# Discussion about $k$-Means and $1D$ Random Projections

Guilherme França

## I. PROCEDURE

Given data $X = \{x_i\}_{i=1}^n$, where $x_i \in \mathbb{R}^D$, and the number of clusters $k$, we perform the following experiments:

1. Run $k$-means++ on the original data space. This is the column named "$k$-means" in the following tables.

2. Use PCA to project the data in the first principal component, $Y = \{y_i\}_{i=1}^n$ where $y_i = u_1 \cdot x_i \in \mathbb{R}$, then apply $k$-means in this 1-dimensional space. This is the column named "PCA" in the following tables.

3. We randomly project the data in one dimension by picking a vector $w$ such that $w_i \sim \mathcal{N}(0,1)$ and normalize it $\|w\| = 1$. Thus $Y = \{y_i\}_{i=1}^n$ where $y_i = w \cdot x_i \in \mathbb{R}$. We apply $k$-means in this randomly projected 1-dimensional space. We do this several times and pick the best answer. This is the column named "Random" in the fllowing tables.

The evaluation of the clustering procedure will be based on the true labels by the following quantity, called accuracy:

$$a(z, \hat{z}) = \frac{1}{n} \sum_{i=1}^{n} \mathbb{1}\left(z_i = \pi(\hat{z}_i)\right) \tag{1}$$

where $z$ is an $n$-dimensional vector containing the true labels, entry $z_i$ corresponds to point $x_i$, and $\hat{z}$ is the estimated labels through the clustering procedure. $\pi$ is a permutation of the labels. Thus the above formula gives 1 if all points were correctly classified and 0 if all points were wrongly classified. In a two class problem with the same number of points, $a = 1/2$ corresponds to picking the points in each cluster at random. This quantity $a$ is the number shown in the following tables.

*How to choose the best answer for random projections?* Consider $k$-means objective function

$$J(X) = \frac{1}{2} \sum_{j=1}^{k} \sum_{x \in \mathcal{C}_j} \|x - m_j\|^2, \qquad m_j = \frac{1}{n_j} \sum_{x \in \mathcal{C}_j} x. \tag{2}$$

Above $m_j$ is the center of cluster $\mathcal{C}_j$, and $n_j$ is the number of elements in cluster $\mathcal{C}_j$. $k$-means algorithm solves the problem $\min_{\{C_j\}} J(X)$.

One might think that a good criteria to choose the best answer is to pick the minimum $J(Y)$ computed in the $1D$ randomly projected space. This doesn't work because each

random projection gives different values for the data $Y$ which in general does not preserve the structure in the original distribution. For instance, considering two random projections yielding $Y_1$ and $Y_2$. It can happen that the clustering on $Y_2$ gives a better accuracy than the clustering on $Y_1$ and even though $J(Y_1) < J(Y_2)$. So we are really comparing apples and bananas here.

Another approach would be to cluster on $Y$ yielding labels $\hat{z}$, then compute $J(X)$ based on these labels, and pick the smallest $J(X)$ computed on the original data. This only works in case where $k$-means in the original space itself provides a good answer. For cases where $k$-means is problematic, e.g. the data are not spherical gaussians, then $J(X)$ itself is not a good function to detect the clustering. This happens for parallel cigars in the example below.

Thus if one still desires to follow this approach, a good function which does not depend on the true labels must be chosen. I tried to use the energy function for this, and still didn't quite work. Also, observe that the energy function on the original space is expensive to compute, $O(n^2)$.

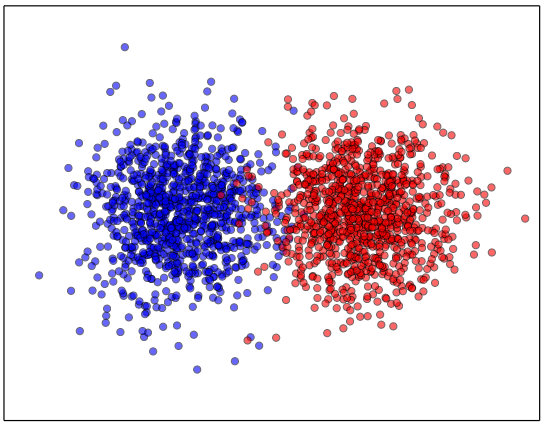
In the following experiments I will *cheat* and use (1) to pick the best answer. The purpose of this is to see if the "truth" can be captured by random projections.

## II. EXPERIMENTS

In the first experiment shown in Fig. 1 we choose two well separated gaussians in $2D$. All of these procedures give good results.

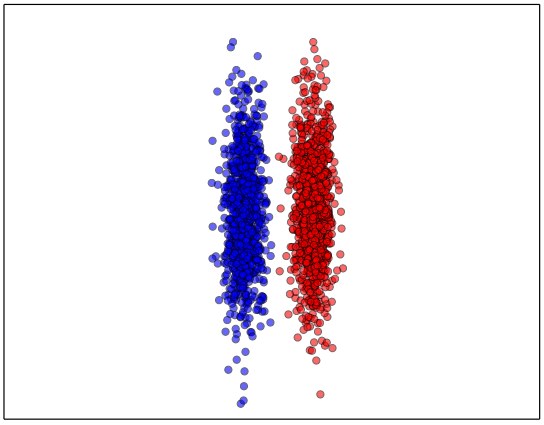
In the experiment of Fig. 2, still in $2D$, we choose parallel cigars. Both $k$-means and PCA cannot perform well, however random projections can do well. This is not surprising because this data can be linearly separable in $1D$. After many tries random projections will find the correct line. Probably, LDA can perform as well on this example.

In the experiment of Fig. 3 we increase the number of dimensions of the gaussian distributions. Both $k$-means and PCA perform well if the dimension is not too high, while $1D$ random projections provide poor results. This is also expected since randomly projecting high dimensional data in a very low dimensional space practically destroy any information about the original distribution.



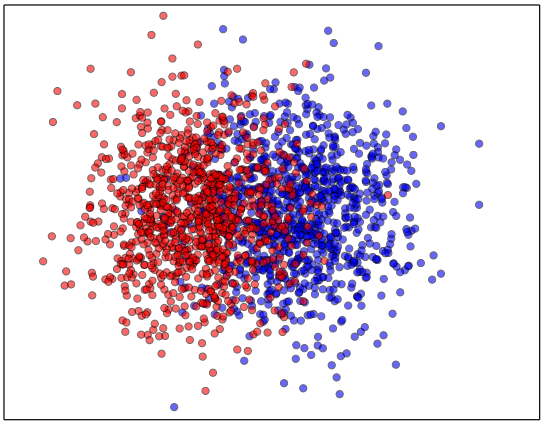
| $k$-means | PCA | Random |
|---|---|---|
| 0.9735 | 0.9735 | 0.9755 |
| 0.978 | 0.978 | 0.979 |
| 0.977 | 0.9775 | 0.978 |

FIG. 1. We have $x \sim \frac{1}{2}\left(\mathcal{N}(\mu_1, I) + \mathcal{N}(\mu_2, I)\right)$ where $\mu_1 = (0,0)^T$ and $\mu_2 = (4,0)^T$, and 1000 points on each cluster. We run the experiment three times.



| $k$-means | PCA | Random |
|---|---|---|
| 0.501 | 0.5075 | 0.9995 |
| 0.522 | 0.515 | 1.0 |
| 0.505 | 0.5055 | 0.9995 |

FIG. 2. We have $x \sim \frac{1}{2}\left(\mathcal{N}(\mu_1, \Sigma) + \mathcal{N}(\mu_2, \Sigma)\right)$ where $\mu_1 = (0,0)^T$, $\mu_2 = (5,0)^T$, and $\Sigma = \begin{pmatrix} 1/2 & 0 \\ 0 & 15 \end{pmatrix}$, and 1000 points on each cluster. We run the experiment three times.



| $D$ | $k$-means | PCA | Random |
|---|---|---|---|
| 5 | 0.84 | 0.8415 | 0.841 |
| 10 | 0.844 | 0.846 | 0.7985 |
| 15 | 0.8325 | 0.8365 | 0.7465 |
| 20 | 0.846 | 0.85 | 0.764 |
| 25 | 0.8555 | 0.8505 | 0.714 |
| 30 | 0.825 | 0.8225 | 0.728 |
| 50 | 0.8485 | 0.8465 | 0.6775 |
| 100 | 0.832 | 0.8325 | 0.644 |
| 200 | 0.8085 | 0.8145 | 0.592 |
| 300 | 0.7645 | 0.794 | 0.5755 |
| 500 | 0.6915 | 0.756 | 0.5615 |
| 1000 | 0.5075 | 0.6965 | 0.562 |
| 2000 | 0.5495 | 0.662 | 0.543 |
| 5000 | 0.531 | 0.5135 | 0.539 |

FIG. 3. High dimensions. We have $x \sim \frac{1}{2}\left(\mathcal{N}(\mu_1, I_D) + \mathcal{N}(\mu_2, I_D)\right)$ where $\mu_1 = (0, 0, \ldots, 0)^T$, $\mu_2 = (1, 0, \ldots, 0)^T$, and 1000 points on each cluster. We show the two principal components of the data in the plot above.