Deriving Quantitative Models for Correlation Clusters

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12th ACM SIGKDD International Conference on Knowledge Discovery and Data Mining, Philadelphia, PA, 2006
Overview

1 Correlation Clustering and Beyond
   - What are Correlation Clusters?
   - Why are Correlation Clusters Interesting?
   - What are Models for?

2 Deriving Quantitative Models for Correlation Clusters
   - Formal Description of Correlation Clusters
   - Quantitative Models for Correlation Clusters
   - Interpretation of Correlation Cluster Models
   - Quantitative Models as Predictive Models

3 Evaluation
   - Identifying Models
   - Predictive Models

4 Conclusions
Correlation Clusters

- hyperplanes exhibiting a high density of data points
- strong correlations between different features
- corresponding linear dependencies
There are certain pathways for degradation of metabolites. Concentrations of input and output metabolites may be correlated, the concentration of alternative intermediate states may vary depending on the environment. Genetic disorders may lead to failure of some pathways, other pathways are used more intensely. The concentrations of more metabolites are correlated if samples suffer from certain diseases.
Example: Metabolic Pathways

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Correlation Clustering

- clustering: find sets of points building a hyperplane of arbitrary dimensionality
  e.g. metabolic pathways: Which patients are suffering from a disease?
- post-clustering: what are the underlying linear dependencies?
  e.g. metabolic pathways: What is the nature of the disease?

\[
\begin{align*}
&\begin{pmatrix}
A \\
- B
\end{pmatrix} = c_1 \\
&\begin{pmatrix}
a_1 \\
-3 \cdot B
\end{pmatrix} = c_2
\end{align*}
\]
Correlation Cluster Model

- A model can describe a cluster.
- A model can possibly be interpreted by domain experts, leading to new insights.
- A model can possibly be used to predict the class of a new point.
decompose covariance matrix of correlation cluster \( C \) to eigenvalues and eigenvectors:

\[
\Sigma_C = V_C \cdot E_C \cdot V_C^T
\]

most of the variance covered by small number of eigenvectors

number of eigenvectors covering most of the variance is called correlation dimensionality \( \lambda_C \) of cluster \( C \)

eigenvectors \( \#1, \ldots, \#\lambda_C \) : strong eigenvectors \( \tilde{V}_C \)

eigenvectors \( \#\lambda_C + 1, \ldots, \#d \) : weak eigenvectors \( \hat{V}_C \)
Strong and Weak Eigenvectors

- Strong eigenvectors span the hyperplane corresponding to a correlation cluster.
- Weak eigenvectors are orthogonal to the hyperplane.

(a) $\lambda = 1$

(b) $\lambda = 2$
Eigenvectors Define a Correlation Cluster

hyperplane of a correlation cluster $\mathcal{C}$ as affine subspace:
- strong eigenvectors $\mathcal{V}_C$ as basis
- an affinity w.r.t. original data space (e.g. centroid $\bar{x}_c$ of the cluster $\mathcal{C}$)

$$x = \bar{x}_c + a_1 v^1_C + \ldots + a_\lambda v^\lambda_C, a_i \in \mathbb{R}$$

equivalent: definition by weak eigenvectors $\hat{\mathcal{V}}_C$ and affinity $\bar{x}_c$
Quantitative Models

- equation system to describe the hyperplane of correlation cluster $C$ based on weak eigenvectors $\hat{V}_C$ and affinity $\bar{x}_C$:

$$\hat{V}_C^T \cdot x = \hat{V}_C^T \cdot \bar{x}_C.$$

- equivalently:

$$v_{(\lambda+1),1}(x_1 - \bar{x}_1) + v_{(\lambda+1),2}(x_2 - \bar{x}_2) + \cdots + v_{(\lambda+1),d}(x_d - \bar{x}_d) = 0$$

$$v_{(\lambda+2),1}(x_1 - \bar{x}_1) + v_{(\lambda+2),2}(x_2 - \bar{x}_2) + \cdots + v_{(\lambda+2),d}(x_d - \bar{x}_d) = 0$$

$$\vdots$$

$$v_{d,1}(x_1 - \bar{x}_1) + v_{d,2}(x_2 - \bar{x}_2) + \cdots + v_{d,d}(x_d - \bar{x}_d) = 0$$

- defect of $\hat{V}_C^T$: number of free attributes
Algorithm

1. run an arbitrary correlation clustering algorithm (e.g. 4C, ORCLUS) on data set $\mathcal{D} \subset \mathbb{R}^d$

2. for each correlation cluster $C_i \subset \mathcal{D}$ found in the first step:
   1. derive covariance matrix $\Sigma_{C_i}$
   2. select weak eigenvectors $\hat{V}_{C_i}$ of $\Sigma_{C_i}$
   3. derive equation system describing the correlation hyperplane:
      \[
      \hat{V}^T_{C_i} \cdot x = \hat{V}^T_{C_i} \cdot \bar{x}_{C_i}
      \]

4. apply Gauss-Jordan elimination to the derived equation system to obtain a unique description of quantitative dependencies by means of the reduced row echelon form
What a Correlation Cluster Model Tells Us

Example Model:

\[
\begin{align*}
1x_1 + 0x_2 + c_1 x_3 + 0x_4 + e_1 x_5 &= f_1 \\
0x_1 + 1x_2 + c_2 x_3 + 0x_4 + e_2 x_5 &= f_2 \\
0x_1 + 0x_2 + 0x_3 + 1x_4 + e_3 x_5 &= f_3
\end{align*}
\]

- correlation dimensionality: 2 (number of free attributes, number of strong eigenvectors)
- linear dependencies by given factors \(c_1, e_1, c_2, e_2,\) and \(e_3\) among: \(\{x_1, x_3,\) and \(x_5\}\) \(\{x_2, x_3,\) and \(x_5\}\) \(\{x_4\) and \(x_5\}\)

Result:

quantitatively and uniquely defined relations between certain attributes
What a Correlation Cluster Model Does Not Tell Us...

Trivially, correlations do not allow to directly conclude causalities.

... and how we can make use of it anyway

BUT: domain experts could make use of the model to refine experiments.
Quantitative Models as Predictive Models

- Refine descriptive model by determining the average distance of cluster members from correlation hyperplane.

- The standard deviation $\sigma$ of the distances of all cluster members defines a Gaussian model of deviations from the common correlation hyperplane.

- for each model: probability for a new data point to be generated by this specific Gaussian distribution

- set of models: convenient instrument for classification in the perspective of different linear dependencies

$$P(C_j | x) = \frac{1}{\sigma_j \sqrt{2\pi}} e^{\frac{-1}{2\sigma_j^2} (d(x,C_j))^2}$$

$$\sum_{i=1}^{n} \frac{1}{\sigma_i \sqrt{2\pi}} e^{\frac{-1}{2\sigma_i^2} (d(x,C_i))^2}$$
A New Type of Classifier

Decision models of different types of classifiers

- Linear decision boundaries
- Axis parallel decision rules
- Density functions
- Deviations from hyperplanes
**Synthetic Data**

Dataset with increasing standard deviation
Created with dependency: $x_1 - 0.5x_2 - 0.5x_3 = 0$

$\sigma = 0$ (no jitter)

$x_1 - 0.5000x_2 - 0.5000x_3 = 0.0000$
Synthetic Data

Dataset with increasing standard deviation
Created with dependency: $x_1 - 0.5x_2 - 0.5x_3 = 0$

$\sigma = 0.0173$ (jitter of 1% of maximum distance in unit cube)

$x_1 - 0.4989x_2 - 0.5002x_3 = 0.0000$
Synthetic Data

Dataset with increasing standard deviation
Created with dependency: $x_1 - 0.5x_2 - 0.5x_3 = 0$

$\sigma = 0.0346$ (jitter of 2% of maximum distance in unit cube)

$x_1 - 0.5017x_2 - 0.4951x_3 = 0.0016$
Synthetic Data

Dataset with increasing standard deviation
Created with dependency: \( x_1 - 0.5x_2 - 0.5x_3 = 0 \)

\[ \sigma = 0.0520 \text{ (jitter of 3\% of maximum distance in unit cube)} \]
\[ x_1 - 0.5030x_2 - 0.5047x_3 = -0.0059 \]
Dataset with increasing standard deviation
Created with dependency: $x_1 - 0.5x_2 - 0.5x_3 = 0$

$\sigma = 0.0693$ (jitter of 4% of maximum distance in unit cube)

$x_1 - 0.4962x_2 - 0.5106x_3 = -0.0040$
Synthetic Data

Dataset with increasing standard deviation
Created with dependency: \( x_1 - 0.5x_2 - 0.5x_3 = 0 \)

\[ \sigma = 0.0866 \text{ (jitter of 5\% of maximum distance in unit cube)} \]

\[ x_1 - 0.4980x_2 - 0.4956x_3 = 0.0064 \]
Models for Real World Data

Wages data

Dependencies among age (A), years of education (YE), years of work experience (YW), and wage (W) found for three clusters in the 1985 Current Population Survey:

1. \[ YE = 12 \]
   \[ YW - 1 \cdot A = -18 \]
   \[ W - 0.07 \cdot A = 5.14 \]

2. \[ YE = 16 \]
   \[ YW - 1 \cdot A = -22 \]

3. \[ YE + 1 \cdot YW - 1 \cdot A = -6 \]
Predictive Models

Our method
kNN
SVM
PART
Naive Bayes
C4.5
Logistic regression

Achtert et al. (LMU)
Conclusions

So far, correlation cluster analysis yields sets of points connected by common correlations.

Based on such approaches, we propose to derive a model to grasp the underlying possible causalities.

Our model is interpretable for domain experts and may help them to refine their experimental setting (descriptive model).

Our model may also be used to classify new data points (predictive model).