Lecture 8. Clustering High-Dimensional Data

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- Challenges of Clustering High-Dimensional Data
- Methods for Clustering High-Dimensional Data
- Subspace Clustering Methods
  - Subspace Clustering I: Subspace Search Methods
  - Subspace Clustering II: Correlation-Based Methods
  - Subspace Clustering III: Bi-Clustering Methods
    - δ-Bi-Clustering
    - δ-pClustering
- Dimensionality Reduction Methods

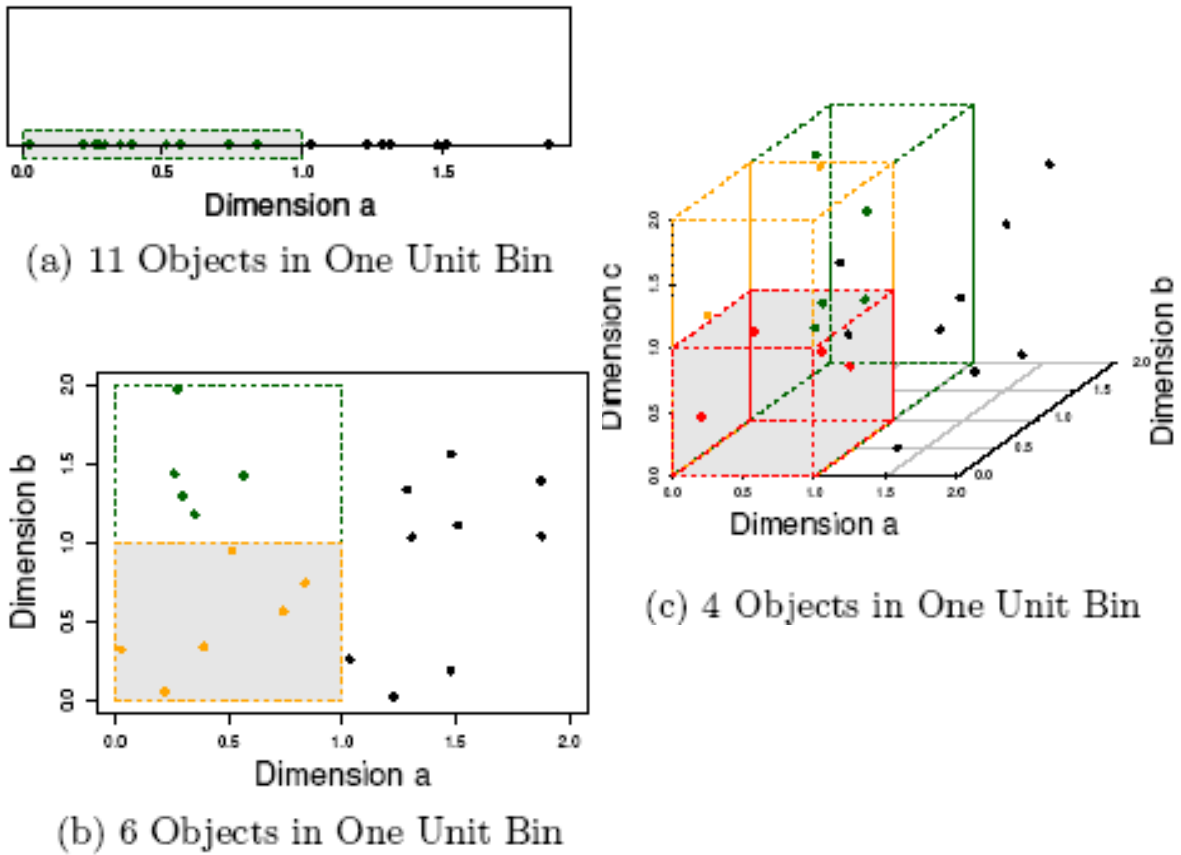
Session 1: Challenges of Clustering High-Dimensional Data

Clustering High-Dimensional Data

- Why cluster high-dimensional data?
  - How high is high-dimension in clustering?
    - Many clustering algorithms deal with 1-3 dimensions
    - These methods may not work well when the number of dimensions grows to 20
  - Many applications, such as text documents or DNA micro-array data, may need to handles tens of thousands of dimensions
- Major challenges of high-dimensional data clustering
    - Many irrelevant dimensions may mask clusters
    - Distance measure becomes meaningless—due to equidistance
    - Clusters may exist only in some subspaces

The Curse of Dimensionality

- Data in only one dimension is relatively packed
- Adding a dimension *stretches* the points across that dimension, making them further apart
- Adding more dimensions will make the points further apart—high dimensional data is extremely sparse
- Distance measure becomes meaningless—due to equidistance
- Traditional distance measure could be dominated by noises in many dimensions



(a) 11 Objects in One Unit Bin

(b) 6 Objects in One Unit Bin

(c) 4 Objects in One Unit Bin

Ack. Graphs adapted from Parsons et al., Subspace clustering for high dimensional data: A review. SIGKDD Explorations 2004)

Curse of Dimensionality: Five Different Aspects

- **Optimization**: The difficulty of global optimization increases exponentially with an increase in the number of dimensions
- **Distance concentration effect** of L_p-norms
  - Distance concentration: Far and close neighbors have similar distances
  - The relative contrast of L_p distances diminishes as dimensionality increases
- **Irrelevant attributes** can interfere with the performance of clustering for that object
  - The relevance of certain attributes may differ for different groups of objects
- **Correlated attributes**: Strong correlation among a subset of attributes can be used to reduce dimensionality
  - The *intrinsic dimensionality* of a dataset can be considerably lower than *embedded dimensionality* (i.e., the number of features of the dataset)
- **Data sparsity**: Data volume in high-dimensional space is extremely sparse

Session 2: Methods for Clustering High-Dimensional Data

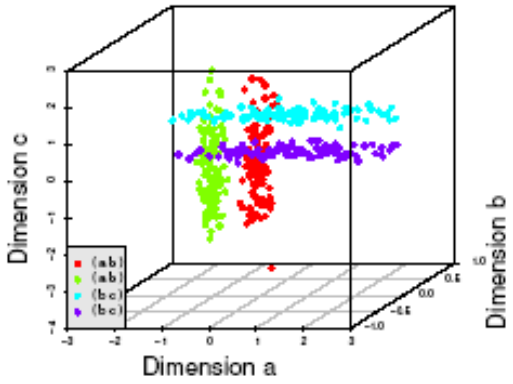
Methods for Clustering High-Dimensional Data

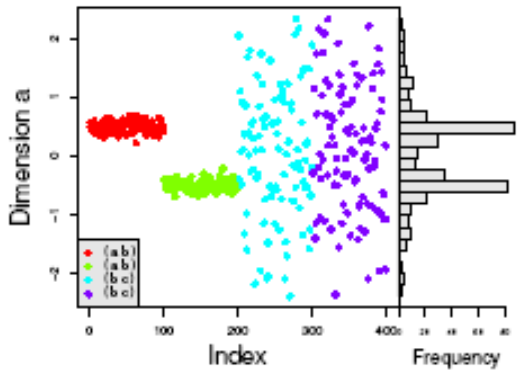
- Methods can be grouped in two categories
  - **Subspace-clustering**: Search for clusters existing in subspaces of the given high dimensional data space
    - CLIQUE, ProClus, and bi-clustering approaches
  - **Dimensionality reduction approaches**: Construct a much lower dimensional space and search for clusters there (may construct new dimensions by combining some dimensions in the original data)
    - Spectral clustering and various dimensionality reduction methods
- Clustering should not only consider dimensions but also attributes (features)
  - **Feature selection:** Useful to find a subspace where the data have nice clusters
  - **Feature transformation:** Effective if most dimensions are relevant
    - PCA (Principal Component Analysis) and SVD (Singular Value Decomposition) are useful when features are highly correlated or redundant

Session 3: Subspace Clustering Methods

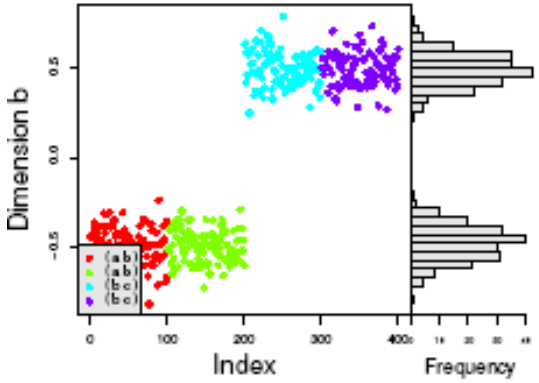
Why Subspace Clustering?

- Clusters may exist only in some subspaces
- Subspace-clustering: Find clusters in all the subspaces

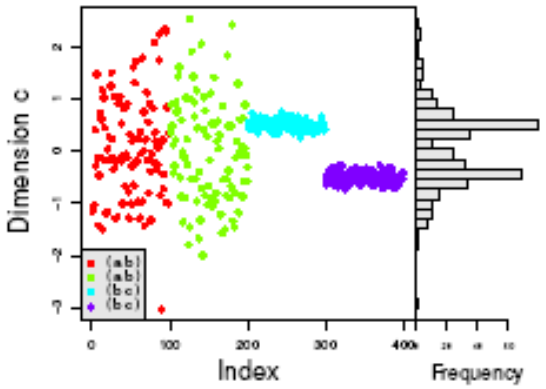




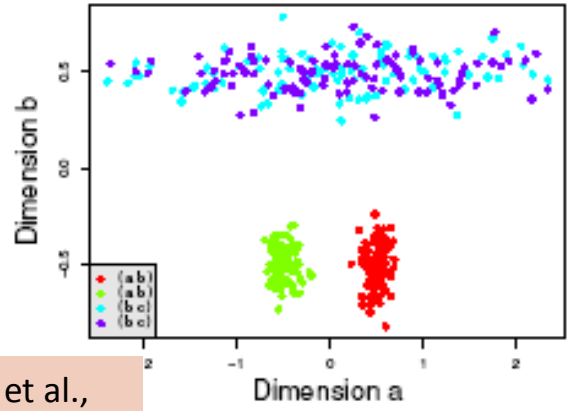
(a) Dimension a



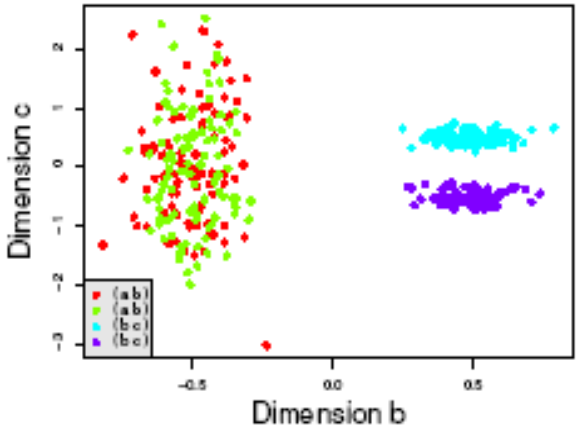
(b) Dimension b



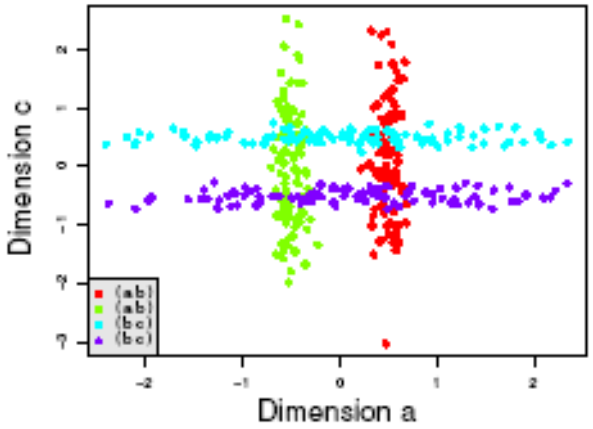
(c) Dimension c



(a) Dims a & b



(b) Dims b & c



(c) Dims a & c

Ack. Graphs adapted from Parsons et al., Subspace clustering for high dimensional data: A review. SIGKDD Explorations 2004)

Subspace Clustering Methods

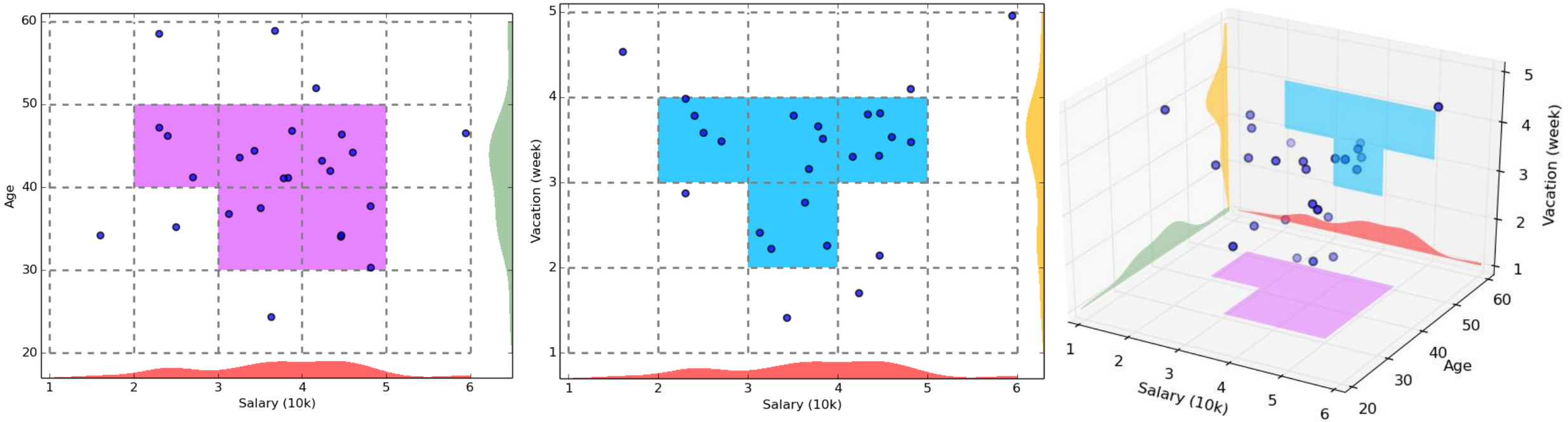
- Axis-parallel vs. arbitrarily oriented subspaces
  - Axis-parallel: Subspaces are in parallel with some axes
  - Arbitrarily oriented subspaces
- **Subspace search methods**: Search in axis-parallel subspaces to find clusters
  - Bottom-up approaches
  - Top-down approaches
- **Search and clustering in arbitrarily oriented subspaces**
  - Correlation-based clustering methods
    - E.g., PCA-based approaches
- **Bi-clustering methods**
  - Optimization-based methods
  - Enumeration methods

Session 4: Subspace Clustering I: Subspace Search Methods

Subspace Clustering: Subspace Search Methods

- Search various subspaces to find clusters
- ***Bottom-up approaches***
  - Start from low-D subspaces and search higher-D subspaces only when there may be clusters in such subspaces
  - Various pruning techniques to reduce the number of higher-D subspaces to be searched
  - Ex. CLIQUE (Agrawal et al. 1998)
- ***Top-down approaches***
  - Start from full space and search smaller subspaces recursively
  - Effective only if the *locality assumption* holds: Restricts that the subspace of a cluster can be determined by the local neighborhood
  - Ex. PROCLUS (Aggarwal et al. 1999): A *k*-medoid-like method

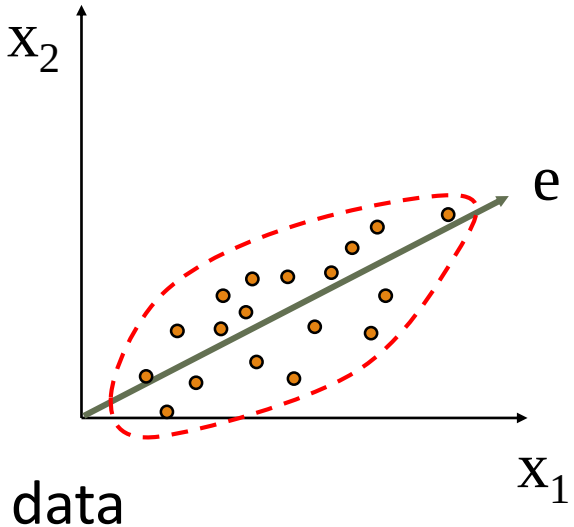
Example of CLIQUE: Density and Grid-Based Subspace Clustering



- Start at 1-D space and discretize numerical intervals in each axis into grid
- Find dense regions in each subspace and generate their minimal descriptions (clusters)
- Use the dense regions to find promising candidates in 2-D space (using Apriori principle)
- CLIQUE automatically identifies subspaces of a high dimensional data space and terminates when no more clusters or cluster candidates can be found

Session 5: Subspace Clustering II: Correlation-Based Methods

Subspace Clustering: Correlation-Based Methods



- **Subspace search method**
  - Similarity measure is based on distance or density
- **Correlation-based method**: Based on advanced correlation models
  - Ex. PCA (Principal Component Analysis)-based approach
    - Find a projection that captures the largest amount of variation in data
    - Apply PCA to derive a set of new, uncorrelated dimensions (*dimensionality reduction*)
    - Then find clusters in the new space or its subspaces
  - Other space transformation methods
    - Hough transform
    - Fractal dimensions

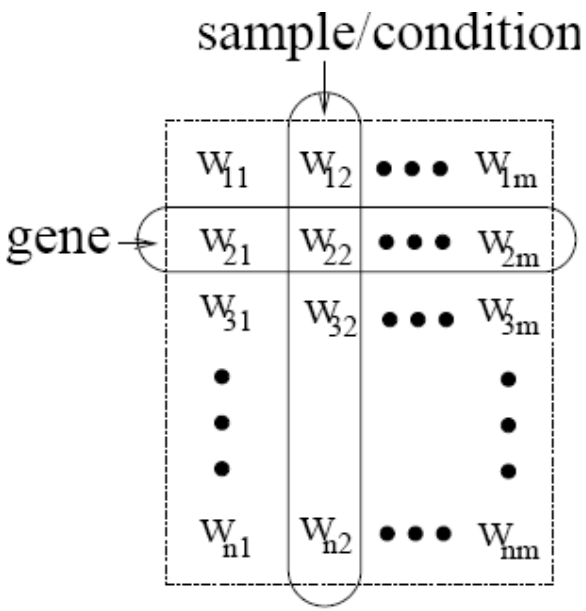
Simple Illustration of Principal Component Analysis

- Given N data vectors (numeric data only) from n-dimensions, find $k \leq n$ orthogonal vectors (*principal components*) that can be best used to represent data
- Normalize input data: Each attribute falls within the same range
- Compute k orthogonal (i.e. linearly uncorrelated) (unit) vectors, i.e., ***principal components***
- Each input vector is a linear combination of the k **principal component vectors**
- The principal components are sorted in order of decreasing "significance" or strength
- Eliminate the *weak components* (i.e., those with low variance)
  - That is, using the strongest principal components, it is possible to reconstruct a good approximation of the original data

Session 6: Subspace Clustering III: Bi-Clustering Methods

Subspace Clustering (III): Bi-Clustering Methods

- Bi-clustering: Cluster both objects and attributes simultaneously (treating objects and attributes in a symmetric way)
- Four requirements:
  1. Only a small set of objects participate in a cluster
  2. A cluster only involves a small number of attributes
  3. An object may participate in multiple clusters or does not participate in any cluster at all
  4. An attribute may be involved in multiple clusters or is not involved in any cluster at all
- Ex 1. *Gene expression* or *microarray data*
  - A gene-sample/condition matrix: Each element in the matrix, a real number, records the expression level of a gene under a specific condition
- Ex. 2. Clustering customers and products



products

customers

$$\begin{matrix} w_{11} & w_{12} & \cdots & w_{1m} \\ w_{21} & w_{22} & \cdots & w_{2m} \\ \cdots & \cdots & \cdots & \cdots \\ w_{n1} & w_{n2} & \cdots & w_{nm} \end{matrix}$$

Types of Bi-Clusters

- Let $A = \{a_1, \ldots, a_n\}$ be a set of genes, $B = \{b_1, \ldots, b_m\}$ a set of conditions
- A bi-cluster: A submatrix where genes and conditions follow some consistent patterns
- 4 types of bi-clusters (ideal cases)
  - Bi-clusters with constant values:
    - for any i in I and j *in* J, $e_{ij} = c$
  - Bi-clusters with constant values in rows:
    - $e_{ij} = c + \alpha_i$
    - Also, it can be constant values in columns
  - Bi-clusters with *coherent values* (i.e., *pattern-based clusters*)
    - $e_{ij} = c + \alpha_i + \beta_j$
  - Bi-clusters with *coherent* evolutions in rows
    - $(e_{i1j1} - e_{i1j2})(e_{i2j1} - e_{i2j2}) \geq 0$
    - i.e., only interested in the up- or down- regulated changes across genes or conditions without constraining on the exact values

10	10	10	10	10
20	20	20	20	20
50	50	50	50	50
0	0	0	0	0

10	50	30	70	20
20	60	40	80	30
50	90	70	110	60
0	40	20	60	10

10	50	30	70	20
20	100	50	1000	30
50	100	90	1200	80
0	80	20	100	10

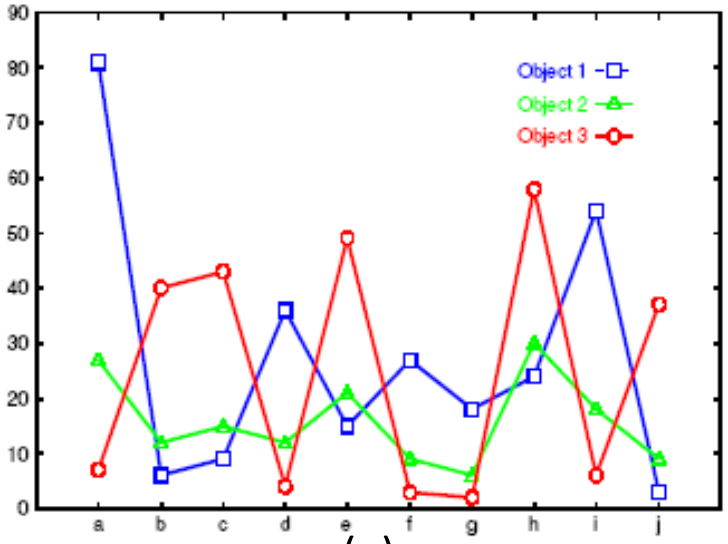
Bi-Clustering Methods

- Real-world data is noisy: Try to find approximate bi-clusters
- Methods: Optimization-based methods vs. enumeration methods
- **Optimization-based methods**
  - Try to find submatrices one at a time to achieve the best significance as a bi-cluster
  - Due to the cost in computation, greedy search is employed to find local optimal bi-clusters
  - Ex. δ-bicluster Algorithm (Cheng and Church, ISMB'2000)
- **Enumeration methods**
  - Use a tolerance threshold to specify the degree of noise allowed in the bi-clusters to be mined
  - Then try to enumerate all submatrices as bi-clusters that satisfy the requirements
  - Ex. δ-pCluster Algorithm (H. Wang et al. SIGMOD'2002, MaPle: Pei et al., ICDM'2003)

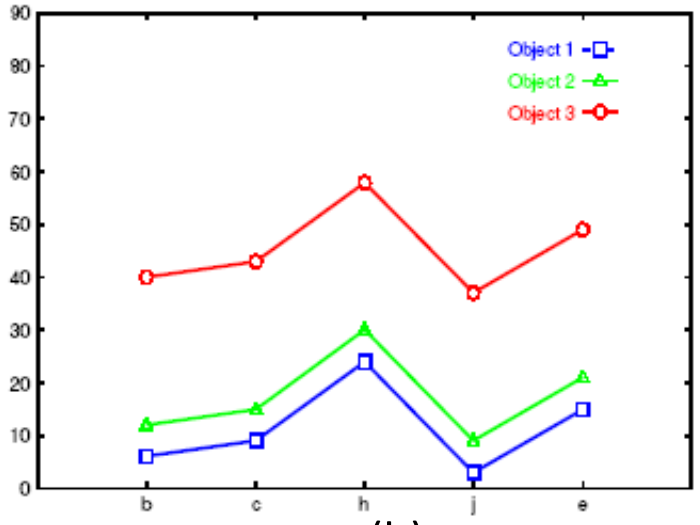
Session 7: Bi-Clustering I: δ-Bi-Clustering

Bi-Clustering for Micro-Array Data Analysis

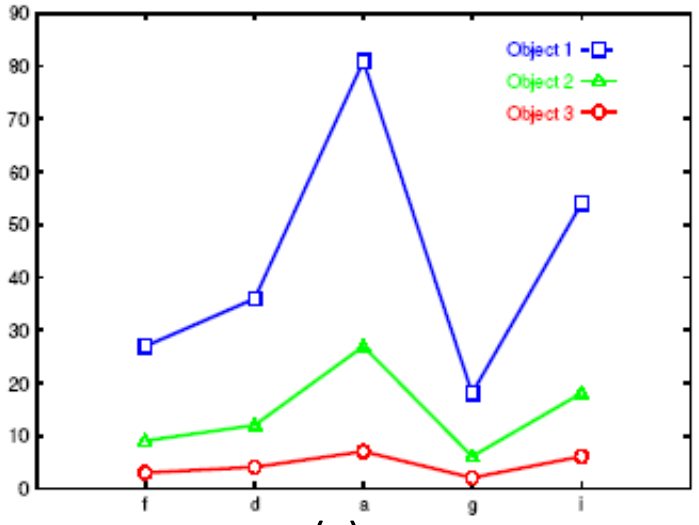
- Figure (a): Micro-array "raw" data shows three objects (e.g., tissues) and their gene values in a multi-dimensional space: Difficult to find their patterns
- Figures (b) and (c): Some subsets of dimensions form nice shift and scaling patterns
- No globally defined similarity/distance measure
- Clusters may not be exclusive
  - A gene can appear in multiple clusters



(a)



(b)



(c)

Bi-Clustering (I): δ-Bi-Cluster

- For a submatrix *I x J*
  - *T*he **mean of the *i*-th row**: $e_{iJ} = \frac{1}{|J|}\sum_{j \in J} e_{ij}$
  - The **mean of the *j*-th column**: $e_{Ij} = \frac{1}{|I|}\sum_{i \in I} e_{ij}$
  - The **mean of all elements in the submatrix**: $e_{IJ} = \frac{1}{|I||J|}\sum_{i \in I, j \in J} e_{ij} = \frac{1}{|I|}\sum_{i \in I} e_{iJ} = \frac{1}{|J|}\sum_{j \in J} e_{Ij}$
- The **quality of the submatrix as a bi-cluster** can be measured by the *mean squared residue* value

$$H(I \times J) = \frac{1}{|I||J|}\sum_{i \in I, j \in J} (e_{ij} - e_{iJ} - e_{Ij} + e_{IJ})^2$$

- A submatrix *I x J* is **δ-bi-cluster** if $H(I \times J) \leq \delta$ where $\delta \geq 0$ is a threshold
  - When $\delta = 0$, *I x J* is a perfect bi-cluster with coherent values
  - By setting $\delta > 0$, a user can specify the tolerance of average noise per element against a perfect bi-cluster
    - residue(e_{ij}) = $e_{ij} - e_{iJ} - e_{Ij} + e_{IJ}$

Bi-Clustering (I): The δ-Bi-Cluster Algorithm

- **Maximal δ-bi-cluster**
  - A δ-bi-cluster *I x J* s.t. no other δ-bi-cluster *I' x J' which* contains *I x J*
- Computing is costly: Use heuristic greedy search to obtain local optimal clusters
- Two phase computation: *Deletion phase* and *addition phase*
  - **Deletion phase:**
    - Start from the whole matrix, iteratively remove rows and columns while the mean squared residue of the matrix is over δ
    - At each iteration, for each row/*column*
      - Compute the *mean squared residue:*

$$d(i) = \frac{1}{|J|}\sum_{j \in J}(e_{ij} - e_{iJ} - e_{Ij} + e_{IJ})^2 \qquad d(j) = \frac{1}{|I|}\sum_{i \in I}(e_{ij} - e_{iJ} - e_{Ij} + e_{IJ})^2$$

      - Remove the row or column of the largest mean squared residue

Bi-Clustering (I): The δ-Bi-Cluster Algorithm (Cont.)

- Two phase computation: *Deletion phase* and *addition phase* (continued)
  - **Addition phase:**
    - Expand iteratively the δ-bi-cluster *I x J* obtained in the deletion phase as long as the δ-bi-cluster requirement is maintained
    - Consider all the rows/columns not involved in the current bi-cluster *I x J* by calculating their mean squared residues
    - A row/column of the smallest mean squared residue is added into the current δ-bi-cluster
- It finds only one δ-bi-cluster, thus needs to run multiple times
  - By replacing the elements in the output bi-cluster by random numbers
- A quite costly search process

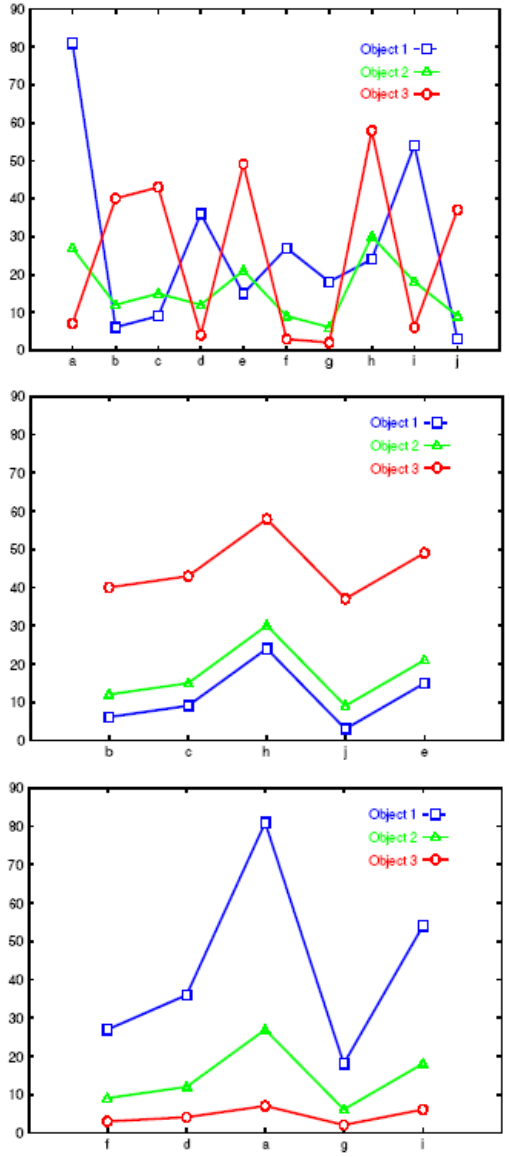
Session 8: Bi-Clustering II: δ-pClustering

Bi-Clustering (II): δ-pCluster: Clustering by Pattern Similarity

- Clustering by pattern similarity (δ-pClusters) [H. Wang, et al., SIGMOD'02]
- A submatrix *I x J* is a bi-cluster with (perfect) coherent values if and only if $e_{i1j1} - e_{i2j1} = e_{i1j2} - e_{i2j2}$
  - For any 2 *x* 2 submatrix of *I x J*, $p\text{-score}\begin{pmatrix} e_{i_1j_1} & e_{i_1j_2} \\ e_{i_2j_1} & e_{i_2j_2} \end{pmatrix} = |(e_{i_1j_1} - e_{i_2j_1}) - (e_{i_1j_2} - e_{i_2j_2})|$
- A submatrix *I x J* is a **δ-pCluster** (pattern-based cluster) if the *p*-score of every 2 *x* 2 submatrix of *I x J* is at most δ, where δ ≥ 0 is a threshold specifying a user's tolerance of noise against a perfect bi-cluster
- The *p*-score controls the noise on every element in a bi-cluster, while the mean squared residue captures the average noise
- **Monotonicity**: If *I* x *J* is a δ-pCluster, every *x* x *y* (*x,y* ≥ 2) submatrix of *I* x *J* is also a δ-pCluster
- A δ-pCluster is **maximal** if no more rows or columns can be added to still make it retain as a δ-pCluster—We only need to compute all maximal δ-pClusters

More on δ-pClustering and Efficiency Improvement (MaPle)

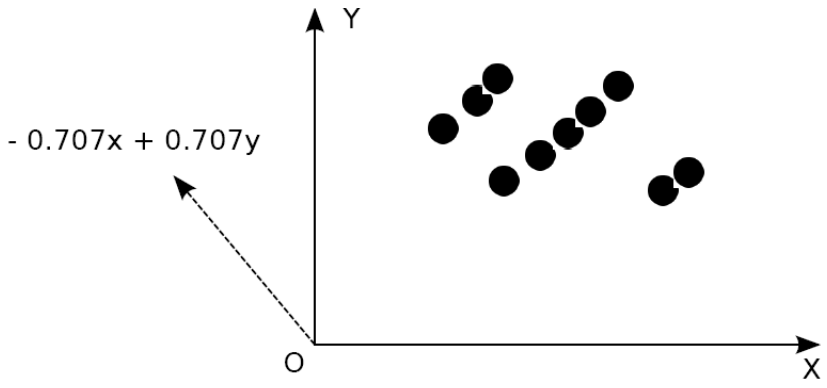
- Additional advantages of *δ-p*Clusters:
  - Containing no outliers: Due to the averaging effect, *δ*-bi-cluster may contain outliers but still within *δ*-threshold
  - For scaling patterns, taking logarithmic on $\frac{d_{xa} / d_{ya}}{d_{xb} / d_{yb}} < \delta$ will lead to the same *p*-score form
- Further improving mining efficiency (MaPle: Pei et al. ICDM'03)
- Framework: A pattern-growth approach in frequent pattern mining (Algorithm is similar to mining frequent closed itemsets)
- For each condition combination J, find the maximal subsets of genes I such that I x J is a *δ-p*Clusters
  - If I x J is not a submatrix of another *δ-p*Clusters
  - then I x J is a maximal *δ-p*Cluster



Session 9: Dimensionality Reduction Methods

Dimensionality Reduction

- Dimensionality reduction
  - In some situations, it is more effective to construct a new space instead of using some subspaces of the original data
  - Ex. To cluster the points in the figure, any subspace of the original one, X and Y, cannot help since all the three clusters projected to X and Y axes will overlap
    - Upon constructing a new dimension such as the dashed one, the three clusters become apparent as the points are projected into the new dimension



Dimensionality-Reduction Methods

- Feature selection and extraction may not focus on clustering structure finding
- Dimensionality reduction: Reduce dimensionality by mathematical transformation
  - **Nonnegative matrix factorization (NMF)** Will briefly outline the idea in the next slide
    - One high-dimensional sparse nonnegative matrix factorizes approximately into two low-rank matrices
  - **Spectral clustering** To be covered in Lecture 10
    - Uses the *spectrum* of the similarity matrix of the data to perform dimensionality reduction for clustering in fewer dimensions
    - Combining feature extraction and clustering
    - **Typical spectral clustering methods**
      - Normalized Cuts (Shi and Malik, CVPR'97 or PAMI'2000)
      - The Ng-Jordan-Weiss algorithm (NIPS'01)

Clustering by Nonnegative Matrix Factorization (NMF)

- Nonnegative matrix factorization (NMF)
  - A nonnegative matrix $A_{n\times d}$ (e.g., word frequencies in documents) can be approximately factorized into two nonnegative lower rank matrices $U_{n\times k}$ and $V_{k\times d}$ $(k << d, n)$:
    - $A_{n\times d} \approx U_{n\times k}\, V_{k\times d}$ (or, $A \approx U\, V$)
  - Residue matrix R represents the noise in the underlying data: $R = A - U\, V$
- Constrained optimization: Determine U and V so that the sum of the square of the residuals in R is minimized
- U and V simultaneously provide the clusters on the rows (docs) and columns (words): Another kind of co-clustering
  - $U_{n\times k}$: the components of each of n objects mapped into each of k newly created dimensions
  - $V_{k\times d}$: Each of k newly created dimensions in terms of the original d dimensions
- Advantage: Interpretability of NMF—A data point can be expressed as a nonnegative linear combination of the concepts in the underlying data

Session 10: Summary

Summary: Clustering High-Dimensional Data

- Challenges of Clustering High-Dimensional Data
- Methods for Clustering High-Dimensional Data
- Subspace Clustering Methods
  - Subspace Clustering I: Subspace Search Methods
  - Subspace Clustering II: Correlation-Based Methods
  - Subspace Clustering III: Bi-Clustering Methods
    - δ-Bi-Clustering
    - δ-pClustering
- Dimensionality Reduction Methods

Recommended Readings

- R. Agrawal, J. Gehrke, D. Gunopulos, and P. Raghavan. Automatic Subspace Clustering of High Dimensional Data for Data Mining Applications. *SIGMOD'98*
- C. C. Aggarwal, C. Procopiuc, J. Wolf, P. S. Yu, and J.-S. Park. Fast Algorithms for Projected Clustering. *SIGMOD'99*
- Y. Cheng and G. Church. Biclustering of Expression Data. *ISMB'00*
- H.-P. Kriegel, P. Kroeger, and A. Zimek. Clustering High Dimensional Data: A Survey on Subspace Clustering, Pattern-Based Clustering, and Correlation Clustering. *TKDD'*09
- S. C. Madeira and A. L. Oliveira. Bi-clustering Algorithms for Biological Data Analysis: A Survey. *IEEE/ACM Trans. Comput. Biol. Bioinformatics*, 1, 2004
- L. Parsons, E. Haque, and H. Liu. Subspace Clustering for High Dimensional Data: A Review. *ACM SIGKDD Explorations*, 6(1):90–105, 2004.
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- H. Wang, W. Wang, J. Yang, and P. S. Yu. Clustering by Pattern Similarity in Large Data Sets. *SIGMOD'02*
- A. Zimek. Clustering High-Dimensional Data (Chapter 9), in C. Aggarwal and C. K. Reddy (eds.), Data Clustering: Algorithms and Applications. CRC Press, 2014