Machine Learning
Clustering I

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Unsupervised learning

Unsupervised Learning:
Given a set of input points $(X_i)_{i=1}^n$:

- **Clustering:** Construction of a grouping of the points into sets of *similar* points, the so called *clusters*.
- **Density Estimation:** Estimation of the distribution of the input points over the input space $\mathcal{X}$. Related problem: **Outlier detection**.
- **Dimensionality Reduction:** Construction of a mapping $\phi : \mathcal{X} \to \mathbb{R}^m$, where the dimensionality m of the target space is usually much smaller than that of the input space $\mathcal{X}$. Generally, the mapping should preserve properties of the input space $\mathcal{X}$ e.g. distances.

Roadmap

Clustering

- Goal of clustering,
- k-means clustering (prototype-based clustering)
- Spectral clustering (graph-based clustering),
- Agglomerative and hierarchical clustering,
- Density based clustering.

Clustering is one instance of unsupervised learning

What is clustering ?

Clustering:

Construction of a grouping of the points into sets of *similar* points, the so called *clusters*.

- no generally accepted objective for clustering $\Longrightarrow$ without specifying a suitable objective clustering is **ill-defined**,
- clustering objective depends usually on application,
- in clustering the modeling aspect is even more important than in supervised learning $\Longrightarrow$ do not use a clustering method if you have not understood what the objective implies !

K-means clustering

- **Goal:** find prototypes μ_i, $i = 1, \ldots, k$ which represent the data in an optimal way (what does that mean ?),
- **Objective:** denote by C_i the i-th cluster (set of points) which is represented by the prototype μ_i,

$$\mathop{\arg\min}_{(C_1,\mu_1),\ldots,(C_k,\mu_k)} \sum_{i=1}^{k} \sum_{x_j \in C_i} \|x_j - \mu_i\|^2 ,$$

  where $\|\cdot\|$ is the Euclidean norm,
- **True Goal:**
  1. finds sphere-like clusters in the data,
  2. heavily influenced by outliers,
  3. non-sphere like clusters are hard to fit.

K-means II

K-means clustering:

- k-means is combinatorial optimization problem,
- simple iterative algorithm - converges fast but finds only local minimum.

Lloyd's algorithm for k-means clustering:

1. initialize centers μ_i,
2. **do** classify all samples according to closest μ_i, $i = 1, \ldots, k$
3. recompute μ_i as the mean of the points in cluster C_i for $i = 1, \ldots, k$
4. **while** no change in μ_i, $i = 1, \ldots, k$,
5. **return** $\mu_1, \ldots, \mu_k$,

Steps are optimal for fixed clusters resp. fixed centers

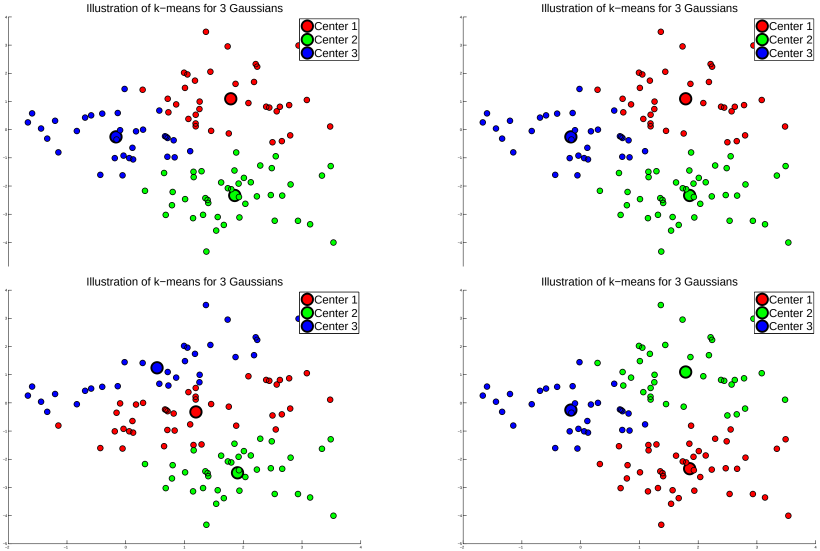
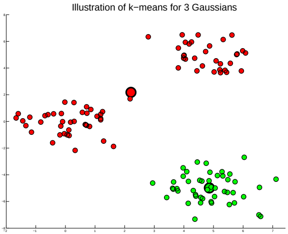
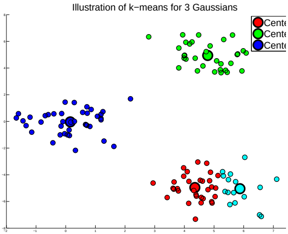
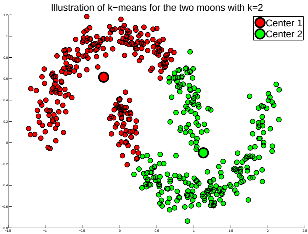


Illustration of k−means for 3 Gaussians
Center 1
Center 2
Center 3
Illustration of k−means for 3 Gaussians
Center 1
Center 2
Center 3
Illustration of k−means for 3 Gaussians
Center 1
Center 2
Center 3
Illustration of k−means for 3 Gaussians
Center 1
Center 2
Center 3

Problems of K-Means







- Left: k is chosen too small.
- Middle: k is chosen too large.
- Right: The two moons dataset - clusters are not of spherical shape.

$$J(k) = \min_{(C_1,\mu_1),\ldots,(C_k,\mu_k)} \sum_{i=1}^{k} \sum_{x_j \in C_i} \left\| x_j - \mu_i \right\|^2 ,$$

$\Longrightarrow$ monotonically decreasing in k - not useful for choosing k !

Spectral Clustering:

- an instance of graph-based clustering,
- First attempts can be traced back to Donath and Hoffman and Fiedler in 1973,
- very popular clustering algorithm since it can find clusters of almost arbitrary shape,
- rich theoretical background.

$\Longrightarrow$ based on eigenvectors of the graph Laplacian.

In the following: we deal with weighted, undirected graphs $G = (V, W)$
$\Rightarrow$ symmetric weight matrix $w_{ij} = w_{ji}$,
$\Rightarrow$ degree of vertex i, $d(i) = \sum_{j=1}^{n} w_{ij}$, degree matrix $D_{ij} = d_i \delta_{ij}$.

Graph Laplacian - Definition

In the literature one can find three types of graph Laplacians:

unnormalized:
$$(\Delta^{(\mathrm{u})} f)(i) = d(i) f(i) - \sum_{j=1}^{n} w_{ij} f(j),$$
$$(\Delta^{(\mathrm{u})} f) = (D - W) f,$$

normalized:
$$(\Delta^{(\mathrm{n})} f)(i) = f(i) - \sum_{j=1}^{n} \frac{w_{ij}}{\sqrt{d_i\, d_j}} f(j),$$
$$(\Delta^{(\mathrm{n})} f) = (\mathbb{1} - D^{-1/2} W D^{-1/2}) f.$$

Caution: often no distinction in the literature - each of them is just called graph Laplacian.

Relation to the continuous Laplacian

The **continuous Laplacian** is a second-order differential operator,

$$\Delta f = \sum_{i=1}^{d} \frac{\partial^2 f}{\partial x_i^2}.$$

It is invariant under rotations and translations ($\Rightarrow$ image processing).

Correspondence: For a grid in $\mathbb{R}^d$ the unnormalized graph Laplacian, $\Delta^{(\mathrm{u})} = D - W$, corresponds up to the sign to the finite difference approximation of the continuous Laplacian.
For the real line with an equidistant discretization of size size h, we get,

$$\frac{d^2 f}{dx^2} \approx \frac{1}{h^2}\Big(f(i+1)+f(i-1)-2f(i)\Big) = -d(i)f(i)+\sum_{j=1}^{m} w_{ij} f(j) = -(\Delta^{(\mathrm{u})} f)(i),$$

where in the grid each point connects to its nearest neighbors and the weights are $1/h^2 \Rightarrow$ degree of each grid point is $2/h^2$.

Properties of the graph Laplacian

- All graph Laplacians are positive semi-definite and self-adjoint,

$$\langle f, \Delta g \rangle_{\mathcal{H}_V} = \langle g, \Delta f \rangle_{\mathcal{H}_V} .$$

- Associated regularization functionals (useful for SSL),

$$\left\langle f, \Delta^{(\mathrm{u})} f \right\rangle = \sum_{i,j=1}^{n} w_{ij} (f_i - f_j)^2,$$

$$\left\langle f, \Delta^{(\mathrm{n})} f \right\rangle = \sum_{i,j=1}^{n} w_{ij} \Big(\frac{f_i}{\sqrt{d_i}} - \frac{f_j}{\sqrt{d_j}} \Big)^2.$$

- The eigenvectors of $\Delta^{(\mathrm{u})}$ and $\Delta^{(\mathrm{n})}$ define an orthonormal basis on $\mathbb{R}^V$.

Key property for Spectral Clustering

- Algebraic connectivity of the graph:

Theorem (Fiedler)

The multiplicity of the first eigenvalue (the first eigenvalue is zero) of the graph Laplacians is equivalent to the number of connected components of the graph.

- Let A_i, $i = 1, \ldots, K$ be the connected components of the graph. $\mathbb{1}_{j \in A_i}$ are eigenvectors of $\Delta^{(\mathrm{u})}$ to the eigenvalue 0. $\sqrt{d_j}\mathbb{1}_{j \in A_i}$ are eigenvectors of $\Delta^{(\mathrm{n})}$ to the eigenvalue 0.
- **Caution:** there is no "first eigenvector" but we have an eigenspace to the eigenvalue zero which has dimension K.

A graph which resolves into disconnected components is the ideal clustering (already the graph reveals the cluster structure - no other clustering method necessary).

Spectral Clustering - Variant I

Chooose the graph Laplacian: unnormalized or normalized and the number of clusters k.

- compute the graph Laplacian,
- compute the first k eigenvectors $\{u_i\}_{i=1}^k$ (each eigenvector is normalized, $\|u_i\|_2 = 1$, $i = 1, \ldots, k$),
- Embedding $\phi : V \to \mathbb{R}^k$, of the n vertices into $\mathbb{R}^k$ by $i \to z_i = (u_1(i), \ldots, u_k(i))$,
- clustering of the resulting n points $\{z_i\}_{i=1}^n$ by k-means into clusters $C_1, \ldots, C_k$.

The embedding: $\phi : V \to \mathbb{R}^k$, $i \to \phi(i) = (u_1(i), \ldots, u_k(i))$ is basically the **Laplacian eigenmap**.

Central Questions

- Is the mapped data in the new space suited for k-means ?
- Why should this yield a good clustering ?

Three different motivations for spectral clustering:

1. Relaxation of graph cuts,
2. Markov random walks,
3. Perturbation theory of the eigenvectors.

Motivation I - Graph Cuts

Partitioning of weighted, undirected graphs

Define: $\overline{C_i} = V \backslash C_i$ and $\mathrm{vol}(C_i) = \sum_{j \in C_i} d_j$ and

$$\mathrm{cut}(C, D) = \sum_{i \in C, j \in D} w_{ij}.$$

Let $(C_1, \ldots, C_k)$ be a partition of V $(\cup_{i=1}^k C_i = V$ and $C_i \cap C_j = \emptyset$, $i \neq j)$

Graph Cut Criteria:

- MinCut: $\mathrm{MinCut}(C_1, \ldots, C_k) = \sum_{i=1}^k \mathrm{cut}(C_i, \overline{C_i})$.
- RatioCut: $\mathrm{RatioCut}(C_1, \ldots, C_k) = \sum_{i=1}^k \frac{\mathrm{cut}(C_i, \overline{C_i})}{|C_i|}$.
- NCut (normalized Cut): $\mathrm{NCut}(C_1, \ldots, C_k) = \sum_{i=1}^k \frac{\mathrm{cut}(C_i, \overline{C_i})}{\mathrm{vol}(C_i)}$.

Goal: find optimal (minimal) Min/Ratio/Normalized-cut among all possible partitions.

Motivation I - Graph Cuts II

Partitioning of weighted, undirected graphs

- MinCut: yields often unbalanced partitions in particular single points become clusters.
- Ratio Cut and Normalized Cut are instances of **balanced graph cut criteria**
  $\Longrightarrow$ enforces balanced partitions (what does balanced mean ?)
  $\Longrightarrow$ Ratio Cut prefers clusters of equal size,
  $\Longrightarrow$ Normalized Cut prefers clusters of equal volume.
- **Problem:** All balanced graph cut criteria are NP-hard.

Spectral clustering is a relaxation of ratio/normalized cut !

Given a partition $(C, \overline{C})$ (two clusters, $k = 2$) define $f^C : V \to \mathbb{R}$,

$$f_i^C = \begin{cases} \sqrt{|\overline{C}|/|C|} & \text{if } i \in C, \\ -\sqrt{|C|/|\overline{C}|} & \text{if } i \in \overline{C}. \end{cases}$$

$$\begin{aligned}\left\langle f^C, \Delta^{(u)} f^C \right\rangle =& \frac{1}{2}\sum_{i,j=1}^{n} w_{ij}(f_i^C - f_j^C)^2 = \sum_{i \in C, j \in \overline{C}} w_{ij}\left(\sqrt{\frac{|\overline{C}|}{|C|}} + \sqrt{\frac{|C|}{|\overline{C}|}}\right)^2 \\ =& \mathrm{cut}(C, \overline{C}) \left(\frac{|\overline{C}|}{|C|} + \frac{|C|}{|\overline{C}|} + 2\right) = \mathrm{cut}(C, \overline{C}) \left(\frac{|C| + |\overline{C}|}{|C|} + \frac{|C| + \overline{C}}{|\overline{C}|}\right) \\ =& |V|\mathrm{cut}(C, \overline{C})\left(\frac{1}{|C|} + \frac{1}{\overline{C}}\right) = |V| \,\mathrm{RatioCut}(C, \overline{C})\end{aligned}$$

$$\sum_{i=1}^{n} f_i^C = \sum_{i \in C} \sqrt{\frac{|\overline{C}|}{|C|}} - \sum_{i \in \overline{C}} \sqrt{\frac{|C|}{|\overline{C}|}} = 0, \quad \left\| f^C \right\|_2^2 = \sum_{i=1}^{n} (f_i^C)^2 = |C|\frac{|\overline{C}|}{|C|} + |\overline{C}|\frac{|C|}{|\overline{C}|} = n.$$

Relaxation of ratio cut II

With the specific form of the function f^C the optimal **ratio cut** can be written as:

$$\min_{C\subset V} \left\{ \left\langle f^C, \Delta^{(\mathrm{u})} f^C \right\rangle \mid \left\langle f^C, \mathbb{1} \right\rangle = 0,\ \left\| f^C \right\| = \sqrt{n} \right\}.$$

This is a discrete combinatorial optimization problem and is NP-hard
$\Rightarrow$ relax problem by allowing f to take arbitrary real values.

$$\min_{f\in\mathbb{R}^V} \left\{ \left\langle f, \Delta^{(\mathrm{u})} f \right\rangle \mid \langle f, \mathbb{1} \rangle = 0,\ \|f\| = \sqrt{n} \right\}.$$

- Rayleigh-Ritz principle $\Rightarrow$ If graph is connected, minimum is the second eigenvalue λ_2 and the minimizer is the second eigenvector u_2 of $\Delta^{(\mathrm{u})} = D - W$.
- Partitioning using optimal threshold t

  $$C_t = \{ j \in V \mid u_2(j) > t \},$$

  by optimizing the Ratio-Cut or alternatively k-means in the embedding.

Relaxation of normalized cut

Given a partition $(C, \overline{C})$ define the function,

$$f_i^C = \begin{cases} \sqrt{\mathrm{vol}(\overline{C})/\,\mathrm{vol}(C)}, & i \in C, \\ -\sqrt{\mathrm{vol}(C)/\,\mathrm{vol}(\overline{C})}, & i \in \overline{C}. \end{cases}$$

$$\left\langle f^C, \Delta^{(\mathrm{u})} f^C \right\rangle = \mathrm{vol}(V)\,\mathrm{NCut}(C, \overline{C}), \quad \left\langle f^C, Df^C \right\rangle = \mathrm{vol}(V) = n, \quad \left\langle \mathbb{1}, Df^C \right\rangle = 0.$$

The optimal normalized cut:

$$\min_{C \subset V} \Big\{ \left\langle f^C, \Delta^{(\mathrm{u})} f^C \right\rangle \;\big|\; \left\langle Df^C, \mathbb{1} \right\rangle = 0,\ \left\langle f^C, Df^C \right\rangle = n \Big\}.$$

Relaxation of the normalized cut:

$$\min_{f \in \mathbb{R}^V} \Big\{ \left\langle f, \Delta^{(\mathrm{u})} f \right\rangle \;\big|\; \left\langle Df, \mathbb{1} \right\rangle = 0,\ \left\langle f, Df \right\rangle = n \Big\}.$$

$\Rightarrow$ generalized eigenproblem $\Delta^{(\mathrm{u})} f = \lambda D f$.

The general case for the ratio cut

Given a partition $(C_1, \ldots, C_k)$ define the functions h_i,

$$h_i(j) = \begin{cases} \frac{1}{\sqrt{|C_i|}} & j \in C_i, \\ 0 & j \in \overline{C_i}. \end{cases}$$

General normalized cut:

$$\min_{C_1,\ldots,C_k} \{ \operatorname{Tr}(H\Delta^{(\mathrm{u})}H^T) \mid HH^T = \mathbb{1}_k, \}$$

- The minimizer of the relaxation to arbitrary $H = \{h_1, \ldots, h_k\}$, that is $H \in \mathbb{R}^{k \times n}$, yields the smallest k eigenvectors $\{u_i\}_{i=1}^k$ of the unnormalized graph Laplacian $\Delta^{(\mathrm{u})}$. The minimum is the sum of the k-smallest eigenvalues of $\Delta^{(\mathrm{u})}$.
- The conversion of $H = \{u_1, \ldots, u_k\}$ into a partition $(C_1, \ldots, C_k)$ can be done by k-means clustering of the rows of $H \Rightarrow$ no approximation guarantees

Theoretical results for $k = 2$

- Let $\phi^* = \min_C \mathrm{NCut}(C, \overline{C})$ and denote by $\phi_{SPECTRAL}$ the cut obtained by optimal thresholding of the second eigenvector. It holds

$$\phi^* \;\leq\; \phi_{SPECTRAL} \;\leq\; 2\sqrt{\max_i d_i}\,\sqrt{\phi^*}$$

  There exist graphs which get close to upper bound.
- Better worst case guarantees for normalized/ratio cut for relaxation into a semi-definite program (Arora et al (2004)).
- Minimization of nonconvex relaxations based on nonlinear eigenproblems (H., Bühler, 2010, H., Setzer, 2011) yields much better cuts than standard spectral clustering in practice

Conclusion: The graph cuts picture is only a part of the story of spectral clustering.

Spectral Clustering - Variant II (recursive bipartitioning)

Chooose graph Laplacian and the number of clusters k.

- initialize: current paritition V.
- **do** build on each element of the current partition the graph Laplacian,

  1. compute the second eigenvector on each partition,
  2. compute the optimal threshold for dividing each partition,
  3. choose the cut which minimizes the total balanced cut criterion.

- **while** number of elements in the partition is less than k

Discussion:

- **Advantage:** uses original criterion to split - no k-means,
- **Disadvantage:** the embedding integrates global information about the data $\Longrightarrow$ problem if first split is not optimal.

Motivation II - Markov random walks on graphs

Markov random walk for an undirected, weighted graph:
stochastic matrix: $P = D^{-1}W$.
stationary distribution: $\pi_i = \frac{d_i}{\mathrm{vol}(V)}$.

Proposition (Meila, Shi)

Let G be connected. Let $X_0 \sim \pi$ be the random walk started in the stationary distribution and C be a subset of V. Then the normalized cut can be written as

$$\mathrm{NCut}(C, \overline{C}) = \Big[\mathrm{P}(X_1 \in \overline{C} \mid X_0 \in C) + \mathrm{P}(X_1 \in C \mid X_0 \in \overline{C})\Big].$$

Interpretation:
$\Longrightarrow$ find a partitioning such that the random walk stays as long as possible in each cluster.

Motivation III - Perturbation theory

Perfect clusters = disconnected graph

- multiplicity of the eigenvalue, $\lambda = 0$, of the graph Laplacians is equal to the number K of connected components of the graph.
- the K eigenvectors for $\lambda = 0$ are constant on the connected component and zero elsewhere.

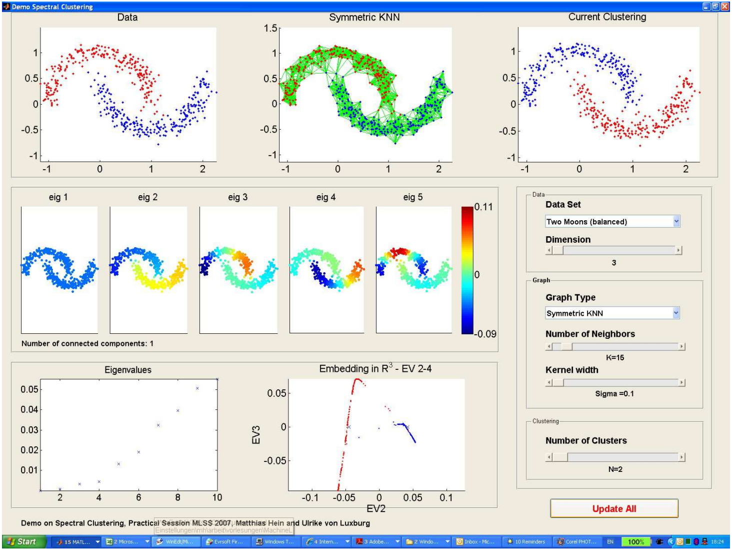
Perturbation of the weight matrix - make the graph connected

$$\tilde{W} = W + \text{ edges such that graph is connected.}$$

- only small change for the weight matrix,
  $\Longrightarrow$ first K eigenvalues should still be very small, $\Longrightarrow$ first K eigenvectors should be only very little perturbed
- each cluster is mapped to a single point (in the embedding).

$\Longrightarrow$ rigorous statements using perturbation theory of symmetric matrices.

DemoSpectralClustering:



Practical issues II

- For sparse graphs (k-NN graphs) the first few eigenvectors can be efficiently computed using the **power or Lanczos method** $\Rightarrow$ spectral clustering can be done for millions of points.
- Spectral Clustering used for image segmentation (Shi and Malik),
- Check the spectrum of the graph Laplacian. Never cut the spectrum where two eigenvalues are close. Always cut at a gap. This can also be formally justified by the stability of eigenvectors and eigenvalues under perturbations.
- Spectral clustering is quite stable against high-dimensional noise.
- Use the normalized graph Laplacian.