VIP Cheatsheet: Unsupervised Learning

Afshine Amidi and Shervine Amidi

August 5, 2018

Introduction to Unsupervised Learning

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

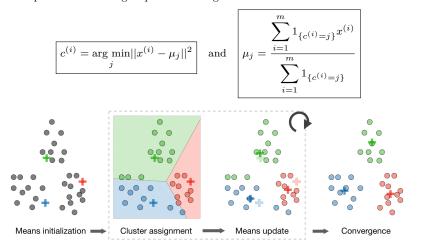
 \Box Jensen's inequality – Let f be a convex function and X a random variable. We have the following inequality:

$$E[f(X)] \geqslant f(E[X])$$

k-means clustering

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

 \square 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:



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

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

Expectation-Maximization

 \Box 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	$\operatorname{Multinomial}(\phi)$	$\mathcal{N}(\mu_j, \Sigma_j)$	$\mu_j \in \mathbb{R}^n, \phi \in \mathbb{R}^k$
Factor analysis	$\mathcal{N}(0,I)$	$\mathcal{N}(\mu + \Lambda z, \psi)$	$\mu_j \in \mathbb{R}^n$

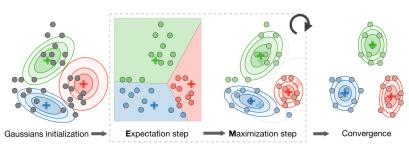
 \square Algorithm – The Expectation-Maximization (EM) algorithm gives an efficient method at estimating the parameter θ through maximum likelihood estimation by repeatedly constructing a lower-bound on the likelihood (E-step) and optimizing that lower bound (M-step) as follows:

• 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:

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

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

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



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

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

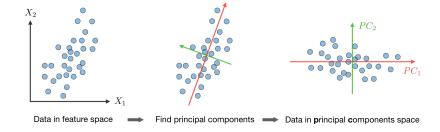
Remark: the eigenvector associated with the largest eigenvalue is called principal eigenvector of matrix A.

 \square 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.

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

- 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 Σ , i.e. the orthogonal eigenvectors of the k largest eigenvalues.
- Step 4: Project the data on $\operatorname{span}_{\mathbb{R}}(u_1,...,u_k)$. 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:

$$x = As$$

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