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# (https://stanford.edu/~shervine/teaching/cs-229/cheatsheet-unsupervised-learning#cheatsheet)Unsupervised Learning cheatsheet



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## (https://stanford.edu/~shervine/teaching/cs-229/cheatsheet-unsupervised-learning#intro) Introduction to Unsupervised Learning

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

❒ **Jensen's inequality** — Let $f$ be a convex function and $X$ a random variable. We have the following inequality:

$$\boxed{E[f(X)] \geqslant f(E[X])}$$

[https://stanford.edu/~shervine/teaching/cs-229/cheatsheet-unsupervised-learning#clustering)

# Clustering

## Expectation-Maximization

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

| Setting | Latent variable $z$ | $x|z$ | Comments |
|---|---|---|---|
| Mixture of $k$ Gaussians | $\text{Multinomial}(\phi)$ | $\mathcal{N}(\mu_j, \Sigma_j)$ | $\mu_j \in \mathbb{R}^n, \phi \in \mathbb{R}^k$ |
| Factor analysis | $\mathcal{N}(0, I)$ | $\mathcal{N}(\mu + \Lambda z, \psi)$ | $\mu_j \in \mathbb{R}^n$ |

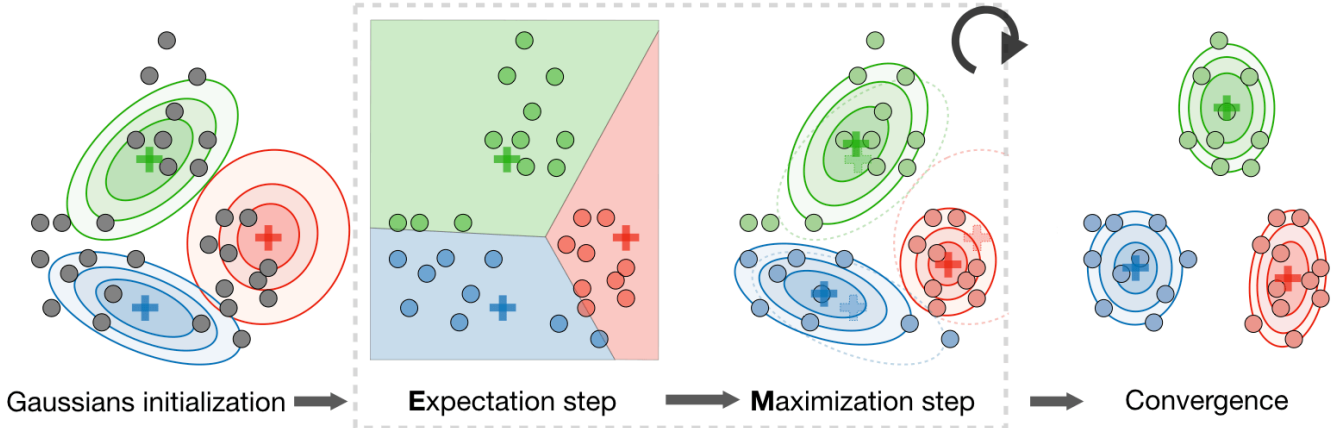
❒ **Algorithm** — The Expectation-Maximization (EM) algorithm gives an efficient method at estimating the parameter $\theta$ through maximum likelihood estimation by repeatedly constructing a lower-bound on the likelihood (E-step) and optimizing that lower bound (M-step) as follows:

- E-step: Evaluate the posterior probability $Q_i(z^{(i)})$ that each data point $x^{(i)}$ came from a particular cluster $z^{(i)}$ as follows:

$$\boxed{Q_i(z^{(i)}) = P(z^{(i)}|x^{(i)};\theta)}$$

- M-step: Use the posterior probabilities $Q_i(z^{(i)})$ as cluster specific weights on data points $x^{(i)}$ to separately re-estimate each cluster model as follows:

$$\boxed{\theta_i = \underset{\theta}{\text{argmax}} \sum_i \int_{z^{(i)}} Q_i(z^{(i)}) \log\left(\frac{P(x^{(i)}, z^{(i)};\theta)}{Q_i(z^{(i)})}\right) dz^{(i)}}$$

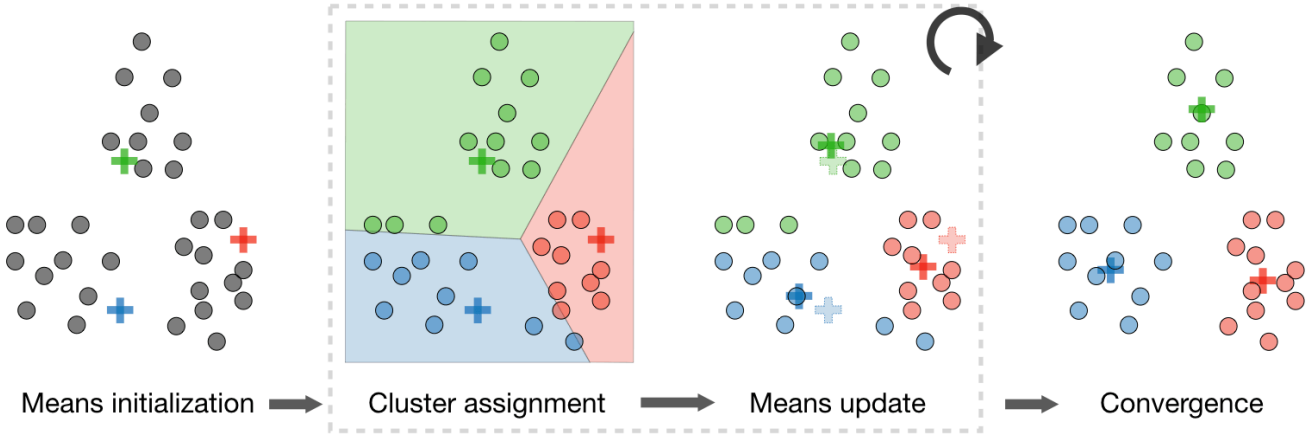


## $k$-means clustering

We note $c^{(i)}$ the cluster of data point $i$ and $\mu_j$ the center of cluster $j$.

❒ **Algorithm** — After randomly initializing the cluster centroids $\mu_1, \mu_2, ..., \mu_k \in \mathbb{R}^n$, the $k$-means algorithm repeats the following step until convergence:

$$\boxed{c^{(i)} = \arg\min_j ||x^{(i)} - \mu_j||^2} \quad \text{and} \quad \boxed{\mu_j = \frac{\sum_{i=1}^{m} 1_{\{c^{(i)}=j\}} x^{(i)}}{\sum_{i=1}^{m} 1_{\{c^{(i)}=j\}}}}$$




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

$$\boxed{J(c, \mu) = \sum_{i=1}^{m} ||x^{(i)} - \mu_{c^{(i)}}||^2}$$

## 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 $a$ and $b$ 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 $s$ for a single sample is defined as follows:

$$\boxed{s = \frac{b-a}{\max(a,b)}}$$

❒ **Calinski-Harabaz index** — By noting $k$ the number of clusters, $B_k$ and $W_k$ the between and within-clustering dispersion matrices respectively defined as

$$B_k = \sum_{j=1}^{k} n_{c^{(i)}} (\mu_{c^{(i)}} - \mu)(\mu_{c^{(i)}} - \mu)^T, \qquad W_k = \sum_{i=1}^{m} (x^{(i)} - \mu_{c^{(i)}})(x^{(i)} - \mu_{c^{(i)}})^T$$

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:

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

## [https://stanford.edu/~shervine/teaching/cs-229/cheatsheet-unsupervised-learning#dimension-reduction) 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 $A \in \mathbb{R}^{n \times n}$, $\lambda$ is said to be an eigenvalue of $A$ if there exists a vector $z \in \mathbb{R}^n \backslash \{0\}$, called eigenvector, such that we have:

$$\boxed{Az = \lambda z}$$

❒ **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 $\Lambda = \text{diag}(\lambda_1, ..., \lambda_n)$, we have:

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

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

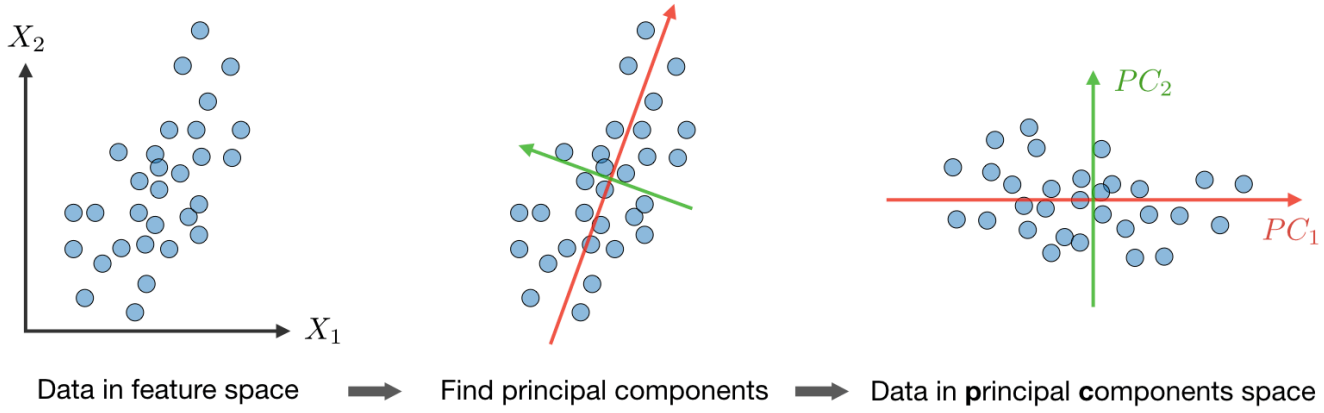
❒ **Algorithm** — The Principal Component Analysis (PCA) procedure is a dimension reduction technique that projects the data on $k$ dimensions by maximizing the variance of the data as follows:

- Step 1: Normalize the data to have a mean of 0 and standard deviation of 1.

$$\boxed{x_j^{(i)} \leftarrow \frac{x_j^{(i)} - \mu_j}{\sigma_j}} \quad \text{where} \quad \boxed{\mu_j = \frac{1}{m} \sum_{i=1}^m x_j^{(i)}} \quad \text{and} \quad \boxed{\sigma_j^2 = \frac{1}{m} \sum_{i=1}^m (x_j^{(i)} - \mu_j)^2}$$

- Step 2: Compute $\Sigma = \frac{1}{m} \sum_{i=1}^m x^{(i)} x^{(i)^T} \in \mathbb{R}^{n \times n}$, which is symmetric with real eigenvalues.
- Step 3: Compute $u_1, ..., u_k \in \mathbb{R}^n$ the $k$ orthogonal principal eigenvectors of $\Sigma$, i.e. the orthogonal eigenvectors of the $k$ largest eigenvalues.
- Step 4: Project the data on $\text{span}_{\mathbb{R}}(u_1, ..., u_k)$.

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 $s = (s_1, ..., s_n)$, where $s_i$ are independent random variables, via a mixing and non-singular matrix $A$ as follows:

$$\boxed{x = As}$$

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:

$$l(W) = \sum_{i=1}^{m} \left( \sum_{j=1}^{n} \log \left( g'(w_j^T x^{(i)}) \right) + \log |W| \right)$$

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

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