Lecture 9: Classic and Modern Data 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

Issues in parametric clustering

- Selecting K
- Outliers

Non-parametric clustering (smoothness given)

- Based on non-parametric density estimation
- Dirichlet process mixture models

Similarity based / graph clustering

- Spectral clustering
- Affinity propagation

Cluster validation

Special topics

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

What is clustering? Problem and Notation

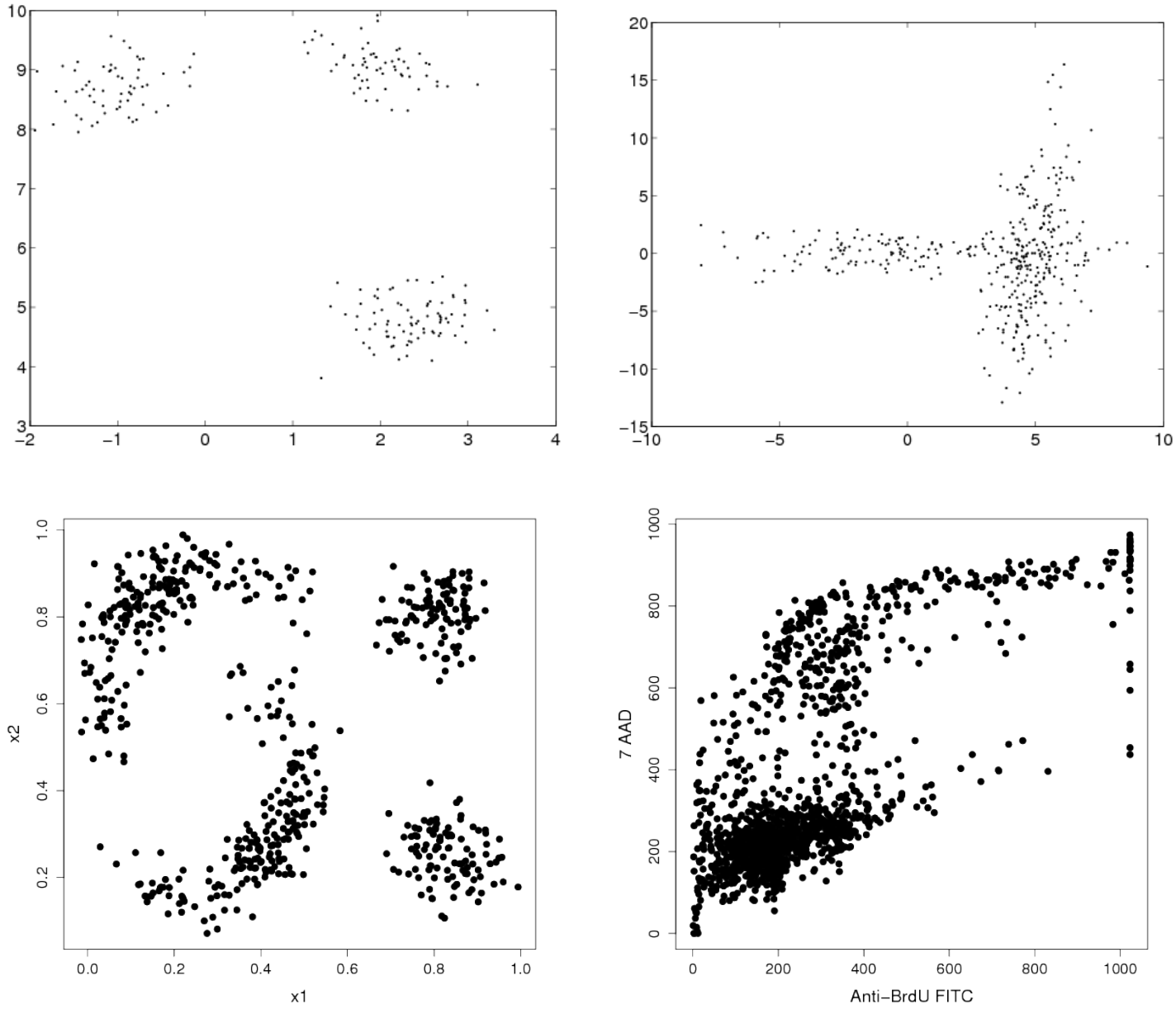
- **Informal definition** **Clustering** = Finding groups in data
- **Notation**

$\mathcal{D}$	=	$\{\mathbf{x}_1, \mathbf{x}_2, \ldots \mathbf{x}_n\}$ 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 [Nugent and Meila, 2010])

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	Cost based [hard]
(K known)	Model based [soft]
Non-parametric	Dirichlet process mixtures [soft]
(K determined	Information bottleneck [soft]
by algorithm)	Modes of distribution [hard]
	Gaussian blurring mean shift[Carreira-Perpinan, 2007] [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

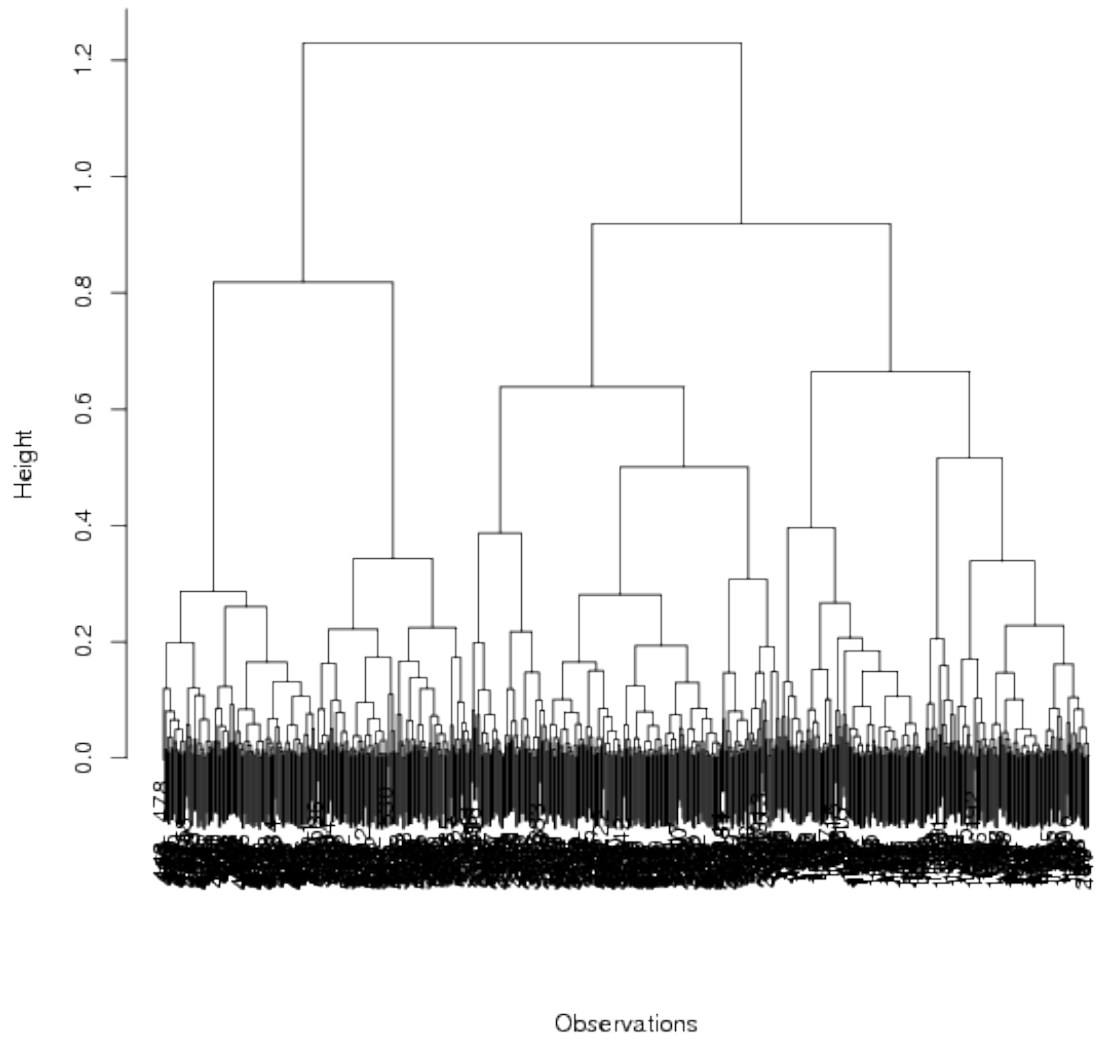
Single Linkage Clustering

Algorithm Single-Linkage

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

1. Construct the Minimum Spanning Tree (MST) of $\mathcal{D}$
2. Delete the largest $K-1$ edges

- **Cost** $\mathcal{L}(\Delta) = -\min_{k,k'} \text{distance}(C_k, C_{k'})$
  where $\text{distance}(A, B) = \underset{x \in A,\, y \in B}{\text{argmin}} ||x - y||$
- Running time $\mathcal{O}(n^2)$ one of the very few costs $\mathcal{L}$ that can be optimized in **polynomial** time
- Sensitive to outliers!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Observations

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** [Hochbaum and Shmoys, 1985] – 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-medians clustering

- **Cost** $\mathcal{L}(\Delta) = \sum_k \sum i \in C_k ||x_i - \mu_k||$ with $\mu_k \in \mathcal{D}$
  - (usually) assumes centers chosen from the data points (analogy to median)

Exercise Show that in 1D $\underset{\mu}{\operatorname{argmin}} \sum_i |x_i - \mu|$ is the median of $\{x_i\}$

  - optimizing this cost is NP-hard

  - has attracted a lot of interest in theoretical CS (general from called "Facility location"

Integer Programming Formulation of K-medians

- Define $d_{ij} = ||x_i - x_j||$,
  $u_{ij} = 1$ iff point i in cluster with center x_j (0 otherwise),
  $y_j = 1$ iff point j is cluster center (0 otherwise)

$$\begin{array}{lll} \min\limits_{u,y} & \sum_{ij} d_{ij} u_{ij} & \\ \text{s.t.} & \sum_j u_{ij} = 1 & \text{point } i \text{ is in exactly 1 cluster for all } i \\ & \sum_j y_j \leq k & \text{there are at most } k \text{ clusters} \\ & u_{ij} \leq y_j & \text{point } i \text{ can only belong to a center for all } i, j \end{array}$$

Linear Programming Relaxation of K-medians

- Define d_{ij}, $y_j = 1, u_{ij}$ as before, but $y_j, u_{ij} \in [0, 1]$

$$\textbf{(LP)} \quad \begin{array}{ll} \min\limits_{u,y} & \sum_{ij} d_{ij} u_{ij} \\ \text{s.t.} & \sum_j u_{ij} = 1 \\ & \sum_j y_j \leq k \\ & u_{ij} \leq y_j \end{array}$$

Algorithm K-Medians (variant of [Bradley and Mangasarian, 2005])

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

1. Solve (LP)

   obtain fractionary "centers" $y_{1:n}$ and "assignments" $u_{1:n,1:n}$
2. Sample K centers $\mu_1 \dots \mu_K$ by
   - $P[\mu_k = \text{pointj}] \propto y_j$ (without replacement)
3. Assign points to centers (deterministically)

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

- Guarantees (Agarwal)
  - **Given** tolerance ε, confidence δ, $K' = K(1 + \frac{1}{\varepsilon}) \ln \frac{n}{K}$, $\Delta_{K'}$ obtained by **K-medians** with K' centers

$$\mathcal{L}(\Delta_{K'}) \;\leq\; (1+\varepsilon)\mathcal{L}_K^{opt}$$

K-means clustering

Algorithm K-Means[Lloyd, 1982]

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)

$$\mu_k = \frac{1}{|C_k|} \sum_{i \in C_k} x_i \tag{1}$$

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  - if Δ doesn't change at iteration m it will never change after that
  - convergence in finite number of steps

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- 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

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

- 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

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

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

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

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

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

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

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

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

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

$$\mathcal{L}(\Delta) = \operatorname{trace} Z^T A Z \qquad \text{with } A_{ij} = ||x_i - x_j||^2 \tag{7}$$

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

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

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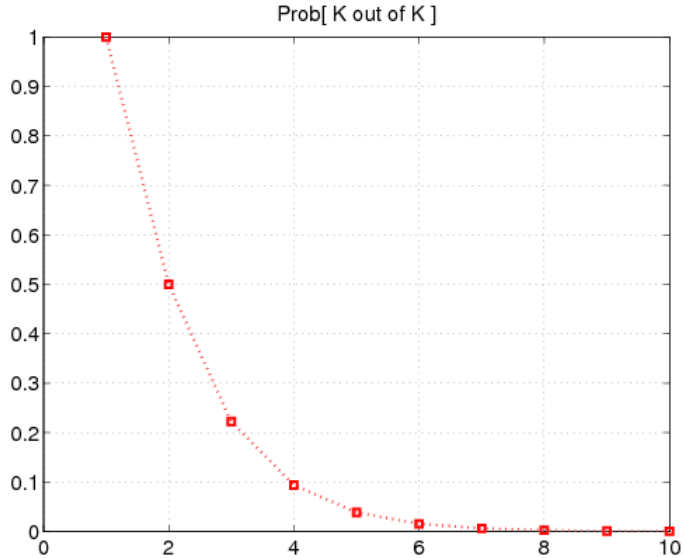
  What's wrong with chosing K data points at random?



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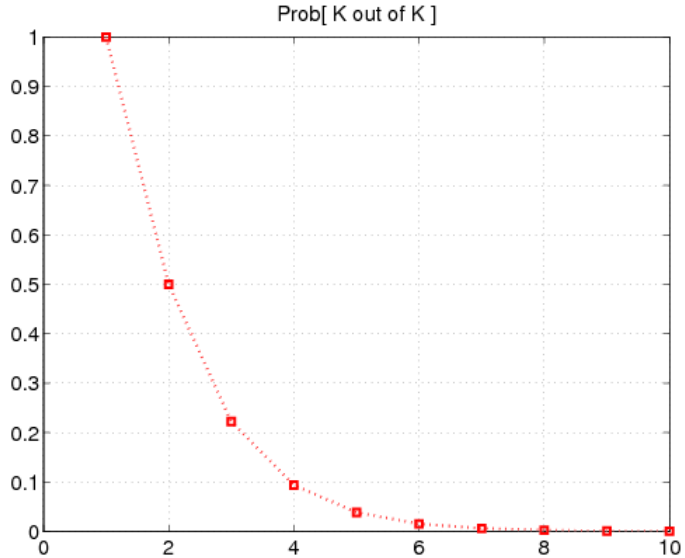

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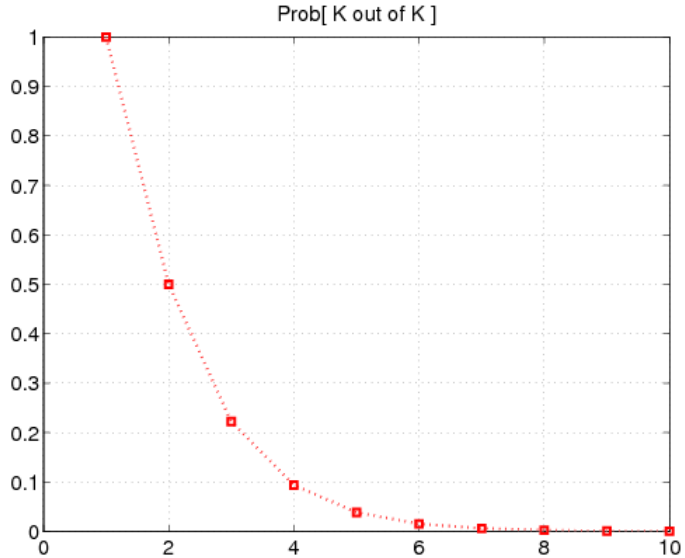

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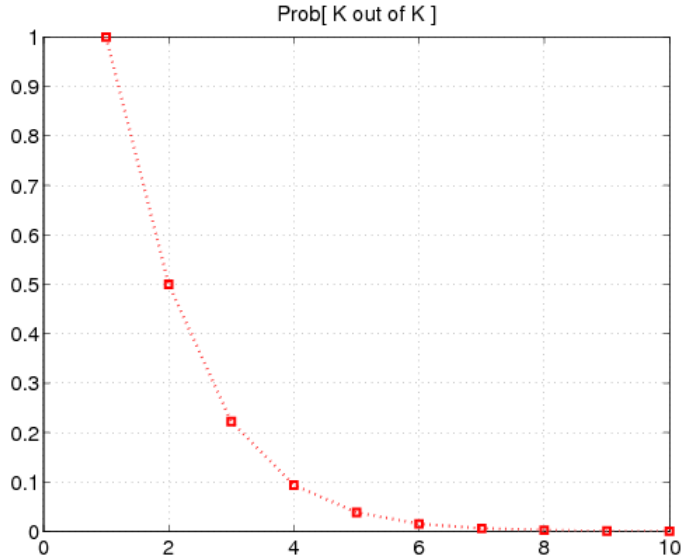

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- Idea 4: **k-means++** [] (randomized, theoretically backed approach to spread out centers)
- Idea 5: **"K-logK" Initialization** (start with enough centers to hit all clusters, then prune down to K)
  For EM Algorithm [], for K-means [Bubeck et al., 2009]

The "K-logK" initialization

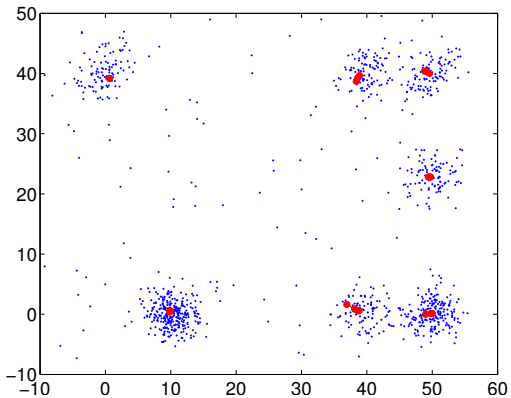
The K-logK Initialization (see also [Bubeck et al., 2009])

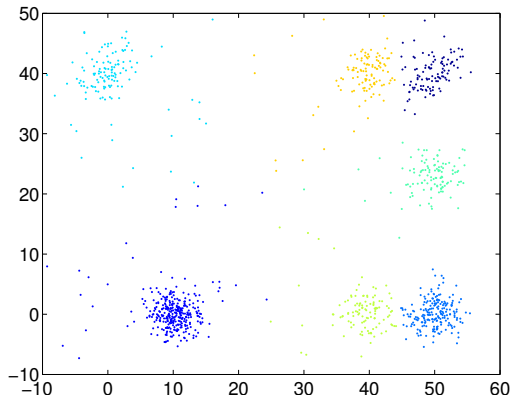
1. pick $\mu^0_{1:K'}$ at random from data set, where $K' = O(K \log K)$
   (this assures that each cluster has at least 1 center w.h.p)
2. run 1 step of K-means
3. remove all centers μ^0_k that have few points, e.g $|C_k| < \frac{n}{eK'}$
4. from the remaining centers select K centers by **Fastest First 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

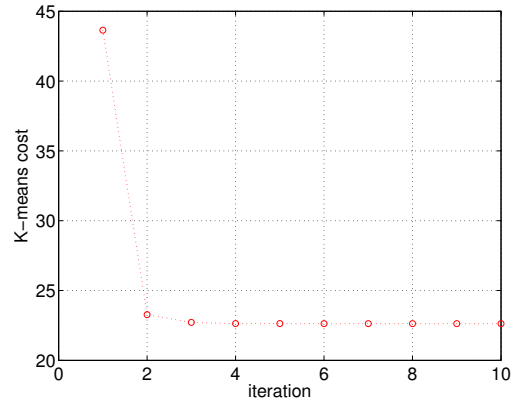
K-means clustering with K-logK Initialization

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

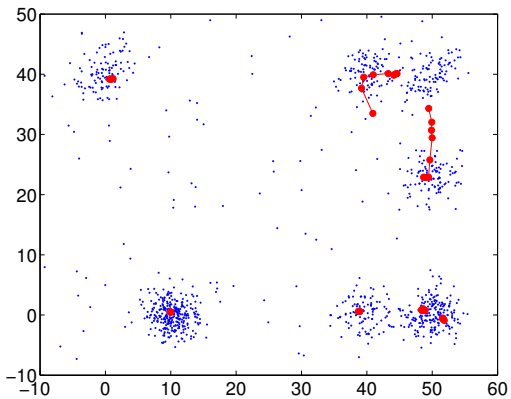
K-LOGK $K = 7,\ T = 100,\ n = 1100,\ c = 1$

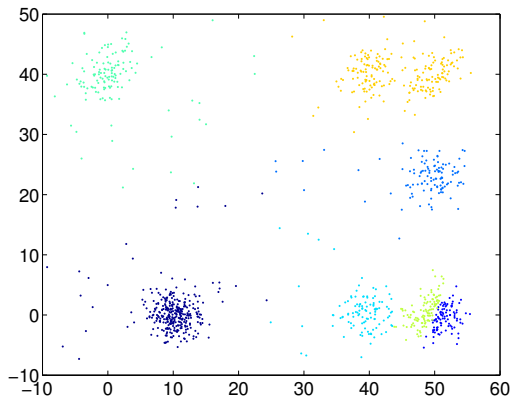


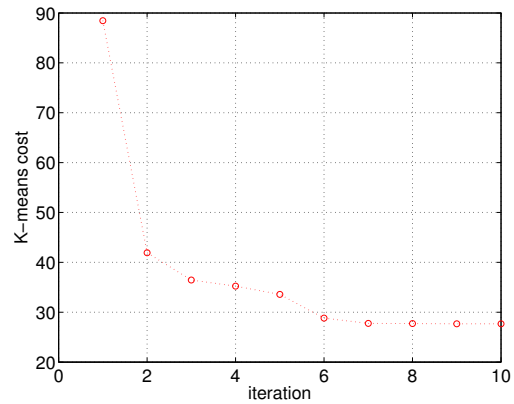




NAIVE $K = 7\ T = 100,\ n = 1100$







Coresets approach to K-medians and K-means

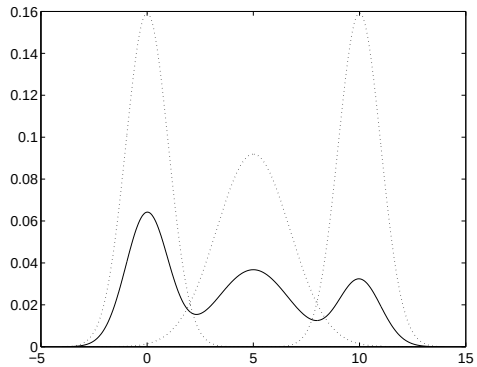
- A weighted subset of $\mathcal{D}$ is a (K, ε) **coreset** iff for any $\mu_{1:K}$,

$$|\mathcal{L}(\mu_{1:K}, A) - \mathcal{L}(\mu_{1:K}; \mathcal{D})| \leq \varepsilon \mathcal{L}(\mu_{1:K}; \mathcal{D})$$

- Note that the size of A is not K
- Finding a coreset (fast) lets use find fast algorithms for clustering a large $\mathcal{D}$
  - "fast" $=$ linear in n, exponential in ε^{-d}, polynomial in K
- **Theorem**[Har-Peled and Mazumdar, 2004],Theorem 5.7
  One can compute an $(1+\varepsilon)$-approximate K-median of a set of n points in time $\mathcal{O}(n + K^5 \log^9 n + gK^2 \log^5 n)$ where $g = e^{[C/\varepsilon \log(1+1/\varepsilon)]^{d-1}}$ (where d is the dimension of the data)
- **Theorem**[Har-Peled and Mazumdar, 2004],Theorem 6.5
  One can compute an $(1+\varepsilon)$-approximate K-means of a set of n points in time $\mathcal{O}(n + K^5 \log^9 n + K^{K+2} \varepsilon^{-(2d+1)} \log^{K+1} n \log^K \frac{1}{\varepsilon})$.

Model based clustering: Mixture models

Mixture in 1D

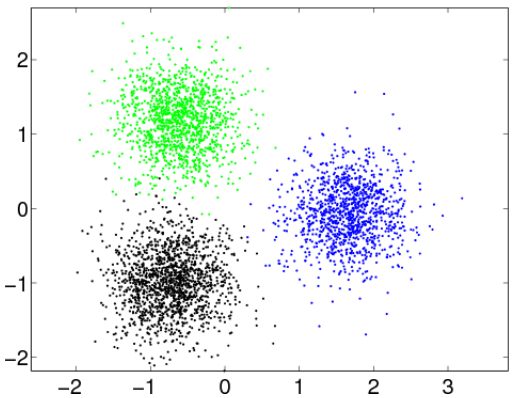


- The **mixture density**

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

- $f_k(x)$ = 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**, $\sum_k = 1^K \pi_k = 1, \quad \pi_k \geq 0.$
- **model parameters** $\theta = (\pi_{1:K}, \mu_{1:K}, \Sigma_{1:K})$

Mixture in 2D



Model based clustering: Mixture models

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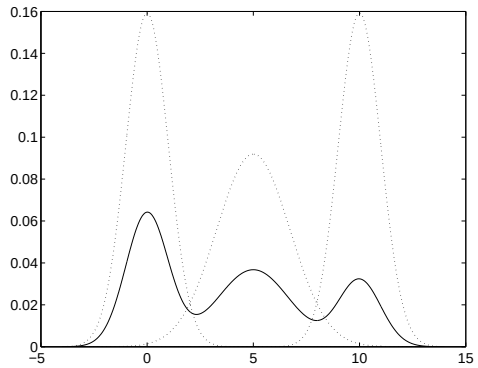

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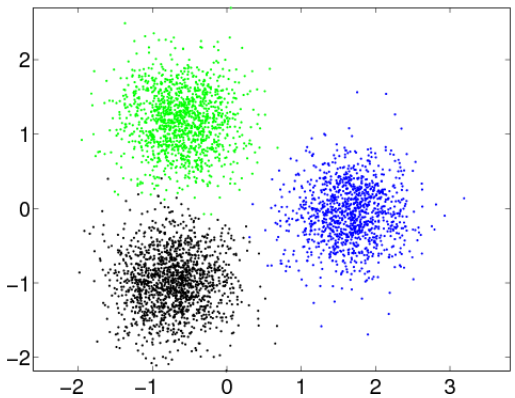
- **model parameters** $\theta = (\pi_{1:K}, \mu_{1:K}, \Sigma_{1:K})$

Mixture in 2D



- 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 $\theta \longrightarrow \theta^{ML}$ [McLachlan and Krishnan, 1997]
- the E and M steps can be seen as projections [Neal and Hinton, 1998]

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

Probablistic alternate projection view of EM[Neal and Hinton, 1998]

- 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

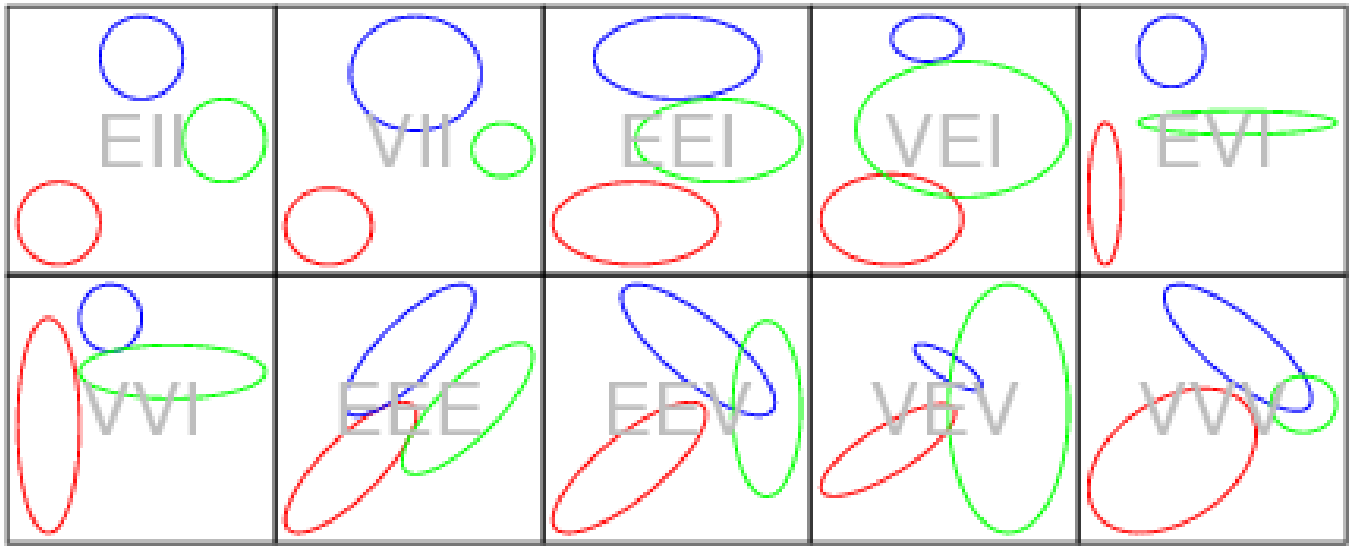
The M step in special cases

- 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



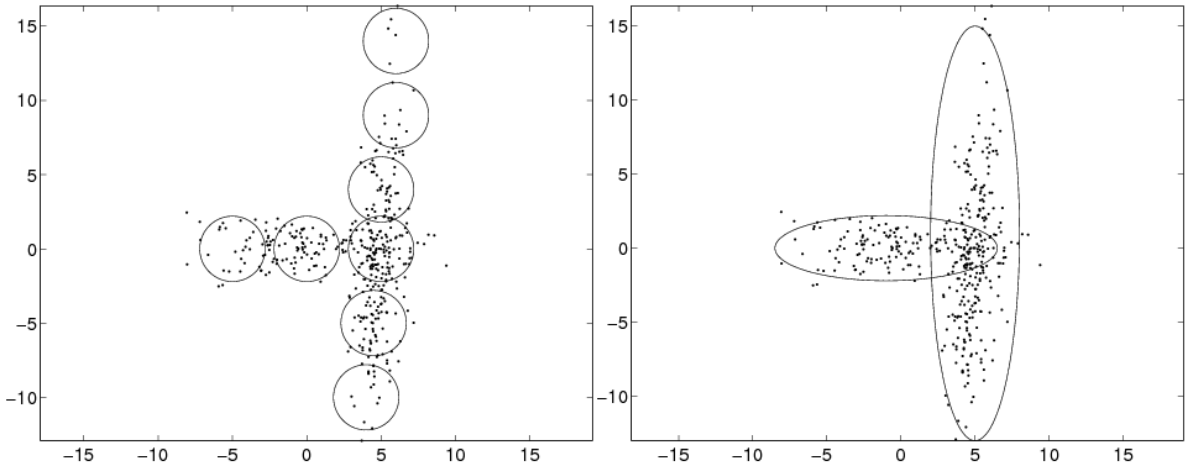
More special cases [Banfield and Raftery, 1993] introduce the following description for a covariance matrice in terms of *volume, shape, alignment with axes* (=determinant, trace, e-vectors). The letters below mean: I=unitary (shape, axes), E=equal (for all k), V=unequal

- 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 [Nugent and Meila, 2010])

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 [Vempala and Wang, 2004]
  - 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)

The Vempala-Wang algorithm[Vempala and Wang, 2004]

Idea

Let $\mathcal{H} = \mathrm{span}(\mu_{1:K})$

Projecting data on $\mathcal{H}$

- $\approx$ preserves $||x_i - x_j||$ if $k(i) \neq k(j)$
- $\approx$ reduces $||x_i - x_j||$ if $k(i) = k(j)$
- density at μ_k increases

(Proved by Vempala & Wang, 2004[Vempala and Wang, 2004]) $\mathcal{H} \approx K$-th principal subspace of data

Algorithm Vempala-Wang (sketch)

1. Project points $\{x_i\} \in \mathbb{R}^d$ on $K-1$-th principal subspace $\Rightarrow$ $\{y_i\} \in \mathbb{R}^K$
2. do distance-based "harvesting" of clusters in $\{y_i\}$

Other "CS" algorithms I

- [Dasgupta, 2000] round, equal sized Gaussian, random projection
- [Arora and Kannan, 2001] arbitrary shaped Gaussian, distances
- [Achlioptas and McSherry, 2005] 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 $u, v \in V$,

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

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
- [Dasgupta and Gupta, 2002] 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 [Dasgupta and Schulman, 2007]

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 $\Longrightarrow \{\pi_k^2, \mu_k^2, \sigma_k^2\}_{k=1:K}$

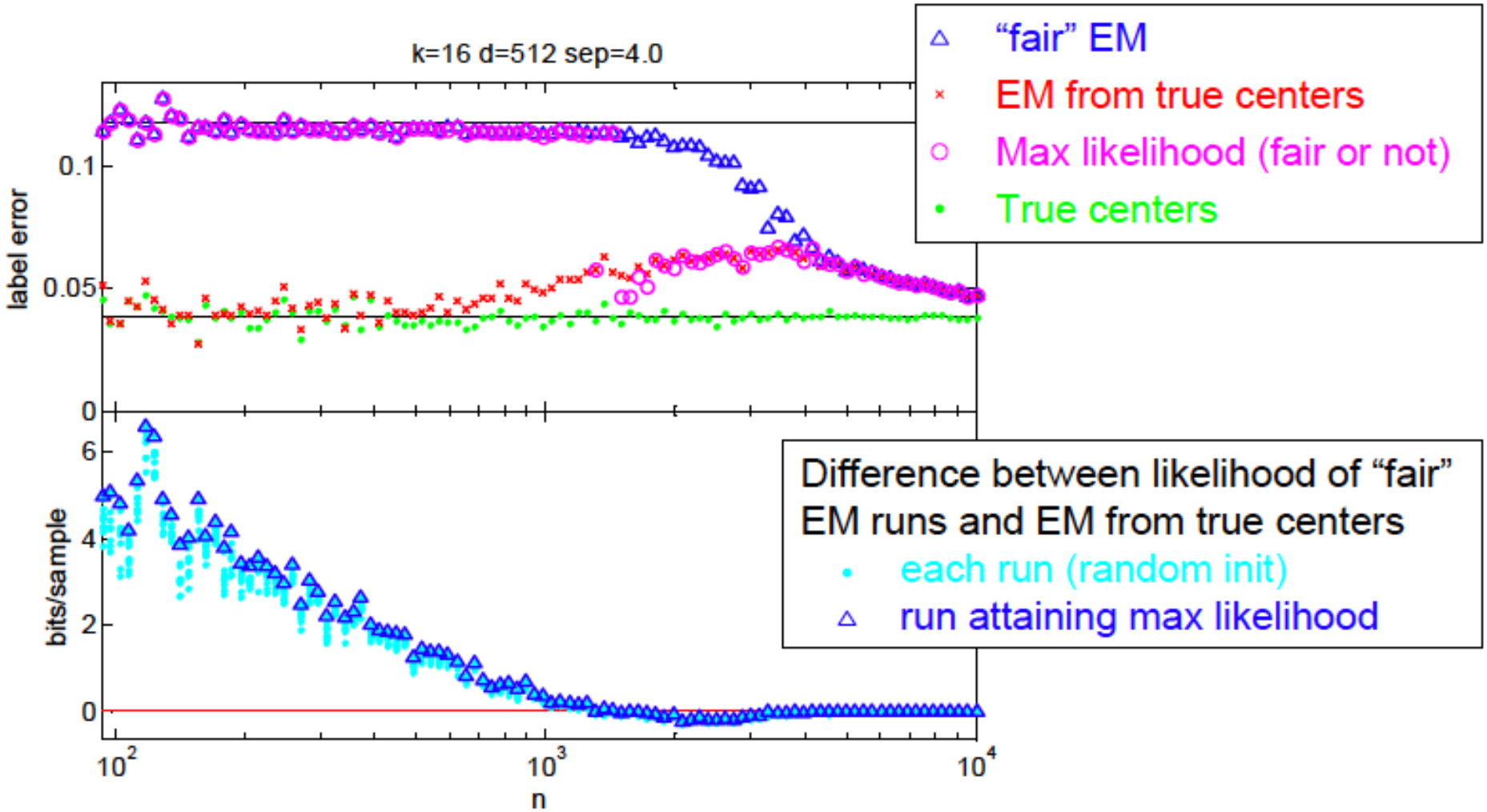
Theorem For any $\delta, \varepsilon > 0$ if d large, n large enough, separation $C \geq d^{1/4}$ the **Two step EM** algorithm obtains centers μ_k so that

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

Experimental exploration [Srebro et al., 2006] I

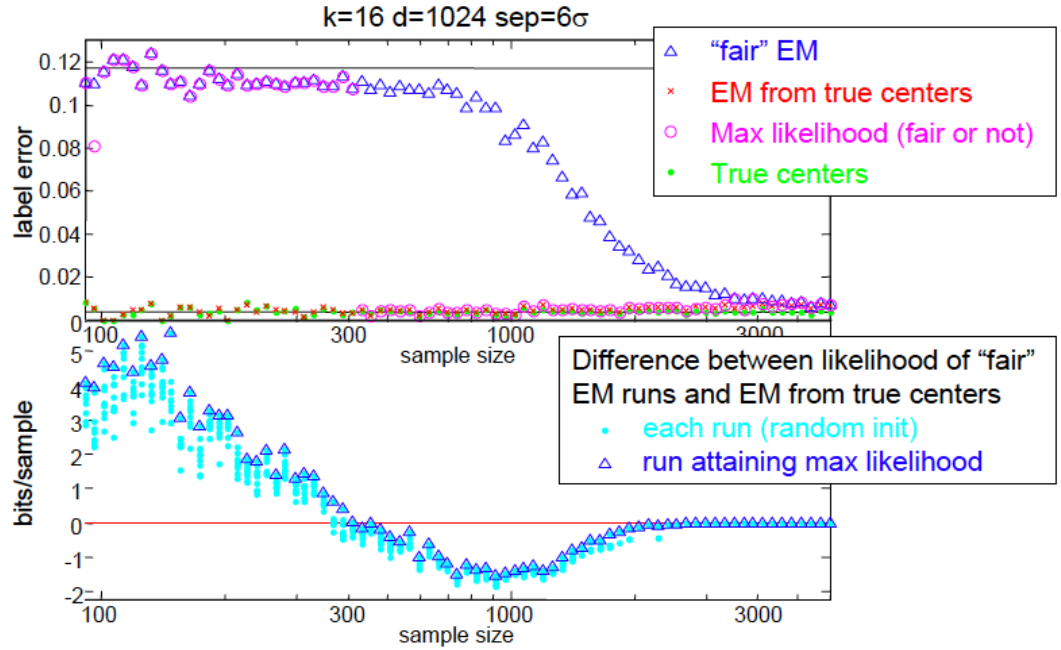
- High d
- True model: centers μ_k^* at corners of hypercube, $\Sigma_k^* = \sigma I_d$ spherical equal covariances, $\pi_k^* = 1/K$
- n, K, separation variable
- Algorithm: EM with Power initialization and projection on $(K-1)$-th principal subspace

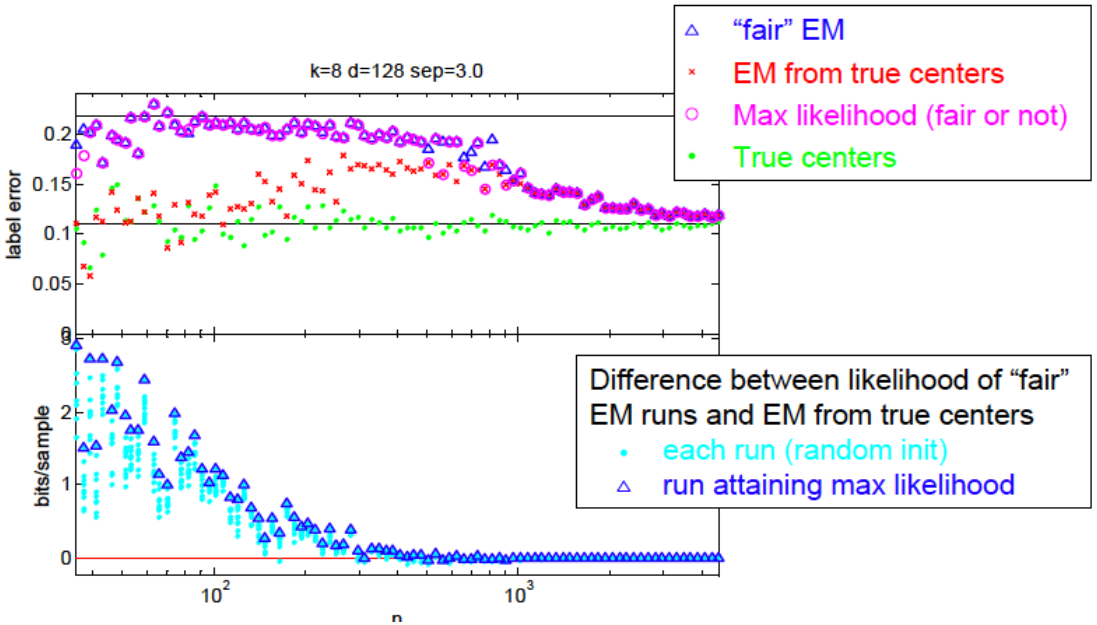
Experimental exploration [Srebro et al., 2006] II



figures from [Srebro et al., 2006]

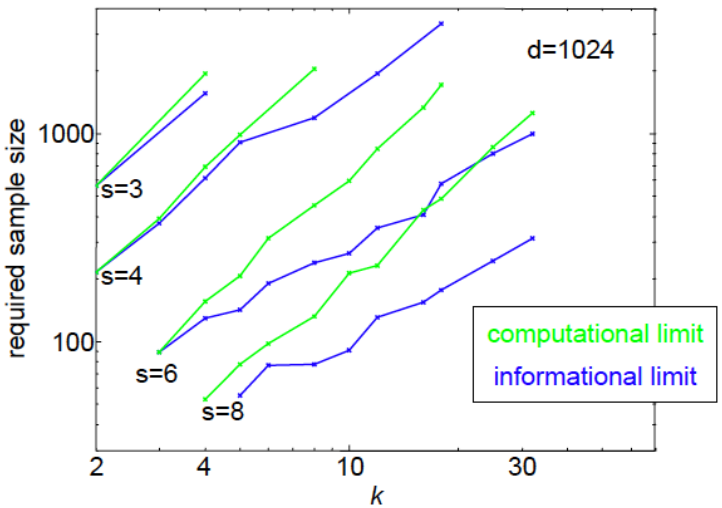
Experimental exploration [Srebro et al., 2006] III





Experimental exploration [Srebro et al., 2006] IV

- Practical limits vs theoretical limits



$n \propto k^{1.5} - k^{1.6}$ for all d, separation

figures from [Srebro et al., 2006]

Dasgupta 1999	$s > 0.5d^{1/2}$	$n = \Omega(k^{\log^2 1/\delta})$	Random projection, then mode finding
Dagupta Schulamn 2000	$s = \Omega(d^{1/4})$ (large d)	$n = poly(k)$	2 round EM with $\Theta(k \cdot \log k)$ centers
Arora Kannan 2001	$s = \Omega(d^{1/4} \log d)$		Distance based
Vempala Wang 2004	$s = \Omega(k^{1/4} \log dk)$	$n = \Omega(d^3k^2\log(dk/s\delta))$	Spectral projection, then distances

General mixture of Gaussians:

[Kannan Salmasian Vempala 2005] $s=\Omega(k^{5/2}\log(kd))$, $n=\Omega(k^2d\cdot\log^5(d))$

[Achliopts McSherry 2005] $s>4k+o(k)$, $n=\Omega(k^2d)$

Selecting K

- Run clustering algorithm for $K = K_{min} : K_{max}$
  - obtain $\Delta_{K_{min}}, \ldots \Delta_{K_{max}}$ or $\gamma_{K_{min}}, \ldots \gamma_{K_{max}}$
  - choose best Δ_K (or γ_K) from among them
- Typically increasing $K \Rightarrow$ cost $\mathcal{L}$ decreases
  - ($\mathcal{L}$ cannot be used to select K)
  - Need to "penalize" $\mathcal{L}$ with function of number parameters

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

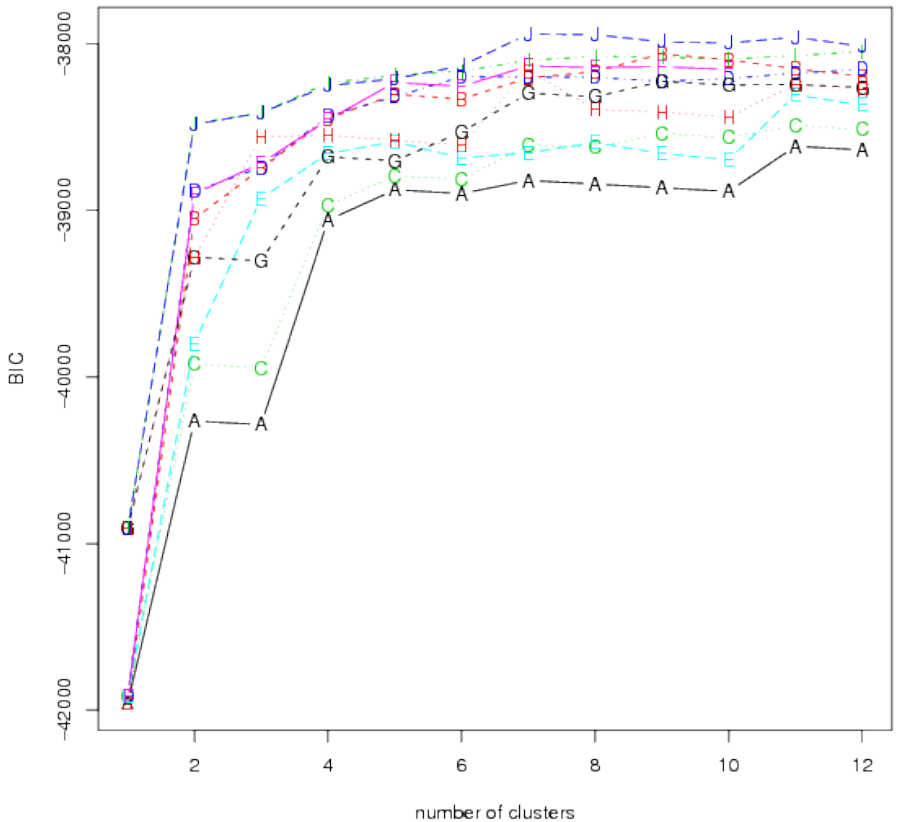
$$\#\theta_K = \underbrace{K-1}_{\pi_{1:K}} + \underbrace{Kd}_{\mu_{1:K}} + \underbrace{Kd(d-1)/2}_{\Sigma_{1:K}}$$

- define

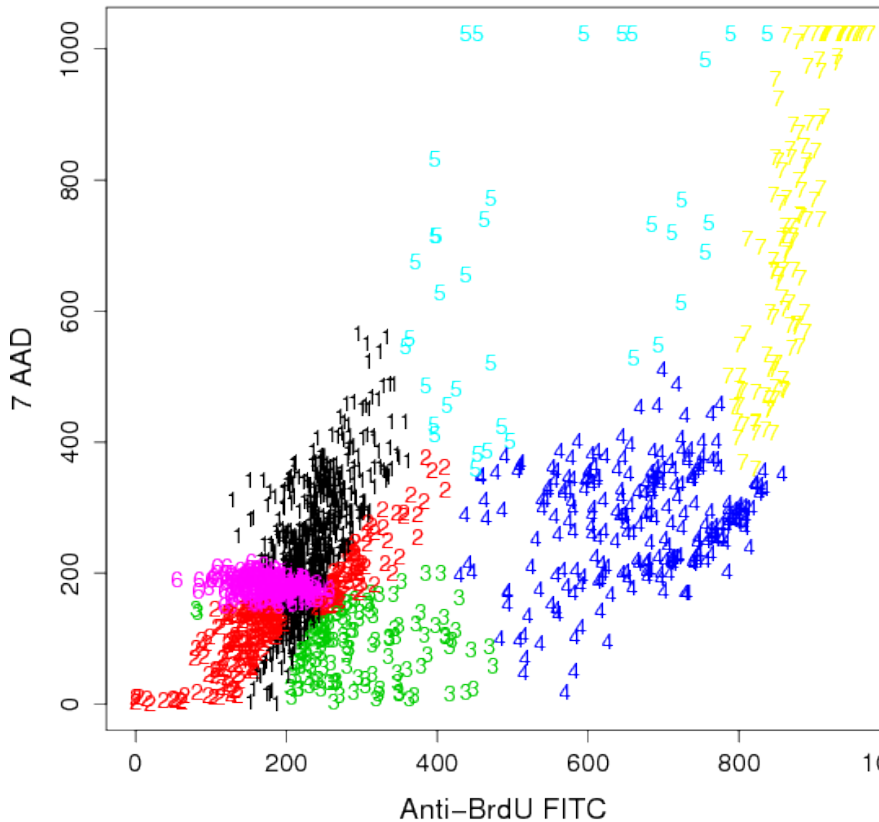
$$BIC(\theta_K) = l(\theta_K) - \frac{\#\theta_K}{2} \ln n$$

- **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)

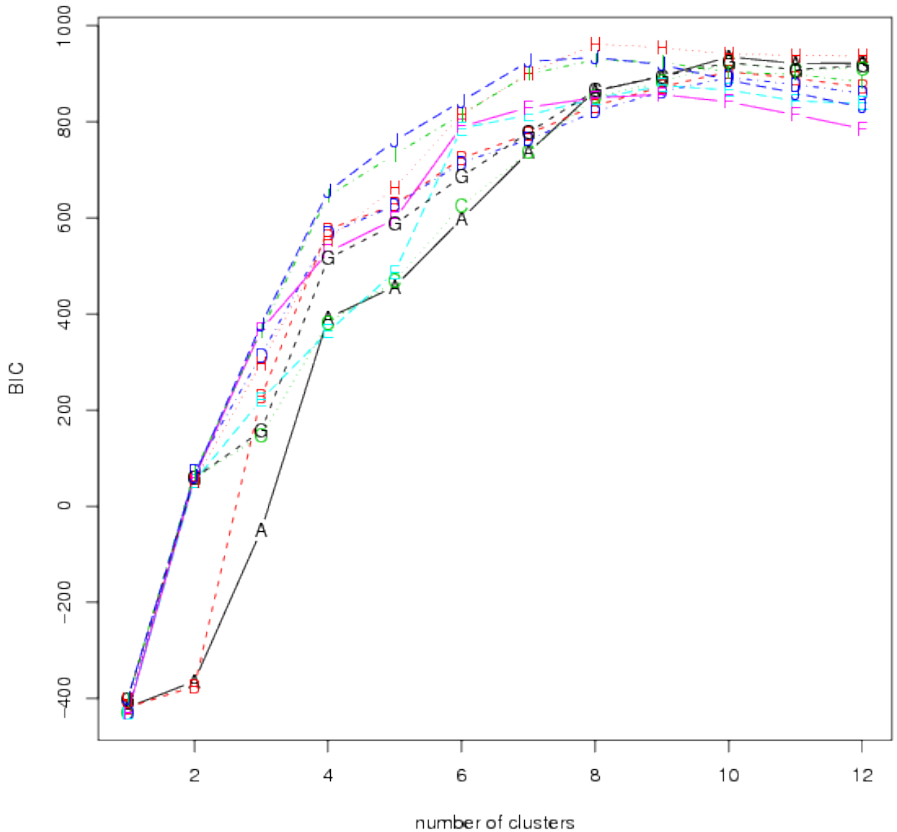


EEV, 8 Cluster Solution

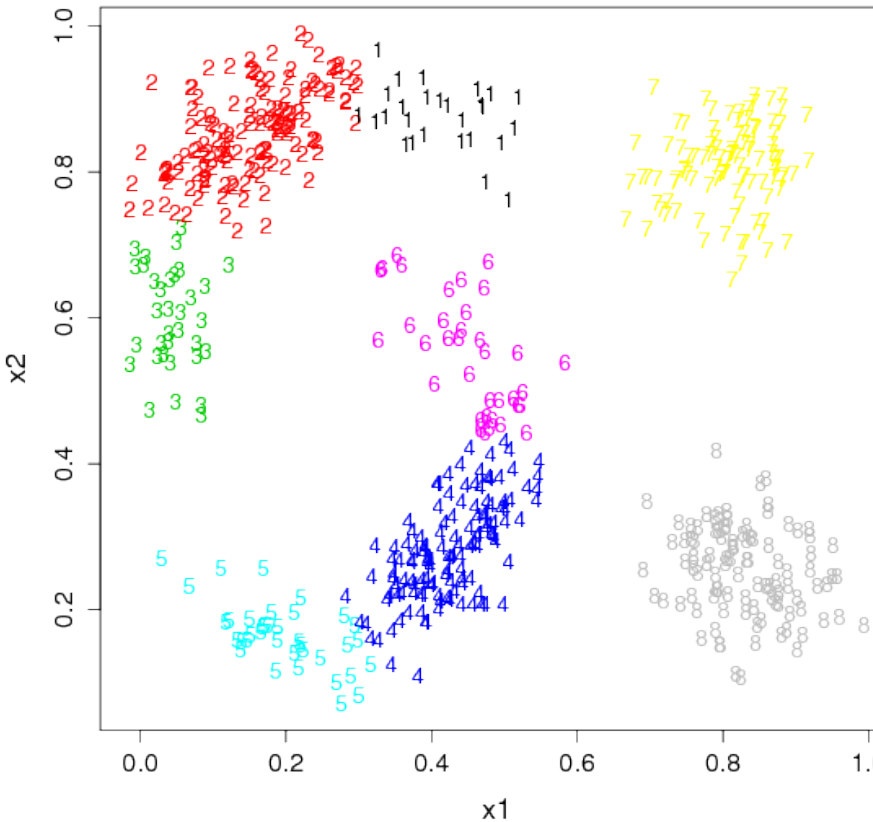


(from [Nugent and Meila, 2010])

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 [Nugent and Meila, 2010])

Selecting K for hard clusterings

- based on statistical testing: the **gap** statistic (Tibshirani, Walther, Hastie, 2000)
- **X-means** [Pelleg and Moore, 2000] heuristic: splits/merges clusters based on statistical tests of Gaussianity
- Stability methods

The gap statistic

Idea

- for some cost $\mathcal{L}$ compare $\mathcal{L}(\Delta_K)$ with its expected value under a null distribution
  - choose null distribution to have no clusters
    - Gaussian (fit to data)
    - uniform with convex support
    - uniform over K_0 principal components of data
  - null value $= E_{P_0}[\mathcal{L}_{K,n}]$ the expected value of the cost of clustering n points from P_0 into K clusters
- the **gap**

$$g(K) = E_{P_0}[\mathcal{L}_{K,n}] - \mathcal{L}(\Delta_K) = \mathcal{L}_K^0 - \mathcal{L}(\Delta_K)$$

- choose K^* corresponding to the largest gap
- nice: it can also indicate that data has no clusters

Practicalities

- $\mathcal{L}_K^0 = E_{P_0}[\mathcal{L}_{K,n}]$ can rarely be computed in closed form (when P_0 very simple)
- otherwise, estimate $\mathcal{L}_K^0$ be Monte-Carlo sampling i.e generate B samples from P_0 and cluster them
- if sampling, variance s_K^2 of estimate $\hat{\mathcal{L}}_K^0$ must be considered s_K^2 is also estimated from the samples
- selection rule: $K^* =$ smallest K such that $g(K) \geq g(K+1) - s_{K+1}$
- favored $\mathcal{L}^V(\Delta) = \sum_k \frac{1}{|C_k|} \sum_{i \in C_k} ||x_i - \mu_k||^2 \approx$ sum of cluster variances

Stability methods for choosing K

- like bootstrap, or crossvalidation
- **Idea** (implemented by [Ben-Hur et al., 2002])

  for each K
  1. perturb data $\mathcal{D} \rightarrow \mathcal{D}'$
  2. cluster $\mathcal{D}' \rightarrow \Delta'_K$
  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 YET supported by theory** . . . see [von Luxburg, 2009] for a summary of the area

A stability based method for model-based clustering

- **The algorithm of [Lange et al., 2004]**
  1. divide data into 2 halves $\mathcal{D}_1$, $\mathcal{D}_2$ at random
  2. cluster (by EM) $\mathcal{D}_1 \rightarrow \Delta_1, \theta_1$
  3. cluster (by EM) $\mathcal{D}_2 \rightarrow \Delta_2, \theta_2$
  4. cluster $\mathcal{D}_1$ using $\theta_2 \rightarrow \Delta_1'$
  5. compare Δ_1, Δ_1'
  6. repeat B times and average the results

  - repeat for each K
  - select K where Δ_1, Δ_1' are closest on average (or most times)

Clustering with outliers

- What are outliers?
- let p = proportion of outliers (e.g 5%-10%)
- Remedies
  - mixture model: introduce a $K+1$-th cluster with large (fixed) Σ_{K+1}, bound Σ_k away from 0
  - K-means and EM
    - **robust** means and variances
      e.g eliminate smallest and largest $pn_k/2$ samples in mean computation (**trimmed mean**)
    - K-medians [Charikar and Guha, 1999]
    - replace Gaussian with a heavier-tailed distribution (e.g. Laplace)
  - single-linkage: do not count clusters with $< r$ points

Is K meaningful when outliers present?

- alternative: non-parametric clustering

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

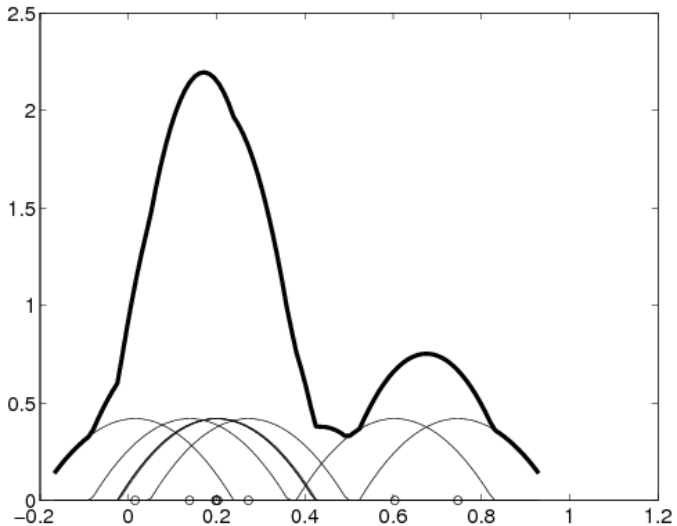
- peak finding algorithms Mean-shift algorithms
- level sets based algorithms
  - Nugent-Stuetzle, Support Vector clustering
- Information Bottleneck [Tishby and Slonim, 2000]

Kernel density estimation

Input
- data $\mathcal{D} \subseteq \mathbb{R}^d$
- **Kernel** function $K(z)$
- parameter **kernel width** h (is a **smoothness parameter**)

Output $f(x)$ a **probability density** over $\mathbb{R}^d$

$$f(x) = \frac{1}{Nh^d} \sum_{i=1}^{n} K\left(\frac{x - x_i}{h}\right)$$



- f is sum of Gaussians centered on each x_i
- f is smoother (less variation) if h larger
- **caveat:** dimension d can't be too large

The kernel function

- Example $K(z) = \frac{1}{(2\pi)^{d/2}} e^{-||z||^2/2}$, $z \in \mathbb{R}^d$ is the Gaussian kernel
- In general
  - $K()$ should represent a density on $\mathbb{R}^d$, i.e $K(z) \geq 0$ for all z and $\int K(z)dz = 1$
  - $K()$ symmetric around 0, decreasing with $||z||$
- In our case, K must be differentiable

Mean shift algorithms

Idea find points with $\nabla f(x) = 0$

Assume $K(z) = e^{-||z||^2/2}/\sqrt{2\pi}$ Gaussian kernel

$$\nabla f(x) = -\frac{1}{Nh^d} \sum_{i=1}^{n} K(\frac{x - x_i}{h})(\mathbf{x} - x_i)/h$$

Local max of f is solution of implicit equation

$$x = \underbrace{\frac{\sum_{i=1}^{n} x_i K(\frac{x-x_i}{h})}{\sum_{i=1}^{n} K(\frac{x-x_i}{h})}}_{\text{the } \mathbf{mean\ shift} m(x)}$$

Algorithm Simple Mean Shift

Input Data $\mathcal{D} = \{x_i\}_{i=1:n}$, kernel $K(z)$, h

1. for $i = 1 : n$
   - 1.1 $x \leftarrow x_i$
   - 1.2 iterate $x \leftarrow m(x)$ until convergence to m_i
2. group points with same m_i in a cluster

Remarks

- mean shift iteration guaranteed to converge to a max of f
- computationally expensive
- a faster variant...

Algorithm Mean Shift (Comaniciu-Meer)

Input Data $\mathcal{D} = \{x_i\}_{i=1:n}$, kernel $K(z)$, h

1. select q points $\{x_j\}_{j=1:q} = \mathcal{D}_q \subseteq \mathcal{D}$ that cover the data well
2. for $j \in \mathcal{D}_q$
   - 2.1 $x \leftarrow x_j$
   - 2.2 iterate $x \leftarrow m(x)$ until convergence to m_j
3. group points in $\mathcal{D}_q$ with same m_j in a cluster
4. assign points in $\mathcal{D} \setminus \mathcal{D}_q$ to the clusters by the **nearest-neighbor** method

$$k(i) = k(\operatorname*{argmin}_{j \in \mathcal{D}_q} ||x_i - x_j||)$$

Gaussian blurring mean shift

Idea

- like **Simple Mean Shift** but points are shifted to new locations
- the density estimate f changes
- becomes concentrated around peaks very fast

Algorithm Gaussian Blurrring Mean Shift (GBMS)

Input Data $\mathcal{D} = \{x_i\}_{i=1:n}$, Gaussian kernel $K(z)$, h

1. Iterate until STOP
   - 1.1 for $i = 1 : n$ compute $m(x_i)$
   - 1.2 for $i = 1 : n$, $x_i \leftarrow m(x_i)$

Remarks

- all x_i converge to a single point

  $\Rightarrow$ need to stop before convergence

Empirical stopping criterion [Carreira-Perpinan, 2007]

- define $e_i^t = ||x_i^t - x_i^{t-1}||$ the change in x_i at t
- define $H(e^t)$ the **entropy** of the **histogram** of $\{e_i^t\}$
- STOP when $\sum_{i=1}^n e_i^t/n <$`tol` OR $|H(e^t) - H(e^{t-1})| <$`tol`'

Convergence rate If true f Gaussian, convergence is **cubic**

$$||x_i^t - x^*|| \leq C||x_i^{t-1} - x^*||^3$$

very fast!!

Algorithm Nugent-Stuetzle

Input Data $\mathcal{D} = \{x_i\}_{i=1:n}$, kernel $K(z)$

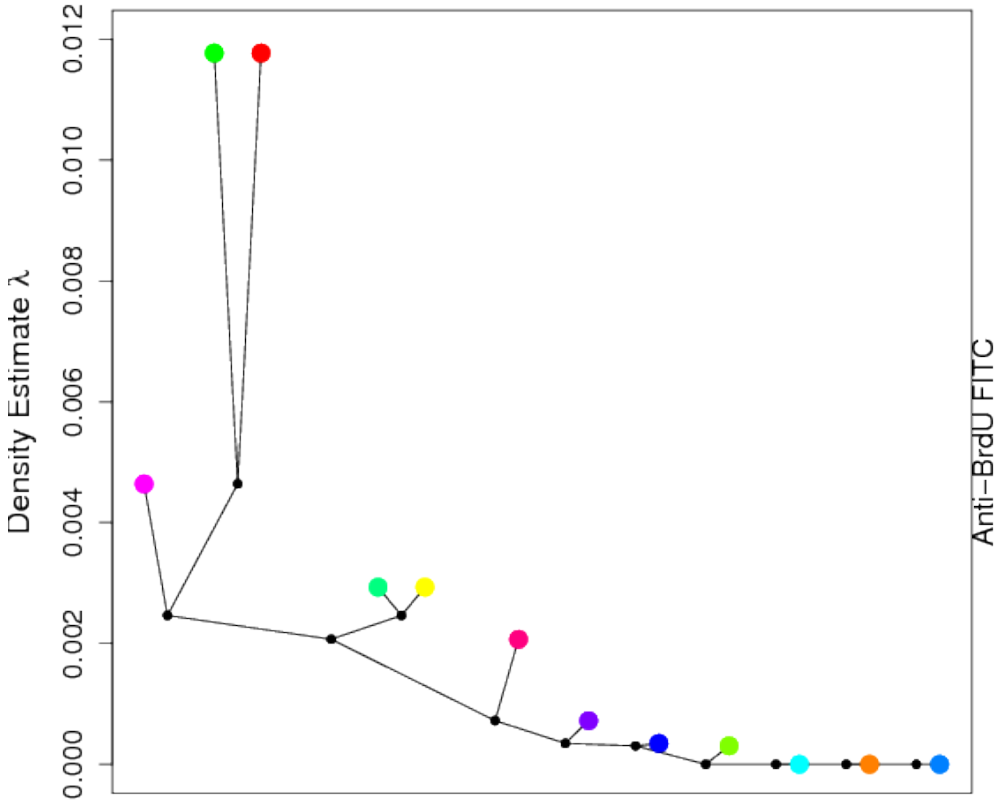
1. Compute KDE $f(x)$ for chosen h
2. for levels $0 < l_1 < l_2 < \ldots < l_r < \ldots < l_R \geq \sup_x f(x)$
   - 2.1 find **level set** $L_r = \{x \mid f(x) \geq l_r\}$ of f
   - 2.2 if L_r **disconnected** then each connected component is a cluster $\rightarrow (C_{r,1}, C_{r,2}, \ldots C_{r,K_r})$

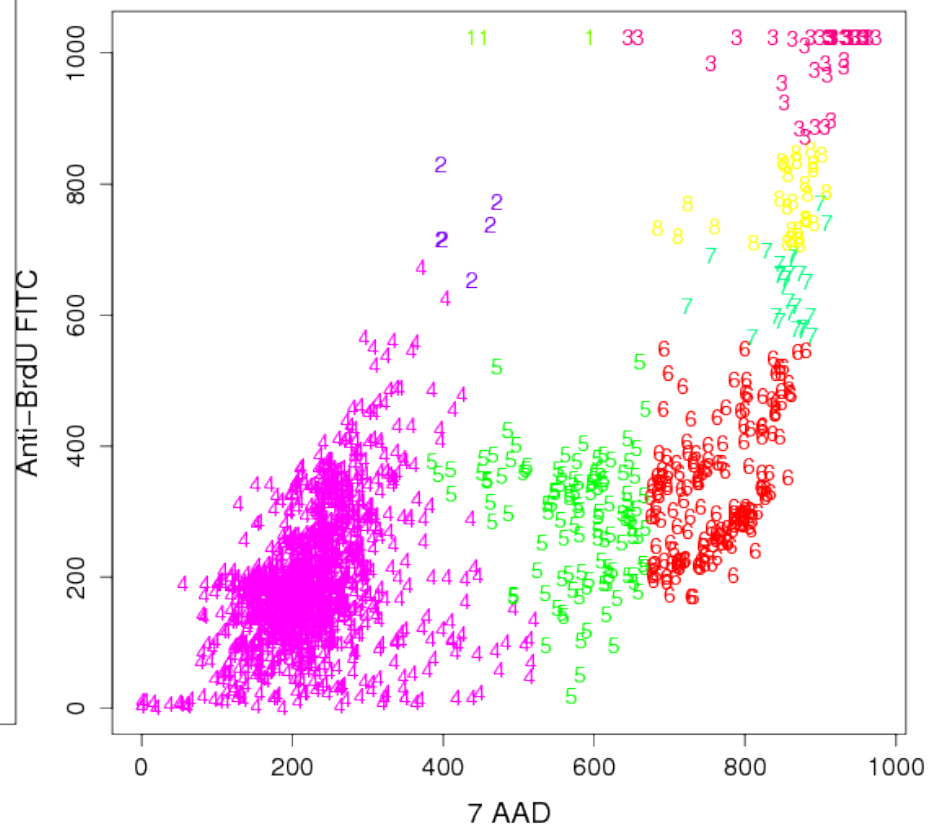
Output clusters $\{(C_{r,1}, C_{r,2}, \ldots C_{r,K_r})\}_{r=1:R}$

Remarks

- every cluster $C_{r,k} \subseteq$ some cluster $C_{r-1,k'}$
- therefore output is hierarchical clustering
- some levels can be pruned (if no change, i.e. $K_r = K_{r-1}$)
- algorithm can be made recursive, i.e. efficient
- finding level sets of f tractable only for $d = 1, 2$
- for larger d, $L_r = \{x_i \in \mathcal{D} \mid f(x_i) \geq l_r\}$
- to find connected components
  - for $i \neq j \in L_r$
    if $f(tx_i + (1-t)x_j) \geq l_r$ for $t \in [0, 1]$
    then $k(i) = k(j)$
- confidence intervals possile by resampling

Cluster tree with 13 leaves (8 clusters, 5 artifacts)





(from [Nugent and Meila, 2010])

Chaudhuri-Dasgupta Algorithm

- Uses k-**nearest neighbor** graphs (filtration)
- Parameters k (nearest neigbhors) and $\alpha \in [1, 2]$
- for $r \geq 0$, $G_r = (V_r, E_r)$ with
  - $x_i \in V_r$ iff **distance to k-nn of x_i** $\leq r$
  - $(x_i, x_j) \in E_r$ iff $||x_i - x_j|| \leq \alpha r$

Consistency Theorem For any ϵ (separation parameter) and δ (confidence), $\alpha \in [\sqrt{2}, 2]$ (graph density), if $k = C \log^2(1/\delta) \frac{d \log n}{\epsilon^2}$
for any two clusters C, C' in cluster tree, there exists a level r so that $C \cap \mathcal{D}, C' \cap \mathcal{D}$ are clusters at level r

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- r depends on $\lambda =$"bridge" between C, C' (and $\sigma > 0$ "tube" width)

$$r^d \omega_d \lambda = \frac{k}{\mathbf{n}} + \ldots \textit{confidence term}$$

- it follows that the needed sample size n at level λ

$$n = \mathcal{O}\left(\frac{d}{\lambda \epsilon^2 (\sigma/2)^d \omega_d} \log \frac{d}{\lambda \epsilon^2 (\sigma/2)^d \omega_d} \right)$$

- this **sample complexity** n is almost tight
- for $\alpha < \sqrt{2}$ sample complexity is exponential in d

- New results **[Kent, B. P., Rinaldo, A. and Verstynen, T. 2013]**

- Remark: algorithm(s) can be applied in any metric space

Support Vector (SV) clustering

Idea same as for Nugent-Stuetzle, but use **kernelized density estimator** instead of KDE

Algorithm SV

Input data $\mathcal{D}$, parameters q kernel width, $p \in (0,1)$ proportion of outliers

1. construct a 1-class SVM with parameters q, $C = 1/np$
   this is equivalent to enclosing the data in a sphere in feature space
   for any x its distance from center of sphere is

$$R^2(x) = K(x,x) - 2\sum_j \alpha_j K(x,x_j) + \sum_{i,j} K(x_i,x_j)$$

   for x_i support vector, $R(x_i) = R$ (same for all)
2. for all pairs $i,j = 1:n$
   - i,j in same cluster if segment $[i,j]$ is within sphere with radius R in feature space
   - practically, test if $R(tx_i + (1-t)x_j) < R$ for t on a grid over [0,1]

Remarks

- the **kernel** used by SV is $K(x, x') = e^{-q||x-x'||^2}$
- q controls boundary smoothness
- SV's lie on cluster boundaries, "margin error" points lie outside clusters (are outliers)
- SV theory $\frac{\text{margin errors}}{n} \rightarrow \frac{1}{nC} = p$ for large n
- hence p controls the proportion of outliers
- p, q together control K
  p larger, q smaller $\Rightarrow$ K smaller

The Dirichlet distribution

- $Z \in \{1 : r\}$ a discrete random variable, let $\theta_j = P_z(j)$, $j = 1, \ldots r$.
- **Multinomial distribution** Probability of i.i.d. sample of size N from P_z

$$P(z^{1,\ldots N}) = \prod_{j=1}^{r} \theta_j^{N_j}$$

  where $N_j = \#$the value j is observed, $j = 1, \ldots r$
- $N_{1:r}$ are the **sufficient statistics** of the data.
- The **Dirichlet distribution** is defined over domain of $\theta_{1,\ldots r}$, with real parameters $N'_{1,\ldots r} > 0$ by

$$D(\theta_{1,\ldots r}; N'_{1,\ldots r}) = \frac{\Gamma(\sum_j N'_j)}{\prod_j \Gamma(N'_j)} \prod_j \theta_j^{N'_j - 1}$$

  where $\Gamma(p) = \int_0^\infty t^{p-1} e^{-t} dt$.

Dirichlet process mixtures

- Model-based
- generalization of mixture models to
  - infinite K
  - Bayesian framework
- denote θ_k = parameters for component f_k
- assume $f_k(x) \equiv f(x, \theta_k) \in \{f(x, \theta)\}$
- assume prior distributions for parameters $g_0(\theta)$
- prior with hyperparameter $\alpha > 0$ on the number of clusters
- very flexible model

A sampling model for the data

- **Example: Gaussian mixtures**, $d = 1$, $\sigma_k = \sigma$ fixed
- $\theta = \mu$
- prior for μ is $Normal(0, \sigma_0^2 I_d)$
- Sampling process
  - for $i = 1 : n$ sample $x_i, k(i)$ as follows

    denote $\{1 : K\}$ the clusters after step $i - 1$
    define n_k the size of cluster k after step $i - 1$

    1. $$k(i) = \begin{cases} k & \text{w.p } \frac{n_k}{i-1+\alpha}, \ k = 1 : K \\ K+1 & \text{w.p } \frac{\alpha}{i-1+\alpha} \end{cases} \tag{15}$$
    2. if $k(i) = K + 1$ sample $\mu_i \equiv \mu_{K+1}$ from $Normal(0, \sigma_0^2)$
    3. sample x_i from $Normal(\mu_{k(i)}, \sigma^2)$
- can be shown that the distribution of $x_{1:n}$ is **interchangeable** (does not depend on data permutation)

The hyperparameters

- σ_0 controls spread of centers
  - should be large
- α controls number of cluster centers
  - α large $\Rightarrow$ many clusters
- cluster sizes non-uniform (larger clusters attract more new points)
- many single point clusters possible

General Dirichlet mixture model

- cluster densities $\{f(x, \theta)\}$
- parameters θ sampled from prior $g_0(\theta, \beta)$
- cluster membership $k(i)$ sampled as in (15)
- x_i sampled from $f(x, \theta_{k(i)})$
- **Model Hyperparameters** α, β

Clustering with Dirichlet mixtures

The clustering problem

- $\alpha, g_0, \beta, \{f\}$ given
- $\mathcal{D}$ given
- wanted $\theta_{1:n}$ (not all distinct!)
- note:
  - $\theta_{1:n}$ determines a hard clustering Δ

Estimating $\theta_{1:n}$ cannot be solved in closed form
Usually solved by MCMC (Markov Chain Monte Carlo) sampling

Clustering with Dirichlet mixtures via MCMC

MCMC estimation for Dirichlet mixture

Input $\alpha, g_0, \beta, \{f\}, \mathcal{D}$

State cluster assignments $k(i)$, $i = 1:n$,
parameters θ_k for all distinct k

Iterate

1. for $i = 1:n$ (reassign data to clusters)
   - 1.1 resample $k(i)$ by

$$k(i) = \begin{cases} \text{existing } k & \text{w.p } \propto \frac{n_k - 1}{n-1+\alpha} f(x_i, \theta_k) \\ \text{new cluster} & \text{w.p } \frac{\alpha}{n-1+\alpha} \int f(x_i, \theta) g_0(\theta) d\theta \end{cases} \tag{16}$$

   - 1.2 if $k(i)$ is new label, sample a new $\theta_{k(i)} \propto g_0 f(x_i, \theta)$
2. for $k \in \{k(1:n)\}$ (resample cluster parameters)
   - 2.1 sample θ_k from posterior $g_k(\theta) \propto g_0(\theta, \beta) \prod_{i \in C_k} f(x_i, \theta)$

   g_k can be computed in closed form if g_0 is conjugate prior

Output a state with high posterior

Summary: Parametric vs. non-parametric

Parametric clustering

- Optimizes a cost $\mathcal{L}$
- Most costs are NP-hard to optimize
- Assumes more detailed knowledge of cluster shapes
- Assumes K known (But there are wrapper methods to select K)
- gets harder with larger K
- Older, more used and studied

Non-parametric clustering

- density-based methods have no cost function

  Dirichlet clustering samplers posterior of $k(1:n), \{\theta_k\}$ given $\mathcal{D}$
- do not depend critically on initialization
- K and outliers selected automatically, naturally
- require hyperparameters (= smoothness parameters)

Note that **Dirichlet mixture** is inbetween parametric and non-parametric

When to use

- Parametric
  - shape of clusters known
  - K not too large or known
  - clusters of comparable sizes
- Non-parametric (density based)
  - shape of clusters arbitrary
  - K large or many outliers
  - clusters sizes in large range (a few large clusters and many small ones)
  - dimension d small (except for **SV**)
  - lots of data
- Dirichlet mixtures
  - shape of clusters known
  - clusters sizes in large range

Similarity based clustering

- **Paradigm:** the features we observe are measures of **similarity/dissimilarity** between pairs of data points, e.g

	points	features
Image segmentation	pixels	distance in color space or location, separated by a contour, belong to same texture
Social network	people	friends, coworkers, phone calls, emails
Text analysis	words	appear in same context

- The features are summarized by a single **similarity measure** S_{ij}
  - e.g $S_{ij} = e^{\sum_k \alpha_k \text{feature}_k(i,j)}$ for all points i, j
  - symmetric $S_{ij} = S_{ji}$
  - non-negative $S_{ij} \geq 0$
- We want to put points that are similar to each other in the same cluster, dissimilar points in different clusters
- Problem is often cast as a **graph cut** problem
  - points = graph nodes, similarity S_{ij} = weight of edge ij
  -

Paradigms for grouping

- Graph cuts

  remove some edges $\Longrightarrow$ disconnected graph

  the groups are the connected components

- By similar behavior

  nodes i, j in the same group iff i, j have the same pattern of connections w.r.t other nodes

- By Embedding

- map nodes $V = \{1, 2, \ldots, n\} \longrightarrow \{x_1, x_2, \ldots, x_n\} \in \mathbb{R}^d$ then use standard classification and clustering methods

Definitions

- $V = \{1, 2, \ldots, n\}$
- node **degree** or **volume**

$$D_i = \sum_{j \in V} S_{ij}$$

- **volume** of cluster $C \subseteq V$

$$D_C = \sum_{i \in C} D_i$$

- **cut** between subsets $C, C' \subseteq V$

$$\sum_{i \in C} \sum_{j \in C'} S_{ij}$$

- **Multiway Normalized Cut** of a partition $\Delta = \{C_{1:K}\}$ of V

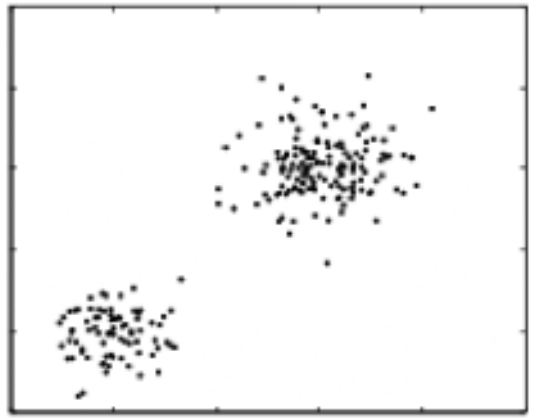
$$MNCut(\Delta) = \sum_{k=1}^{K} \sum_{k' \neq k} \frac{Cut(C_k, C_{k'})}{D_{C_k}}$$

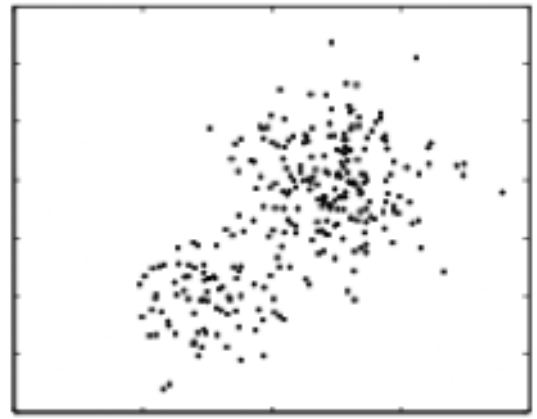
in particular, for $K = 2$,

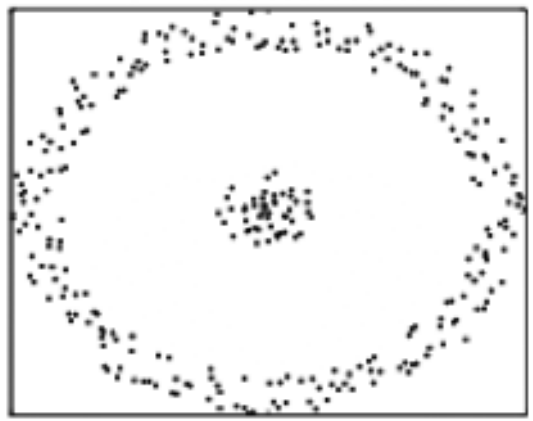
$$MNCut(C, C') = Cut(C, C') \left(\frac{1}{D_C} + \frac{1}{D_{C'}} \right)$$

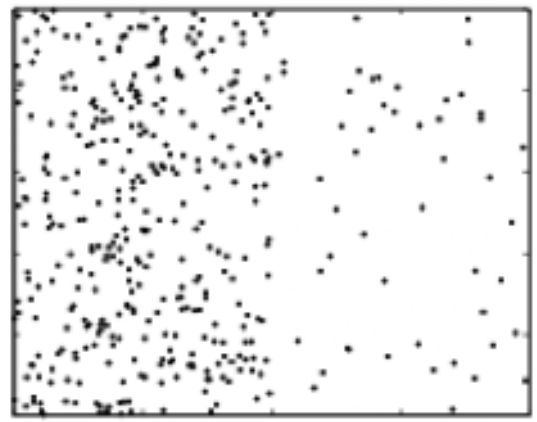
Motivation for MNCut

$S_{ij} \propto 1/\text{dist}(i,j)$

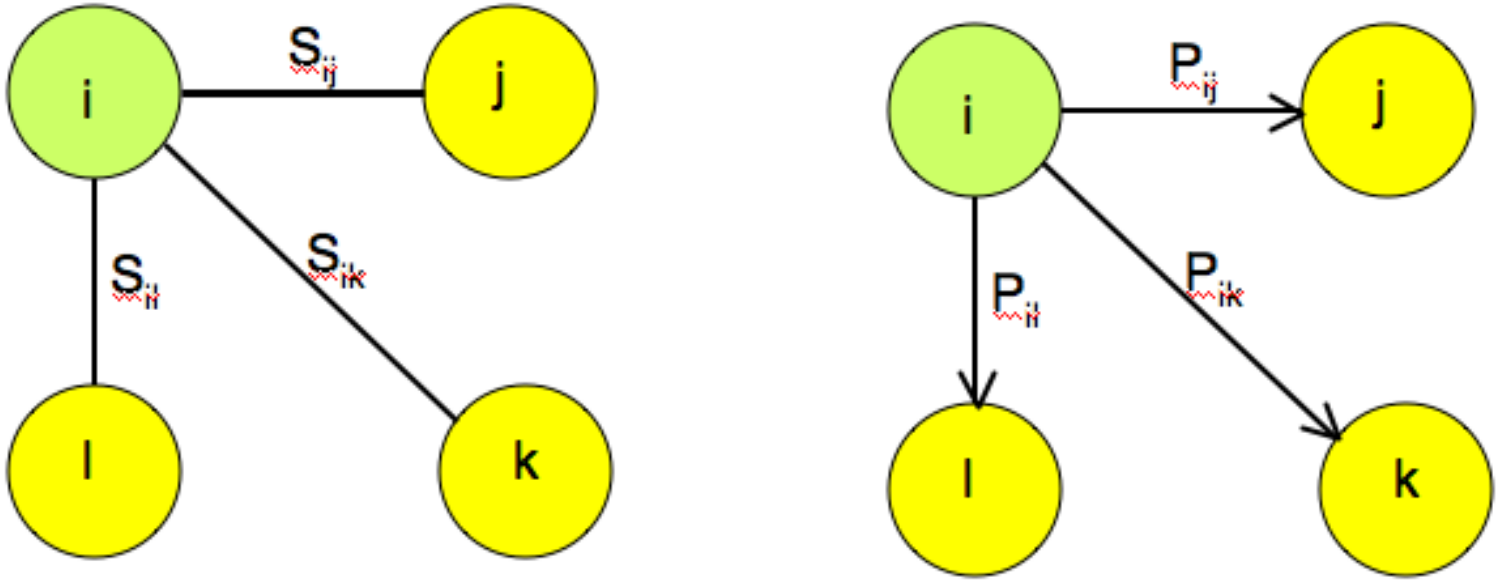








A random walks view



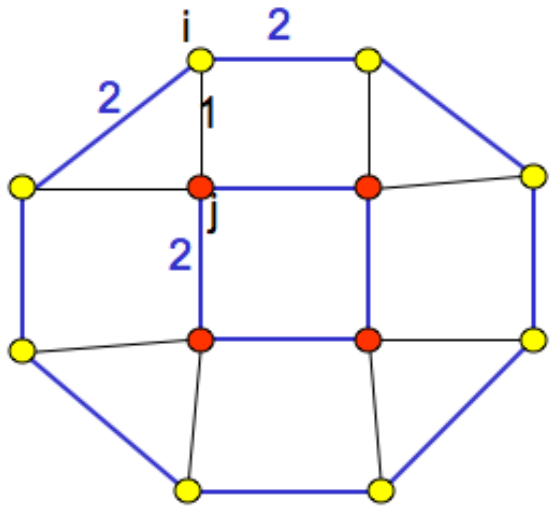
- Define

$$P_{ij} = \frac{S_{ij}}{D_i} \quad \text{for all } i, j \in V$$

- in matrix notation $P = D^{-1}S$ where $P = [P_{ij}]$, $D = \text{diag}(D_1, \ldots D_n)$
- P defines a **random walk** over the graph nodes V

Grouping from the random walks point of view

- Idea: group nodes together if they transition in the same way to other clusters



$$P_{i,red} = Pr[\, i \rightarrow red \,|\, i] = \sum_{j \in red} P_{ij}$$

i	$P_{i,red}$	$P_{i,yellow}$
●	1/5	4/5
●	1/5	4/5
●	1/5	4/5
●	1/5	4/5
●	1/5	4/5
●	1/5	4/5
●	1/5	4/5
●	1/5	4/5
●	2/3	1/3
●	2/3	1/3
●	2/3	1/3
●	2/3	1/3

... is the same as grouping by embedding

- **embedding** of V = mapping from V into $\mathbb{R}^d$
- Wanted: similar points embedded near each other

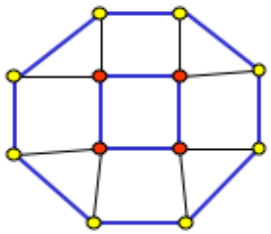
  ideally, points in the same cluster mapped to the same point in $\mathbb{R}^d$

Another look at $P_{i,c}$

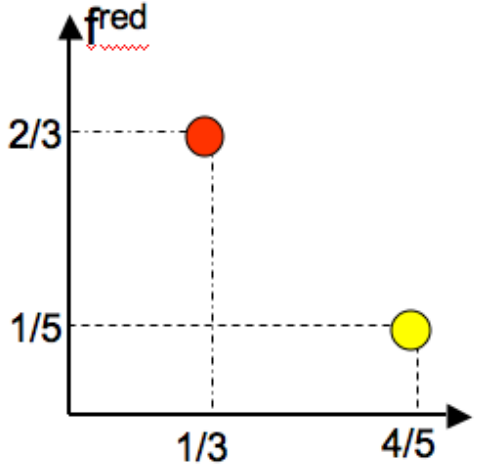
$P_{\cdot,red} \equiv f^{red}$

$P_{\cdot,yel} \equiv f^{yel}$

a **piecewise constant** function

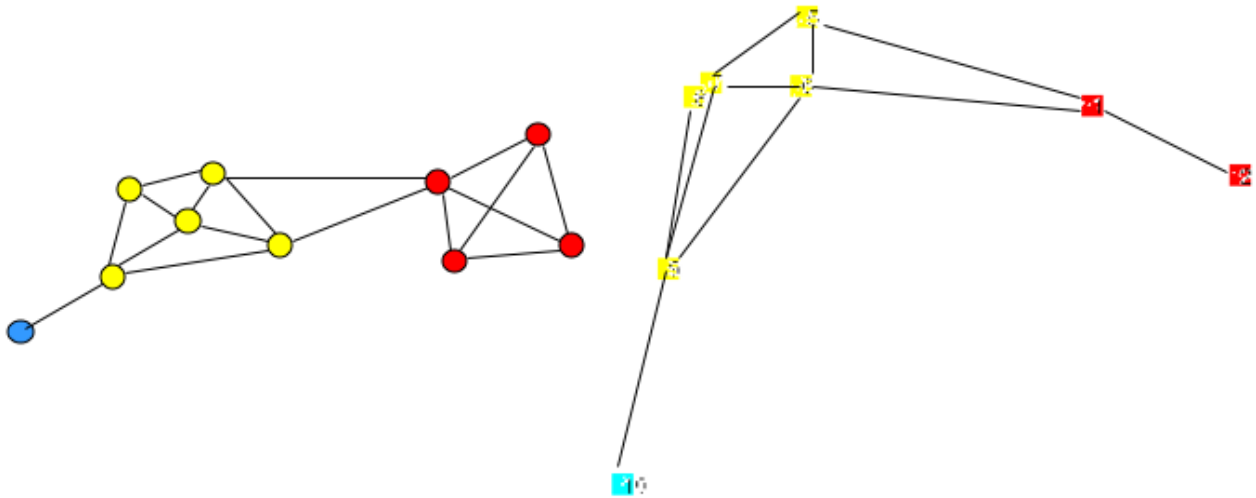


i	$P_{i,red}$	$P_{i,yellow}$
	1/5	4/5
	1/5	4/5
	1/5	4/5
	1/5	4/5
	1/5	4/5
	1/5	4/5
	1/5	4/5
	1/5	4/5
	2/3	1/3
	2/3	1/3
	2/3	1/3
	2/3	1/3



Some questions

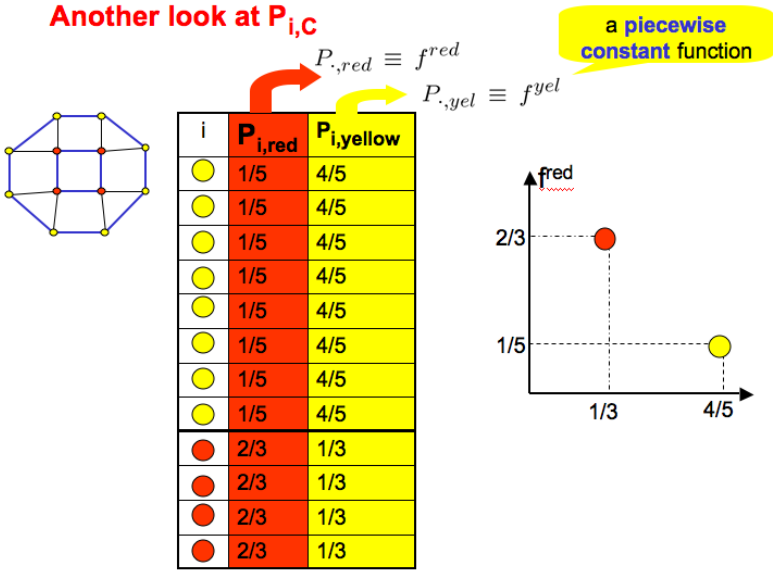
- Not all graphs embed perfectly



- How many dimensions do we need?
- Nice, but we need to know the clusters in advance...

Lumpability

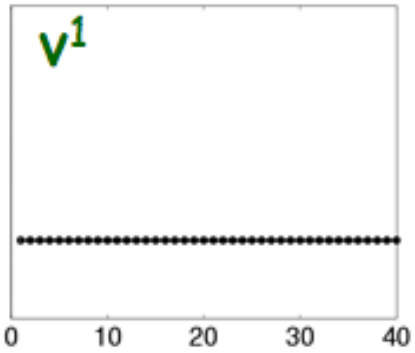
- A vector v is **piecewise constant** w.r.t a clustering Δ iff $v_i = v_j$ whenever i, j in same $C \in \Delta$

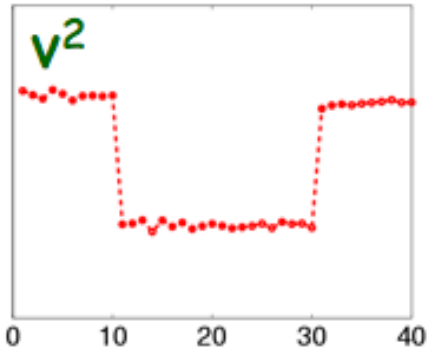


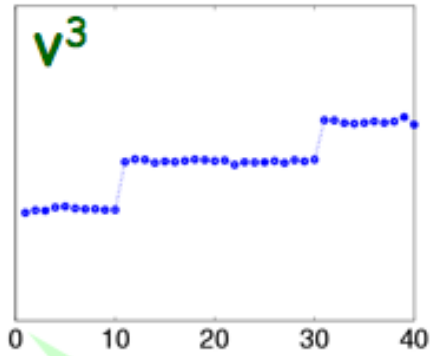
- **Theorem [Lumpability]**[Meila&Shi 2001] Let S be a similarity matrix and Δ a clustering with K clusters. Then P has K **piecewise constant** eigenvectors w.r.t Δ **iff**

$$\sum_{j \in C'} P_{ij} = R_{CC'} \text{ whenver } i \in C, \text{ for all } C, C' \in \Delta$$

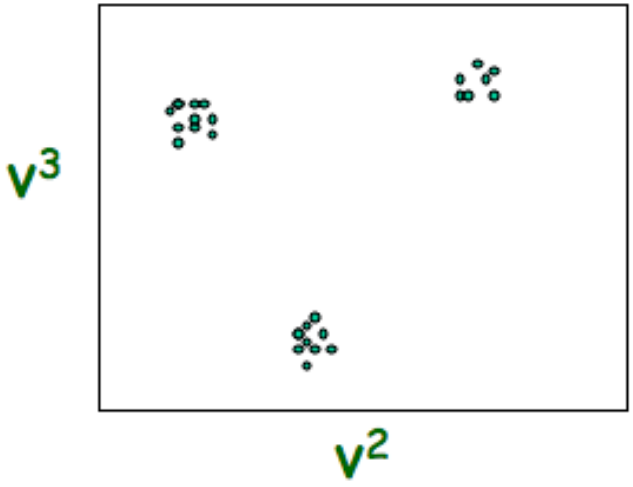
The spectral mapping





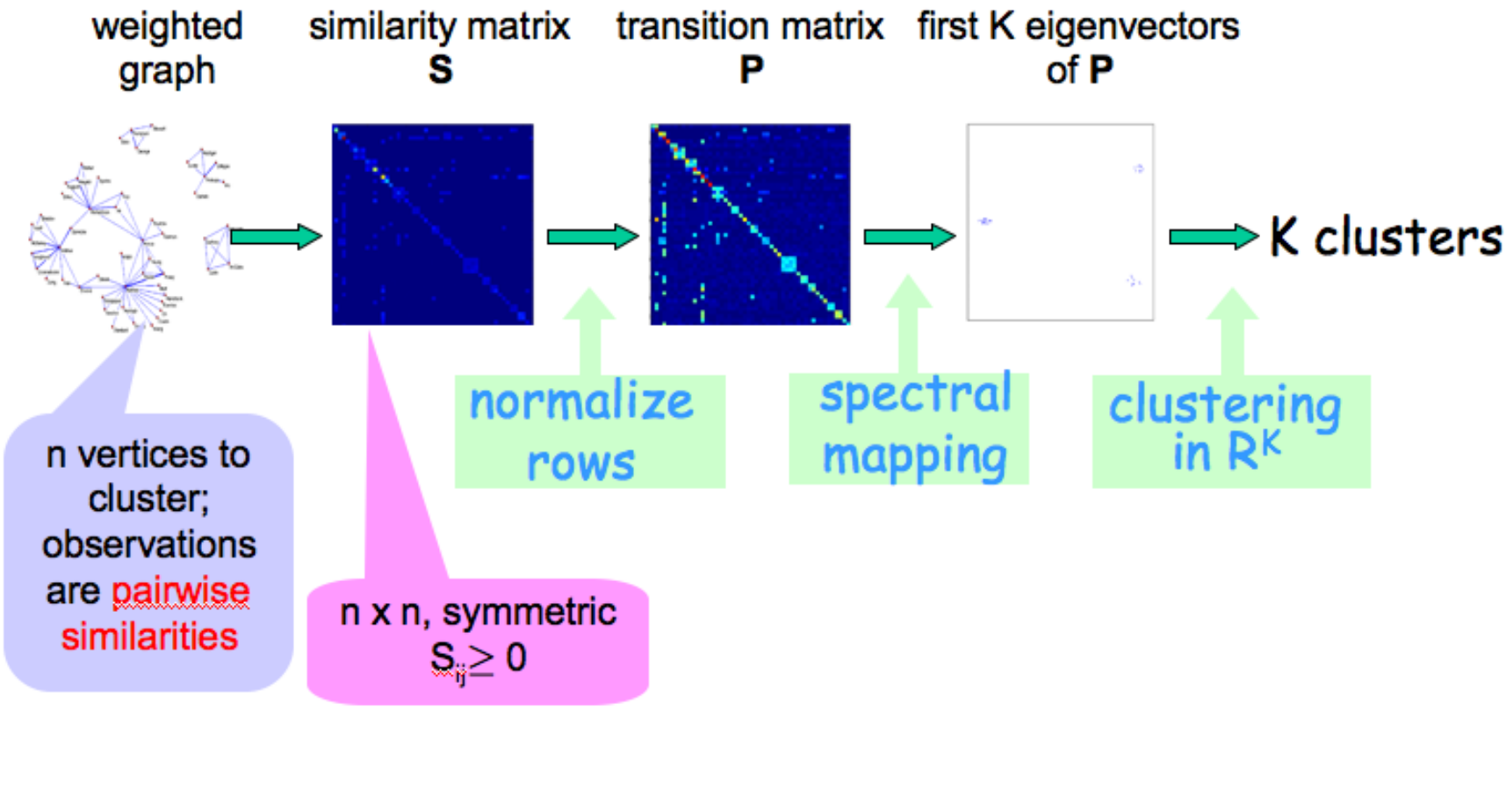


The **spectral mapping**: Data as elements of v^2, v^3



These eigenvectors are called **piecewise constant (PC)**

Spectral clustering in a nutshell



Spectral clustering

An algorithm based on [Meilă and Shi, 2001b] and [Ng et al., 2002].

Spectral Clustering Algorithm

Input Similarity matrix S, number of clusters K

1. Transform S: Set $D_i = \sum_{j=1}^{n} S_{ij}$, $j = 1 : n$ the **node degrees**.
   Form the **transition matrix** $P = [P_{ij}]_{ij=1}^{n}$ with

$$P_{ij} \leftarrow S_{ij}/D_i, \text{ for } i, j = 1 : n$$

2. Compute the largest K eigenvalues $\lambda_1 = 1 \geq \lambda_2 \geq \ldots \geq \lambda_K$ and eigenvectors $\mathbf{v}_1, \ldots \mathbf{v}_K$ of P.
3. Embed the data in principal subspace Let $V = [\mathbf{v}_2\ \mathbf{v}_3\ \ldots\ \mathbf{v}_K] \in \mathbb{R}^{n \times K}$, $\mathbf{x}_i \leftarrow$ i-th row of V.
4. (orthogonal initialization) Find K initial centers by
   4.1 take μ_1 randomly from $\mathbf{x}_1, \ldots \mathbf{x}_n$
   4.2 for $k = 2, \ldots K$ set $\mu_k = \operatorname{argmin}_{\mathbf{x}_i} \max_{k' < k} \mu_{k'}^T \mathbf{x}_i$.
5. Run the K-means algorithm on the "data" $\mathbf{x}_{1:n}$ starting from the centers $\mu_{1:K}$.

Properties of spectral clustering

- Arbitrary cluster shapes (main advantage)
- Elegant mathematically
- Practical up to medium sized problems
  - Running time (by Lanczos algorithm) $\mathcal{O}(nk)$/iteration.
- Works well when K known, not too large

  estimating K [Azran and Ghahramani, 2006]
- Depend heavily on the similarity function (main problem)

  learning the similarities
  [Meilă and Shi, 2001a],[Bach and Jordan, 2006],[Meilă et al., 2005],[Shortreed and Meilă,
- Outliers become separate clusters (user must adjust K accordingly!)
- Very popular, many variants which aim to improve on the above

  Diffusion maps [Nadler et al., 2006]: normalize the eigenvectors $\lambda_k^t v^k$
- Practical fix, when K large: only compute a fixed number of eigenvectors $d < K$.
  This avoids the effects of noise in lower ranked eigenvectors

Affinity propagation

- **Idea** Each item $i \in \mathcal{D}$ finds an **exemplar** item $k \in \mathcal{D}$ to "represent" it
- Affinity Propagation is to spectral clustering what Mean Shift is to K-means
- number of exemplars not fixed in advance
- quantities of interest
  - similarities s_{ij}, $i \neq j$ (given)
  - **availability** a_{ik} of k for i = how much support there is from other items for k to be an exemplar
  - **responsibility** r_{ik} that measures how fit is k to represent i, as compared to other possible candidates k'.
  - diagonal elements s_{ii} represent **self-similarities**
    - larger s_{ii} $\Rightarrow$ more likely i will become an exemplar $\Rightarrow$ more clusters

Affinity Propagation

Affinity Propagation Algorithm [Frey and Dueck, 2007]

Input Similarity matrix $S = [s_{ik}]_{ik=1}^{n}$, parameter $\lambda = 0.5$

Iterate the following steps until convergence

1. $a_{ik} \leftarrow 0$ for $i, k = 1 : n$
2. for all i
   - 2.1 Find the best exemplar for i: $s^* \leftarrow \max_k (s_{ik} + a_{ik})$, $A_i^* \leftarrow \underset{k}{\operatorname{argmax}} (s_{ik} + a_{ik})$ (can be a set of items)
   - 2.2 for all k update responsibilities

$$r_{ik} \leftarrow \begin{cases} s_{ik} - s^*, & \text{if } k \notin A_i^* \\ s_{ik} - \max_{k' \notin A_i^*} (s_{ik} + a_{ik}) & \text{otherwise} \end{cases}$$

3. for all k update availabilities
   - 3.1 $a_{kk} \leftarrow \sum_{i \neq k} [r_{ik}]_+$ where $[r_{ik}]_+ = r_{ik}$ if $r_{ik} > 0$ and 0 otherwise.
   - 3.2 for all i, $a_{ik} \leftarrow \min\{0, r_{kk} + \sum_{i' \neq i,k} [r_{i'k}]_+\}$
4. Assign an exemplar to i by $k(i) \leftarrow \underset{k'}{\operatorname{argmax}} (r_{ik'} + a_{ik'})$

Cluster validation

- External
  - when the true clustering Δ^* is known
  - compares result(s) Δ obtained by algorithm **A** with Δ^*
  - validates algorithms/methods
- Internal - no external reference

External cluster validation

Scenarios

- given data $\mathcal{D}$, truth Δ^*; algorithm **A** produces Δ
  is Δ close to Δ^*?
- given data $\mathcal{D}$, truth Δ^*; algorithm **A** produces Δ, algorithm **A'** produces Δ'
  which of Δ, Δ' is closer to Δ^*?
- multiple datasets, multiple algorithms
  which algorithm is better?

A **distance between clusterings** $d(\Delta, \Delta')$ needed

Requirements for a distance

Depend on the application

- Applies to any two partitions of the same data set
- Makes no assumptions about how the clusterings are obtained
- Values of the distance between two pairs of clusterings comparable under the weakest possible assumptions
- Metric (triangle inequality) desirable
- **understandable, interpretable**

The confusion matrix

- Let $\Delta = \{C_{1:K}\},\ \Delta' = \{C'_{1:K'}\}$
- Define $n_k = |C_k|,\ n'_{k'} = |C'_{k'}|$
- $m_{kk'} = |C_k \cap C'_{k'}|,\ k = 1:K, k' = 1:K'$
- note: $\sum_k m_{kk'} = n'_{k'},\ \sum_{k'} m_{kk'} = n_k,\ \sum_{k,k'} m_{kk'} = n$
- The **confusion matrix** $M \in \mathbb{R}^{K \times K'}$ is

$$M = [m_{kk'}]_{k=1:K}^{k'=1:K'}$$

- all distances and comparison criteria are based on M
- the **normalized confusion matrix** $P = M/n$

$$p_{kk'} = \frac{m_{kk'}}{n}$$

- The **normalized cluster sizes** $p_k = n_k/n,\ p'_{k'} = n'_{k'}/n$ are the **marginals** of P

$$p_k = \sum_{k'} p_{kk'} \quad p_{k'} = \sum_{k} p_{kk'}$$

The Misclassification Error (ME) distance

- Define the **Misclassification Error (ME)** distance d_{ME}

$$d_{ME} = 1 - \max_{\pi} \sum_{k=1}^{K} p_{k,\pi(k)} \quad \pi \in \{\text{all } K-\text{permutations}\},\ K \leq K' \text{w.l.o.g}$$

- Interpretation: treat the clusterings as classifications, then minimize the classification error over all possible label matchings
- Or: nd_{ME} is the Hamming distance between the vectors of labels, minimized over all possible label matchings
- can be computed in polynomial time by **Max bipartite matching** algorithm (also known as Hungarian algorithm)
- Is a metric: symmetric, ≥ 0, triangle inequality

$$d_{ME}(\Delta_1, \Delta_2) + d_{ME}(\Delta_1, \Delta_3) \geq d_{ME}(\Delta_2, \Delta_3)$$

- easy to understand (very popular in computer science)
- $d_{ME} \leq 1 - 1/K$
- bad: if clusterings not similar, or K large, d_{ME} is coarse/indiscriminative
- recommended: for small K

The Variation of Information (VI) distance
Clusterings as random variables

- Imagine points in $\mathcal{D}$ are picked randomly, with equal probabilities
- Then $k(i), k'(j)$ are random variables
  with $Pr[k] = p_k$, $Pr[k, k'] = p_{kk'}$

Incursion in information theory I

- **Entropy** of a random variable/clustering $H_\Delta = -\sum_k p_k \ln p_k$
- $0 \leq H_\Delta \leq \ln K$
- Measures uncertainty in a distribution (amount of randomness)
- **Joint entropy** of two clusterings

$$H_{\Delta,\Delta'} = -\sum_{k,k'} p_{kk'} \ln p_{kk'}$$

- $H_{\Delta',\Delta} \leq H_\Delta + H_{\Delta'}$ with equality when the two random variables are independent
- **Conditional entropy** of Δ' given Δ

$$H_{\Delta'|\Delta} = -\sum_k p_k \sum_{k'} \frac{p_{kk'}}{p_k} \ln \frac{p_{kk'}}{p_k}$$

- Measures the expected uncertainty about k' when k is known
- $H_{\Delta'|\Delta} \leq H_{\Delta'}$ with equality when the two random variables are independent
- **Mutual information** between two clusterings (or random variables)

$$\begin{aligned} I_{\Delta,\Delta} &= H_\Delta + H_{\Delta'} - H_{\Delta',\Delta} \\ &= H_{\Delta'} - H_{\Delta'|\Delta} \end{aligned}$$

- Measures the amount of information of one r.v. about the other
- $I_{\Delta,\Delta} \geq 0$, symmetric. Equality iff r.v.'s independent

The VI distance

- Define the **Variation of Information (VI)** distance

$$\begin{aligned} d_{VI}(\Delta, \Delta') &= H_\Delta + H_{\Delta'} - 2I_{\Delta',\Delta} \\ &= H_{\Delta|\Delta'} + H_{\Delta'|\Delta} \end{aligned}$$

- Interpretation: d_{VI} is the sum of information gained and information lost when labels are switched from $k()$ to $k'()$
- d_{VI} symmetric, ≥ 0
- d_{VI} obeys triangle inequality (is a metric)

Other properties

- Upper bound
  $d_{VI} \leq 2 \ln K_{max}$ if $K, K' \leq K_{max} \leq \sqrt{n}$
  (asymptotically attained)
- $d_{VI} \leq \ln n$ over all partitions (attained)
- Unbounded! and grows fast for small K

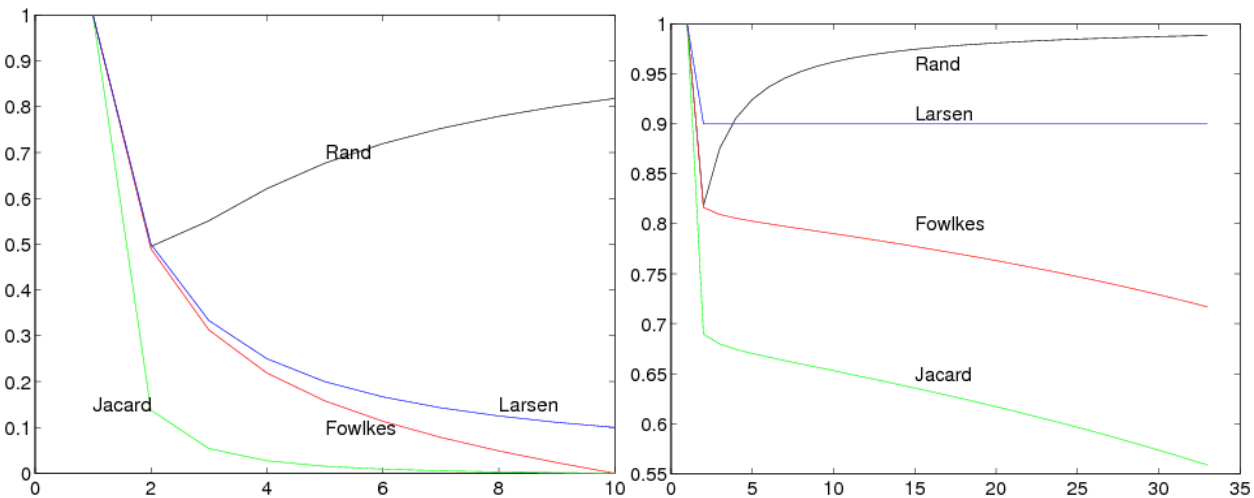
Other criteria and desirable properties

- Comparing clustering by **indices of similarity** $i(\Delta, \Delta')$
  - from statistics (Rand, adjusted Rand, Jaccard, Fowlkes-Mallows ...)
  - range=[0,1], with $i(\Delta, \Delta') = 1$ for $\Delta = \Delta'$
  - the properties of these indices not so good
  - any index can be transformed into a "distance" by $d(\Delta, \Delta') = 1 - i(\Delta, \Delta')$
- Other desirable properties of indices and distances between clusterings
  - n-invariance
  - locality
  - convex additivity

- Define $N_{11} = \#$ pairs which are together in both clusterings, $N_{12} = \#$ pairs together in Δ, separated in Δ', N_{21} (conversely), $N_{22} =$#number pairs separated in both clusterings
- Rand index $= \frac{N_{11}+N_{22}}{\#\text{pairs}}$
- Jaccard index $= \frac{N_{11}}{\#\text{pairs}}$
- Fowlkes-Mallows $=$ Precision$\times$ Recall

- all vary strongly with K. Thereforek, **Adjusted** indices used mostly

$$adj(i) = \frac{i - \bar{i}}{\max(i) - \bar{i}}$$



Internal cluster(ing) validation

Why?

- Most algorithms output a clustering even if no clusters in data (parametric algorithms)

  How to decide whether to accept it or not?
- related to selection of K
- Some algorithms are run multiple times (e.g EM)

  How to select the clustering(s) to keep?
- Validate by the cost $\mathcal{L}$
  - Δ is valid if $\mathcal{L}(\Delta)$ is "small"
- but how small is "small"?
- Note: rescaling data may change $\mathcal{L}(\Delta)$

Heuristics

- **Gap** heuristic
- single linkage:
  - define l_r length of r-th edge added to MST

$$\underbrace{l_1 \leq l_2 \leq \ldots l_{n-K}}_{\text{intracluster}} \leq \underbrace{l_{n-K+1} \leq \ldots}_{\text{deleted}}$$

  - $l_{n-K}/l_{n-K+1} \leq 1$ should be small
- min diameter:

$$\frac{\mathcal{L}(\Delta)}{\max_{i,j \in \mathcal{D}} ||x_i - x_j||}$$

$$\frac{\mathcal{L}(\Delta)}{\min_{k,k'} \text{distance}(C_k, C_{k'})}$$

- etc

Quadratic cost

- $\mathcal{L}(\Delta) = const - \operatorname{trace} X^T(\Delta) A X(\Delta)$
- with $X =$ matrix reprentation for Δ
- then, if cost value $\mathcal{L}(\Delta)$ small, we can prove that clustering Δ is almost optimal
- This holds for K-means (weighted, kernelized) and several graph partioning costs (normalized cut, average association, correlation clustering, etc)

Matrix Representations

- matrix reprentations for Δ
  - unnormalized (redundant) representation

$$\tilde{X}_{ik} = \begin{cases} 1 & i \in C_k \\ 0 & i \notin C_k \end{cases} \qquad \text{for } i = 1:n, k = 1:K$$

  - normalized (redundant) representation

$$X_{ik} = \begin{cases} 1/\sqrt{|C_k|} & i \in C_k \\ 0 & i \notin C_k \end{cases} \qquad \text{for } i = 1:n, k = 1:K$$

  therefore $X_k^T X_{k'} = \delta(k, k')$, X orthogonal matrix
  $X_k =$ column k of X
- normalized non-redundant reprentation
  - X_K is determined by $X_{1:K-1}$
  - hence we can use $Y \in \mathbb{R}^{n \times (K-1)}$ orthogonal representation
  - intuition: Y represents a subspace (is an orthogonal basis)
  - K centers in $\mathbb{R}^d$, $d \geq K$ determine a $K-1$ dimesional subspace plus a translation

- Example: the K-means cost
  - remember
$$\mathcal{L}(\Delta) = \sum_{k=1}^{K} \sum_{i,j \in C_k} \frac{1}{2|C_k|} ||x_i - x_j||^2 + \text{constant}$$
  - in matrix form
$$\mathcal{L}(\Delta) = -\frac{1}{2} X^T A X + \text{constant}$$
    where
$$A_{ij} = x_i^T x_j$$
    is the Gram matrix of the data
  - if data centered, ie $\sum_i x_i = 0$ and Y rotated appropriately (see Meila, 2006)[Meilă, 2006]
$$\mathcal{L}(\Delta) = -\frac{1}{2} Y^T A Y + \text{constant}$$
- Assume k-means cost from now on

A spectral lower bound

- minimizing $\mathcal{L}(\Delta)$ is equivalent to

$$\max Y^T A Y$$

  over all $Y \in \mathbb{R}^{n \times (K-1)}$ that represent a clustering

- a relaxation

$$\max Y^T A Y$$

  over all $Y \in \mathbb{R}^{n \times (K-1)}$ orthogonal

- solution to relaxed provlem is

$$Y^* = \text{eigenvectors}_{1:K-1} \text{ of } A$$

$$\mathcal{L}^* = \sum_{k=1}^{K-1} \lambda_k(A)$$

- $\mathcal{L}^* = \textit{constant} - L^* = \operatorname{trace} A - L^*$ is lower bound for $\mathcal{L}$

$$\mathcal{L}^* \leq \mathcal{L}(\Delta) \text{ for all } \Delta$$

A theorem (Meila, 2006)

Theorem

- define

$$\delta = \frac{Y^T A Y - \sum_{k=1}^{K-1} \lambda_k}{\lambda_{K-1} - \lambda_K} \qquad \varepsilon(\delta) = 2\delta[1 - \delta/(K-1)]$$

- define $p_{min}, p_{max} = \frac{\min,\max |C_k|}{n}$
- then, whenever $\varepsilon(\delta) \leq p_{min}$, we have that

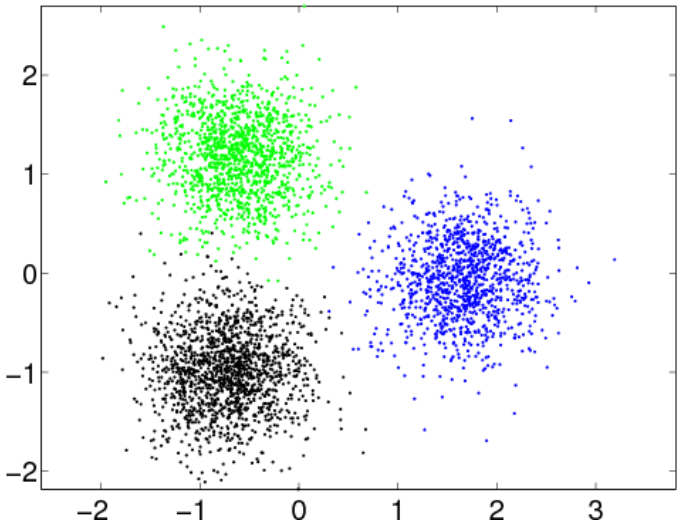
$$d_{ME}(\Delta, \Delta^{opt}) \leq \varepsilon(\delta) p_{max}$$

where d_{ME} is misclassification error distance

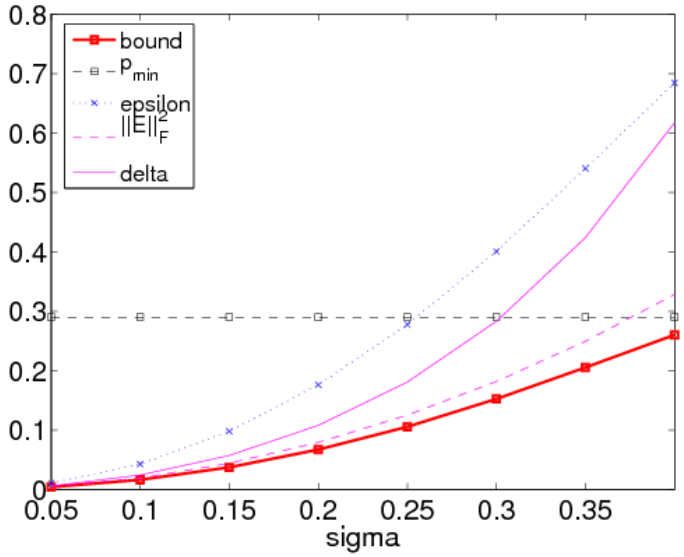
Remarks

- it is a worst-case result
- makes no (implicit) distributional assumptions
- when theorem applies, bound is good $d_{ME}(\Delta, \Delta^{opt}) \leq p_{min}$
- applies only if a good clustering is found (not all data, clusterings)
- intuiton: if data well clustered, $K-1$ principal subspace is aligned with cluster centers

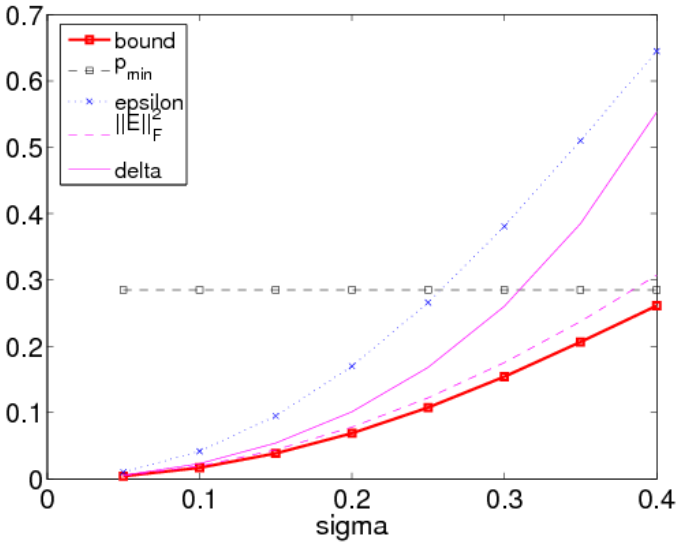
data $d = 35$, $\sigma = 0.4$



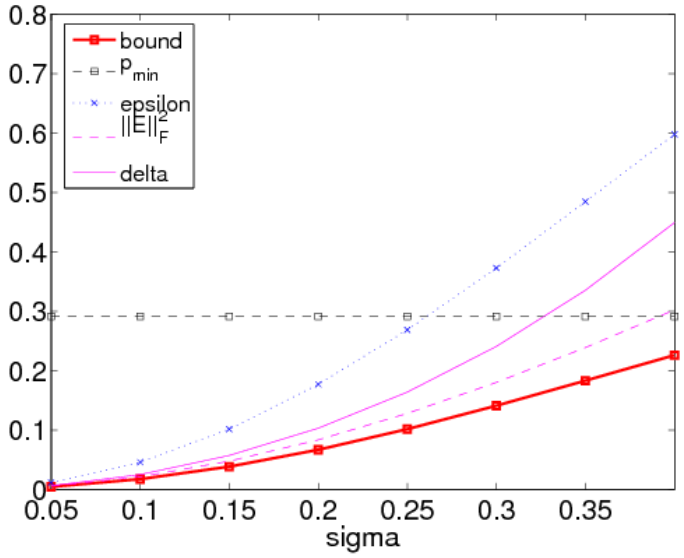
$n = 100$



$n = 200$



$n = 1000$



What I didn't talk about

- Hierarchical clustering
- Subspace clustering (or clustering on subsets of attributes)
- Bi-clustering (and multi-way-clustering)
- Partial clustering
- Ensembles of clusterings, consensus clustering, and clustering clusterings

Hierarchical clustering

- **Divisive** (top down)
  - starts with all data in one cluster, divides recursively into 2 (or more) clusters
  - Example: spectral clustering, min diameter
- **Agglomerative** (bottom up)
  - starts n cluster containing 1 item, merges 2 clusters recursively
  - Example: Ward algorithm, single linkage
- **Hierarchical Dirichlet processes**
- Remarks
  - Any cost based clustering paradigm can produce a hierarchical clustering
  - Any non-parametric level-sets paradigm can produce a hierarchical clustering
  - Mixture models (finite or not) can also be defined hierarchically. Issues of identifyability appear

The Ward agglomerative algoritm [Ward, 1963]

- Cost $=$ same as K-means
- Algorithm idea:
  - Start with n single point clusters
  - Merge the two clusters that increase $\mathcal{L}$ the least, until K clusters left
- **Greedy**, recursive algorithm, $\mathcal{O}(n^3)$ operations

Subspace clustering

- Problem: each cluster is defined by a subset of relevant attributes (features)
  - Examples: user modeling (clusters of users vs clusters of products/services), gene expression data
- Known as **Clustering on Subsets of Attributes (COSA) Biclustering (and Multiway Clustering), Subspace clustering**
- Amounts to clustering both the data exemplars and the data features
- Approaches
  - **COSA** [Friedman and Meulman, 2004] cost based, + additional entropy term. Alternate minimization algorithm.
  - **[?]** Dirichlet process mixtures approach. Each $f(.;\theta_k)$ samples a set of relevant features. Estimated by MCMC
  - **Multivariate Information Bottleneck** [Friedman et al., 2001] Information theory based. Estimation by alternate (KL-divergence) projections.
  - many others. . . see IEEE TKDE

Partial clustering

- Problem: Given a node, find its cluster
- Premise: the data set is extremely large, there are many small clusters, possibly $\mathcal{O}(n)$
- **Nibble** algorithm of [Spielman and Teng, 2008]

  Given: a graph, by its Markov transition matrix P
  Start with node i, tolerance ε, number steps t
  Initialize $p \in \mathbb{R}^n$ with $p_i = 1$, $p_j = 0$ for $j \neq i$
  - Iterate for t steps
    1. $p \leftarrow Pp$
    2. for $j = 1 : n$, if $p_j < \varepsilon$ set $p_j = 0$

  Output $C(i) = \{ j \mid p_j > 0 \}$
- $C(i)$ is the set of items attainable from i by a "likely" path
- Original algorithm has sparsest cut guarantees
  Used as subroutine by other algorithms.

Links

- Yee Whye Teh's tutorial on DP Mixtures http://mlg.eng.cam.ac.uk/tutorials/07/ywt.pdf
- Lecture on exponential family models http: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