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

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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. 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 "k-random" in the following tables. We will choose 100 random projections.

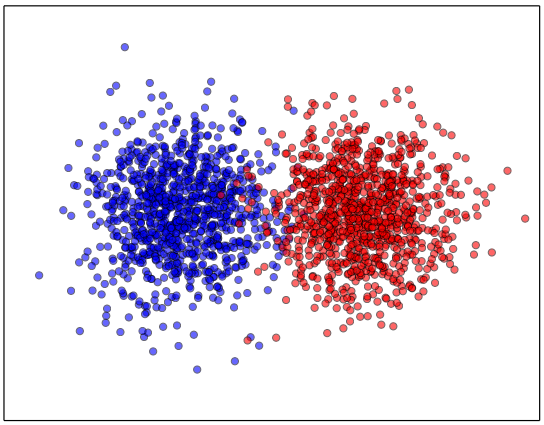
4. We use random projections as in the previous item, but use the T-test from energy statistics. In $1D$ we can compute the energy distance in an efficient manner if we sort the data Y. This is the column called "$\mathcal{E}$-random" in the following tables. We will choose 100 random projections.

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. π is a permutation of the labels. Thus the above formula gives $a = 1$ if all points were correctly classified and $a = 0$ 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? In the following experiments we are going to cheat and pick the best answer according to the highest value of (1). This is



k-means	PCA	k-random	$\mathcal{E}$-random
0.9735	0.9735	0.9745	0.976
0.9745	0.975	0.976	0.975
0.973	0.9735	0.976	0.976

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.

cheating because we are using the true labels, however, this test allows us to easily check if the "truth" can be captured by these procedures involving random projections. If the results are poor in this way, no matter what criteria we choose, optimizing $\mathcal{E}$ or any other function will also not work.

Note: The procedures involving random projections are much slower than simple k-means in the original data. It is also much slower than PCA+k-means. Moreover, computing random projections in high dimensions is also a little expensive. Doing this many times can make the algorithm really slow.

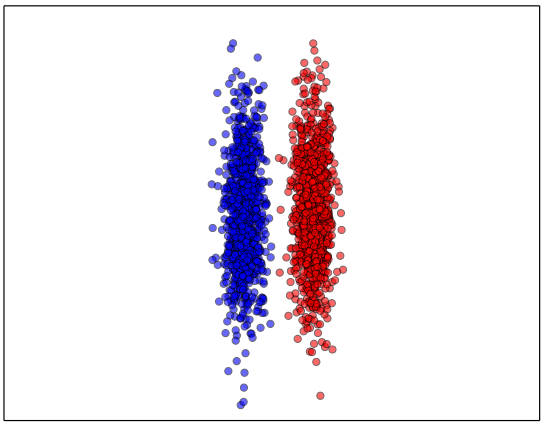
II. FIRST EXPERIMENTS

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.

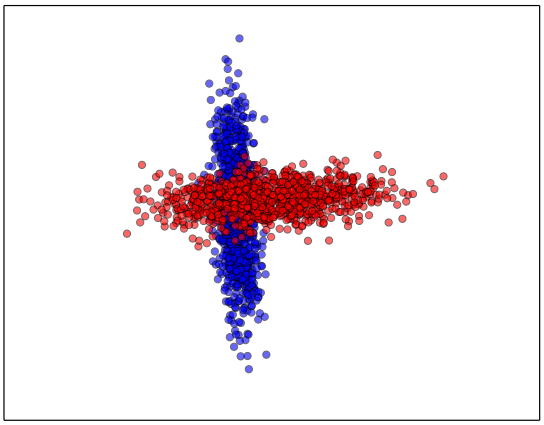
In the experiment of Fig. 3 notice that the k-means with random projections performs better than any other method.

In the experiment of Fig. 4 we increase the number of dimensions of the gaussian distri-



k-means	PCA	k-random	$\mathcal{E}$-random
0.5085	0.5025	1.0	1.0
0.5025	0.5035	1.0	1.0
0.503	0.5	1.0	1.0

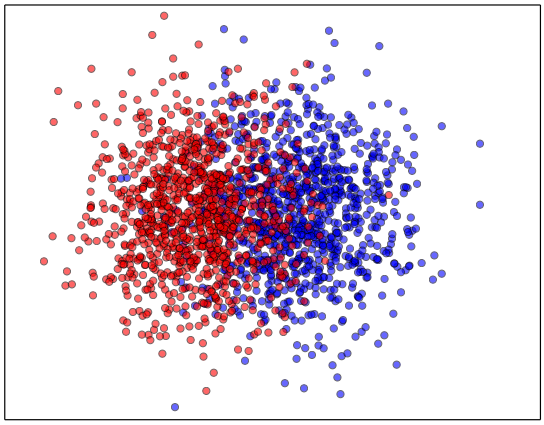
FIG. 2. We have $x \sim \frac{1}{2}\left(\mathcal{N}(\mu_1, \Sigma) + \mathcal{N}(\mu_2, \Sigma)\right)$ where $\mu_1 = (0,0)^T$, $\mu_2 = (5,0)^T$, and $\Sigma = \begin{pmatrix} 1/2 & 0 \\ 0 & 15 \end{pmatrix}$, and 1000 points on each cluster. We run the experiment three times.



k-means	PCA	k-random	$\mathcal{E}$-random
0.6315	0.6295	0.7235	0.66
0.725	0.7065	0.726	0.678
0.6405	0.6465	0.724	0.679

FIG. 3. We have $x \sim \frac{1}{2}\left(\mathcal{N}(\mu_1, \Sigma_1) + \mathcal{N}(\mu_2, \Sigma_2)\right)$ where $\mu_1 = (0,0)^T$, $\mu_2 = (2,1)^T$, $\Sigma_1 = \begin{pmatrix} 0.5 & -0.8 \\ -0.8 & 15 \end{pmatrix}$, $\Sigma_2 = \begin{pmatrix} 15 & 1 \\ 1 & 1 \end{pmatrix}$, and 1000 points on each cluster. We run the experiment three times.

butions. 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.



D	k-means	PCA	k-random	$\mathcal{E}$-random
5	0.934500	0.934500	0.919000	0.924000
10	0.939500	0.941500	0.912000	0.856000
15	0.933000	0.935000	0.882000	0.816000
20	0.940000	0.942000	0.762000	0.817000
25	0.931500	0.933500	0.767000	0.759000
30	0.936000	0.934000	0.754000	0.725000
50	0.946000	0.942500	0.718500	0.741000
100	0.926500	0.927000	0.658500	0.647000
200	0.940000	0.940000	0.604000	0.647000
300	0.918000	0.921500	0.592500	0.602000
500	0.915000	0.922000	0.596500	0.576000
1000	0.874000	0.890500	0.552000	0.574000
2000	0.597000	0.863500	0.542000	0.554000
5000	0.509000	0.788000	0.543000	0.540000

FIG. 4. High dimensions. We have $x \sim \frac{1}{2}\left(\mathcal{N}(\mu_1, I_D) + \mathcal{N}(\mu_2, I_D)\right)$ where $\mu_1 = (0, 0, \ldots, 0)^T$, $\mu_2 = (3, 0, \ldots, 0)^T$, and 1000 points on each cluster. We show the two principal components of the data in the plot above.

III. SECOND EXPERIMENTS

We repeated the experiments above using the objective function as a criteria instead of the accuracy (1) so we do not use the true labels. We computed the objective function in the $1D$ projected space.

For k-means the function is the sum of squared distances from the points to the centers of the clusters, and for energy statistics we compute the "energy" $\mathcal{E}$ in the $1D$ space, which can be done in $O(n \log n)$. The results are just slightly worse than before because not always the optimal function coincides with the best clustering. Notice that we are comparing these functions on different data sets, one for each projection. Thus this is not a very consistent way of doing the test.

IV. CONCLUSIONS

These are just my thoughts about why random projections in $1D$ does not work for *clustering*—it surely must work with random projections in higher dimensions though, since we have Johnson-Lindenstrauss lemma that guarantees that distances are preserved in lower dimensional spaces, but they are not so low-dimensional—regardless of the function you are trying to optimize, e.g. k-means objective function, energy statistics, whatever, etc.

In $1D$, random projections just seems to me a more expensive way of doing LDA. In $1D$ the best line which separates the data (I believe) is the line passing through the means of each cluster (I'm thinking about two clusters only). If data is not linearly separable in $1D$, neither of both methods work.

Although $\mathcal{E}$ seems a nice function, which can distinguish different distributions in a non-parametric way, random projections in general destroy a lot of information from the original distribution. Therefore, it does not matter which function you try to optimize, the information was already lost. Moreover, projecting data in $1D$ clumps data together, which is the opposite of separating the data, which can be achieved only in higher dimensions.

Also, $1D$ random projections are not necessarily cheap. Suppose we have n points in D dimensions, k clusters, and we compute p random projections. The cost of each $1D$ random projection is $O(dn)$. Suppose the cost of optimizing the function is $O(n)$ (which is the best possible scenario). The total cost would be $O(pDn)$ in the best possible case. Roughly, k-means on the original data can be $O(kDn)$. Since $p \gg k$ usually random projections may be more expensive than pure k-means. In our experiment this was always the case.

One may think about this criteria as an initialization procedure. I still believe this is not so good (hope to be wrong though). I think a way better proposal would be the following. Suppose we have N data points in D-dimensions where both can be really large, so k-means++ initialization is not feasible. Then sample $M \lll N$ points uniformly. Now do a few random projections in $O(\log(M/\epsilon^2)$ dimensions, thus obeying the Johnson-Lindenstrauss lemma which assures that in this case we preserve distances in the original space. Now apply initialization procedure in this reduced number of points and in lower dimensions. Also, applying the whole clustering procedure in this new data set should give a descent estimate for clustering in the entire data set.