Achieving near-perfect clustering for high dimension, low sample size data

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1.1 Geometric representation of HDLSS data

- **Notation and General setting**

  - \( K \) : Number of clusters, \( N \) : Sample size, \( p \) : dimensions,

  - \( n_k \) : Sample size of Cluster \( k \), \( N = \sum_{k=1}^{K} n_k \),

  - \( X^{(p)}_k \) : \( p \) -dimensional random vector of Cluster \( k \),

  - \( X^{(p)}_k := (X_{k1}, \ldots, X_{kp})^T \), \( d_{ij}^{(p)} := \|X_i^{(p)} - X_j^{(p)}\| \)

  - \( X^{(p)}_k \) (\( k = 1, \ldots, K \)) are independent.
1.1 Geometric representation of HDLSS data

- **Notation and General setting** \((k = 1, \ldots, K)\)

  (a) \(\exists M > 0; \forall s \in \mathbb{N}; \mathbb{E}\left[|X_{ks}|^4\right] < M\)

  (b) \(\frac{1}{p} \sum_{s=1}^{p} \mathbb{E}[X_{ks}]^2 \to \mu_k^2 \quad \text{as} \quad p \to \infty\)

  (c) \(\frac{1}{p} \sum_{s=1}^{p} \text{Var}(X_{ks}) \to \sigma_k^2 \quad \text{as} \quad p \to \infty\)

  (d) \(\frac{1}{p} \sum_{s=1}^{p} \{\mathbb{E}[X_{ks}] - \mathbb{E}[X_{ls}]\}^2 \to \delta_{kl}^2 \quad \text{as} \quad p \to \infty\)
1.1 Geometric representation of HDLSS data

- **Notation and General setting** \((k = 1, \ldots, K)\)

\[
\frac{1}{p} \sum_{s=1}^{p} \mathbb{E}[X_{ks}] \mathbb{E}[X_{ls}] \rightarrow \eta_{kl} \quad \text{as} \quad p \rightarrow \infty
\]

(f) There is some permutation of \(X_k^{(\infty)}\),

which is \(\rho\)-mixing*.

*The concepts of \(\rho\)-mixing is useful as a mild condition for the development of laws of large number.
1.1 Geometric representation of HDLSS data

- Hall et al. (2005; JRSS B)
  - The distance between data vectors from a same cluster is approximately-constant after scaled by $\sqrt{p}$!

- The distance between data vectors from different clusters is also approximately constant after scaled by $\sqrt{p}$!
1.2. Difficulty of clustering for HDLSS data

- Hierarchical clustering in HDLSS contexts

\[ U_1^{(p)}, U_2^{(p)}, U_3^{(p)} \overset{i.i.d.}{=} X_1^{(p)}; V^{(p)} \overset{i.i.d.}{=} X_2^{(p)} \]

\[ \sqrt{2\sigma_1} \geq \sqrt{\delta^2_{12} + \sigma^2_1 + \sigma^2_2} \]

- In some cases, classical methods do not work well...

\[ 2\sigma^2_k < \mu^2_{kl} + \sigma^2_k + \sigma^2_l \]

Condition for label consistency
2. Previous study (MDP clustering)

- **Maximal data piling (MDP) distance** (Ahn and Marron, 2007)
  
  - The orthogonal distance between the affine subspaces generated by the data vectors in each cluster.

\[
U_1^{(p)}, U_2^{(p)}, U_3^{(p)} \overset{i.i.d.}{\sim} X_1^{(p)}; \quad V^{(p)} \overset{i.i.d.}{\sim} X_2^{(p)}
\]
2. Previous study (MDP clustering)

- Clustering with MDP distance (Ahn, et al., 2013)
  - Find successive binary split, each of which creates two clusters in such a way that the MDP distance between them is as large as possible.
2. Previous study (MDP clustering)

• **MDP distance Clustering (Ahn, et al., 2013)**

  - A sufficient condition for the label consistency

\[
\delta_{12}^2 + \frac{\sigma_1^2}{n_1} + \frac{\sigma_2^2}{n_2} > \max \left\{ \frac{n_1 + G}{n_1 G} \sigma_1^2, \frac{n_2 + G}{n_2 G} \sigma_2^2 \right\}
\]

  - where \( G \leq \max\{n_1, n_2\} \).

  - If \( \delta_{12}^2 > 0 \) is sufficient large, the label consistency holds.
2. Previous study (MDP clustering)

- **Some problems of MDP clustering**

  - The sufficient condition depends on variances (and sample sizes).
  
  - Cannot discover differences between variances in each cluster.

  Avoiding stereotypes of clustering method, we can conduct simple and effective methods based on a distance matrix or an inner product matrix.
3. Clustering with distance vectors

3.1 Main idea

– Toy example:

• $X_1 \sim N_p(0, I_p)$

• For $c \neq 1$, $X_2 \sim N_p(0, cI_p)$,

• The condition of Ahn et al. (2013) dose not hold.

\[
\delta_{12}^2 + \frac{\sigma_1^2}{n_1} + \frac{\sigma_2^2}{n_2} > \max \left\{ \frac{n_1 + G}{n_1G} \sigma_1, \frac{n_2 + G}{n_2G} \sigma_2 \right\}
\]
3. Clustering with distance vectors

3.1 Main idea

Standardized distances converge to some constants in prob.

*Distance “vectors” have the cluster information!*
3. Clustering with distance vectors

**Proposed method**

– **Step 1.** Compute the distance matrix $D$ from the data matrix $X$ (or the inner product matrix $S := XX^T$).

– **Step 2.** Calculate the following distances ($\Xi := (\xi_{ij})_{n \times n}$),

$$\xi_{ij} = \sqrt{\sum_{s \neq i, s \neq j} (d_{is} - d_{js})^2} \quad \left( \text{or} \quad := \sqrt{\sum_{t \neq i, t \neq j} (s_{it} - s_{jt})^2} \right).$$

– **Step 3.** For the matrix $\Xi$, apply a usual clustering method.
3. Clustering with distance vectors

- **K-means Type**

\[
Q_p(C \mid K) := \sum_{i=1}^{N} \min_k \sum_{j \neq i} \left( d_{ij}^{(p)} - \bar{d}_{kj}^{(p)} \right)^2,
\]

where \( \bar{d}_{kj}^{(p)} := \frac{1}{n_k - 1} \sum_{i \neq j} d_{ij}^{(p)}. \)

- We can optimize this by the usual \( k \)-means algorithm.

- **Important property**

- Under the assumptions a) \( \sim \) f), for all \( K^* \geq K \),

\[
\min_C Q_p(C \mid K^*) \xrightarrow{\mathbb{P}} 0 \quad \text{as} \quad p \to \infty.
\]
3. Clustering with distance vectors

• Theoretical results of the $k$-means type
  – In the case of using a distance matrix

Assume $a) \sim f) \Rightarrow$

\[
\delta_{12}^2 + \frac{\sigma_1^2}{n_1} + \frac{\sigma_2^2}{n_2} > \max \left\{ \frac{n_1 + G}{n_1 G} \sigma_1^2, \frac{n_2 + G}{n_2 G} \sigma_2^2 \right\}
\]

then the estimate label vector converges to the true label vector in probability as $p \to \infty$.

– Ahn et al., 2013
3. Clustering with distance vectors

• Theoretical results of the $k$-means type
  – In the case of using an inner product matrix

Assume $a) \sim f)$.

If $\delta_{12}^2 > 0$,

then the estimate label vector converges to the true label vector in probability as $p \to \infty$.

– Ahn et al., 2013

$$\delta_{12}^2 + \frac{\sigma_1^2}{n_1} + \frac{\sigma_2^2}{n_2} > \max \left\{ \frac{n_1 + G}{n_1G} \sigma_1^2, \frac{n_2 + G}{n_2G} \sigma_2^2 \right\}$$
3. Clustering with distance vectors

Application to Cancer Microarray data (Leukemia data)

➢ Summary:
  – The number of labels: 2
  – Sample size: 72
  – Dimensions: 3571

➢ Comparison
  – Reg. k-means: 2/72 (2)
  – MDP: 2/72 (2)
  – Proposal method: 1/72 (2)
4. Conclusion

• In this presentation,
  – Introduce geometric representations of HDLSS data,
  – Propose a new efficient clustering method for HDLSS data.

• Remark:
  – In HDLSS contexts,
    the closeness between data points may not be meaningful,
    but “vectors” of distances have the cluster information!


A. Definition of $\rho$-mixing

- **$\rho$-mixing** (Kolmogorov and Rozanov, 1960; Theor. Probab. Appl.)
  - For $-\infty \leq J \leq L \leq \infty$,
    \[ \mathcal{F}_j^L : \text{the } \sigma \text{-field of events generated by the r.v.s } (Z_i, J \leq i \leq L). \]
  - For any $\sigma$-field $\mathcal{A}$,
    \[ L_2(\mathcal{A}) : \text{the space of square-integrable, } \mathcal{A}\text{-measurable r.v.s.} \]
  - For each $m \geq 1$, define the maximal correlation coefficient
    \[ \rho(m) := \sup |\text{Corr}(f, g)|, \quad f \in L_2(\mathcal{F}_{-\infty}^j), \quad g \in L_2(\mathcal{F}_{j+m}^\infty), \]
    where $j \in \mathbb{Z}$.
  - The sequence $\{Z_i\}$ is said to be $\rho$-mixing if
    \[ \rho(m) \to 0 \quad \text{as} \quad m \to \infty. \]