Clustering Data: Does Theory Help?

Ravi Kannan

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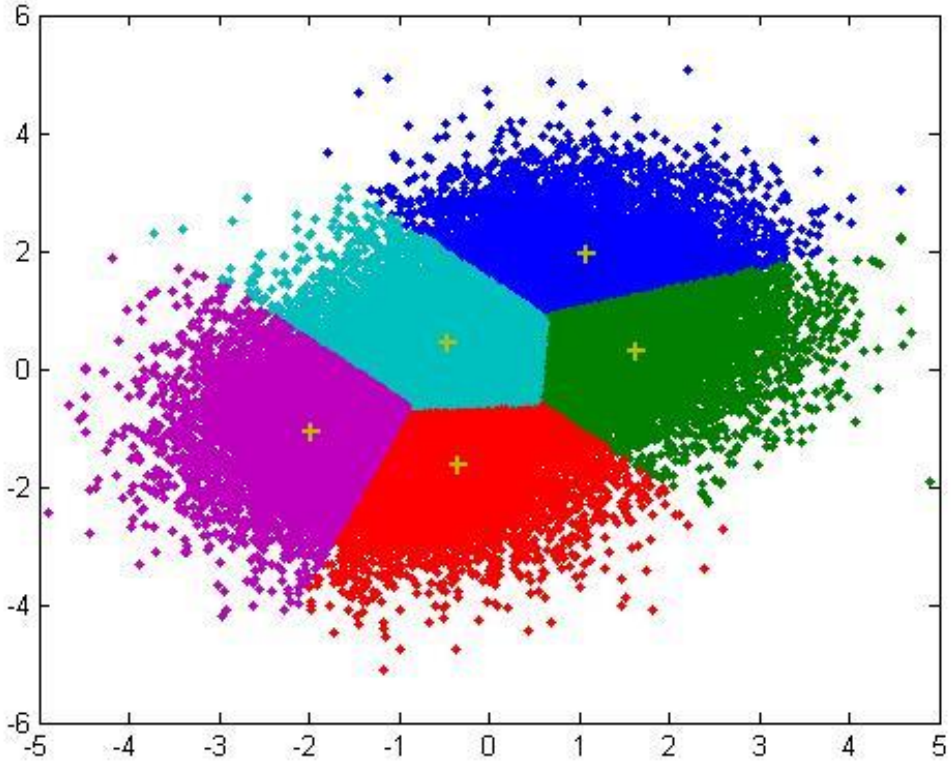
- Many headaches of this talk (and the field) would be gone if we can exactly optimize. Alas Exact Optimization is NP-Hard, so can only approx optimize.

Picture

5 clusters



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The Invisible Hand

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- Random sample (of all data) contains subset from largest cluster.
  - Try all subsets. Peel off cluster "close to" centroid of subset. Repeat.
- Cannot go beyond constant size subsets, so cannot beat constant (small) factor error.

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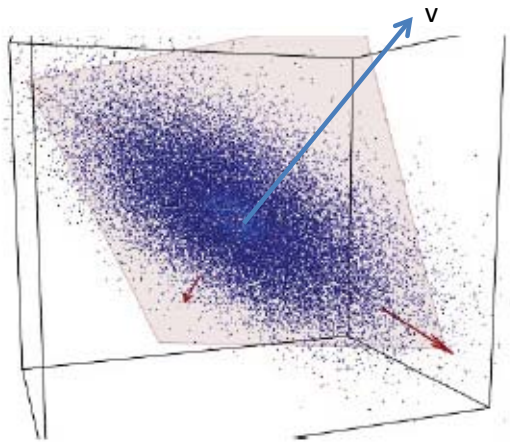

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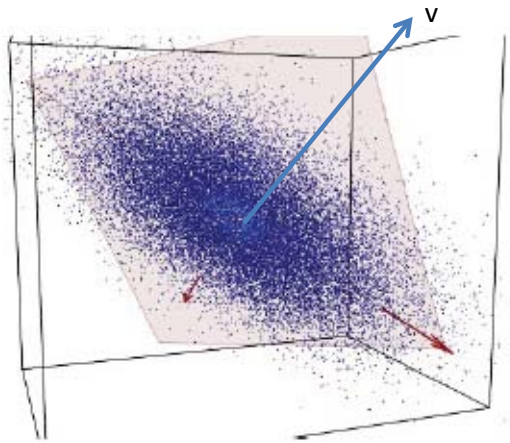

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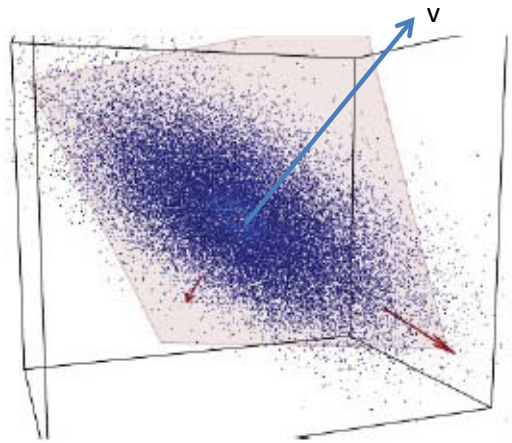
- Relax to rank$(C) \leq k$ instead of k distinct rows.
- Then, space spanned by C_i is the least-squares-fit $k-$dimensional space to $A_1, A_2, \ldots, A_n$. It can be found by Singular Value Decomposition. Principal Component Analysis - PCA.



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- First: The glories of PCA.
- There is also a different way to do spectral clustering- by repeatedly using a 1-d projections, Fiedler; Shi, Malik; ... which we do not discuss here.

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- $\sum_i |\bar{A}_i - C_i|^2 \leq \frac{8k}{d} \sum_i |B_i|^2$.
- Big gain if $k << d$.

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- One $\bar{A}$ is close to EVERY C !!!

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- If data was generated by a mixture model (of spherical gaussians), then this does the job.
- Indeed, even if the data was not generated from a mixture model, will see that this provides a good start for $k-$means (from which we get rapid convergence).

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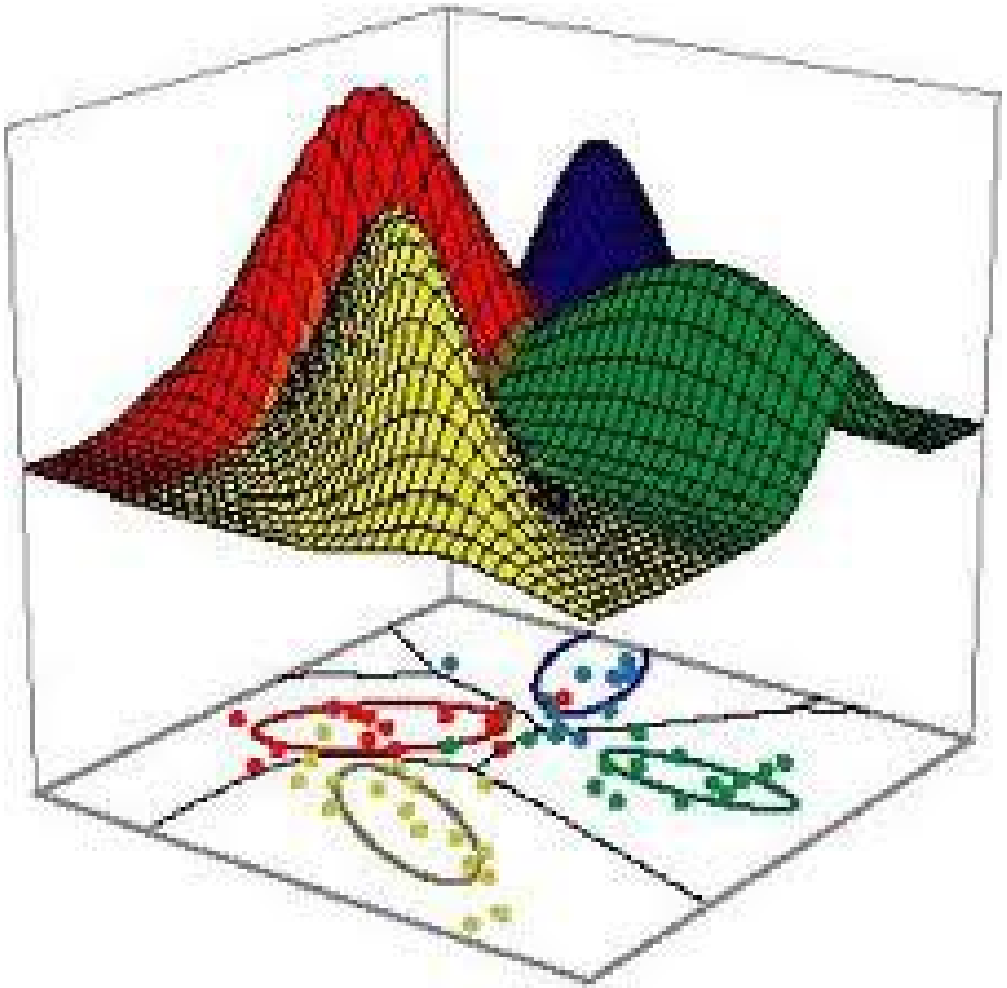
- Using Subspace Embeddings: If S is a $r \times n$ matrix ($r << n$) with one ± 1 entry per column chosen at random, then simultaneously for all vectors x,
  $|SAx|$ is within relative error ε of $|Ax|$

Mixture Models

Stochastic Model of data for clustering problems.



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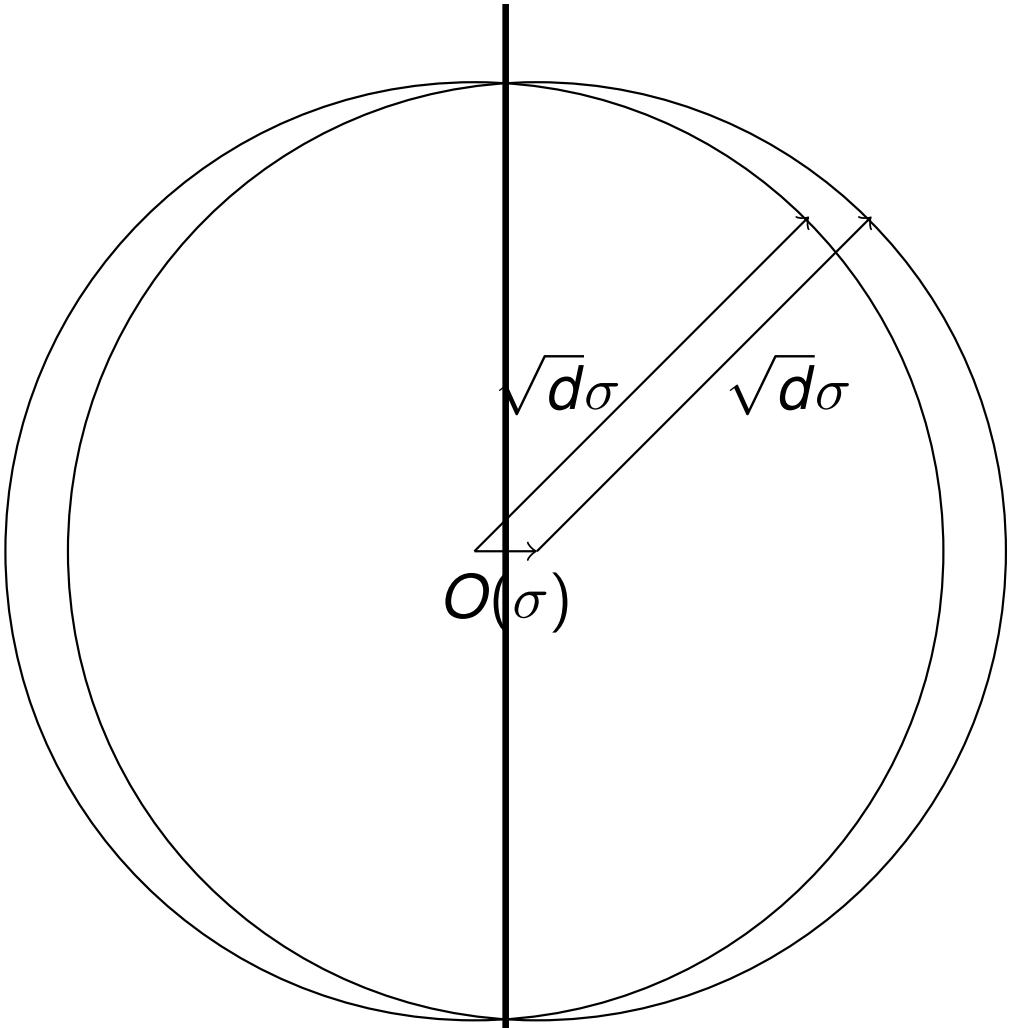
- Data points are n i.i.d. samples, each drawn according to F.
- Given data points, cluster them into k clusters corresponding to $F_1, F_2, \ldots, F_k$. Then it is easy fit a Gaussian to each cluster.

Two Gaussians of S.D. σ



Pts of Gaussian 1 $\leftrightarrow$ Pts of Gaussian 2

Typical picture in d dimensions

MSD is $O(d\sigma^2)$

Inter-center Sep is $O(\sigma)$

Error of $\varepsilon d\sigma^2$
Can mis-cluster many points !!

Correct Unit: σ

Correct Units in space of centers

***PICTURE OF TWO GAUSSIANS WITH PROJECTION

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  - Use Singular Value Decomposition)(PCA) crucially. An elegant argument.

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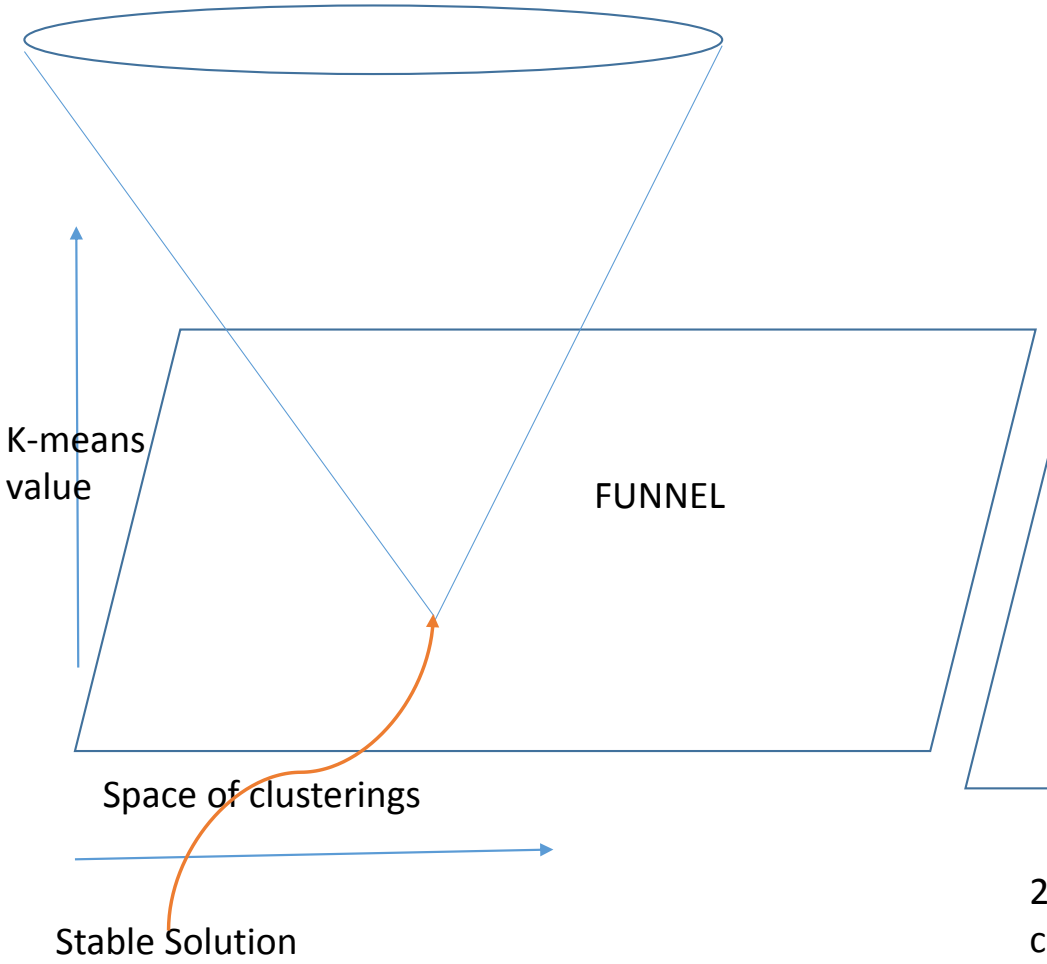
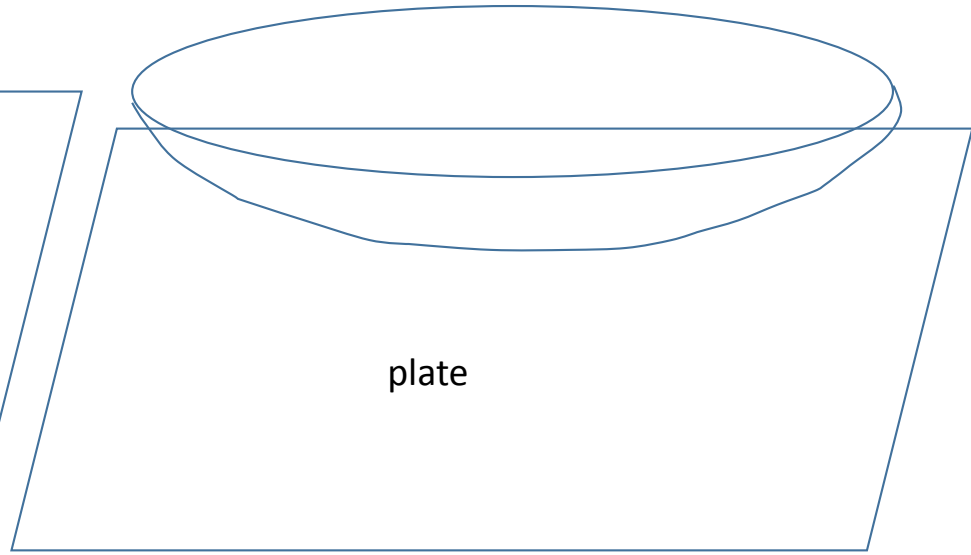
- Promising approaches and many open questions. But for the notorious two Gaussian picture, the correct solution is not stable!

Stability in Pictures





2-Gaussians. K-means value so large that mis-clustering points costs (relatively) little. So many clusterings of roughly the same value.

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- Harder Theorem: Kumar, Kannan: If there is a clustering C^* such that when data points are projected to space of centers, each projected data point is closer to its own center than any other center by at least $\Omega(\sigma(C^*))$, then Project and Cluster followed by Llyod's algorithm converges exponentially fast to the centers of C^*.

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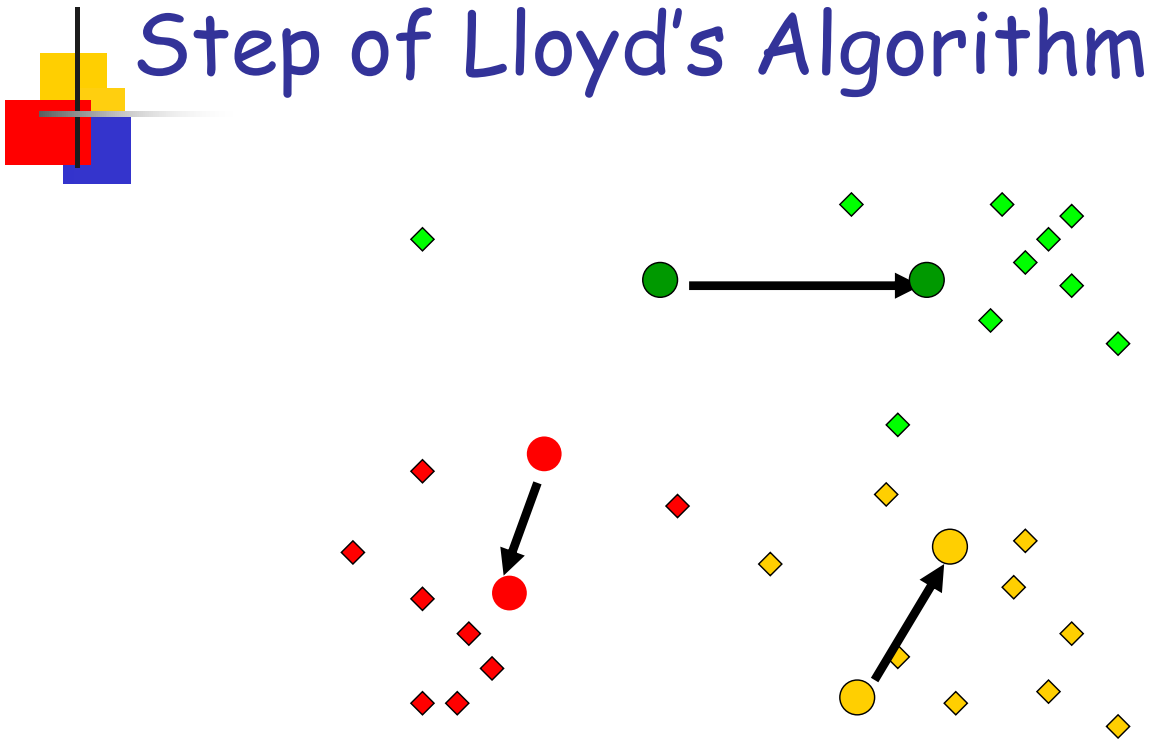
- Mean Squared Distance of data point to its cluster center = MSD (aka: k-means)
  - Lloyd's improves MSD at each step (SIMPLE).
  - Thus converges (to something).

Lloyd's Algorithm-Pictures

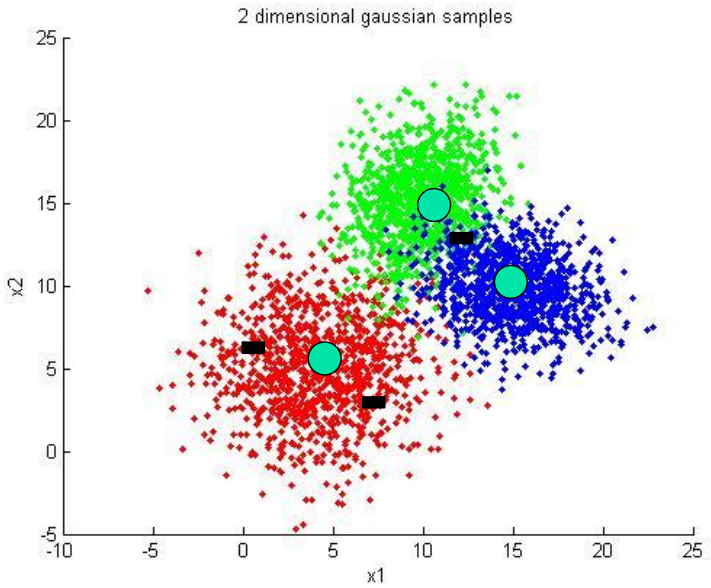


41

Pictures-II

Importance of a good start

- Good start
- Bad Start



More General Gaussians

Algorithm for fitting a general Mixture of k Gaussians

- Start with a initial guess of k (general) Gaussians: $(\mu_1, \Sigma_1), (\mu_2, \Sigma_2), \ldots, (\mu_k, \Sigma_k)$.

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- Kleinberg; Indyk, Motwani Project Data points into a random low dimensional subspace and find NN to query point in the projection.

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- Prove that PCA does the job in NNS and other applications.
- Difficulty: Whereas Random Projections preserve EVERY (pairwise) distance, PCA does not. But surely, data independent random projection just cannot always be that good?

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- Hopcroft, Kannan: Theorem: Balanced $k-$means (Minimum sum of dist squared to cluster centers among all partitions into k clusters, each of size n/k) satisfies all the axioms.