Notes about Statistics, Clustering, Graphs, . . .

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Abstract

In this document we collect notes about our experiments and theories for discussion.

I. EXPERIMENTS USING ENERGY STATISTICS AND ONE-DIMENSIONAL RANDOM PROJECTIONS

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.

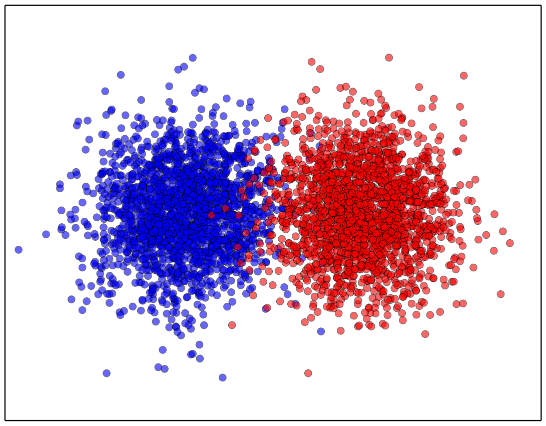
3. We randomly project the data in one dimension by picking a vector w such that $w_i \sim \mathcal{N}(0, 1)$ and normalize it $\|w\| = 1$. Thus $Y = \{y_i\}_{i=1}^n$ where $y_i = w \cdot x_i \in \mathbb{R}$. We apply k-means++ in this randomly projected 1-dimensional space. We do this several times and pick the best answer,i.e. the one which has minumim objective function in the *original* space, since it is cheap to compute this objective function. This is the column named "k-random" in the following tables.

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 accomplished in $O(n \log n)$. This is the column called "$\mathcal{E}$-random" in the following tables. We pick the best answer by computing the largest T, in the one-dimensional space.

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

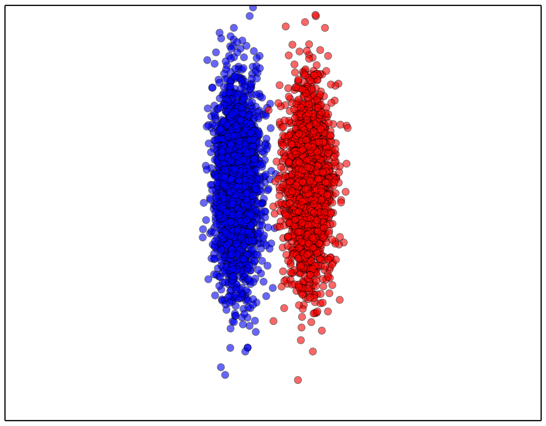
$$a(z, \hat{z}) = \frac{1}{n} \sum_{i=1}^{n} \mathbb{1}\left(z_i = \pi(\hat{z}_i)\right) \tag{1}$$

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.



k-means	PCA	k-random	$\mathcal{E}$-random
0.97775	0.97825	0.79925	0.977
0.975	0.975	0.7305	0.976
0.9765	0.9765	0.9655	0.9605

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. We choose only 20 random projections.

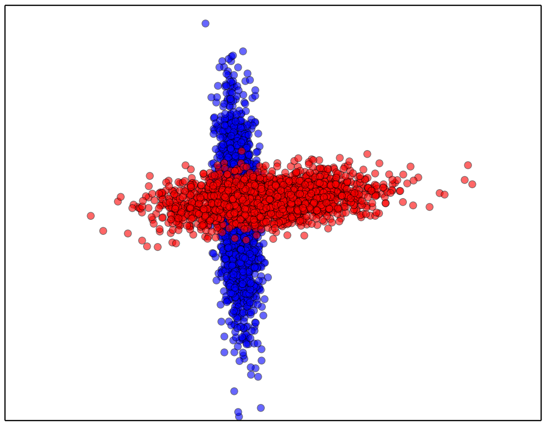


k-means	PCA	k-random	$\mathcal{E}$-random
0.51325	0.506	0.70325	0.977
0.52175	0.5105	0.54725	0.7295
0.53325	0.53175	0.9785	0.998

FIG. 2. We have $x \sim \frac{1}{2}\left(\mathcal{N}(\mu_1, \Sigma) + \mathcal{N}(\mu_2, \Sigma)\right)$ where $\mu_1 = (0,0)^T$, $\mu_2 = (6,0)^T$, and $\Sigma = \left(\begin{smallmatrix} 1 & 0 \\ 0 & 20 \end{smallmatrix}\right)$, and 2000 points on each cluster. We run the experiment three times. We use 30 random projections.

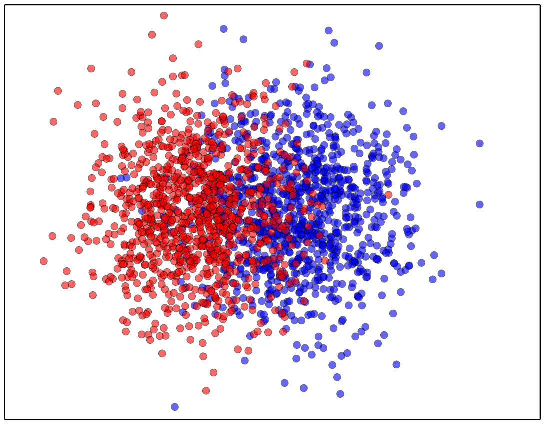
In the first experiment shown in Fig. 1 we choose two well separated gaussians in $2D$. All of these procedures give good results.

In the experiment of Fig. 5 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	k-random	$\mathcal{E}$-random
0.71275	0.68675	0.51275	0.6505
0.7235	0.6645	0.6095	0.641
0.72575	0.68475	0.60975	0.509

FIG. 3. We have $x \sim \frac{1}{2}\left(\mathcal{N}(\mu_1,\Sigma_1)+\mathcal{N}(\mu_2,\Sigma_2)\right)$ where $\mu_1=(0,0)^T$, $\mu_2=(2,1)^T$, $\Sigma_1=\left(\begin{smallmatrix}0.5 & -0.8\\ -0.8 & 15\end{smallmatrix}\right)$, $\Sigma_2=\left(\begin{smallmatrix}15 & 1\\ 1 & 1\end{smallmatrix}\right)$, and 2000 points on each cluster. We run the experiment three times, with 30 random projections.

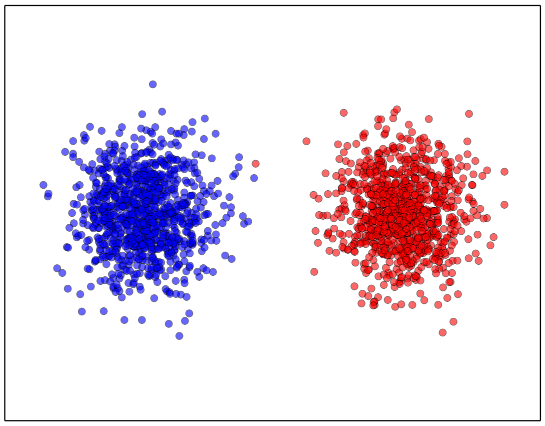


D	k-means	PCA	k-random	$\mathcal{E}$-random
5	0.928000	0.928000	0.689500	0.859000
10	0.935500	0.935500	0.551000	0.890000
15	0.929000	0.930000	0.580500	0.839000
20	0.938000	0.940000	0.647000	0.741000
25	0.937500	0.936500	0.576500	0.801000
30	0.939000	0.938500	0.545000	0.565000
50	0.933500	0.930000	0.505500	0.701000
100	0.928500	0.932000	0.624500	0.565000
200	0.935000	0.935000	0.502000	0.528000
300	0.922500	0.924500	0.508500	0.527000
500	0.916500	0.923500	0.509000	0.513000
1000	0.881000	0.889500	0.503000	0.501000
2000	0.615000	0.867000	0.509500	0.505000
5000	0.534500	0.780000	0.514000	0.511000

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 $\mu_1=(0,0,\dots,0)^T$, $\mu_2=(3,0,\dots,0)^T$, and 1000 points on each cluster. We do 100 random projections. We show the two principal components of the data in the plot above.

A. Conclusions

If we have enough signal, even in high dimensions random projections with energy statistics seems like a good thing. I believe that at least for a initialization procedure this can be usefull. It will be interesting to have a benchmark of how many random projections



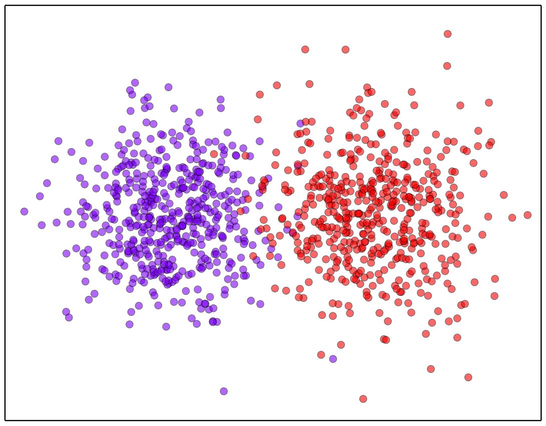
D	k-means	PCA	k-random	$\mathcal{E}$-random
5	0.963000	0.963000	0.615000	0.921000
10	0.985500	0.985000	0.758000	0.957000
15	0.998000	0.998000	0.537500	0.919000
20	0.998500	0.998500	0.505500	0.889000
25	1.000000	1.000000	0.530000	0.968000
30	1.000000	1.000000	0.733500	0.978000
50	1.000000	1.000000	0.640000	0.957000
100	1.000000	1.000000	0.887500	0.972000
200	1.000000	1.000000	0.708500	0.964000
300	1.000000	1.000000	0.549000	0.967000
500	1.000000	1.000000	0.653000	0.968000
1000	1.000000	1.000000	0.604500	0.983000
2000	1.000000	1.000000	0.535000	0.967000
5000	1.000000	1.000000	0.727500	0.949000

FIG. 5. High dimensions. We have $x \sim \frac{1}{2}\left(\mathcal{N}(\mu_1, I_D) + \mathcal{N}(\mu_2, I_D)\right)$ where $\mu_1 = (1, 0, 1, \dots, 0, 1)^T$, $\mu_2 = (-1, 0, -1, \dots, 0, -1)^T$, i.e. the even dimensions are shifted at $+1$ and -1, respectivelly. We have 1000 points on each cluster. We do 100 random projections. We show the two principal components of the data in the plot above. When we have more signal we can see that random projections with $\mathcal{E}$ is much superior to random projections and k-means++.

we need. Too many is expensive, however, if this is an initialization procedure, it will be required only once. Maybe we can compare just $\mathcal{E}$-random with the initialization provided by k-means++.

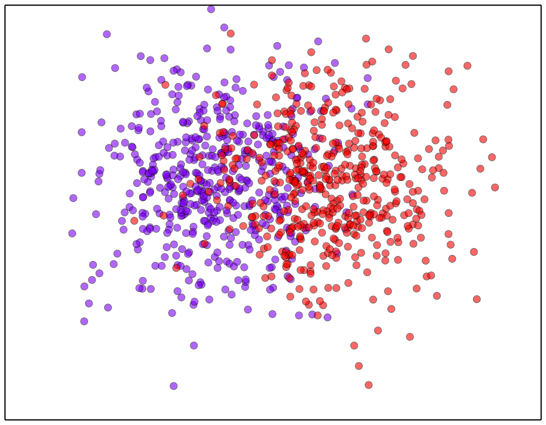
II. ENERGY STATISTICS BASED CLUSTERING

We show some experiments regarding our method for clustering using energy statistics. We have a QCQP approximation to the original problem, and we solve this QCQP through a relaxation, thus there are two approximations going on here. We solve this through a kernel approach. The function has a maximum, but it is really sensitive to initialization, since apparently there are lots of local minima. We use energy statistics in $1D$ with random projections for initialization. This seems to provide a better initialization than pure random or even k-means.



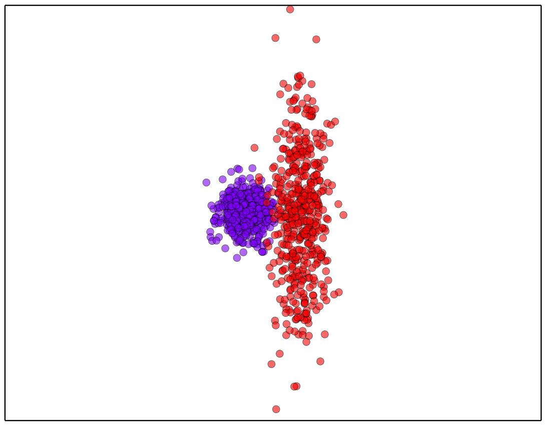
Ker/$\mathcal{E}$	Ker/Gauss	Ker/Poly	GMM	k-means
0.97	0.965	0.863	0.969	0.971
0.98	0.98	0.878	0.982	0.98
0.982	0.982	0.877	0.983	0.983

FIG. 6. We have $x \sim \frac{1}{2}\left(\mathcal{N}(\mu_1, \Sigma_1) + \mathcal{N}(\mu_2, \Sigma_2)\right)$ where $\mu_1 = (0,0)^T$, $\mu_2 = (4,0)^T$, $\Sigma_1 = \Sigma_2 = I$, and 500 points on each cluster. We run the experiment three times, with 20 random projections as initialization.



Ker/$\mathcal{E}$	Ker/Gauss	Ker/Poly	GMM	k-means
0.844	0.829	0.688	0.841	0.843
0.834	0.836	0.695	0.835	0.834
0.843	0.813	0.68	0.805	0.841

FIG. 7. We have $x \sim \frac{1}{2}\left(\mathcal{N}(\mu_1, \Sigma_1) + \mathcal{N}(\mu_2, \Sigma_2)\right)$ where $\mu_1 = (0,0)^T$, $\mu_2 = (2,0)^T$, $\Sigma_1 = \Sigma_2 = I$, and 500 points on each cluster. We run the experiment three times, with 20 random projections as initialization.

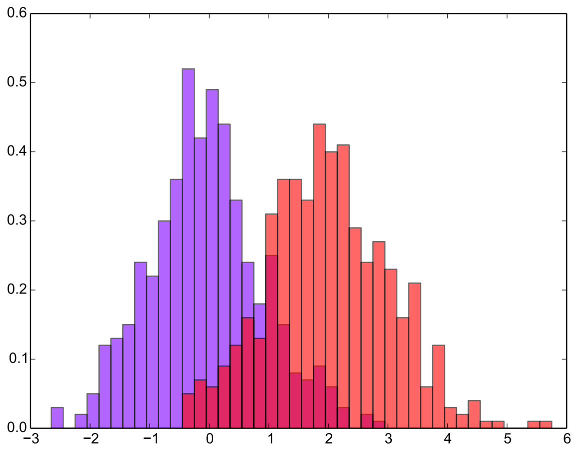


Ker/$\mathcal{E}$	Ker/Gauss	Ker/Poly	GMM	k-means
0.988	0.807	0.603	0.988	0.7
0.981	0.831	0.603	0.983	0.698
0.731	0.789	0.626	0.986	0.717

FIG. 8. We have $x \sim \frac{1}{2}\left(\mathcal{N}(\mu_1, \Sigma_1) + \mathcal{N}(\mu_2, \Sigma_2)\right)$ where $\mu_1 = (0,0)^T$, $\mu_2 = (4,0)^T$, $\Sigma_1 = I$, $\Sigma_2 = \left(\begin{smallmatrix} 1 & 0 \\ 1 & 20 \end{smallmatrix}\right)$ and 500 points on each cluster. We run the experiment three times, with 20 random projections as initialization.

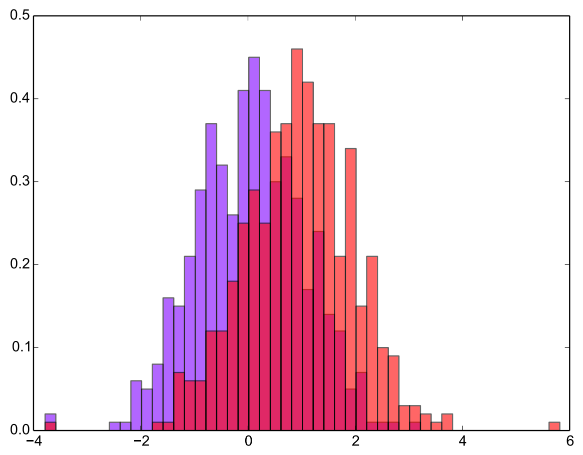
III. $1D$ ENERGY CLUSTERING

Now we do energy clustering in $1D$ ($\mathcal{E}1D$), which in this case we can optimize the function exactly. We also compare with the Kernel approach (Ker/$\mathcal{E}$)to energy statistics, and also the graph partitioning approach (EClust). One can see that these results agree between themselves.



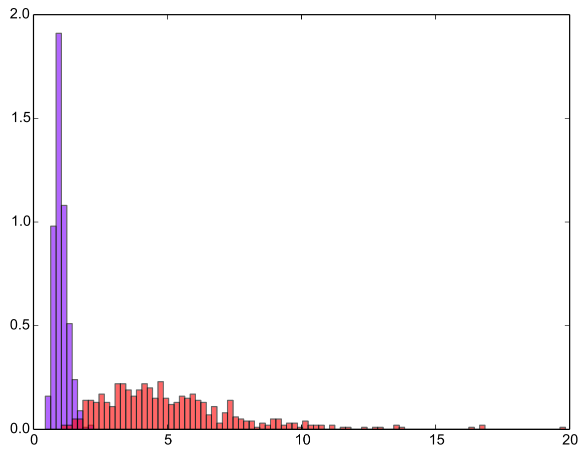
Ker/$\mathcal{E}$	$\mathcal{E}1D$	EClust	GMM	k-means
0.823	0.823	0.823	0.798	0.826
0.852	0.852	0.852	0.852	0.853
0.842	0.841	0.841	0.842	0.839

FIG. 9. We have $x \sim \frac{1}{2}\left(\mathcal{N}(\mu_1, \Sigma_1) + \mathcal{N}(\mu_2, \Sigma_2)\right)$ where $\mu_1 = 0$, $\mu_2 = 2$, $\Sigma_1 = \Sigma_2 = 1$, and 500 points on each cluster. We run the experiment three times, using k-means++ as initialization in kernel.



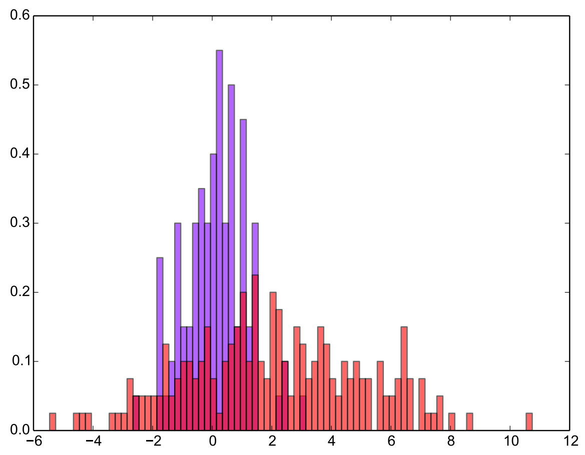
Ker/$\mathcal{E}$	$\mathcal{E}1D$	EClust	GMM	k-means
0.704	0.704	0.704	0.703	0.704
0.693	0.686	0.686	0.688	0.686
0.687	0.688	0.688	0.691	0.691

FIG. 10. We have $x \sim \frac{1}{2}\left(\mathcal{N}(\mu_1, \Sigma_1) + \mathcal{N}(\mu_2, \Sigma_2)\right)$ where $\mu_1 = 0$, $\mu_2 = 1$, $\Sigma_1 = \Sigma_2 = 1$, and 500 points on each cluster. We run the experiment three times, using k-means++ as initialization in kernel.



Ker/$\mathcal{E}$	$\mathcal{E}1D$	EClust	GMM	k-means
0.914	0.921	0.921	0.978	0.762
0.894	0.894	0.894	0.979	0.8
0.877	0.877	0.877	0.972	0.794

FIG. 11. We have $x \sim \frac{1}{2}\left(\log \mathcal{N}(\mu_1, \Sigma_1) + \log \mathcal{N}(\mu_2, \Sigma_2)\right)$ where $\mu_1 = 0$, $\mu_2 = 1.5$, $\Sigma_1 = 0.25$, $\Sigma_2 = 0.5$, and 500 points on each cluster. We run the experiment three times, using k-means++ as initialization in kernel.

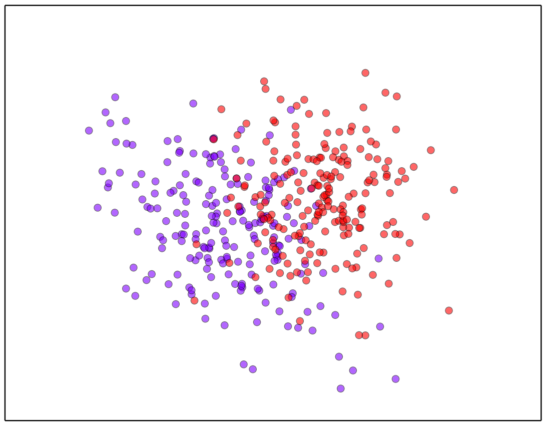


Ker/$\mathcal{E}$	$\mathcal{E}1D$	GMM	k-means
0.663	0.653	0.606	0.606
0.726	0.723	0.793	0.71
0.663	0.666	0.593	0.66
0.653	0.62	0.653	0.603
0.676	0.63	0.72	0.62

FIG. 12. We have $x \sim \frac{1}{2}\left(\mathcal{N}(\mu_1, \Sigma_1) + \mathcal{N}(\mu_2, \Sigma_2)\right)$ where $\mu_1 = 0$, $\mu_2 = 2$, $\Sigma_1 = 1$, $\Sigma_2 = 3$, $n_1 = 100$, $n_2 = 200$. For each experiment we run several times and pick the answer with optimal objective function.

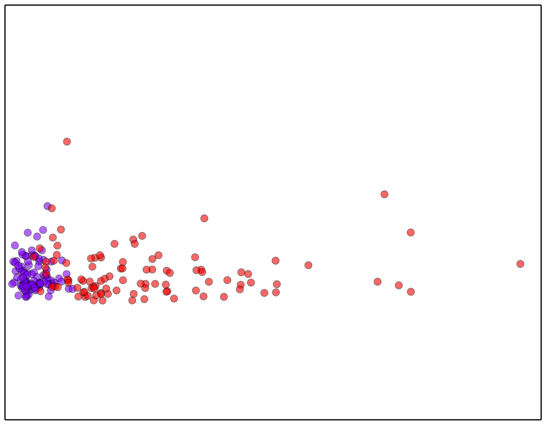
IV. ENERGY CLUSTERING HIGHER D

Same as before but in higher dimensions.



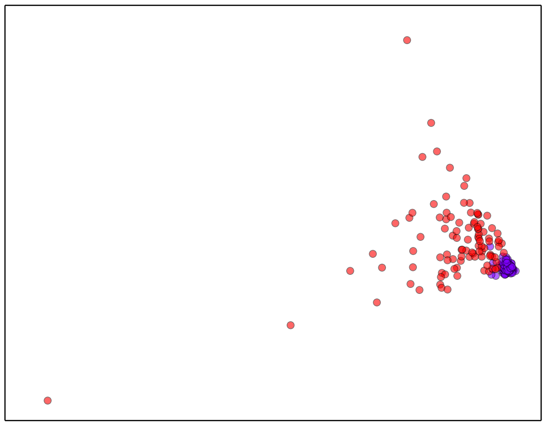
Ker/$\mathcal{E}$	Spectral/$\mathcal{E}$	GMM	k-means
0.7825	0.7175	0.6	0.7675
0.815	0.77	0.665	0.8175
0.8325	0.7825	0.685	0.8175
0.835	0.7675	0.8	0.83

FIG. 13. We have $x \sim \frac{1}{2}\left(\mathcal{N}(\mu_1,\Sigma_1)+\mathcal{N}(\mu_2,\Sigma_2)\right)$ where $\mu_1 = (0,0,0,0)^T$, $\mu_2 = (1.5,0,0,0)^T$, $\Sigma_1 = \left(\begin{smallmatrix} 0.6 & 0.2 & 0.2 & 0.2 \\ 0.2 & 0.6 & 0.2 & 0.2 \\ 0.2 & 0.2 & 0.6 & 0.2 \\ 0.2 & 0.2 & 0.2 & 0.6 \end{smallmatrix}\right)$, $\Sigma_2 = \left(\begin{smallmatrix} 0.5 & 0 & 0 & 0 \\ 0 & 0.5 & 0 & 0 \\ 0 & 0 & 0.5 & 0 \\ 0 & 0 & 0 & 0.5 \end{smallmatrix}\right)$, $n_1 = 200$, $n_2 = 200$. We run the experiments few times and pick the answer with best objective function.



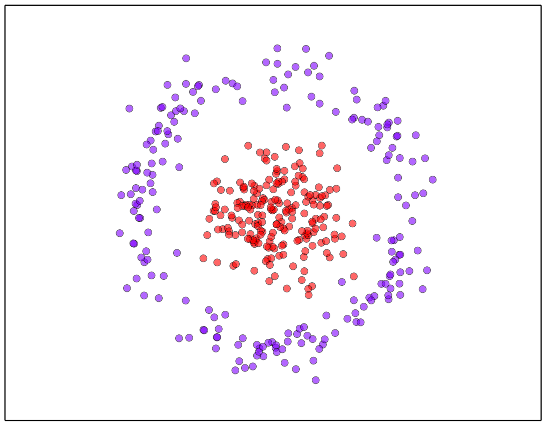
Ker/$\mathcal{E}$	EClust	GMM	k-means
0.755	0.755	0.71	0.585
0.74	0.745	0.81	0.575
0.775	0.775	0.805	0.635

FIG. 14. We have $x \sim \frac{1}{2}\left(\log\mathcal{N}(\mu_1,\Sigma_1)+\log\mathcal{N}(\mu_2,\Sigma_2)\right)$ where $\mu_1 = (0,0)^T$, $\mu_2 = (1.5,0)^T$, $\Sigma_1 = \left(\begin{smallmatrix} 0.25 & 0 \\ 0 & 0.25 \end{smallmatrix}\right)$, $\Sigma_2 = \left(\begin{smallmatrix} 0.5 & 0 \\ 0 & 0.5 \end{smallmatrix}\right)$, and 100 points on each cluster. We run the experiment three times, using k-means++ as initialization in kernel. EClust is extremelly slow.



Ker/$\mathcal{E}$	EClust	GMM	k-means
0.895	0.895	0.95	0.715
0.91	0.91	0.955	0.8
0.815	0.815	0.93	0.69

FIG. 15. We have $x \sim \frac{1}{2}(\log \mathcal{N}(\mu_1, \Sigma_1) + \log \mathcal{N}(\mu_2, \Sigma_2))$ where $\mu_1 = (0,0,0,0)^T$, $\mu_2 = (1.5, 1.5, 0, 0)^T$, $\Sigma_1 = \begin{pmatrix} 0.25 & 0 & 0 & 0 \\ 0 & 0.25 & 0 & 0 \\ 0 & 0 & 0.25 & 0 \\ 0 & 0 & 0 & 0.25 \end{pmatrix}$, $\Sigma_2 = \begin{pmatrix} 0.5 & 0 & 0 & 0 \\ 0 & 0.5 & 0 & 0 \\ 0 & 0 & 0.5 & 0 \\ 0 & 0 & 0 & 0.5 \end{pmatrix}$, and 100 points on each cluster. We run the experiment three times, using k-means++ as initialization in kernel. EClust is extremelly slow.



Ker/$\mathcal{E}$	EClust	GMM	k-means
0.74	0.516	0.516	0.536
0.583	0.513	0.52	0.556
0.706	0.503	0.516	0.503
0.633	0.5	0.553	0.52

FIG. 16. We generate two circles with random noise. First circle has radius 1 and a gaussian noise of size 0.2. Second circle has radius .2 and a gaussian noise of size 0.2. We have 200 points on each class.