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

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0. Contents

1. Introduction

1.1 Geometric representation of HDLSS data

(Hall et al., 2005; JRSS B)

1.2 Difficulty of clustering HDLSS data

2. Previous study

2.1 Clustering with MDP distance (Ahn et al, 2013; Statist. Sinica)

3. Clustering with distance (or inner product) vectors

3.1 Main idea

3.2 Proposal method

3.3 Theoretical result of the proposal methods

4. Conclusion

1.1 Geometric representation of HDLSS data

- **<u>Notation and General setting</u>**
  - K : Number of clusters, N : Sample size, p : dimensions,
  - n_k : Sample size of Cluster k, $N = \sum_{k=1}^{K} n_k$,
  - $\boldsymbol{X}_k^{(p)}$: p -dimensional random vector of Cluster k ,
  - $\boldsymbol{X}_k^{(p)} := (X_{k1}, \ldots, X_{kp})^T$, $d_{ij}^{(p)} := \left\| \boldsymbol{X}_i^{(p)} - \boldsymbol{X}_j^{(p)} \right\|$
  - $\boldsymbol{X}_k^{(p)}$ $(k = 1, \ldots, K)$ 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) $$\frac{1}{p}\sum_{s=1}^{p} \mathrm{Var}(X_{ks}) \to \sigma_k^2 \quad \text{as} \quad p \to \infty$$

(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** $(k = 1, \ldots, K)$

  (e) $\displaystyle \frac{1}{p}\sum_{s=1}^{p} \mathbb{E}[X_{ks}]\mathbb{E}[X_{ls}] \to \eta_{kl} \quad \text{as} \quad p \to \infty$

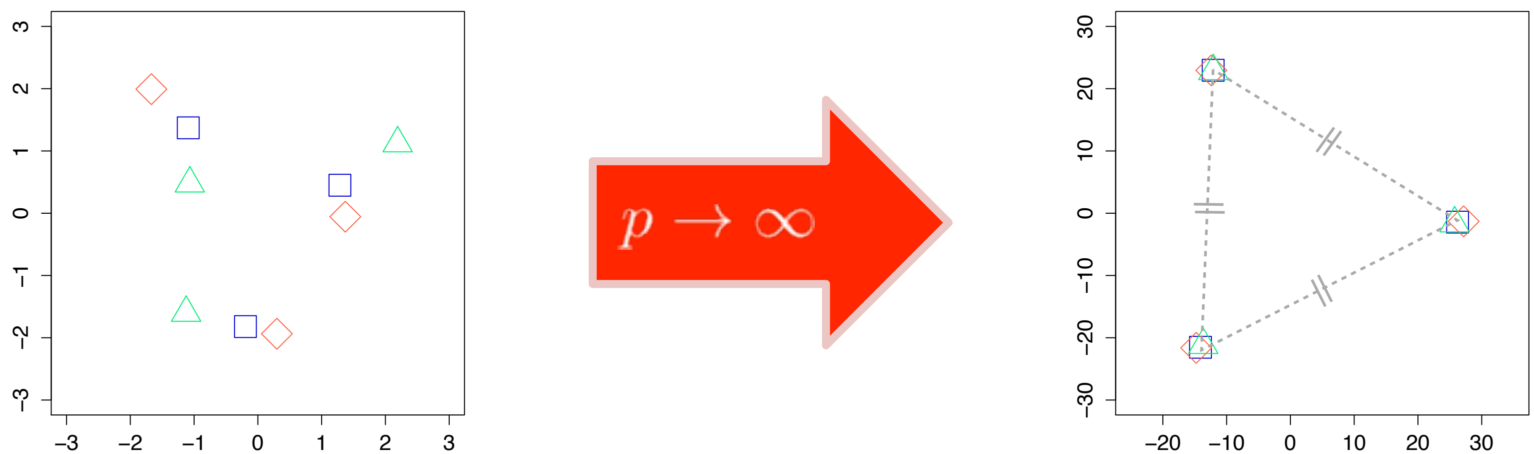
  (f) There is some permutation of $\boldsymbol{X}_k^{(\infty)}$,

  which is ρ -mixing*.

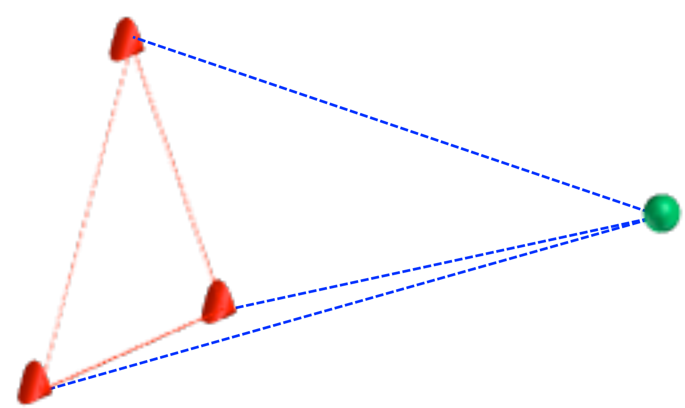
  *The concepts of ρ -mixing is useful as a mild condition for the development of laws of large number.

1.1 Geometric representation of HDLSS data

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

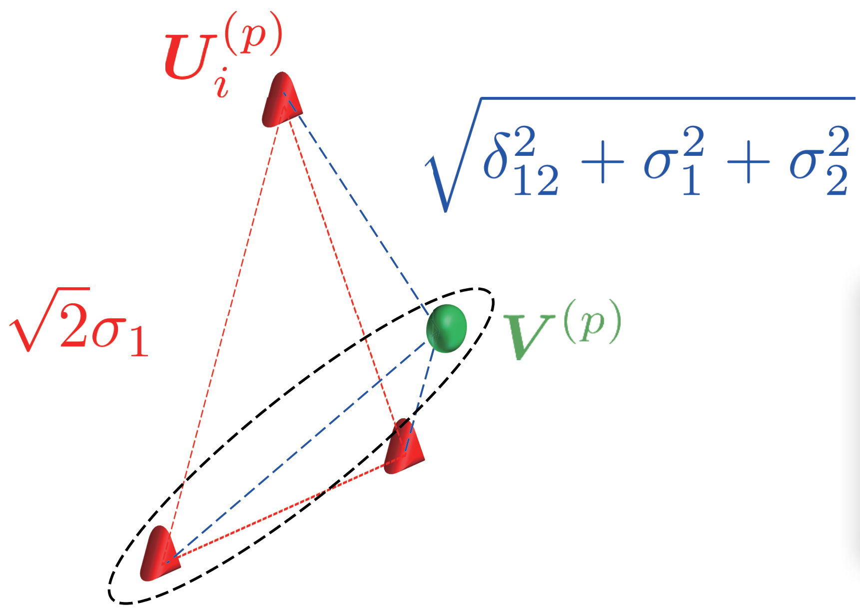


  - The distance between data vectors from different clusters is also approximately constant after scaled by $\sqrt{p}$!



1.2. Difficulty of clustering for HDLSS data

- **Hierarchical clustering in HDLSS contexts**
  - $\boldsymbol{U}_1^{(p)}, \boldsymbol{U}_2^{(p)}, \boldsymbol{U}_3^{(p)} \overset{\text{i.i.d.}}{\sim} \boldsymbol{X}_1^{(p)}$; $\boldsymbol{V}^{(p)} \overset{\text{i.i.d.}}{\sim} \boldsymbol{X}_2^{(p)}$



$$\sqrt{2}\sigma_1 \geq \sqrt{\delta_{12}^2 + \sigma_1^2 + \sigma_2^2}$$

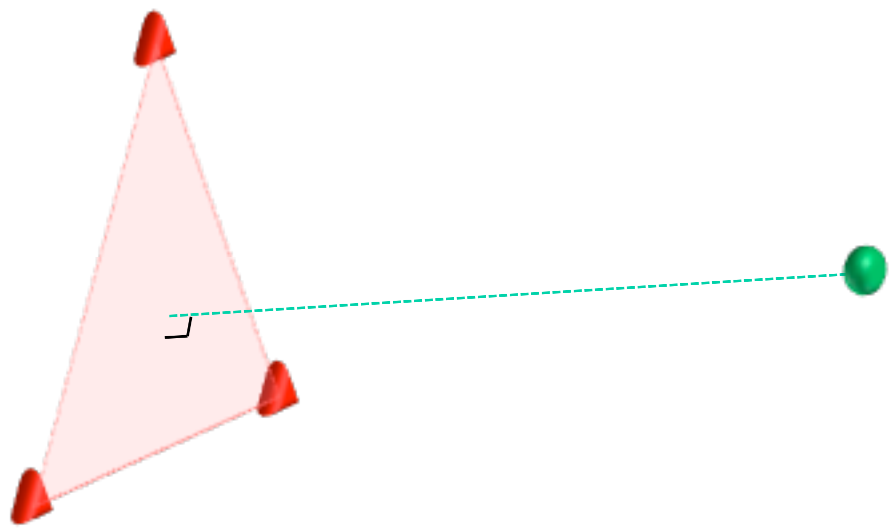
Condition for label consistency

$$2\sigma_k^2 < \mu_{kl}^2 + \sigma_k^2 + \sigma_l^2$$

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

2. Previous study (MDP clustering)

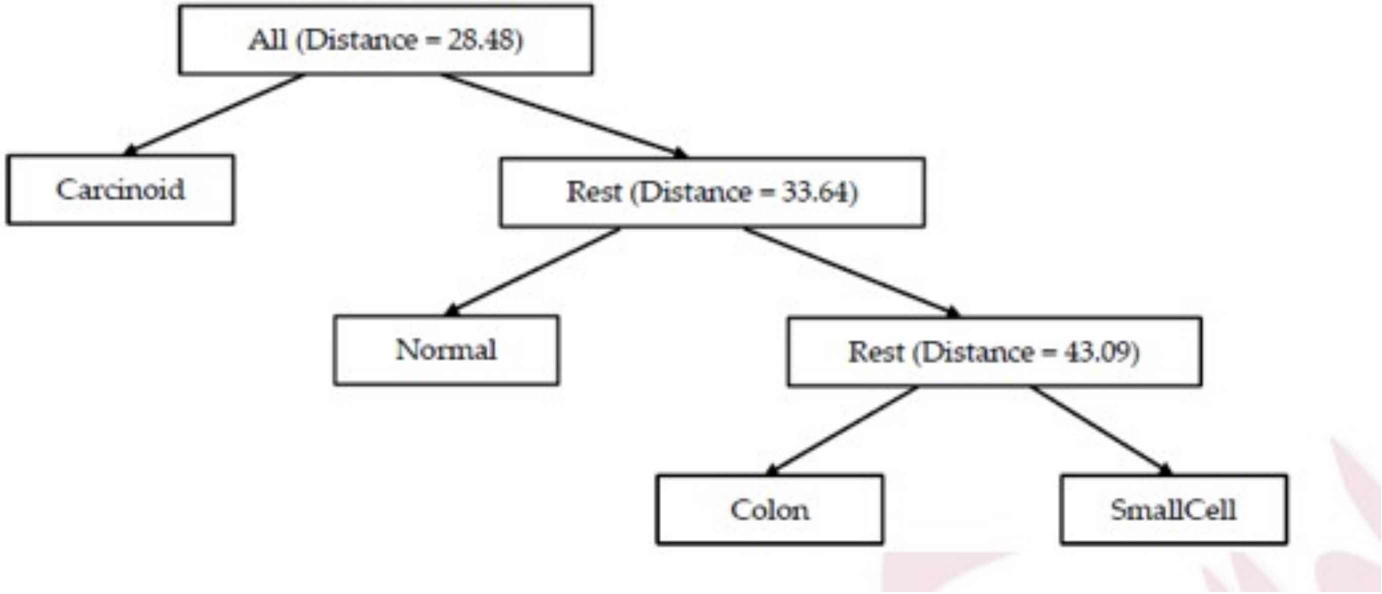
- **Maximal data piling (MDP) distance (Ahn and Marron, 2007)**
  - The orthogonal distance between the affine subspaces generated by the data vectors in each cluster.



$$\boldsymbol{U}_1^{(p)}, \boldsymbol{U}_2^{(p)}, \boldsymbol{U}_3^{(p)} \overset{\text{i.i.d.}}{\sim} \boldsymbol{X}_1^{(p)};\ \boldsymbol{V}^{(p)} \overset{\text{i.i.d.}}{\sim} \boldsymbol{X}_2^{(p)}$$

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

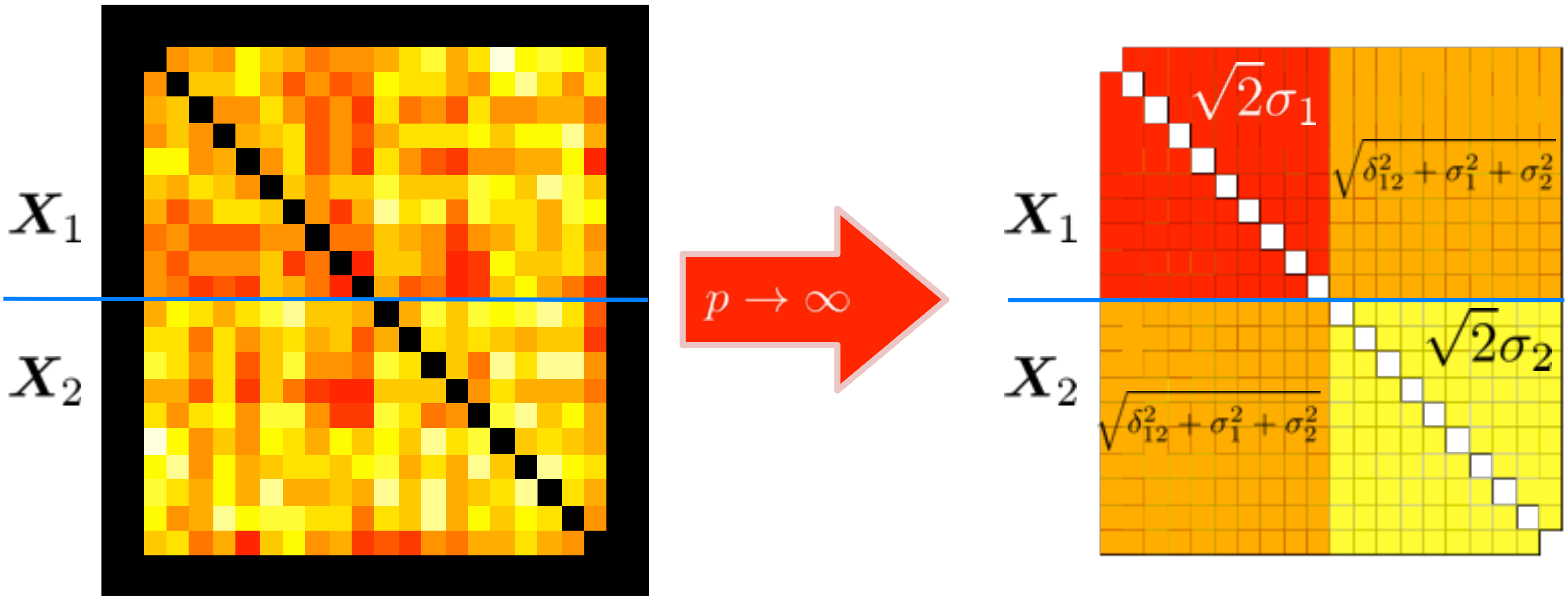
– Toy example:

- $\boldsymbol{X}_1 \sim N_p(\mathbf{0},\ I_p)$
- For $c \neq 1$, $\boldsymbol{X}_2 \sim N_p(\mathbf{0},\ cI_p)$,
- The condition of Ahn et al. (2013) dose not hold.

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

3. Clustering with distance vectors

3.1 Main idea



Standardized distances converge to some constants in prob.

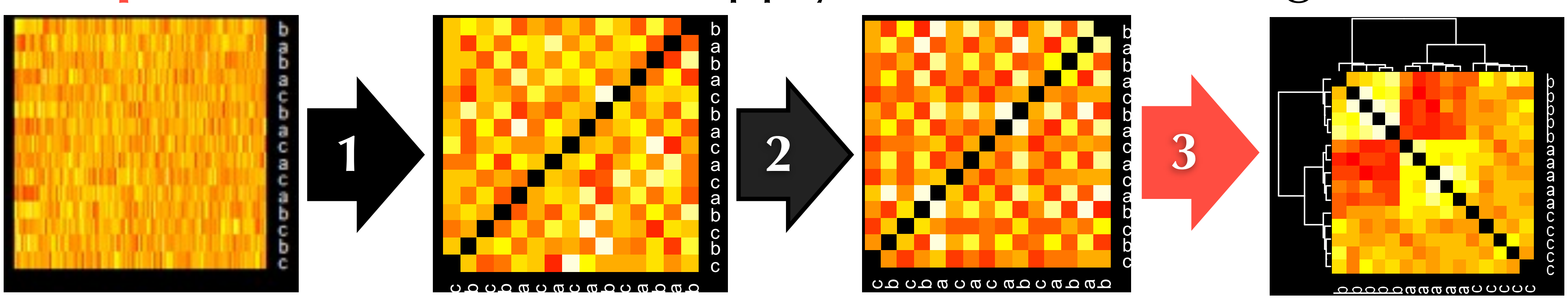
Distance "*vectors*" have the cluster information!

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 ($\Xi := (\xi_{ij})_{n \times n}$),

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

  - <u>**Step 3.**</u> For the matrix Ξ, apply a usual clustering method.



Data matrix X — Inner product S — Distance matrix Ξ — Inner product S

3. Clustering with distance vectors

- ***K*-means Type**

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

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 $K^* \geq K$,

$$\min_{\mathscr{C}} Q_p(\mathscr{C} \mid K^*) \xrightarrow{\mathbb{P}} 0 \quad \text{as} \quad p \to \infty.$$

3. Clustering with distance vectors

- **Theoretical results of the *k*-means type**
  - **In the case of using a distance matrix**

Assume a) $\sim$ f) .

If $\forall k,\ l\ (k \neq l);\ \sigma_k \neq \sigma_l \text{ or } \delta_{kl}^2 > 0,$

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

- Ahn et al., 2013

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

3. Clustering with distance vectors

- **Theoretical results of the *k*-means type**
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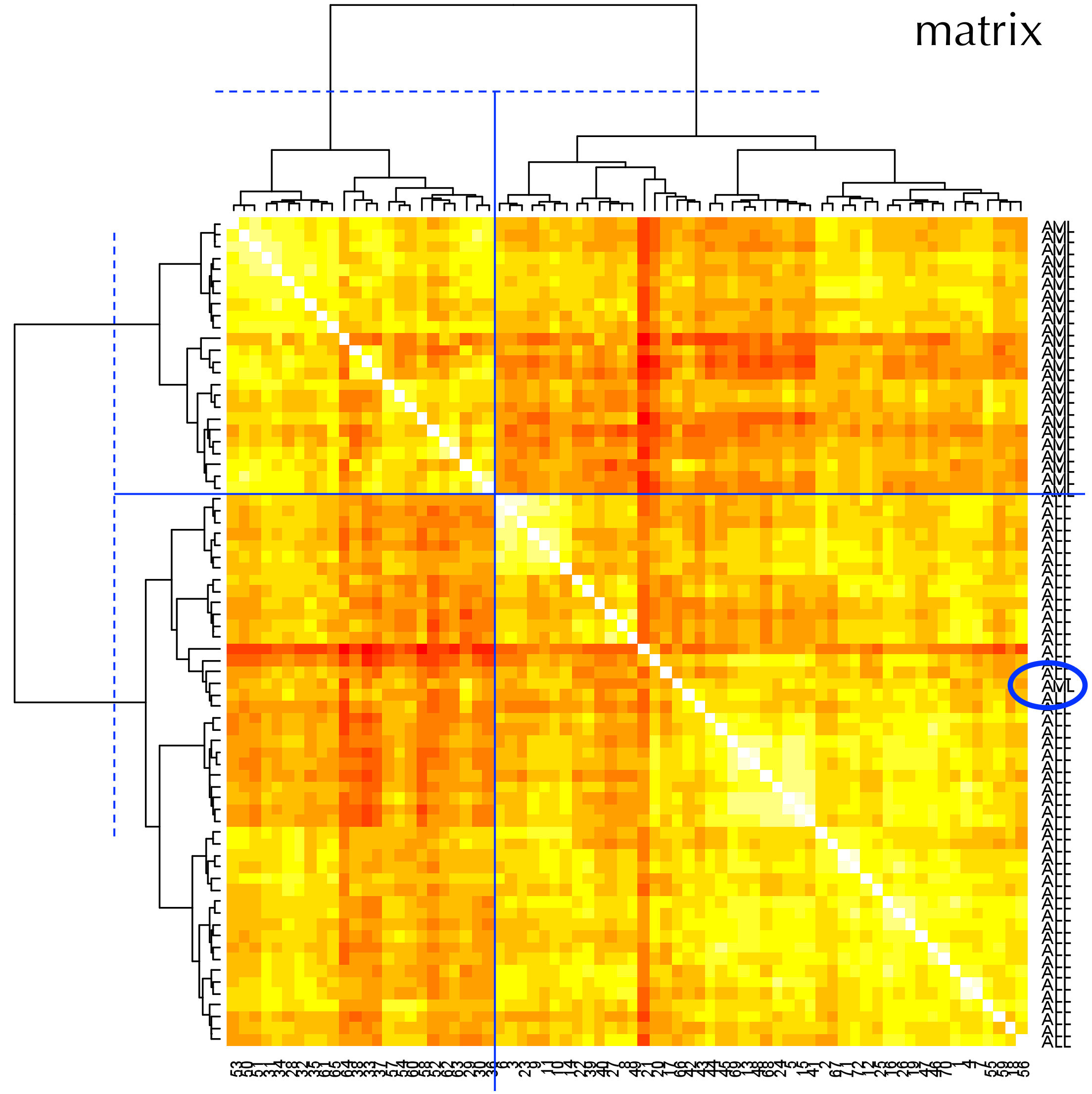
3. Clustering with distance vectors

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)

Inner product matrix



4. Conclusion

Thank you for your attention!

- In this presentaion,
  - 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!

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A. Definition of ρ-mixing

- **ρ-mixing** (Kolmogorov and Rozanov, 1960; Theor. Probab. Appl.)
  - For $-\infty \leq J \leq L \leq \infty$,

    $\mathcal{F}_J^L$: the σ-field of events generated by the r.v.s $(Z_i,\ J \leq i \leq L)$.
  - For any σ-field $\mathcal{A}$,

    $L_2(\mathcal{A})$: the space of square-integrable, $\mathcal{A}$-measurable r.v.s.
  - For each $m \geq 1$, define the maximal correlation coefficient

    $$\rho(m) := \sup |\mathrm{Corr}(f,\ g)|, \quad f \in L_2(\mathcal{F}_{-\infty}^{j}),\ g \in L_2(\mathcal{F}_{j+m}^{\infty}),$$

    where $j \in \mathbb{Z}$.
  - The sequence $\{Z_i\}$ is said to be ρ**-mixing** if

    $$\rho(m) \to 0 \quad \text{as} \quad m \to \infty.$$