Lecture II: Introduction to Clustering – Parametric clustering

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Paradigms for clustering

Parametric clustering algorithms (K given)

- Cost based / hard clustering

Basic algorithms

- K-means clustering and the quadratic distortion
- Model based / soft clustering

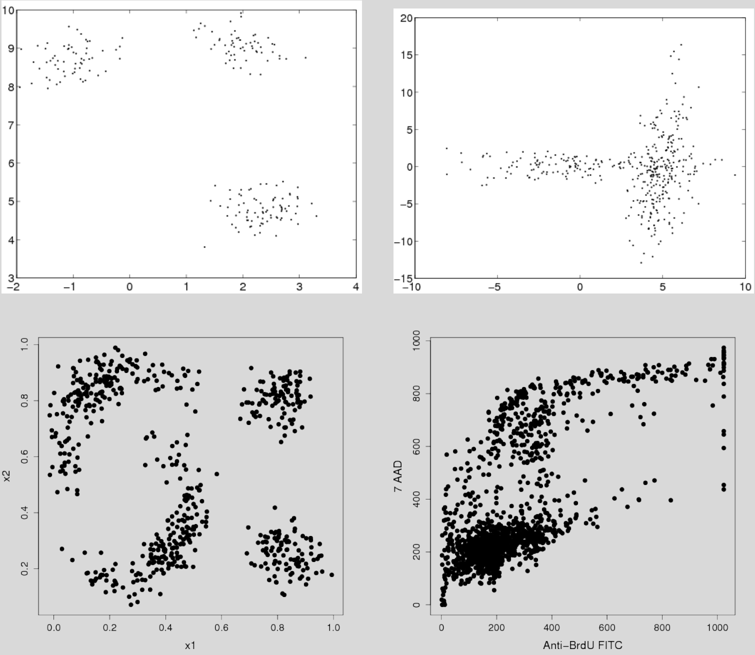
Reading HTF Ch.: 14.3, Murphy Ch.: Ch 11.[1], 11.2.1-3, 11.3, Ch 25, Bach Ch.:

What is clustering? Problem and Notation

- **Informal definition** **Clustering** = Finding groups in data
- **Notation**
  $\mathcal{D}$ = $\{x_1, x_2, \ldots x_n\}$ a **data set**
  n = number of **data points**
  K = number of **clusters** ($K << n$)
  Δ = $\{C_1, C_2, \ldots, C_K\}$ a partition of $\mathcal{D}$ into disjoint subsets
  $k(i)$ = the **label** of point i
  $\mathcal{L}(\Delta)$ = cost (loss) of Δ (to be minimized)
- **Second informal definition** **Clustering** = given n **data points**, separate them into K **clusters**
- Hard vs. soft clusterings
  - **Hard** clustering Δ: an item belongs to only 1 cluster
  - **Soft** clustering $\gamma = \{\gamma_{ki}\}_{k=1:K}^{i=1:n}$
    γ_{ki} = the **degree of membership** of point i to cluster k

$$\sum_k \gamma_{ki} = 1 \quad \text{for all } i$$

(usually associated with a probabilistic model)



(from [?])

Paradigms

Depend on type of data, type of clustering, type of cost (probabilistic or not), and constraints (about K, shape of clusters)

- Data = vectors $\{x_i\}$ in $\mathbb{R}^d$

Parametric (K known)	Cost based [hard] Model based [soft]
Non-parametric (K determined by algorithm)	Dirichlet process mixtures [soft] Information bottleneck [soft] Modes of distribution [hard] Gaussian blurring mean shift[?] [hard]

- Data = similarities between pairs of points $[S_{ij}]_{i,j=1:n},\ S_{ij} = S_{ji} \geq 0$ **Similarity based clustering**

Graph partitioning	spectral clustering [hard, K fixed, cost based] typical cuts [hard non-parametric, cost based]
Affinity propagation	[hard/soft non-parametric]

Classification vs Clustering

	Classification	Clustering
Cost (or Loss) $\mathcal{L}$	Expectd error	many! (probabilistic or not)
	Supervised	Unsupervised
Generalization	Performance on new data is what matters	Performance on current data is what matters
K	Known	Unknown
"Goal"	Prediction	Exploration Lots of data to explore!
Stage of field	Mature	Still young

Parametric clustering algorithms

- Cost based
  - Single linkage (min spanning tree)
  - Min diameter
    - Fastest first traversal (HS initialization)
  - K-medians
  - K-means
- Model based (cost is derived from likelihood)
  - EM algorithm
  - "Computer science"/"Probably correct" algorithms

Minimum diameter clustering

- **Cost** $\mathcal{L}(\Delta) = \max_k \underbrace{\max_{i,j \in C_k} ||x_i - x_j||}_{\text{diameter}}$
  - Mimimize the diameter of the clusters
  - Optimizing this cost is NP-hard
- **Algorithms**
  - **Fastest First Traversal** [?] – a factor 2 approximation for the min cost

For every $\mathcal{D}$, FFT produces a Δ so that

$$\mathcal{L}^{opt} \leq \mathcal{L}(\Delta) \leq 2\mathcal{L}^{opt}$$

  - rediscovered many times

Algorithm Fastest First Traversal

Input Data $\mathcal{D} = \{x_i\}_{i=1:n}$, number clusters K

defines **centers** $\mu_{1:K} \in \mathcal{D}$

(many other clustering algorithms use centers)

1. pick μ_1 at random from $\mathcal{D}$
2. for $k = 2 : K$

   $$\mu_k \leftarrow \operatorname*{argmax}_{\mathcal{D}} \text{distance}(x_i, \{\mu_{1:k-1}\})$$

3. for $i = 1 : n$ (assign points to centers)

   $k(i) = k$ if μ_k is the nearest center to x_i

K-means clustering

Algorithm K-Means[?]

Input Data $\mathcal{D} = \{x_i\}_{i=1:n}$, number clusters K
Initialize **centers** $\mu_1, \mu_2, \ldots \mu_K \in \mathbb{R}^d$ at random
Iterate until convergence

1. for $i = 1 : n$ (assign points to clusters $\Rightarrow$ new clustering)

$$k(i) = \operatorname*{argmin}_k ||x_i - \mu_k||$$

2. for $k = 1 : K$ (recalculate centers)

$$\mu_k = \frac{1}{|C_k|} \sum_{i \in C_k} x_i \qquad (1)$$

- Convergence
  - if Δ doesn't change at iteration m it will never change after that
  - convergence in finite number of steps to local optimum of cost $\mathcal{L}$ (defined next)
  - therefore, initialization will matter

The K-means cost

$$\mathcal{L}(\Delta) = \sum_{k=1}^{K} \sum_{i \in C_k} ||x_i - \mu_k||^2 \qquad (2)$$

- K-means solves a **least-squares** problem
- the cost $\mathcal{L}$ is called **quadratic distortion**

Proposition The K-means algorithm decreases $\mathcal{L}(\Delta)$ at every step.

Sketch of proof

- step 1: reassigning the labels can only decrease $\mathcal{L}$
- step 2: reassigning the centers μ_k can only decrease $\mathcal{L}$ because μ_k as given by (1) is the solution to

$$\mu_k = \min_{\mu \in \mathbb{R}^d} \sum_{i \in C_k} ||x_i - \mu||^2 \qquad (3)$$

Equivalent and similar cost functions

- The distortion can also be expressed using intracluster distances

$$\mathcal{L}(\Delta) \;=\; \sum_{k=1}^{K} \frac{1}{n_k} \sum_{i,j \in C_k} ||x_i - x_j||^2 \tag{4}$$

- **Correlation clustering** is defined as optimizing the related criterion

$$\mathcal{L}(\Delta) \;=\; \sum_{k=1}^{K} \sum_{i,j \in C_k} ||x_i - x_j||^2$$

- This cost is equivalent to the (negative) sum of (squared) intercluster distances

$$\mathcal{L}(\Delta) \;=\; -\sum_{k=1}^{K} \sum_{i \in C_k} \sum_{j \notin C_k} ||x_i - x_j||^2 + \text{constant} \tag{5}$$

Proof of (6) Replace μ_k as expressed in (1) in the expression of $\mathcal{L}$, then rearrange the terms

Proof of (5) $\sum_k \sum_{i,j \in C_k} ||x_i - x_j||^2 \;=\; \underbrace{\sum_{i=1}^{n} \sum_{j=1}^{n} ||x_i - x_j||^2}_{\text{independent of } \Delta} - \sum_k \sum_{i \in C_k} \sum_{j \notin C_k} ||x_i - x_j||^2$

The K-means cost in matrix form – the assignment matrix

- $\mathcal{L}$ as sum of squared intracluster distances

$$\mathcal{L}(\Delta) \;=\; \sum_{k=1}^{K} \frac{1}{|C_k|} \sum_{i,j \in C_k} ||x_i - x_j||^2 \qquad (6)$$

-
- Define the **assignment matrix** associated with Δ by $Z(\Delta)$
  Let $\Delta = \{C_1 = \{1,2,3\},\ C_2 = \{4,5\}\}$

$$Z^{unnorm}(\Delta) \;=\; \begin{array}{c} \begin{array}{cc} C_1 & C_2 \end{array} \\ \begin{bmatrix} 1 & 0 \\ 1 & 0 \\ 1 & 0 \\ 0 & 1 \\ 0 & 1 \end{bmatrix} \end{array} \text{ point } i \qquad Z(\Delta) \;=\; \begin{array}{c} \begin{array}{cc} C_1 & C_2 \end{array} \\ \begin{bmatrix} 1/\sqrt{3} & 0 \\ 1/\sqrt{3} & 0 \\ 1/\sqrt{3} & 0 \\ 0 & 1/\sqrt{2} \\ 0 & 1/\sqrt{2} \end{bmatrix} \end{array}$$

  Then Z is an orthogonal matrix (columns are orthornormal) and

$$\mathcal{L}(\Delta) \;=\; \mathrm{trace}\, Z^T D Z \qquad \text{with } D_{ij} = ||x_i - x_j||^2 \qquad (7)$$

$$\text{Let } \mathcal{Z} \;=\; \{\, Z \in \mathbb{R}^{n \times K},\ K \text{ orthonormal} \,\}$$

Proof of (7) Start from (2) and note that $\mathrm{trace}\, Z^T A Z = \sum_k \sum_{i,j \in C_k} Z_{ik} Z_{jk} A_{ij} = \sum_k \sum_{i,j \in C_k} \frac{1}{|C_k|} A_{ij}$

The K-means cost in matrix form – the co-ocurrence matrix

$$n = 5,\ \Delta = (1, 1, 1, 2, 2), \qquad X(\Delta) = \begin{bmatrix} \frac{1}{3} & \frac{1}{3} & \frac{1}{3} & 0 & 0 \\ \frac{1}{3} & \frac{1}{3} & \frac{1}{3} & 0 & 0 \\ \frac{1}{3} & \frac{1}{3} & \frac{1}{3} & 0 & 0 \\ 0 & 0 & 0 & \frac{1}{2} & \frac{1}{2} \\ 0 & 0 & 0 & \frac{1}{2} & \frac{1}{2} \end{bmatrix}$$

1. $X(\Delta)$ is symmetric, positive definite, ≥ 0 elements
2. $X(\Delta)$ has row sums equal to 1
3. trace $X(\Delta) = K$

$$\begin{aligned} \|X(\Delta)\|_F^2 &= \langle X, X\rangle = K \\ X(\Delta) &= Z(\Delta)Z^T(\Delta) \end{aligned}$$

$$2\mathcal{L}(\Delta) = \sum_{k=1}^{K} \frac{1}{|C_k|} \sum_{i,j\in C_k} ||x_i - x_j||^2 = \frac{1}{2}\langle D, X(\Delta)\rangle$$

with $D_{ij} = ||x_i - x_j||^2$

Spectral and convex relaxations

$$\begin{aligned}
\mathcal{L}(\Delta) &= \frac{1}{2}\langle D, X(\Delta)\rangle, \quad D = \text{squared distance matrix} \in \mathbb{R}^{n\times n} \\
\mathcal{X} &= \{\, X \in \mathbb{R}^{n\times n},\; X \succeq 0,\; X_{ij} \geq 0,\; \operatorname{trace} X = K,\; X1 = 1 \,\} \\
\mathcal{Z} &= \{\, Z \in \mathbb{R}^{n\times K},\; K \text{ orthonormal} \,\}
\end{aligned}$$

Spectral relaxation of the K-means problem

$$\min_{Z\in\mathcal{Z}} \operatorname{trace} Z^T D Z$$

This is solved by an **eigendecomposition** $Z^* =$ top K eigenvectors of D

Convex relaxation of the K-means problem

$$\min_{X\in\mathcal{X}} \langle D, X\rangle$$

This is a **Semi-Definite Program (SDP)**
Minimizing $\mathcal{L}$

- By K-means – clustering Δ, local optima
- By convex/spectral relaxation – matrix Z, X, global optimum

Symmetries between costs

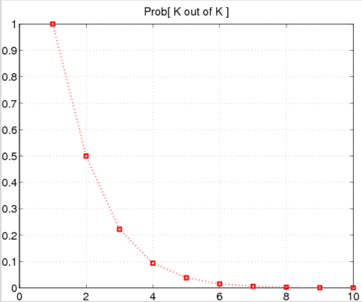
- K-means cost $\mathcal{L}(\Delta) = \min_{\mu_{1:K}} \sum_k \sum_{i \in C_k} ||x_i - \mu_k||^2$
- K-medians cost $\mathcal{L}(\Delta) = \min_{\mu_{1:K}} \sum_k \sum_{i \in C_k} ||x_i - \mu_k||$

- Correlation clustering cost $\mathcal{L}(\Delta) = \sum_k \sum_{i,j \in C_k} ||x_i - x_j||^2$
- min Diameter cost $\mathcal{L}^2(\Delta) = \max_k \max_{i,j \in C_k} ||x_i - x_j||^2$

Initialization of the centroids $\mu_{1:K}$

- Idea 1: start with K points at random
- Idea 2: start with K data points at random

  What's wrong with chosing K data points at random?



  The probability of hitting all K clusters with K samples approaches 0 when $K > 5$
- Idea 3: start with K data points using Fastest First Traversal [] (greedy simple approach to spread out centers)
- Idea 4: **k-means++** [] (randomized, theoretically backed approach to spread out centers)
- Idea 5: **"K-logK" Initialization** (start with enough centers to hit all clusters, then prune down to K)

  For EM Algorithm [], for K-means [**?**]

The "K-logK" initialization

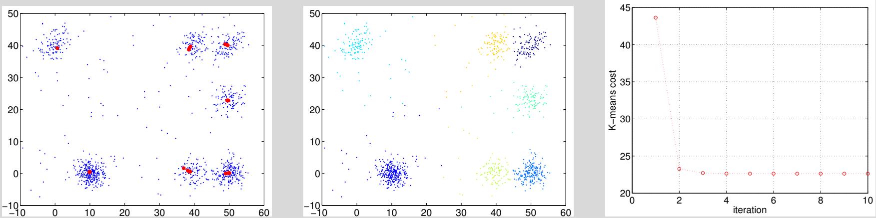
The K-logK Initialization (see also [?])

1. pick $\mu^0_{1:K'}$ at random from data set, where $K' = O(K \log K)$
   (this assures that each cluster has at least 1 center w.h.p)
2. run 1 step of K-means
3. remove all centers μ^0_k that have few points, e.g $|C_k| < \frac{n}{eK'}$
4. from the remaining centers select K centers by **Fastest First Traversal**
   - 4.1 pick μ_1 at random from the remaining $\{\mu^0_{1:K'}\}$
   - 4.2 for $k = 2 : K$, $\mu_k \leftarrow \underset{\mu^0_{k'}}{\operatorname{argmax}} \min_{j=1:k-1} ||\mu^0_{k'} - \mu_j||$, i.e next μ_k is furthest away from the already chosen centers
5. continue with the standard **K-means** algorithm

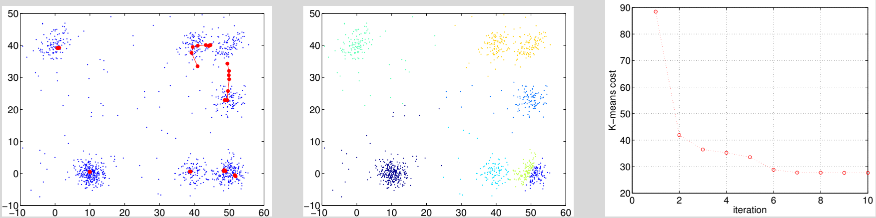
K-means clustering with K-logK Initialization

Example using a mixture of 7 Normal distributions with 100 outliers sampled uniformly

K-LOGK $K = 7,\ T = 100,\ n = 1100,\ c = 1$

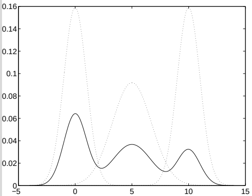


NAIVE $K = 7\ T = 100,\ n = 1100$

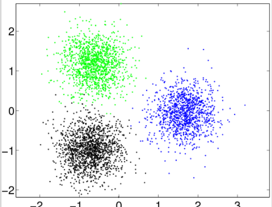


Model based clustering: Mixture models

Mixture in 1D



Mixture in 2D



- The **mixture density**

$$f(x) \;=\; \sum_{k=1}^{K} \pi_k f_k(x)$$

- $f_k(x)$ = the **components** of the mixture
  - each is a density
  - f called **mixture of Gaussians** if $f_k = Normal_{\mu_k, \Sigma_k}$
- π_k = the **mixing proportions**, $\sum_k = 1^K \pi_k = 1, \;\; \pi_k \geq 0$.
- **model parameters** $\theta = (\pi_{1:K}, \, \mu_{1:K}, \, \Sigma_{1:K})$
- The **degree of membership** of point i to cluster k

$$\gamma_{ki} \stackrel{\text{def}}{=} P[x_i \in C_k] \;=\; \frac{\pi_k f_k(x)}{f(x)} \text{ for } i = 1:n, k = 1:K \tag{8}$$

- depends on x_i and on the model parameters

Criterion for clustering: Max likelihood

- denote $\theta = (\pi_{1:K}, \mu_{1:K}, \Sigma_{1:K})$ (the parameters of the mixture model)
- Define **likelihood** $P[\mathcal{D}|\theta] = \prod_{i=1}^{n} f(x_i)$
- Typically, we use the **log likelihood**

$$l(\theta) = \ln \prod_{i=1}^{n} f(x_i) = \sum_{i=1}^{n} \ln \sum_k \pi_k f_k(x_i) \tag{9}$$

- denote $\theta^{ML} = \operatorname*{argmax}_\theta l(\theta)$
- θ^{ML} determines a soft clustering γ by (8)
- a soft clustering γ determines a θ (see later)
- Therefore we can write

$$\mathcal{L}(\gamma) = -l(\theta(\gamma))$$

Algorithms for model-based clustering

Maximize the (log-)likelihood w.r.t θ

- directly - (e.g by gradient ascent in θ)
- by the EM algorithm (very popular!)
- indirectly, w.h.p. by "computer science" algorithms

w.h.p = with high probability (over data sets)

The Expectation-Maximization (EM) Algorithm

Algorithm Expectation-Maximization (EM)

Input Data $\mathcal{D} = \{x_i\}_{i=1:n}$, number clusters K

Initialize parameters $\pi_{1:K} \in \mathbb{R},\ \mu_{1:K} \in \mathbb{R}^d,\ \Sigma_{1:K} \in \mathbb{R}^{d\times d}$ at random[1]

Iterate until convergence

E step (Optimize clustering) for $i = 1:n,\ k = 1:K$

$$\gamma_{ki} = \frac{\pi_k f_k(x)}{f(x)}$$

M step (Optimize parameters) set $\Gamma_k = \sum_{i=1}^n \gamma_{ki},\ k = 1:K$ (number of points in cluster k)

$$\pi_k = \frac{\Gamma_k}{n},\quad k = 1:K$$

$$\mu_k = \sum_{i=1}^n \frac{\gamma_{ki}}{\Gamma_k} x_i$$

$$\Sigma_k = \frac{\sum_{i=1}^n \gamma_{ki}(x_i-\mu_k)(x_i-\mu_k)^T}{\Gamma_k}$$

- $\pi_{1:K}, \mu_{1:K}, \Sigma_{1:K}$ are the maximizers of $l_c(\theta)$ in (13)
- $\sum_k \Gamma_k = n$

[1] Σ_k need to be symmetric, positive definite matrices

The EM Algorithm – Motivation

- Define the **indicator variables**

$$z_{ik} = \begin{cases} 1 & \text{if } i \in C_k \\ 0 & \text{if } i \notin C_k \end{cases} \tag{10}$$

denote $\bar{z} = \{z_{ki}\}_{k=1:K}^{i=1:n}$

- Define the **complete log-likelihood**

$$l_c(\theta, \bar{z}) = \sum_{i=1}^{n} \sum_{k=1}^{K} z_{ki} \ln \pi_k f_k(x_i) \tag{11}$$

- $E[z_{ki}] = \gamma_{ki}$
- Then

$$E[l_c(\theta, \bar{z})] = \sum_{i=1}^{n} \sum_{k=1}^{K} E[z_{ki}][\ln \pi_k + \ln f_k(x_i)] \tag{12}$$

$$= \sum_{i=1}^{n} \sum_{k=1}^{K} \gamma_{ki} \ln \pi_k + \sum_{i=1}^{n} \sum_{k=1}^{K} \gamma_{ki} \ln f_k(x_i)] \tag{13}$$

- If θ known, γ_{ki} can be obtained by (8)
  (Expectation)
- If γ_{ki} known, π_k, μ_k, Σ_k can be obtained by separately maximizing the terms of $E[l_c]$
  (Maximization)

Brief analysis of EM

$$Q(\theta, \gamma) = \sum_{i=1}^{n} \sum_{k=1}^{K} \gamma_{ki} \ln \underbrace{\pi_k f_k(x_i)}_{\theta}$$

- each step of EM increases $Q(\theta, \gamma)$
- Q converges to a local maximum
- at every local maxi of Q, $\theta \leftrightarrow \gamma$ are fixed point
- $Q(\theta^*, \gamma^*)$ local max for $Q \Rightarrow l(\theta^*)$ local max for $l(\theta)$
- under certain regularity conditions $\theta \longrightarrow \theta^{ML}$ [?]
- the E and M steps can be seen as projections [?]

- Exact maximization in **M step** is not essential.
  Sufficient to increase Q.
  This is called **Generalized EM**

Probablistic alternate projection view of EM[?]

- let z_i = which gaussian generated i? (random variable), $X = (x_{1:n})$, $Z = (z_{1:n})$
- Redefine Q
$$Q(\tilde{P}, \theta) \;=\; \mathcal{L}(\theta) - KL(\tilde{P} || P(Z|X, \theta))$$
where $P(X, Z|\theta) = \prod_i \prod_k P[z_i = k] P[x_i|\theta_k]$
$\tilde{P}(Z)$ is any distribution over Z,
$KL(P(w)||Q(w)) = \sum_w P(w) \ln \frac{P(w)}{Q(w)}$ the **Kullbach-Leibler divergence**

  Then,
  - **E step** $\max_{\tilde{P}} Q \Leftrightarrow KL(\tilde{P}||P(Z|X, \theta)$
  - **M step** $\max_\theta Q \Leftrightarrow KL(P(X|Z, \theta^{old})||P(X|\theta))$
- Interpretation: KL is "distance", "shortest distance" = projection

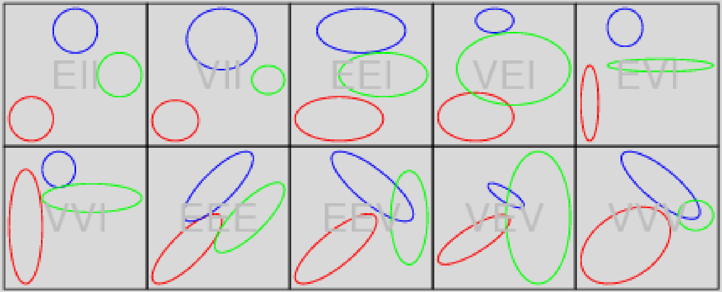
The M step in special cases

- Note that the expressions for μ_k, Σ_k = expressions for μ, Σ in the normal distribution, with data points x_i weighted by $\frac{\gamma_{ki}}{\Gamma_k}$

	M step
general case	$\Sigma_k = \sum_{i=1}^n \frac{\gamma_{ki}}{\Gamma_k}(x_i - \mu_k)(x_i - \mu_k)^T$
$\Sigma_k = \Sigma$ "same shape & size" clusters	$\Sigma \leftarrow \frac{\sum_{i=1}^n \sum_{k=1}^K \gamma_{ki}(x_i-\mu_k)(x_i-\mu_k)^T}{n}$
$\Sigma_k = \sigma_k^2 I_d$ "round" clusters	$\sigma_k^2 \leftarrow \frac{\sum_{i=1}^n \gamma_{ki}\|\|x_i-\mu_k\|\|^2}{d\Gamma_k}$
$\Sigma_k = \sigma^2 I_d$ "round, same size" clusters	$\sigma^2 \leftarrow \frac{\sum_{i=1}^n \sum_{k=1}^K \gamma_{ki}\|\|x_i-\mu_k\|\|^2}{nd}$

Exercise Prove the formulas above

- Note also that **K-means** is **EM** with $\Sigma_k = \sigma^2 I_d,\ \sigma^2 \to 0$ Exercise Prove it



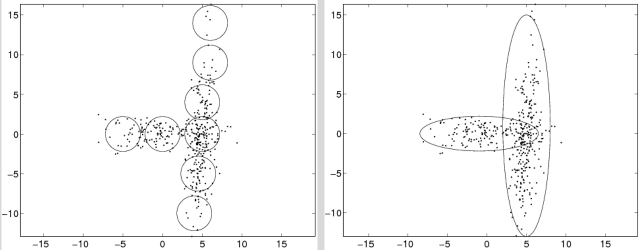
More special cases [?] introduce the following description for a covariance matrice in terms of *volume, shape, alignment with axes* (=determinant, trace, e-vectors). The letters below mean: I=unitary (shape, axes), E=equal (for all k), V=unequal

- EII: equal volume, round shape (spherical covariance)
- VII: varying volume, round shape (spherical covariance)
- EEI: equal volume, equal shape, axis parallel orientation (diagonal covariance)
- VEI: varying volume, equal shape, axis parallel orientation (diagonal covariance)
- EVI: equal volume, varying shape, axis parallel orientation (diagonal covariance)
- VVI: varying volume, varying shape, equal orientation (diagonal covariance)
- EEE: equal volume, equal shape, equal orientation (ellipsoidal covariance)
- EEV: equal volume, equal shape, varying orientation (ellipsoidal covariance)
- VEV: varying volume, equal shape, varying orientation (ellipsoidal covariance)
- VVV: varying volume, varying shape, varying orientation (ellipsoidal covariance)

(from [?])

EM versus K-means

- Alternates between cluster assignments and parameter estimation
- Cluster assignments γ_{ki} are probabilistic
- Cluster parametrization more flexible



- Converges to local optimum of **log-likelihood**
  Initialization recommended by K-logK method []

- **Modern algorithms with guarantees** (for e.g. mixtures of Gaussians)
  - Random projections
  - Projection on principal subspace [**?**]
  - Two step EM (=K-logK initialization + one more EM iteration) []

"Computer science" algorithms for mixture models

- Assume clusters well-separated **(S)**
  - e.g $||\mu_k - \mu_l|| \geq C \max(\sigma_k, \sigma_l)$
  - with $\sigma_k^2 = \max \text{eigenvalue}(\Sigma_k)$
- true distribution is mixture
  - of Gaussians
  - of **log-concave** f_k's (i.e. $\ln f_k$ is concave function)
- then, w.h.p. (n, K, d, C)
  - we can label all data points correctly
  - $\Rightarrow$ we can find good estimate for θ

Even with **(S)** this is not an easy task in high dimensions
Because $f_k(\mu_k) \to 0$ in high dimensions (i.e there are few points from Gaussian k near μ_k)

Other "CS" algorithms

- [?] round, equal sized Gaussian, random projection
- [?] arbitrary shaped Gaussian, distances
- [?] log-concave, principal subspace projection

Example Theorem (Achlioptas & McSherry, 2005) If data come from K Gaussians, $n >> K(d + \log K)/\pi_{min}$, and

$$||\mu_k - \mu_l|| \geq 4\sigma_k\sqrt{1/\pi_k + 1/\pi_l} + 4\sigma_k\sqrt{K \log nK + K^2}$$

then, w.h.p. $1 - \delta(d, K, n)$, their algorithm finds true labels

Good

- theoretical guarantees
- no local optima
- suggest heuritics for EM K-means
  - project data on principal subspace (when $d >> K$)

But

- strong assuptions: large separation (unrealistic), concentration of f_k's (or f_k known), K known
- try to find perfect solution (too ambitious)

A fundamental result

The Johnson-Lindenstrauss Lemma For any $\varepsilon \in (0,1]$ and any integer n, let d' be a positive integer such that $d' \geq 4(\varepsilon^2/2 - \varepsilon^3/3)^{-1} \ln n$. Then for any set $\mathcal{D}$ of n points in $\mathbb{R}^d$, there is a map $f : \mathbb{R}^d \to \mathbb{R}^{d'}$ such that for all $u, v \in V$,

$$(1-\varepsilon)||u-v||^2 \leq ||f(u)-f(v)||^2 \leq (1+\varepsilon)||u-v||^2 \quad (14)$$

Furthermore, this map can be found in randomized polynomial time.

- note that the **embedding dimension** d' does not depend on the original dimension d, but depends on n, ε
- [?] show that: the mapping f is linear and that w.p. $1 - \frac{1}{n}$ a random projection (rescaled) has this property
- their proof is elementary Projecting a fixed vector v on a a random subspace is the same as projecting a random vector v on a fixed subspace. Assume $v = [v_1, \ldots v_d]$ with $v \sim$ i.i.d. and let $\tilde{v} =$ projection of v on axes $1 : d'$. Then $E[||\tilde{v}||^2 = d' E[v_j^2] = \frac{d'}{d} E[||v||^2]$. The next step is to show that the variance of $||\tilde{v}||^2$ is very small when d' is sufficiently large.

A two-step EM algorithm [?]

Assumes K spherical gaussians, separation $||\mu_k^{true} - \mu_{k'}^{true} \geq C\sqrt{d}\sigma_k$

1. Pick $K' = \mathcal{O}(K \ln K)$ centers μ_k^0 at random from the data
2. Set $\sigma_k^0 = \frac{d}{2} \min_{k \neq k'} ||\mu_k^0 - \mu_{k'}^0||^2$, $\pi_k^0 = 1/K'$
3. Run one E step and one M step $\Longrightarrow \{\pi_k^1, \mu_k^1, \sigma_k^1\}_{k=1:K'}$
4. Compute "distances" $d(\mu_k^1, \mu_{k'}^1) = \frac{||\mu_k^1 - \mu_{k'}^1||}{\sigma_k^1 - \sigma_{k'}^1}$
5. Prune all clusters with $\pi_k^1 \leq 1/4K'$
6. Run Fastest First Traversal with distances $d(\mu_k^1, \mu_{k'}^1)$ to select K of the remaining centers. Set $\pi_k^1 = 1/K$.
7. Run one E step and one M step $\Longrightarrow \{\pi_k^2, \mu_k^2, \sigma_k^2\}_{k=1:K}$

Theorem For any $\delta, \varepsilon > 0$ if d large, n large enough, separation $C \geq d^{1/4}$ the **Two step EM** algorithm obtains centers μ_k so that

$$||\mu_k - \mu_k^{true}|| \leq ||\mathrm{mean}(C_k^{true}) - \mu_k^{true}|| + \varepsilon\sigma_k\sqrt{d}$$

Selecting K for mixture models

The **BIC (Bayesian Information) Criterion**

- let θ_K = parameters for γ_K
- let $\#\theta_K$=number independent parameters in θ_K
  - e.g for mixture of Gaussians with full Σ_k's in d dimensions

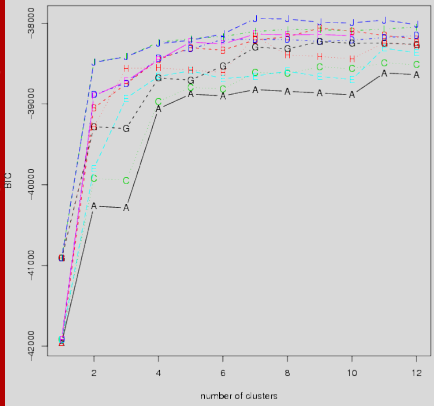
$$\#\theta_K = \underbrace{K-1}_{\pi_{1:K}} + \underbrace{Kd}_{\mu_{1:K}} + \underbrace{Kd(d-1)/2}_{\Sigma_{1:K}}$$

- define

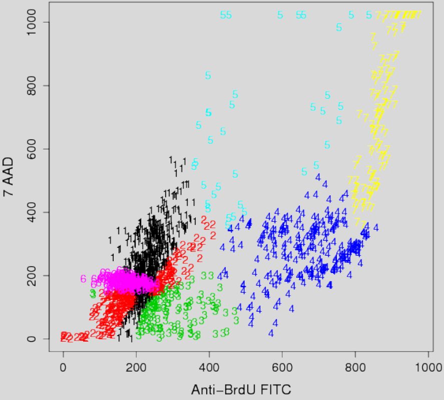
$$BIC(\theta_K) \;=\; l(\theta_K) - \frac{\#\theta_K}{2}\ln n$$

- **Select** K that maximizes $BIC(\theta_K)$
- selects true K for $n \to \infty$ and other technical conditions (e.g parameters in compact set)
- but theoretically not justified (and overpenalizing) for finite n

Number of Clusters vs. BIC EII (A), VII (B), EEI (C), VEI (D), EVI (E), VVI (F), EEE (G), EEV (H), VEV (I), VVV (J)

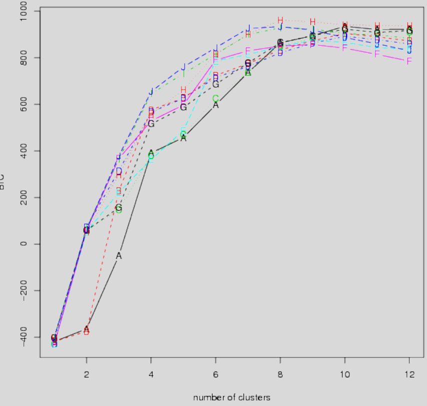


EEV, 8 Cluster Solution

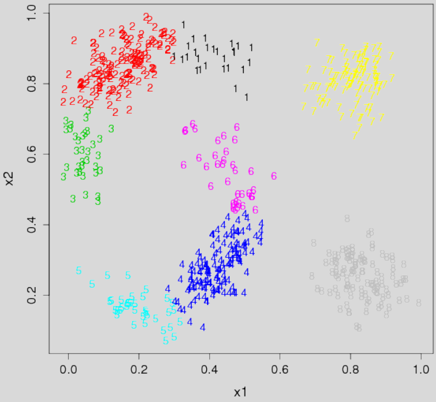


(from [?])

Number of Clusters vs. BIC EII (A), VII (B), EEI (C), VEI (D), EVI (E), VVI (F), EEE (G), EEV (H), VEV (I), VVV (J)



EEV, 8 Cluster Solution



(from [?])

Selecting K for hard clusterings

- based on statistical testing: the **gap** statistic (Tibshirani, Walther, Hastie, 2000)
- **X-means** [?] heuristic: splits/merges clusters based on statistical tests of Gaussianity
- Stability methods
  - Empirical – prove instability
  - Optimization based – prove stability

Empirical Stability methods for choosing K

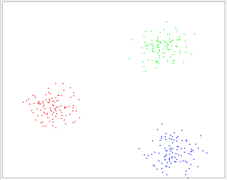
- like bootstrap, or crossvalidation
- **Idea** (implemented by [?])

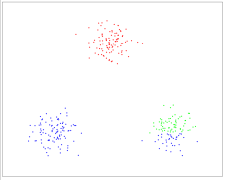
  for each K
  1. perturb data $\mathcal{D} \to \mathcal{D}'$
  2. cluster $\mathcal{D}' \to \Delta'_K$
  3. compare Δ_K, Δ'_K. Are they similar?
     If yes, we say Δ_K is **stable to perturbations**

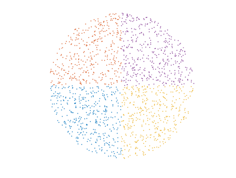
Fundamental assumption If Δ_K is stable to perturbations then K is the correct number of clusters

- these methods are supported by experiments (not extensive)
- **not directly supported by theory** ... see [?] for a summary of the area

Is this clustering approximately correct?



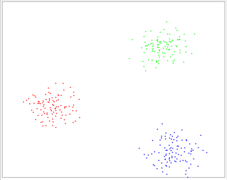


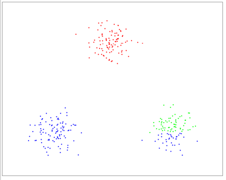


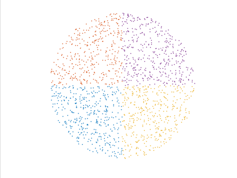
SS method	Yes, OI=$1e^{-4}$	Don't know	Don't know

- Given data $\mathcal{D}$, clustering Δ
- $\mathcal{L}($ data, clustering$)$ (e.g. K-means)
- **"correct"**
    - $=$ the "only" "good" clustering supported by $\mathcal{D}$
    - $\Leftrightarrow$ any other Δ' with smaller $\mathcal{L}$ is ε-close to Δ

Is this clustering approximately correct?







SS method	Yes, OI=$1e^{-4}$	Don't know	Don't know
	good, stable	bad	unstable

- Given data $\mathcal{D}$, clustering Δ
- $\mathcal{L}($ data, clustering$)$ (e.g. K-means)
- **"correct"**

  = the "only" "good" clustering supported by $\mathcal{D}$

  $\Leftrightarrow$ any other Δ' with smaller $\mathcal{L}$ is ε-close to Δ

What is an **Optimality Interval (OI)**?

Theorem (Meta-theorem)

If Δ fits the data $\mathcal{D}$ well, then we shall prove that any other clustering Δ' that also fits $\mathcal{D}$ well will be a small perturbation of Δ.

- Δ' is **good** if
$$\mathcal{L}(\Delta') \leq \mathcal{L}(\Delta) + \alpha.$$
- δ is **OI**: for all good Δ',
$$d_{ME}(\Delta', \Delta) \leq \delta$$
where d_{ME} is the misclassification error/earth mover distance
- if OI exists we say Δ is **stable**

How? 1. Mapping a clustering to a matrix

$$n = 5,\ \Delta = (1, 1, 1, 2, 2), \qquad X(\Delta) = \begin{bmatrix} \frac{1}{3} & \frac{1}{3} & \frac{1}{3} & 0 & 0 \\ \frac{1}{3} & \frac{1}{3} & \frac{1}{3} & 0 & 0 \\ \frac{1}{3} & \frac{1}{3} & \frac{1}{3} & 0 & 0 \\ 0 & 0 & 0 & \frac{1}{2} & \frac{1}{2} \\ 0 & 0 & 0 & \frac{1}{2} & \frac{1}{2} \end{bmatrix}$$

1. $X(\Delta)$ is symmetric, positive definite, ≥ 0 elements
2. $X(\Delta)$ has row sums equal to 1
3. trace $X(\Delta) = K$

$$\|X(\Delta)\|_F^2 = K$$

Let $\mathcal{X}$ be the space $n \times n$ of matrices with Properties 1, 2, 3 above

- $\mathcal{X}$ is convex
- $X(C)$ are extreme points of $\mathcal{X}$

How? 2. Convex relaxations

Original clustering problem Given data $\mathcal{D}$, K, $\mathcal{L}()$

$$\text{minimize}_\Delta \quad \mathcal{L}(\mathcal{D}, \Delta) \quad \text{with solution } \Delta^{\text{opt}}$$

Convex relaxation

- map clustering $\Delta \rightarrow$ matrix $X(\Delta) \in \mathcal{X}$
- so that $\mathcal{L}(X)$ convex in X
- Relaxed problem

$$L^* = \min_{X \in \mathcal{X}} \mathcal{L}(X), \quad \text{with solution } X^* \tag{15}$$

The Sublevel Set (SS) method

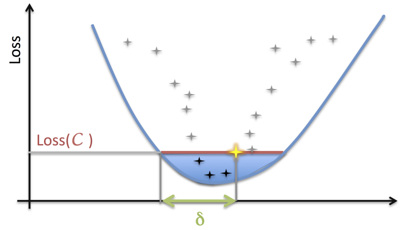
ework Given data, L , convex relaxation
Step 0 Cluster data, obtain a clustering Δ.

Step 1 Use convex relaxation to define new optimization problem

$$\text{SS} \quad \delta \;=\; \max_{X' \in \mathcal{X}} \|X(\Delta) - X'\|_F, \quad \text{s.t. } \mathcal{L}(X') \le \mathcal{L}(\Delta).$$

Step 2 Prove that $\| \;\|_F \le \delta \Rightarrow d_{ME}(\;) \le \epsilon$ M, MLJ 2012
Done: ϵ is a Optimality Interval (OI) for Δ.

$\mathcal{X}\mathcal{X}_{\le l} = \{X \in \mathcal{X},\, \mathcal{L}(X) \le c\}$ is **sublevel set** of L



Two technical bits

1. SS is convex only if $||X' - X(\Delta)||$ concave
   - Use $|| \ ||_F$ Frobenius norm. $||X(\Delta)||_F^2 = K$ for any clustering.

2. Relating $\| \ \|_F$ to distance between clusterings.

$$\|X(\Delta) - X(\Delta)'\|_F^2 \leq \delta \quad \Rightarrow \quad d_{ME}(\Delta, \Delta') \leq \epsilon$$

distance between matrices — "misclassification error" metric between clusterings

- Theorem proved in M, Machine Learning Journal, 2012 with $\epsilon = 2\delta p_{\max}$.
- The tightest result known. Upper/lower bounds between d_{ME}, $\| \ \|_F$ and Rand Index
- Proofs use geometry of convex sets + refined analysis for small distances
- Example from Wan,M NIPS16 OI by existing results Rohe et al. 2011 $\sim 10^2$ OI by our method

Relation with other work

- **Previous ideas on OI**
  - Spectral bounds for Spectral Clustering M,Shortreed,Xu AISTATS05
  - Spectral bounds for K-means, NCut and other quadratic costs M, ICML06 and JMVA 2018
  - Spectral bounds for networks model based clustering: Stochastic Block Model and Preference Frame Model Wan,M NIPS2016
- **Previous work we build on**
  - Convex relaxations for clustering MANY! here we use SDP for K-means Peng, Wei 2007
  - Transforming bound on $||X - X'||_F$ into bound on d_{ME} M MLJ 2012
- **Contrast with** work on Clusterability and resilience, e.g. Ben-David, 2015,Bilu,Linial 2009
  - "Their" work: assume $\exists$ stable Δ, prove it can be found efficiently
  - This work: given Δ, prove it is stable

For what clustering paradigms can we obtain OI's?

"All" ways to map Δ to a matrix

space	matrix	definition	size
$\mathcal{X}$	$X(\Delta)$	$X_{ij} = 1/n_k$ iff $i, j \in C_k$	$n \times n$, block-diagonal
$\tilde{\mathcal{X}}$	$\tilde{\mathcal{X}}(\Delta)$	$\tilde{\mathcal{X}}_{ij} = 1$ iff $i, j \in C_k$	$n \times n$, block-diagonal
$\mathcal{Z}$	$Z(\Delta)$	$Z_{ik} = 1/\sqrt{n_k}$ iff $i \in C_k$	$n \times K$, orthogonal

Theorem

M NeurIPS 2018 If L has a convex relaxation involving one of $X, \tilde{\mathcal{X}}, Z$, then

(1) There exists a convex SS problem

$$(SS) \quad \delta = \min_{X' \in \mathcal{X}\mathcal{X}_{\leq l}} \langle X(\Delta), X' \rangle \quad \text{(similarly for } \tilde{\mathcal{X}}, Z).$$

(2) From optimal δ an OI ε can be obtained, valid when $\varepsilon \leq p_{\min}$.

$$X : X_{ij} = 1/n_k \text{ iff } i, j \in C_k \qquad \varepsilon = (K - \delta) p_{\max}$$

$$\tilde{\mathcal{X}} : \tilde{\mathcal{X}}_{ij} = 1 \text{ iff } i, j \in C_k \qquad \varepsilon = \frac{\sum_{k \in [K]} n_k^2 + (n-K+1)^2 + (K-1) - 2\delta}{2 p_{\min}}$$

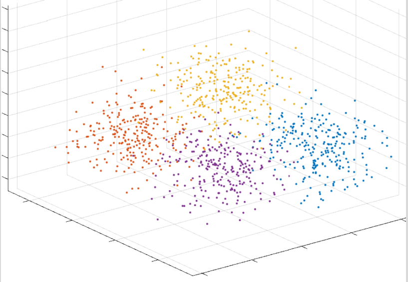
$$Z : Z_{ik} = 1/\sqrt{n_k} \text{ iff } i \in C_k \qquad \varepsilon = (K - \delta^2/2) p_{\max}$$

Existence of guarantee depends only on space of convex relaxation.

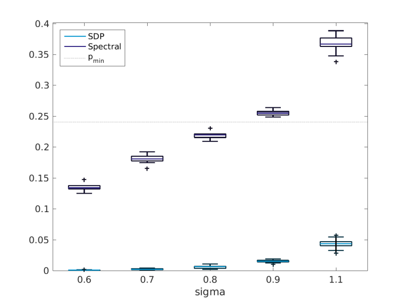
Results for K-means clusterings

$K = 4$ equal Gaussian clusters, $n = 1024$, $||\mu_k - \mu_l|| = 4\sqrt{2} \approx 5.67$

data for $\sigma = 0.9$

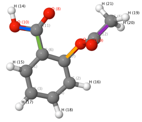


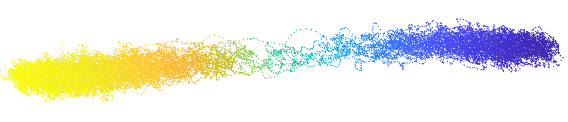
Values of ϵ vs cluster spread σ



Spectral=M ICML06, SDP=M NeurIPS 2018

Aspirin ($C_9O_4H_8$) molecular simulation data Chmiela et al. 2017



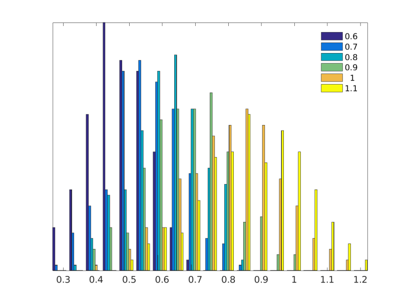


$n = 2118$ $\varepsilon = 0.065$

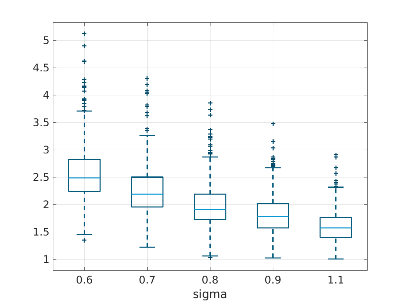
$K = 2$
$p_{\min} = .26$
$p_{\max} = .74$

Separation statistics

distance to own center over min center separation, colored by σ.



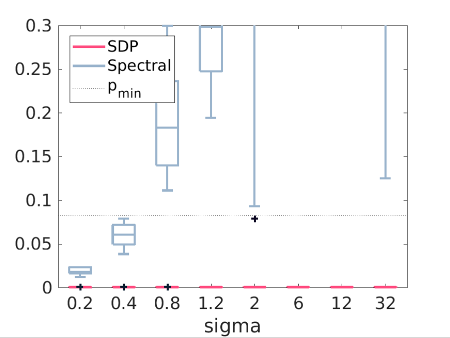
distance to second closest center over distance to own center, versus σ



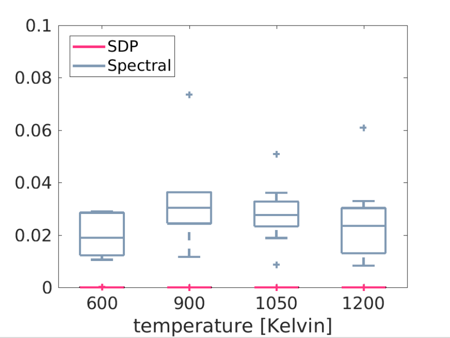
Results for Spectral Clustering by Normalized Cut

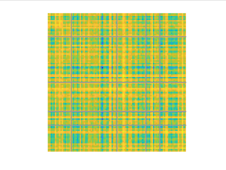
Spectral=M AISTATS05, SDP=M NeurIPS 2018

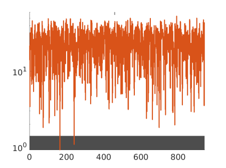
Synthetic S, $n = 100$

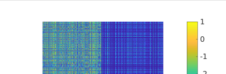


Chemical reaction data, $n \approx 1000$

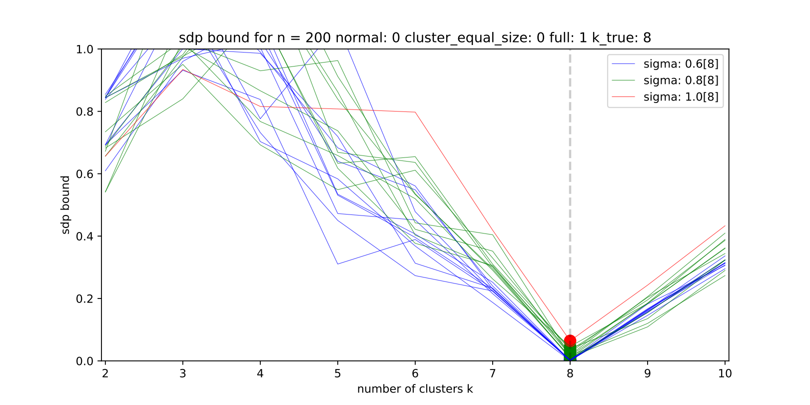








Stability and the selection of K Cheng,M,Harchaoui (in preparation)



Summary of SS method

1. Cluster data
2. Set up and solve SS problem
3. If solution δ small enough, **guarantee** Δ is approximately optimal and all other good clusterings are near it

- without any model assumptions, practically applicable
- not all Δ can have guarantees

Methods based on non-parametric density estimation

Idea The clusters are the isolated peaks in the (empirical) data density

- group points by the peak they are under
- some outliers possible
- $K = 1$ possible(no clusters)
- shape and number of clusters K determined by algorithm
- **structural parameters**
  - **smoothness** of the **density estimate**
  - what is a peak

Algorithms

- peak finding algorithms Mean-shift algorithms
- level sets based algorithms
  - Nugent-Stuetzle, Support Vector clustering
- Information Bottleneck [?]