}_j$ positive.
- Different losses L have been proposed:
  - Quadratic, Guassian noise [Lee and Seung, 2000].
  - Kullback–Leibler divergence, Poisson noise [Dhillon and Sra, 2005].
  - Itakura-Saito, audio spectrum [Févotte et al., 2009]).
- Optimization problem can be solved with gradient descent, block coordinate descent and multiplicative updates.
- Sparsity regularization can also be used similarly to SparseDL.
- Scikit-learn implementation : sklearn.decomposition.NMF.

Matrix factorization (collaborative filtering)

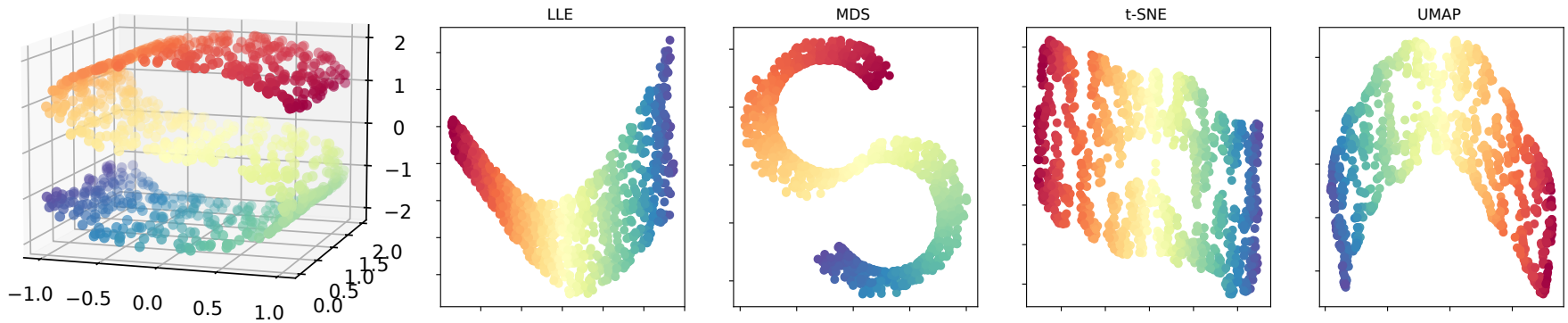


Principle (Survey [Bokde et al., 2015])

$$\min_{\mathbf{D},\mathbf{A}} \quad \sum_{i=1}^{n} \|\mathbf{m}_i \odot (\mathbf{x}_i - \mathbf{D}\mathbf{a}_i)\|^2 \tag{11}$$

- $\odot$ is the pointwise multiplication and $\mathbf{m}_i \in \{0,1\}^d$ is a binary mask denoting which features in $\mathbf{x}_i$ that are observed for sample $\mathbf{x}_i$.
- Data is only partially observed but one wants to predict the values for all components of the matrix $\mathbf{X}$ (observed values are stored in a sparse matrix).
- Solved using truncated Singular Vector Decomposition that return a low rank $p < \min(d, n)$ factorization $\mathbf{X} \approx \mathbf{A}\mathbf{D}^T$.
- Used in recommender systems for user/product recommendation.

Nonlinear dimension reduction methods (manifold learning)



Nonlinear subspaces

- The dataset often lies in a nonlinear subspace (a manifold) of $\mathbb{R}^d$.
- Manifold learning method aim at recovering this low dimensional manifold.
- Example above of 2D manifold in a 3D ambient space and the projection of the samples in 2D for different methods (colors only to check that the relation between samples are preserved).

Manifold learning problems

- **Projection** $\{\mathbf{x}_i\}_{i=1}^n \Rightarrow \{\tilde{\mathbf{x}}_i \in \mathbb{R}^p\}_{i=1}^n$ with $p \ll d$: Project dataset in low dimension (visualization).
- **Inductive** $\{\mathbf{x}_i\}_{i=1}^n \Rightarrow g : \mathbb{R}^d \to \mathbb{R}^p$: learn a nonlinear projection function.
- **Inductive+Invertible** $\{\mathbf{x}_i\}_{i=1}^n \Rightarrow g : \mathbb{R}^d \to \mathbb{R}^p, f : \mathbb{R}^p \to \mathbb{R}^d, f(g(\mathbf{x})) \approx \mathbf{x}$: learn both projection and reconstruction nonlinear functions.

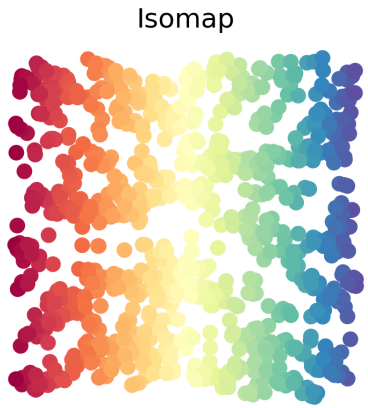
Common manifold learning methods

Multi-Dimensional Scaling (MDS) [Kruskal, 1964]

- Search for positions $\{\tilde{\mathbf{x}}_i\}$ that have a similar pairwise distance matrix as the original data $\{\mathbf{x}_i\}$.
- Solved with eigendecomposition (PCA on distances).
- Scikit-learn : sklearn.manifold.MDS.

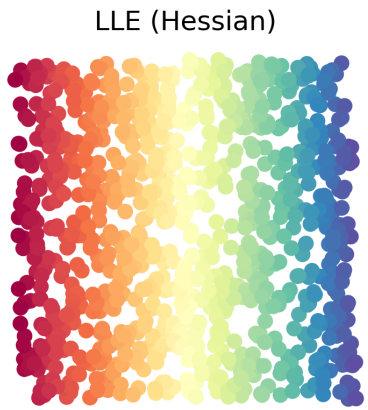
ISOMAP [Tenenbaum et al., 2000]

- Estimate a graph of neighbors in the ambient space.
- Use the geodesic distance on the graph between samples and perform MDS (preserve distance on the manifold).
- Scikit-learn : sklearn.manifold.Isomap.

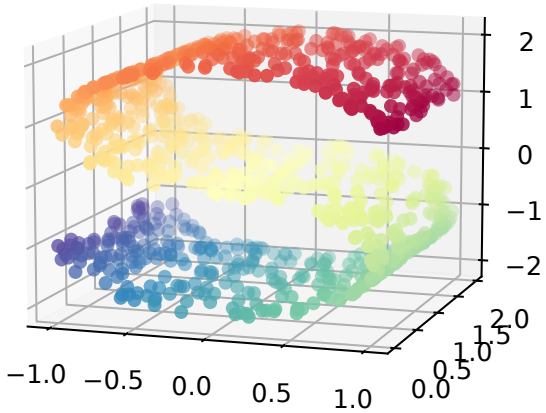


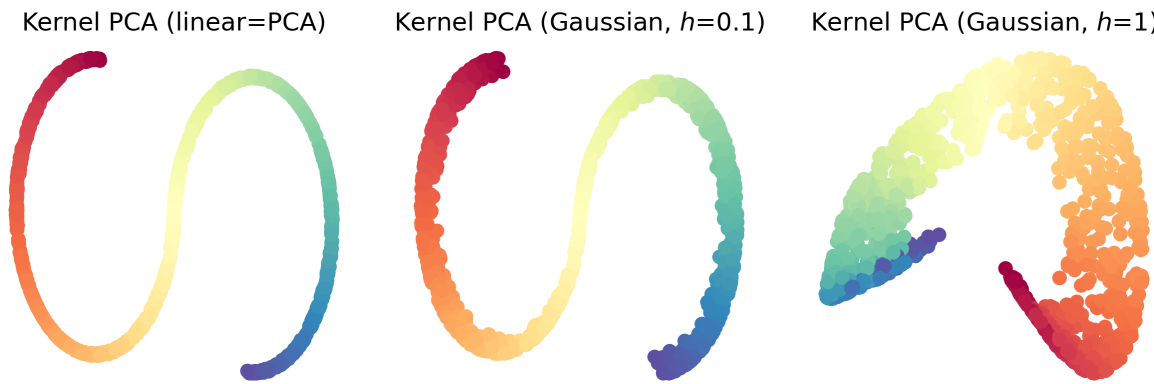
Locally Linear Embedding (LLE) [Roweis and Saul, 2000]

- Find an embedding that preserve distance in local neighborhood (many PCA).
- Regularized LLE : modified [Zhang and Wang, 2007], Hessian [Donoho and Grimes, 2003] .
- Scikit-learn : sklearn.manifold.LocallyLinearEmbedding.



Kernel PCA (KPCA)

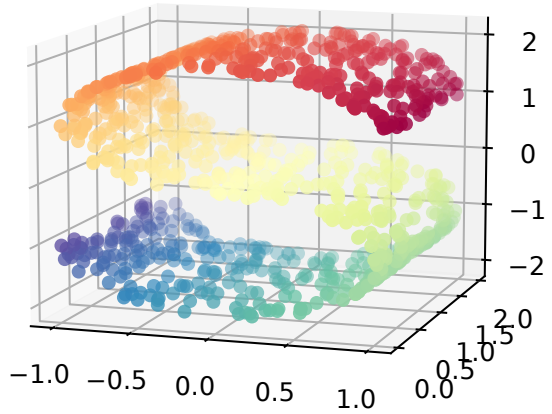


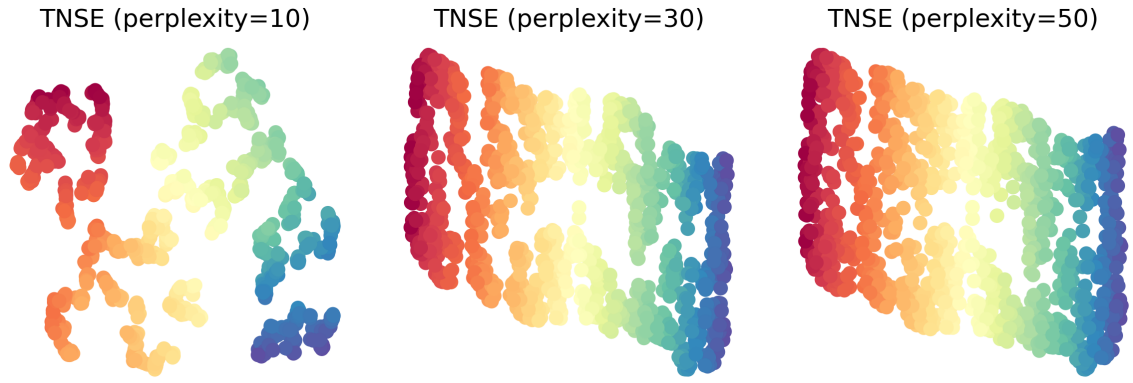


Principle [Schölkopf et al., 1997]

- Perform PCA in a high-dimensional non-linear embedding $\phi(\mathbf{x})$ of the data.
- Embedding is implicit, thanks to the use of a kernel $k(\mathbf{x}, \mathbf{x}') =< \phi(\mathbf{x}), \phi(\mathbf{x}') >$, only the kernel matrix between samples is necessary. This is called the "kernel trick"(used also for SVM classification).
- Inductive method, reconstruction is possible but requires solving an inverse problem (kernel pre-image problem [Kwok and Tsang, 2004]).
- Classical kernels are linear kernel (equivalent to PCA) and Gaussian kernel (Radial Basis Function RBF in Sckikit-learn).
- LLE and ISOMAP are actually special cases of KPCA with specifically designed kernels [Ham et al., 2004]
- Scikit-learn implementation : sklearn.decomposition.KernelPCA.

t-Stochastic Neighbor Embedding (TSNE)





Principle [Van der Maaten and Hinton, 2008]

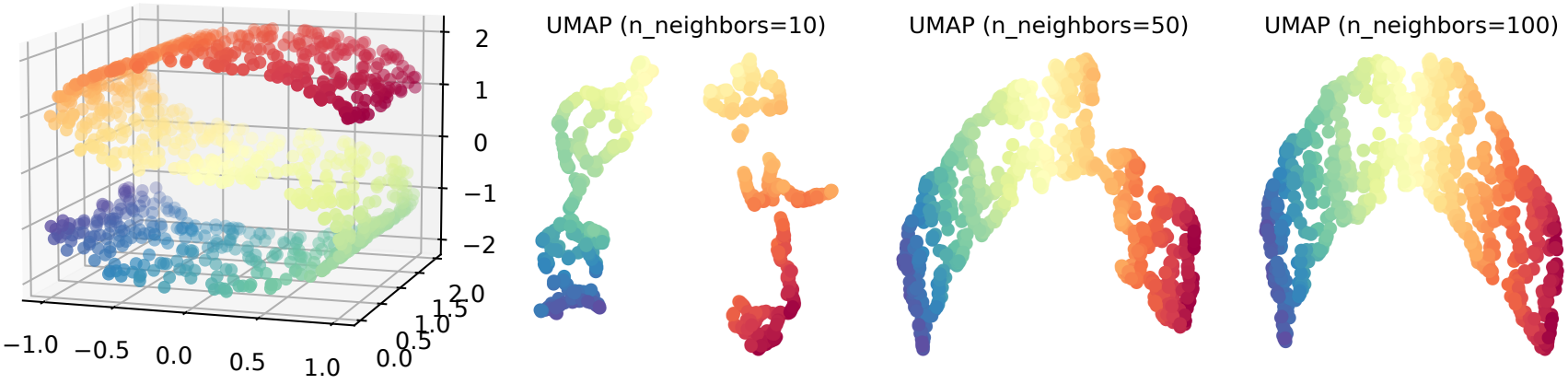
$$\min_{\tilde{\mathbf{x}}_i, \forall i} \sum_{i,j} KL(p_x(\mathbf{x}_i|\mathbf{x}_j)||q_{\tilde{x}}(\tilde{\mathbf{x}}_i|\tilde{\mathbf{x}}_j))$$

- KL is the Kullback–Leibler divergence and the distributions p and q are the probability that two samples are neighbors expressed as:

$$p_x(\mathbf{x}_i|\mathbf{x}_j) = \frac{\exp(-\|\mathbf{x}_i - \mathbf{x}_j\|^2/2\sigma_i^2)}{\sum_{k\neq i}\exp(-\|\mathbf{x}_i - \mathbf{x}_k\|^2/2\sigma_i^2)}, \quad q_{\tilde{x}}(\tilde{\mathbf{x}}_i|\tilde{\mathbf{x}}_j) = \frac{(1+\|\tilde{\mathbf{x}}_i - \tilde{\mathbf{x}}_j\|^2)^{-1}}{\sum_k \sum_{l\neq k}(1+\|\tilde{\mathbf{x}}_k - \tilde{\mathbf{x}}_l\|^2)^{-1}}$$

- The bandwith σ_i are set to provide a given perplexity parameter (accuracy of density estimation on training data).
- t-SNE uses a t-Student distribution on the projected samples instead of the Gaussian kernel in classical SNE [Hinton and Roweis, 2002].
- Warning: TNSE has a tendency to show non-existent clusters for small perplexity.
- Scikit-learn implementation : `sklearn.manifold.TSNE(n_components=2,perplexity=50)`.

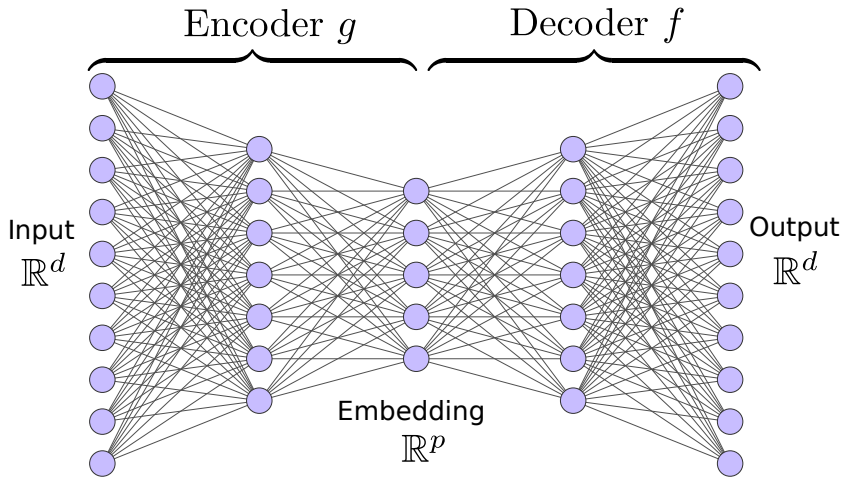
Uniform Manifold Approximation and Projection (UMAP)



Principle [McInnes et al., 2018]

- Suppose that the data is uniformly distributed on Riemannian manifold and this manifold is locally connected.
- Construct a graph of neighbors (`n_neighbors` parameter) and approximate the manifold with a Fuzzy topological structure.
- Can be adapted to non-uniform densities [Narayan et al., 2020].
- While not designed to be inductive and invertible, UMAP implementation provide numerical estimation for both.
- More efficient that TSNE on large dataset because does not a requires normalization step to compute pairwise relations.
- Implementation in `umap-learn` : `umap.UMAP(n_components = 2, n_neighbors=n_neighbors)`

Auto-Encoder (AE)



Principle (Tutorial [Goodfellow et al., 2016, Chapter 14])

$$\min_{f,g} \quad \sum_{i=1}^{n} L(\mathbf{x}_i, f(g(\mathbf{x}_i)))$$

- Train two neural networks : $g : \mathbb{R}^d \to \mathbb{R}^p$ the encoder and $f : \mathbb{R}^p \to \mathbb{R}^d$ the decoder such that $f(g(\mathbf{x})) \approx \mathbf{x}$.
- Models are often deep neural networks such as $g(\mathbf{x}) = g_K(g_{K-1}(\dots g_1(\mathbf{X})))$ where $g_k(\mathbf{x}) = \sigma(\mathbf{W}_k\mathbf{x} + \mathbf{b}_k)$ and σ is a nonlinear activation function.
- When $p < d$ the AE searches for a nonlinear subspace (manifold) that optimize data reconstruction *w.r.t.* the loss L.
- Sparse AE use a regularization (KL [Makhzani and Frey, 2013] or L1/L2 [Arpit et al., 2016]) to promote sparse activations $g(\mathbf{x})$.

Variational Auto-Encoders (VAE)

Principle [Kingma and Welling, 2013]

- Estimate probabilistic encoder $q(\mathbf{z}|\mathbf{x})$ and decoder $p(\mathbf{x}|\mathbf{z})$ that model the dataset.
- Optimize the MAP on the data with a Bayesian prior on the embedding is $p(\mathbf{z})$.
- The embedding $q(\mathbf{z}|\mathbf{x})$ of sample $\mathbf{x}$ is a distribution (usually a Normal distribution).
- The reconstruction is also probabilistic : one can generate several reconstructions from and embedding for instance to model uncertainty.

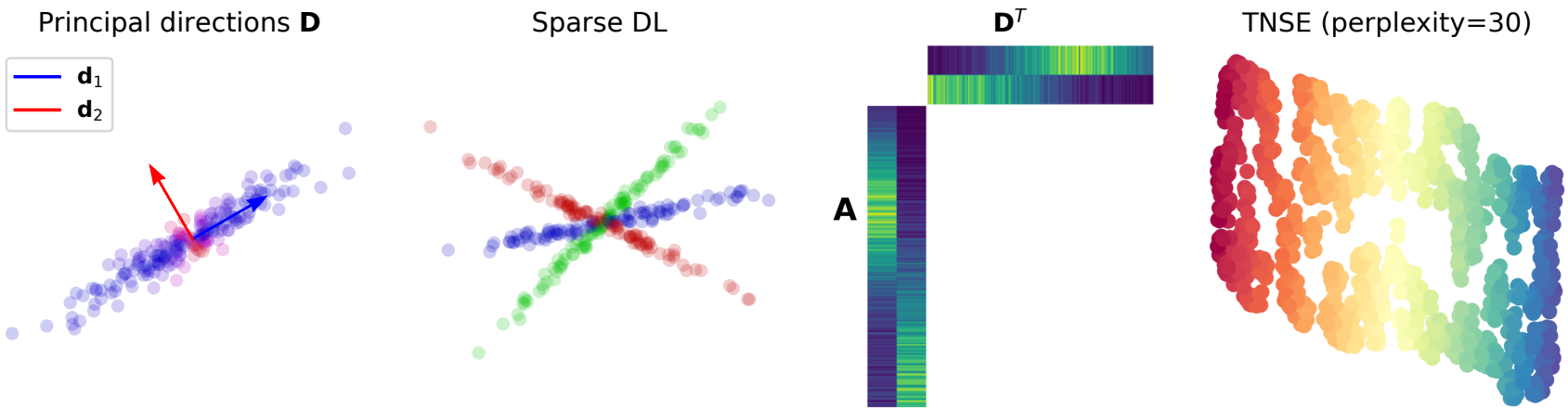
VAE in practice

- In practice optimization of the Evidence Lower BOund (ELBO) that is a variational lower bound of the MLE or MAP.
- The embedding if often modeled with $z \sim q(\mathbf{z}|\mathbf{x}) = \mathcal{N}(m(\mathbf{x}), \text{diag}(s(\mathbf{x})))$ where m and s are deep neural network predicting the mean and variances respectively.
- The reparametrization trick allows to propagate the gradients with Stochastic Gradient Descent (SGD) by generating samples :

$$\mathbf{z} = m(\mathbf{x}) + s(\mathbf{x}) \odot \boldsymbol{\epsilon}, \qquad \boldsymbol{\epsilon} \sim \mathcal{N}(\mathbf{0}_p, \mathbf{I}_p)$$

- VAE can be used for data imputation when data is partially observed [Mattei and Frellsen, 2019].

Dimensionality Reduction (DR) in practice

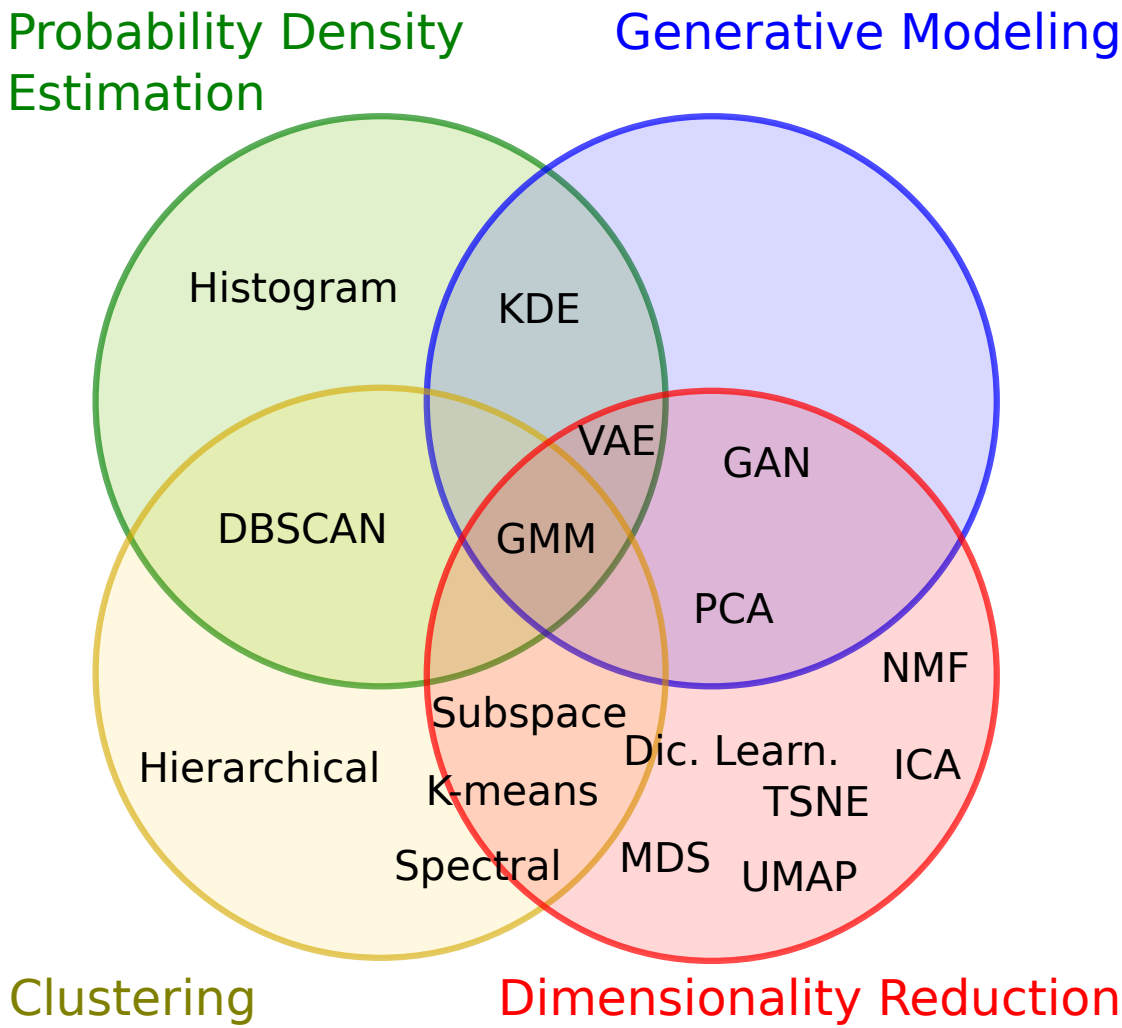


Why and when?

- Dimensionality reduction is a classical tool for visualizing high dimensional data in 2D but always comes with loss of information ($d = 2$ is very small).
- Inductive and invertible DR methods can be used for denoising because noise is high dimensional and data is usually low dimensional.
- Standard 2D visualization for data/feature manifolds are TSNE and more recently UMAP but beware of false clusters.
- PCA is a classical pre-processing step but quantization with K-means or dictionary learning (bag of visual words) also used in practice.

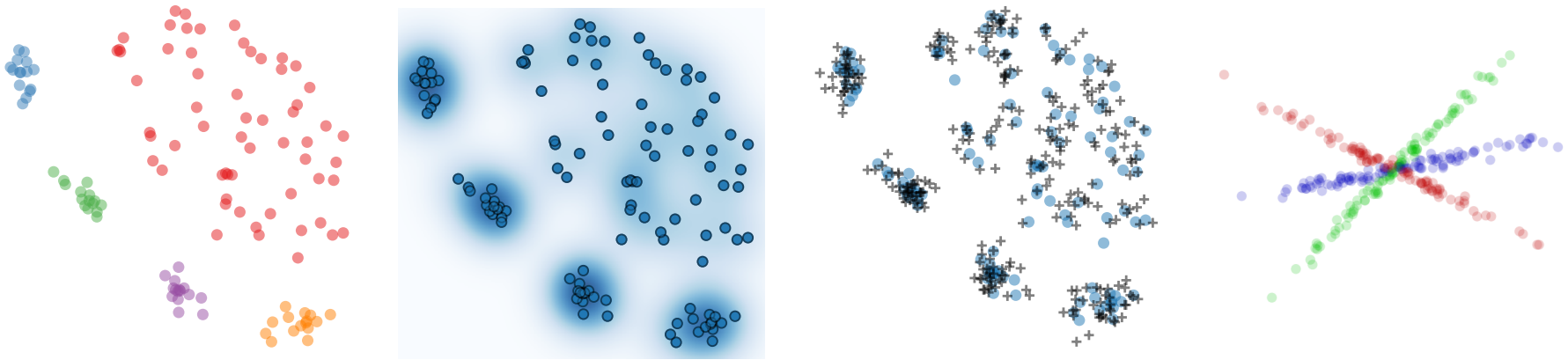
Section

Unsupervised learning problems VS methods



Most methods can be used to solve several ML problems.

Conclusion



Unsupervised learning

- Most datasets are unlabeled because labeling is expensive (requires humans).
- Unsupervised learning aim at modeling and interpreting the data without human annotations.
- It's difficult to measure and evaluate the quality of the models in unsupervised learning (the criterion is often optimized).
- Numerous research in self-supervised learning (learning representations that are good for predictions without labels, invariant to some variability).
- Most unsupervised learning methods can be used for pre-processing and feature extraction before supervised learning (when inductive).

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