How Many Clusters: An algorithmic answer Chiranjib Bhattacharyya, Ravi Kannan, Amit Kumar

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- Notation Set S of points (in R^d), μ(S), σ(S) are respy their mean and (maximum) standard deviation (in a 1-d projection).

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- Special methods for GMM's: Kalai, Moitra, Valiant; Regev, Vijayaraghavan; Kwan, Caramanis;... need *k*.

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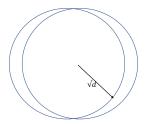
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• 2 Gaussians $\Omega(\sigma)$ apart. In most 1-d projections close to k = 1.



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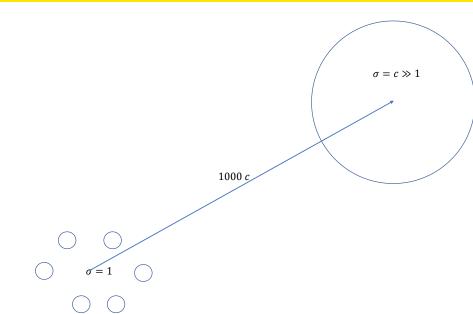
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- Gap Statistic Take *k* with good ratio of *k*-means cost to 1-means under a prior. Tibshirani; . Proofs for special cases.
- Even for spherical Gaussian mixtures, not true that largest drop occurs at correct k. In fact, for every m, there is a m-component spherical GMM with largest drop at k = 2

k in spherical Gaussian Mixtures



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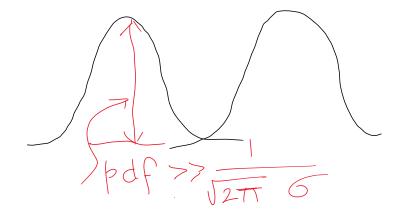
Conditions for "nice" GT

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- Here: A proper answer.

Baby Eg.: d = 1, one or two Gaussians

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d = 1 GT mixture of one or 2 Gaussians satisfying Mean Sep and Min



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- Considerably harder. Here, some intuition/ideas behind it.

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$$\forall T \subseteq S, |T| \ge c\sqrt{n}, \sigma(T) \ge \frac{|T|}{12|S|}\sigma(S).$$

• Lemma Anti-concentration implies NLSC.

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- **Corollary** For stochastic mixture of pdf's, each pdf satisfying anti-concentration, mixture satisfying Mean Sep. and Min wt. can find *k* exactly and GT approximately provided number of samples is at least $O^*(1/w_0)$ times max no. of samples needed to learn mean and Std. Dev. of a single component.
- **Corollary** For any log-concave mixture satisfying Mean Sep and Min Wt., the algorithm finds *k* exactly and GT approximately.

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- All Steps use quantities determined by DATA+ w_0 . Except step 2, all doable with some technical work. Focus now on Step 2.

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- Via Semi-Definite-Programming relaxation Plus Rounding.

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- Aside: Role of Spectral Norm instead of Frobenius norm in Clustering not studied enough.

Expanders and Spectrally tight sets

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- Cheeger \implies for every unit vector *u*, an upper bound on (*) in terms of the sum over only the edges of *H* (instead of all (*i*,*j*).)

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- Can substitute "expander" by "dense" in (5)

Dense graphs Via Semi-Definite Program

 v_i vector label on data point a_i . $u_{ij} = |(a_i - a_j) \cdot u|$. Solve SDP below. $\{(i,j) : v_i \cdot v_j \ge \Omega(1)\} \in \Omega(n^2) \rightarrow \text{dense.}$ (4) says (*) summed over edges small.

$$\begin{array}{ll} \min & \sigma^2 \\ & \sum\limits_{i=1}^n v_i \cdot v_i = \alpha n \\ & \sum\limits_{i,j} v_i \cdot v_j \ge \alpha^2 n^2 \end{array} (1) \\ & \sum\limits_{i,j} v_i \cdot v_j \ge \alpha^2 n^2 \\ & |v_i| \le 1 \quad \forall i \in [n]. \\ & \sum\limits_{i,j} u_{ij}^2 v_i \cdot v_j \le 2\alpha^2 \sigma^2 n^2 \quad \forall \quad \text{unit directions } u. \end{aligned} (2) \\ & \sum\limits_{i,j} v_i \cdot v_j \ge 2\alpha^2 \sigma^2 n^2 \quad \forall \quad \text{unit directions } u. \end{aligned} (3) \\ & \sum\limits_{i,j} v_i \cdot v_j \ge 0 \quad \forall i,j \end{aligned} (5)$$

Getting by with just data, w₀ not given

Try w = 1, 1 - (1/n), 1 - (2/n), When we hit the correct w₀, the correct k would be found by above. What can go wrong before that ? Recall our alg finds nuclii of clusters.

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- Failure 1 ⇒ NLSC violted. Failure 2 ⇒ the two nuclii have μ too close. Failure 3 ⇒ ???? NOT enough to deal only with nuclii... Complexity...

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- Analog of k-means: Find the partition into k subsets which minimizes weighted sum of spectral norms of the sets. Algorithm ? Hueristic ? For k-means, it is not true in general that for data from a mixture of k Mean-Separated spherical Gaussians, approximate optimal k- means partition finds the correct clustering. Prove it is true for spectral norm based measure in some generality. A. Sinop