Unsupervised Learning cheatsheet

stanford.edu/~shervine/teaching/cs-229/cheatsheet-unsupervised-learning

Introduction to Unsupervised Learning

Motivation — The goal of unsupervised learning is to find hidden patterns in unlabeled data {x(1),...,x(m)}{x(1),...,x(m)}.

Jensen's inequality — Let ff be a convex function and XX a random variable. We have the following inequality:

E[f(X)]⩾f(E[X])E[f(X)]⩾f(E[X])

Clustering

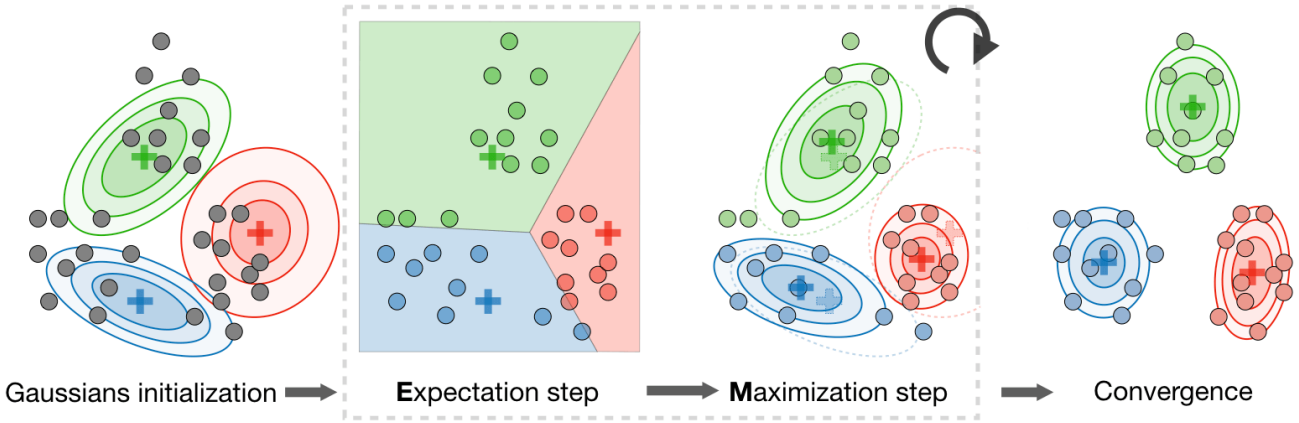
Expectation-Maximization

Latent variables — Latent variables are hidden/unobserved variables that make estimation problems difficult, and are often denoted zz. Here are the most common settings where there are latent variables:

Setting	Latent variable zz	x|zx|z	Comments
Mixture of kk Gaussians	Multinomial(ϕ)Multinomial(ϕ)	N(μj,Σj)N(μj,Σj)	μj∈Rn,ϕ∈Rkμj∈Rn,ϕ∈Rk
Factor analysis	N(0,I)N(0,I)	N(μ+Λz,ψ)N(μ+Λz,ψ)	μj∈Rnμj∈Rn

Algorithm — The Expectation-Maximization (EM) algorithm gives an efficient method at estimating the parameter θθ through maximum likelihood estimation by repeatedly constructing a lower-bound on the likelihood (E-step) and optimizing that lower bound (M-step) as follows:

- E-step: Evaluate the posterior probability Qi(z(i))Qi(z(i)) that each data point x(i)x(i) came from a particular cluster z(i)z(i) as follows:
  Qi(z(i))=P(z(i)|x(i);θ)Qi(z(i))=P(z(i)|x(i);θ)
- M-step: Use the posterior probabilities Qi(z(i))Qi(z(i)) as cluster specific weights on data points x(i)x(i) to separately re-estimate each cluster model as follows:
  θi=argmax θ∑i∫z(i)Qi(z(i))log(P(x(i),z(i);θ)Qi(z(i)))dz(i)θi=argmax θ∑i∫z(i)Qi(z(i))log(P(x(i),z(i);θ)Qi(z(i)))dz(i)

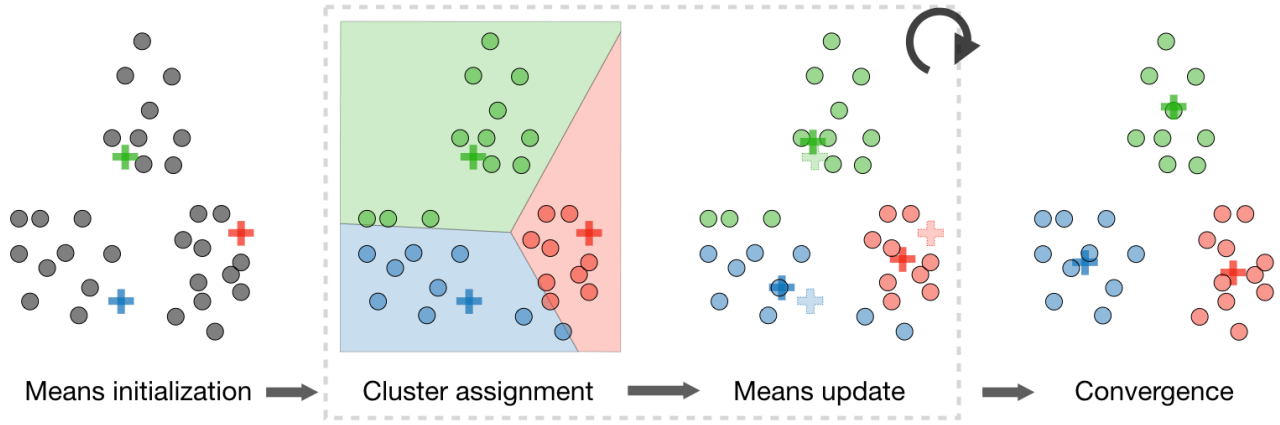


kk-means clustering

We note c(i)c(i) the cluster of data point ii and μjμj the center of cluster jj.

Algorithm — After randomly initializing the cluster centroids μ1,μ2,...,μk∈Rnμ1,μ2,...,μk∈Rn, the kk-means algorithm repeats the following step until convergence:

c(i)=arg minj||x(i)−μj||2andμj=m∑i=11{c(i)=j}x(i)m∑i=11{c(i)=j}c(i)=arg minj||x(i)−μj||2andμj=∑i=1m1{c(i)=j}x(i)∑i=1m1{c(i)=j}



Distortion function — In order to see if the algorithm converges, we look at the distortion function defined as follows:

J(c,μ)=m∑i=1||x(i)−μc(i)||2J(c,μ)=∑i=1m||x(i)−μc(i)||2

Hierarchical clustering

Algorithm — It is a clustering algorithm with an agglomerative hierarchical approach that build nested clusters in a successive manner.

Types — There are different sorts of hierarchical clustering algorithms that aims at optimizing different objective functions, which is summed up in the table below:

Ward linkage	Average linkage	Complete linkage
Minimize within cluster distance	Minimize average distance between cluster pairs	Minimize maximum distance of between cluster pairs

Clustering assessment metrics

In an unsupervised learning setting, it is often hard to assess the performance of a model since we don't have the ground truth labels as was the case in the supervised learning setting.

Silhouette coefficient — By noting aa and bb the mean distance between a sample and all other points in the same class, and between a sample and all other points in the next nearest cluster, the silhouette coefficient ss for a single sample is defined as follows:

s=b−amax(a,b)s=b−amax(a,b)

Calinski-Harabaz index — By noting kk the number of clusters, BkBk and WkWk the between and within-clustering dispersion matrices respectively defined as

$$B_k = \sum_{j=1}^{k} n_c(i)(\mu_c(i)-\mu)(\mu_c(i)-\mu)^T, \quad W_k = m\sum_{i=1}(x(i)-\mu_c(i))(x(i)-\mu_c(i))^T$$

the Calinski-Harabaz index $s(k)$ indicates how well a clustering model defines its clusters, such that the higher the score, the more dense and well separated the clusters are. It is defined as follows:

$$s(k) = \frac{Tr(B_k)}{Tr(W_k)} \times \frac{N-k}{k-1}$$

Dimension reduction

Principal component analysis

It is a dimension reduction technique that finds the variance maximizing directions onto which to project the data.

Eigenvalue, eigenvector — Given a matrix $A \in \mathbb{R}^{n \times n}$, λ is said to be an eigenvalue of A if there exists a vector $z \in \mathbb{R}^n \setminus \{0\}$, called eigenvector, such that we have:

$$Az = \lambda z$$

Spectral theorem — Let $A \in \mathbb{R}^{n \times n}$. If A is symmetric, then A is diagonalizable by a real orthogonal matrix $U \in \mathbb{R}^{n \times n}$. By noting $\Lambda = diag(\lambda_1, ..., \lambda_n)$, we have:

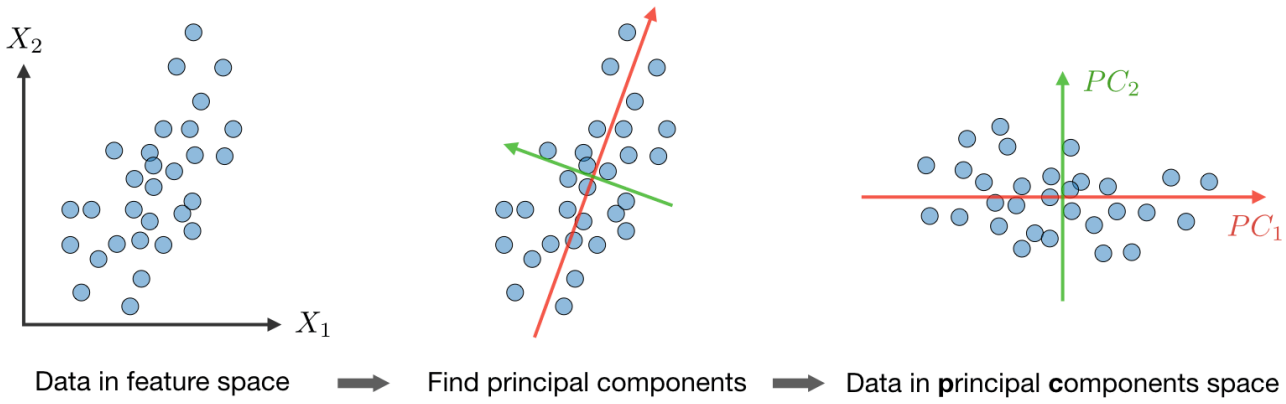
$$\exists \Lambda \text{ diagonal}, A = U\Lambda U^T$$

Remark: the eigenvector associated with the largest eigenvalue is called principal eigenvector of matrix A.

Algorithm — The Principal Component Analysis (PCA) procedure is a dimension reduction technique that projects the data on k dimensions by maximizing the variance of the data as follows:

- Step 1: Normalize the data to have a mean of 0 and standard deviation of 1.
$$x(i)_j \leftarrow \frac{x(i)_j - \mu_j}{\sigma_j} \text{ where } \mu_j = \frac{1}{m}\sum_{i=1} x(i)_j \text{ and } \sigma_j^2 = \frac{1}{m}\sum_{i=1}(x(i)_j - \mu_j)^2$$
$$x_j(i) \leftarrow \frac{x_j(i) - \mu_j}{\sigma_j} \text{ where } \mu_j = \frac{1}{m}\sum_{i=1} x_j(i) \text{ and } \sigma_j^2 = \frac{1}{m}\sum_{i=1}(x_j(i) - \mu_j)^2$$
- Step 2: Compute $\Sigma = \frac{1}{m}\sum_{i=1} x(i)x(i)^T \in \mathbb{R}^{n \times n}$, which is symmetric with real eigenvalues.
- Step 3: Compute $u_1, ..., u_k \in \mathbb{R}^n$ the k orthogonal principal eigenvectors of Σ, i.e. the orthogonal eigenvectors of the k largest eigenvalues.
- Step 4: Project the data on $span_{\mathbb{R}}(u_1, ..., u_k)$.

This procedure maximizes the variance among all k-dimensional spaces.



Independent component analysis

It is a technique meant to find the underlying generating sources.

Assumptions — We assume that our data x has been generated by the n-dimensional source vector $s=(s_1,\dots,s_n)$, where s_i are independent random variables, via a mixing and non-singular matrix A as follows:

$$x=As$$

The goal is to find the unmixing matrix $W=A^{-1}$.

Bell and Sejnowski ICA algorithm — This algorithm finds the unmixing matrix W by following the steps below:

- Write the probability of $x=As=W^{-1}s$ as:
  $$p(x)=\prod_{i=1}^{n} p_s(w_i^T x)\cdot |W|$$
- Write the log likelihood given our training data $\{x^{(i)}, i\in[[1,m]]\}$ and by noting g the sigmoid function as:
  $$l(W)=\sum_{i=1}^{m}\left(\sum_{j=1}^{n}\log(g'(w_j^T x^{(i)}))+\log|W|\right)$$

Therefore, the stochastic gradient ascent learning rule is such that for each training example $x^{(i)}$, we update W as follows:

$$W \longleftarrow W+\alpha\begin{pmatrix}1-2g(w_1^T x^{(i)})\\ 1-2g(w_2^T x^{(i)})\\ \vdots\\ 1-2g(w_n^T x^{(i)})\end{pmatrix} x^{(i)T}+(W^T)^{-1}$$