Non-exhaustive, Overlapping k-means

J. J. Whang, I. S. Dhilon, and D. F. Gleich

Teresa Lebair

University of Maryland, Baltimore County

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Outline

Introduction

- NEO-K-Means Objective Functional
- NEO-K-Means Algorithm
- Graph Clustering using NEO-K-Means
- Experimental Results
- Conclusions and Future Work

Introduction

- The traditional k-means clustering algorithm is
 - exhaustive (every point is put into a cluster), and
 - non-overlapping (no point belongs to more than one cluster).
- There are many applications in which
 - there are outliers (points do not belong to any cluster) and / or
 - some points belong to multiple clusters.
- Application examples:
 - Outlier detection in datasets.
 - Popular *EachMovie* dataset: some movies belong to multiple genres.
 - Biology: clustering genes by function results in overlapping clusters.

Introduction

- Many papers on clustering consider either cluster outliers, or overlapping clusters, but not both.
- This paper is one of the first to consider both cluster outliers and overlapping clusters in a unified manner.
- One popular application is community detection (e.g., detecting clusters or communities of users in social networks.)
- In this paper, the objective functional for traditional clustering is modified to produce the NEO-K-Means objective functional.

• A NEO-K-Means Algorithm is proposed to minimize the NEO-K-Means objective functional.

• NEO-K-Means is also used to solve graph clustering problems.

• NEO-K-Means is tested experimentally on both vector and graph data

Traditional k-means

- $\mathcal{X} := \{x_1, x_2, \dots, x_n\}$ is a set of data points.
- We want to partition \mathcal{X} into k clusters $\mathcal{C}_1, \mathcal{C}_2, \dots, \mathcal{C}_k$, i.e., $\cup_j \mathcal{C}_j = \mathcal{X}$ and $i \neq j \implies \mathcal{C}_i \cap \mathcal{C}_j = \emptyset$.
- The goal of *k*-means is to pick the clusters to minimize the sum of the distances of the clusters from the cluster centroids, i.e., solve the minimization problem

$$\min_{\{C_j\}_{j=1}^k} \sum_{j=1}^k \sum_{x_i \in \mathcal{C}_j} \|x_i - m_j\|^2, \text{ where } m_j := \frac{\sum_{x_i \in \mathcal{C}_j} x_i}{|\mathcal{C}_j|}$$

- This is an NP-hard problem.
- However, the traditional *k*-means algorithm monotonically decreases the objective functional.

k-means Extension

- Define the assignment matrix $U = (u_{ij}) \in \mathbb{R}^{n \times k}$ such that $u_{ij} = \begin{cases} 1 & \text{if } x_i \in \mathcal{C}_j \\ 0 & \text{otherwise.} \end{cases}$
- In the case of traditional disjoint exhaustive clustering, each column of *U* contains exactly one entry of 1; all other entries are zeros. Hence the trace of $U^T U$ is equal to the number of cluster assignments, *n*.
- To control the number of cluster assignments, we introduce the constraint that the trace of U^TU is equal to n(1 + α), where 0 ≤ α ≤ (k − 1).

• First extend the *k*-means objective as follows to minimize over assignment matrices *U*:

$$\min_{U} \sum_{j=1}^{k} \sum_{i=1}^{n} u_{ij} \|x_i - m_j\|^2, \text{ where } m_j = \frac{\sum_{i=1}^{n} u_{ij} x_i}{\sum_{i=1}^{n} u_{ij}}.$$
s.t. trace($U^T U$) = $(1 + \alpha)n$

- Take α << (k 1) to avoid assigning each point as its own cluster.
- New objective functional allows for both outliers and overlapping clusters.

Testing k-means extension

- Tested first extension of the *k*-means objective on synthetic data set:
 - Two over-lapping clusters of ordered pairs, with several additional points as outliers.
 - Each cluster generated from a Gaussian distribution.
- Algorithm similar to *k*-means is used.
- α is set to 0.1, the ground-truth value of α .

Testing k-means extension

- First extension of *k*-means fails to recover ground-truth clusters.
- Too many points are labeled as outliers.



NEO-K-Means Objective

- Necessary to control the degree of non-exhaustiveness.
- Let ${\mathbb I}$ denote the indicator function:

$$\mathbb{I}(ext{expression}) = egin{cases} 1 & ext{if the expression is true} \\ 0 & ext{otherwise.} \end{cases}$$

- Let $\mathbf{1} \in \mathbb{R}^k$ denote the vector of all ones.
- Note that (U1)_i denotes the number of clusters to which x_i belongs.
- We update the objective functional by adding a non-exhaustiveness constraint.

• The NEO-K-Means Objective is defined as follows:

$$\begin{split} \min_{U} & \sum_{j=1}^{k} \sum_{i=1}^{n} u_{ij} \| x_i - m_j \|^2, \text{ where } m_j = \frac{\sum_{i=1}^{n} u_{ij} x_i}{\sum_{i=1}^{n} u_{ij}}.\\ \text{s.t. } & \text{trace}(U^T U) = (1 + \alpha)n, \ \sum_{i=1}^{n} \mathbb{I}((U\mathbf{1})_i = 0) \le \beta n. \end{split}$$

- $0 \leq \beta << 1$ controls the amount of points can be labeled as outliers.
- The choice of $\alpha = \beta = 0$ recovers the traditional *k*-means objective.

Testing NEO-K-Means Objective

- Tested the NEO-K-Means Objective using the previous synthetic data set.
- Outcome is much better than that of the previous *k*-means extension.



- At most βn data points have no cluster membership ⇒ at least n − βn data points belong to a cluster.
- Sketch of NEO-K-Means Algorithm
 - Initialize cluster centroids (use any traditional *k*-means initialization strategy.)
 - Compute d_{ij} , the distance between each point x_i and each cluster C_j , for all i = 1, ..., n and j = 1, ..., k.
 - Sort data points in ascending order by distance to closest cluster.
 - Assign the first $n \beta n$ data points in the sorted list to their closest clusters. Let \overline{C}_j denote the assignments made by this step.

Sketch of NEO-K-Means Algorithm (Continued)

• Note that
$$\sum_{j=1}^{k} |\bar{\mathcal{C}}_j| = n - \beta n$$
.

- Make an additional $\alpha n + \beta n$ assignments based off of the $\alpha n + \beta n$ smallest entries of $D = (d_{ij})$ not already associated with assignments to \overline{C}_j 's. Let \hat{C}_j denote the assignments made by this step.
- Each cluster C_j is then updated to be $C_j := \overline{C_j} \cup \widehat{C_j}$.
- Repeat process until objective function is sufficiently small, or the maximum number of iterations is reached.

Algorithm 1 NEO-K-Means

Input: $\mathcal{X} = \{\mathbf{x}_1, \mathbf{x}_2, \cdots, \mathbf{x}_n\}$, the number of clusters k, the maximum number of iterations t_{max} , α , β **Output:** C_1, C_2, \cdots, C_k 1: Initialize cluster means $\{\mathbf{m}_i\}_{i=1}^k, t = 0.$ 2: while not converged and $t < t_{max}$ do Compute cluster means, and then compute distances 3: between every data point and clusters $[d_{ij}]_{n \times k}$. Initialize $\mathcal{T} = \emptyset$, $\mathcal{S} = \emptyset$, p = 0, and $\overline{C}_i = \emptyset$, $\hat{C}_i = \emptyset \forall i$. 4: while $p < (n + \alpha n)$ do 5: if $p < (n - \beta n)$ then 6: Assign \mathbf{x}_{i^*} to $\overline{\mathcal{C}}_{j^*}$ such that $(i^*, j^*) = \operatorname{argmin} d_{ij}$ 7: where $\{(i, j)\} \notin \mathcal{T}, i \notin \mathcal{S}$. $\mathcal{S} = \mathcal{S} \cup \{i^*\}.$ 8: else 9: Assign \mathbf{x}_{i^*} to $\hat{\mathcal{C}}_{j^*}$ such that $(i^*, j^*) = \operatorname{argmin} d_{ij}$ 10: where $\{(i, j)\} \notin \mathcal{T}$. end if 11: 12: $\mathcal{T} = \mathcal{T} \cup \{(i^*, j^*)\}.$ p = p + 1. 13: 14. end while $\forall j$, update clusters $C_j = \overline{C}_i \cup \hat{C}_i$. 15: 16: t = t + 1. 17: end while

Theorem

The NEO-K-Means objective functional monotonically decreases through the application of the NEO-K-Means Algorithm while satisfying the constraints for fixed α and β .

Proof.

Let $J^{(t)}$ denote the objective at the *t*-th iterations. Then

$$J^{(t)} = \sum_{j=1}^{k} \sum_{x_{i} \in \mathcal{C}_{j}^{(t)}} \|x_{i} - m_{j}^{(t)}\|^{2} \ge \sum_{j=1}^{k} \sum_{x_{i} \in \tilde{\mathcal{C}}_{j}^{(t+1)}} \|x_{i} - m_{j}^{(t)}\|^{2} + \sum_{j=1}^{k} \sum_{x_{i} \in \tilde{\mathcal{C}}_{j}^{(t+1)}} \|x_{i} - m_{j}^{(t)}\|^{2}$$
$$= \sum_{j=1}^{k} \sum_{x_{i} \in \mathcal{C}_{j}^{(t+1)}} \|x_{i} - m_{j}^{(t)}\|^{2} \ge \sum_{j=1}^{k} \sum_{x_{i} \in \mathcal{C}_{j}^{(t+1)}} \|x_{i} - m_{j}^{(t+1)}\|^{2} = J^{(t+1)}.$$

NEO-K-Means Algorithm: Choosing α and β

- Choosing β :
 - Run traditional *k*-means. Let *d_i* be the distance between a data point *x_i* and its closest cluster.
 - Compute the mean μ and standard deviation σ for these set of distances.
 - Consider d_i and outlier if $d_i \notin [\mu \delta \sigma, \mu + \delta \sigma]$ for some fixed $\delta > 0$. ($\delta = 6$ usually leads to reasonable β .)
 - Set β equal to the proportion of d_i 's that are outliers.
- Choosing α :
 - Two different strategies can be used to choose α .

NEO-K-Means Algorithm: Choosing α

- First strategy for choosing α (for small overlap):
 - For each cluster C_j , consider the distances between each $x_i \in C_j$ and C_j . Compute the mean μ_j and standard deviation σ_j of the distances.
 - For each $x_{\ell} \notin C_j$, compute the distance between x_{ℓ} and C_j . If $d_{\ell j}$ is less than $\mu_j + \delta \sigma_j$, consider x_j to be in the overlapped region.
 - Count the points in overlapped regions to estimate α .

NEO-K-Means Algorithm: Choosing α

- Second strategy for choosing α (for large overlap):
 - Let d_{ij} denote the distance between the point x_i and the cluster C_j .
 - Compute the normalized distance between each point x_i and cluster C_j : $\bar{d}_{ij} := \frac{d_{ij}}{\sum_{\ell=1}^k d_{i\ell}}$
 - Count the number of d
 _{ij}'s whose value is less than 1/(k+1). Divide by n to obtain α.
 - Note that if a point x_i is equidistant from all clusters C_{ℓ} , we have $\overline{d}_{i\ell} = \frac{1}{k}$ for all ℓ . Using a threshold of $\frac{1}{k+1}$ gives us a stronger bound.

Weighted Kernel K-Means

- In kernel k-means, each point is mapped into a higher dimensional feature space via the mapping φ.
- Additionally, weights ω_i ≥ 0 can be introduced to differentiate each point's contribution to the objective functional.
- The weighted kernel k-means objective functional is

$$\min_{\{\mathcal{C}_j\}_{j=1}^k} \sum_{j=1}^k \sum_{x_i \in \mathcal{C}_j} \omega_i \|\phi(x_i) - m_j\|^2, \text{ where } m_j = \frac{\sum_{x_i \in \mathcal{C}_j} \omega_i \phi(x_i)}{\sum_{x_i \in \mathcal{C}_j} \omega_i}.$$

 Can define an analogous weighted kernel NEO-K-Means objective functional:

$$\min_{U} \sum_{c=1}^{k} \sum_{i=1}^{n} u_{ic} \omega_{i} \|\phi(x_{i}) - m_{c}\|^{2}, \text{ where } m_{c} = \frac{\sum_{i=1}^{n} u_{ic} \omega_{i} \phi(x_{i})}{\sum_{i=1}^{n} u_{ic} \omega_{i}},$$

s.t. trace $(U^{T}U) = (1 + \alpha)n, \sum_{i=1}^{n} \mathbb{I}((U\mathbf{1})_{i} = 0) \leq \beta n$

• This NEO-K-Means extension allows us to consider non-exhaustive overlapping graph clustering / overlapping community detection.

- A graph $G = (\mathcal{V}, \mathcal{E})$ is a collection of vertices and edges.
- We can define an adjacency matrix A = (a_{ij}), such that a_{ij} is equal to the weight of the edge between vertices i and j.
- Example:





The adjacency matrix is A B L P E $A \begin{pmatrix} 0 & 8 & 2 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 \end{pmatrix}$

$$A = \begin{matrix} A \\ B \\ A \\ P \\ E \end{matrix} \begin{pmatrix} 0 & 8 & 2 & 0 & 0 \\ 8 & 0 & 0 & 1 & 0 \\ 2 & 0 & 0 & 4 & 0 \\ 0 & 1 & 4 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \end{matrix} \right).$$

- We assume that there are no connections between any vertex i and itself $\implies a_{ii} = 0$ for all i = 1, ..., n.
- Also assume that graph is unidirected (so A is symmetric).
- Traditional graph partitioning problem groups vertices into k pairwise disjoint clusters C₁ ∪ ... C_k = V.
- Define the 'links' function between two clusters as the sum of the edge weights between the clusters: links(C_j, C_ℓ) := ∑_{x_{i1} ∈C_j} ∑_{x_{i2} ∈C_ℓ} a_{i1i2}
- Example: If $C_1 := \{ Alice, Bob \}$ and $C_2 = \{ Linda, Paul \}$, then $links(C_1, C_2) = a_{AL} + a_{BL} + a_{AP} + a_{BP} = 2 + 0 + 0 + 1 = 3$.

• The cut (popular measure of evaluating graph partitioning) of a graph G is defined as

$$\mathsf{Cut}(G) = \sum_{j=1}^k rac{\mathsf{links}(\mathcal{C}_j, \mathcal{V} \setminus \mathcal{C}_j)}{\mathsf{links}(\mathcal{C}_j, \mathcal{V})}.$$

• The normalized cut of a graph partition is the partition of \mathcal{V} that minimizes Cut(G) over all possible partitions, i.e.

$$\operatorname{NCut}(G) = \min_{\mathcal{C}_1,\ldots,\mathcal{C}_k} \operatorname{Cut}(G).$$

• Let D be the diagonal matrix such that $d_{ii} = \sum_{j=1}^{n} a_{ij}$, i.e., the matrix of vertex degrees.

• We can rewrite $\mathsf{NCut}(G) = \min_{\mathcal{C}_1, \dots, \mathcal{C}_k} \sum_{j=1}^k \frac{\mathsf{links}(\mathcal{C}_j, \mathcal{V} \setminus \mathcal{C}_j)}{\mathsf{links}(\mathcal{C}_j, \mathcal{V})}$ as

$$\operatorname{NCut}(G) = \min_{y_1, \dots, y_k} \sum_{j=1}^k \frac{y_j^T (D - A) y_j}{y_j^T D y_j} = \max_{y_1, \dots, y_k} \sum_{j=1}^k \frac{y_j^T A y_j}{y_j^T D y_j},$$

where y_j denotes the indicator vector for the cluster C_j , i.e., $y_j(i) = 1$ if $v_i \in C_j$, and zero otherwise.

• This traditional normalized cut objective is for disjoint, exhaustive graph clustering.

• For NEO-K-Means graph clustering, consider the maximization problem

$$\max_{Y} \sum_{j=1}^{\kappa} \frac{y_j^T A y_j}{y_j^T D y_j}$$

s.t. trace $(Y^T Y) = (1 + \alpha)n, \sum_{i=1}^{n} \mathbb{I}((Y\mathbf{1})_i = 0) \le \beta n,$

where Y is an assignment matrix, with the *j*th column of Y given by y_j .

- Just as with the vector data, we may adjust α and β to control the degree of non-exhaustiveness.
- This optimization problem for graph partitioning can be reformulated as weighted kernel NEO-K-Means problem.

- Let W ∈ ℝ^{n×n} be the diagonal matrix such that w_{ii} is equal to the vertex degree/weight for each i = 1,..., n.
- Let K be a kernel matrix given by $K_{ij} = \phi(x_i)\phi(x_j)$.
- Finally, let u_c be the column of the assignment matrix U.
- The weighted kernel NEO-K-Means objective can be rewritten as

$$\min_{U} \sum_{c=1}^{k} \sum_{i=1}^{n} u_{ic} \omega_{i} \|\phi(x_{i}) - m_{c}\|^{2} =$$
$$\min_{U} \sum_{c=1}^{k} \left(\sum_{i=1}^{n} u_{ic} \omega_{i} \mathcal{K}_{ii} - \frac{u_{c}^{T} \mathcal{W} \mathcal{K} \mathcal{W} u_{c}}{u_{c}^{T} \mathcal{W} u_{c}} \right).$$

- Define the kernel as $K = \gamma W^{-1} + W^{-1}AW^{-1}$, where $\gamma > 0$ is chosen so that K is positive definite.
- Then

$$\begin{split} \min_{U} & \sum_{c=1}^{k} \left(\sum_{i=1}^{n} u_{ic} \omega_{i} K_{ii} - \frac{u_{c}^{T} A u_{c}}{u_{c}^{T} W u_{c}} \right) \\ &= & \min_{U} \left(\gamma (1+\alpha) n - \sum_{c=1}^{k} \frac{u_{c}^{T} A u_{c}}{u_{c}^{T} W u_{c}} \right) \\ &= & \max_{U} \sum_{c=1}^{k} \frac{u_{c}^{T} A u_{c}}{u_{c}^{T} W u_{c}}. \end{split}$$

 Letting W = D and noting that U = Y demonstrates that the extended normalized cut objective can be formulated as a weighted kernel NEO-K-Means objective.

Authors use the following distance function between a vertex v_i and a cluster C_j:

$$\mathsf{dist}(v_i,\mathcal{C}_j) = -\frac{2\mathsf{links}(v_i,\mathcal{C}_j)}{\mathsf{deg}(v_i)\mathsf{deg}(\mathcal{C}_j)} + \frac{\mathsf{links}(\mathcal{C}_j,\mathcal{C}_j)}{\mathsf{deg}(\mathcal{C}_j)^2} + \frac{\gamma}{\mathsf{deg}(v_i)} - \frac{\gamma}{\mathsf{deg}(\mathcal{C}_j)}$$

- deg(v_i) denotes the degree of the vertex v_i, and deg(C_j) denotes the sum of the edge weights connecting vertices in C_j.
- The NEO-K-Means Algorithm can then be applied to the graph data using this distance function.

- To measure the effectiveness of the NEO-K-Means algorithm, we use the average *F*₁ score:
 - Define F_1 score of the the ground-truth cluster S_i as $F_1(S_i) = \frac{2r_{S_i}p_{S_i}}{r_{S_i}+p_{S_i}}$, where $p_{S_i} = \frac{|\mathcal{C}_{j^*} \cap S_i|}{|\mathcal{C}_{j^*}|}$, $r_{S_i} = \frac{|\mathcal{C}_{j^*} \cap S_i|}{|S_i|}$ and j^* corresponds to the cluster \mathcal{C}_{j^*} which makes $F_1(S_i)$ as large as possible out of all the clusters.
 - The average F_1 score is then

$$ar{F}_1 = rac{1}{|\mathcal{S}|} \sum_{\mathcal{S}_i \in \mathcal{S}} F_1(\mathcal{S}_i),$$

where ${\cal S}$ is the set of ground-truth clusters.

• Higher $\bar{F}_1 \in [0,1]$ score indicates better clustering.

• Tested NEO-K-Means Algorithm on several vector data sets.

| Table 1: Vector datasets. | | | | | | |
|---------------------------|-------|------|-----------------------|----------|------------------|--|
| | n | dim. | $ \bar{\mathcal{C}} $ | outliers | \boldsymbol{k} | |
| synth1 | 5,000 | 2 | 2,750 | 0 | 2 | |
| synth2 | 1,000 | 2 | 550 | 5 | 2 | |
| synth3 | 6,000 | 2 | 3,600 | 6 | 2 | |
| yeast | 2,417 | 103 | 731.5 | 0 | 14 | |
| music | 593 | 72 | 184.7 | 0 | 6 | |
| scene | 2,407 | 294 | 430.8 | 0 | 6 | |

• Compared effectiveness of NEO-K-Means to that of several other algorithms.

Table 2: F_1 scores on vector datasets. NEO-K-Means (the last column) achieves the highest F_1 score across all the datasets while the performance of other existing algorithms is not consistent across all the datasets.

| | moc | fuzzy | esp | isp | okm | rokm | NEO |
|--------|-------|-------|-------|-------|-------|-------|-------|
| synth1 | 0.833 | 0.959 | 0.977 | 0.985 | 0.989 | 0.969 | 0.996 |
| synth2 | 0.836 | 0.957 | 0.952 | 0.973 | 0.967 | 0.975 | 0.996 |
| synth3 | 0.547 | 0.919 | 0.968 | 0.952 | 0.970 | 0.928 | 0.996 |
| yeast | - | 0.308 | 0.289 | 0.203 | 0.311 | 0.203 | 0.366 |
| music | 0.534 | 0.533 | 0.527 | 0.508 | 0.527 | 0.454 | 0.550 |
| scene | 0.467 | 0.431 | 0.572 | 0.586 | 0.571 | 0.593 | 0.626 |

 NEO-K-Means consistently outperforms the other algorithms for this data set. • Additionally test NEO-K-Means with large graph data sets:

| Table 4: Graph datasets | | | | | |
|-------------------------|-----------------|--------------|--|--|--|
| | No. of vertices | No. of edges | | | |
| Amazon | 334,863 | 925,872 | | | |
| DBLP | 317,080 | 1,049,866 | | | |
| Flickr | 1,994,422 | 21,445,057 | | | |
| LiveJournal | 1,757,326 | 42,183,338 | | | |

• Compare the average normalized cut of each algorithm when applied to large real-world datasets.

| better clustering. NEO-IN-Means achieves the lowest hormanzed cut on an the datasets. | | | | | | | |
|---|-------|-------|---------|-------|-------|--|--|
| | demon | oslom | bigclam | sse | NEO | | |
| Amazon | 0.555 | 0.221 | 0.392 | 0.116 | 0.105 | | |
| DBLP | 0.606 | 0.355 | 0.617 | 0.204 | 0.188 | | |
| Flickr | - | - | 0.596 | 0.515 | 0.331 | | |
| LiveJournal | - | - | 0.912 | 0.643 | 0.373 | | |

Table 3: Average normalized cut of each algorithm on large real-world networks. Lower normalized cut indicates better clustering NEO-K-Means achieves the lowest normalized cut on all the datasets

 Also consider (i) average F₁ score of different algorithms, and (ii) average normalized cut and F₁ NEO-K-Means for different α's and β's.

| and comparable F_1 score with sse on DBLP. | | | | | | | |
|---|-------------------------|-------------------------|-------------------------|------------------------------|------------------------------|--------------------------------|--|
| | ۵ | lemon | oslom | bigclam | sse | NEO | |
| Amaze | on 0 |).165 | 0.318 | 0.269 | 0.467 | 0.490 | |
| DBLP | ° 0 | 0.137 | 0.132 | 0.151 | 0.176 | 0.174 | |
| Table 6: Average normalized cut and F_1 score of NEO-K-Means with different α and β on Amazon dataset. | | | | | | | |
| | $\alpha{=}30,\beta{=}0$ | $\alpha{=}35,\beta{=}0$ | $\alpha{=}45,\beta{=}0$ | $\alpha{=}30,\beta{=}0.0001$ | $\alpha{=}35,\beta{=}0.0001$ | $\alpha{=}45, \beta{=}0.0001$ | |
| ncut | 0.107 | 0.104 | 0.104 | 0.106 | 0.104 | 0.104 | |
| F_1 | 0.488 | 0.490 | 0.490 | 0.488 | 0.490 | 0.490 | |

Table 5: F_1 score of each algorithm on Amazon and DBLP. NEO-K-Means shows the highest F_1 score on Amazon, and comparable F_1 score with sse on DBLP.

Conclusions and Future Work

- NEO-K-Means simultaneously considers non-exhaustive and overlapping clusters.
- New method outperforms state-of-the-art methods in terms of finding ground truth clusters.
- Conclude that NEO-K-Means is a useful algorithm.
- Plan to extend this type of clustering to other types of Bregman divergences.

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