

# High-Order Heterogeneous Data Mining

#### Tie-Yan Liu Researcher, Microsoft Research Asia 2006-11-5

# Why High-Order Heterogeneous?

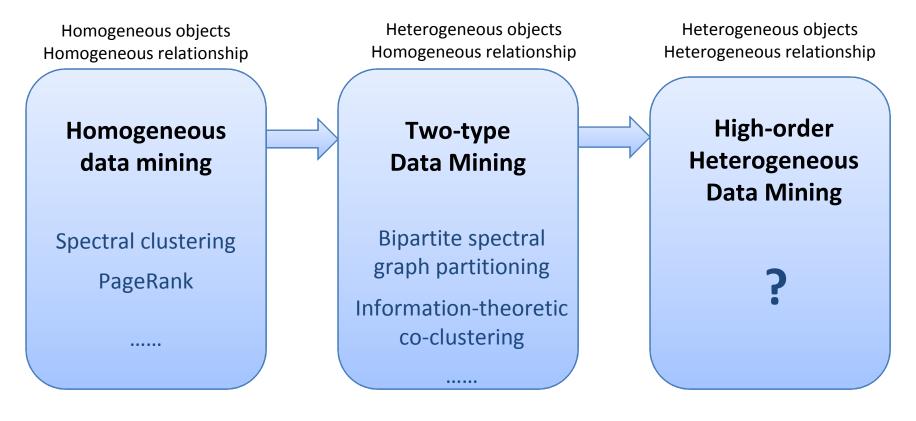
- The world is heterogeneous
  - Objects are heterogeneous:
    - (query, document...), (author, paper...)
- Many applications involve multiple types of objects
  - Web search
    - User  $\leftrightarrow$  Query  $\leftrightarrow$  Web Page
  - Academic society
    - Author  $\leftarrow$  > Paper  $\leftarrow$  > Conference  $\land$

√ Journal

 Relationships among these objects are also heterogeneous: similarity, relevance, endorsement; directed, undirected...

#### However, ...

• Most traditional ML and DM methods focus on homogeneous data, or data of no more than two types.



#### Related Work: Spectral Clustering (PAMI 2000)

- Spectral clustering cuts relationship graph to cluster similar data.
  - Minimize graph cut

$$obj = \frac{cut(V_1, V_2)}{weight(V_1)} + \frac{cut(V_2, V_1)}{weight(V_2)}$$

$$cut(V_1, V_2) = \sum_{i \in V_1, j \in V_2, \in E} e_{ij}$$

and 
$$weight(V_i) = \sum_{j \in V_i} W_j$$
.

$$\min \frac{q^T L q}{q^T D q}$$
, subject to  $q^T D e = 0, q \neq 0$ 

Solution

A

В

- Graph cut can be converted to a generalized eigenvalue problem by using continuous slacking:  $Lq = \lambda Dq$
- The eigenvector associated with the second smallest eigenvalue of the Laplace matrix is an optimal embedding for cut minimization.

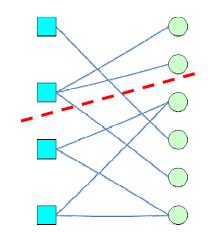
#### Related Work: PageRank (WWW 1998)

- PageRank ranks the popularity of vertices in a directed graph according to their linkage information.
- PageRank of a vertex is proportional to its parents' rank, but inversely proportional to its parents' outdegree.

$$R(u) = d + (1-d) \sum_{v \in B_u} \frac{R(v)}{N_v}$$
$$R = (1-d)AR + d\Pi, A_{u,v} = \frac{1}{N_v}, \Pi = \frac{1}{N} [1, 1, \dots, 1]'$$

 PageRank can be explained using a Markov random surfer model; or be explained as the principal eigenvector of the smoothed adjacency matrix of the Web graph.

# Related Work: Bipartite Graph Partitioning (KDD 2001)



• Cuts bipartite relationship graph to cluster two types of data simultaneously.

$$\begin{array}{ccc} X & Y \\ M = X & \begin{bmatrix} 0 & A \\ \\ Y & \begin{bmatrix} A^T & 0 \end{bmatrix} \end{array}$$

• Due to the bipartite property of the graph, after some trivial deduction, this problem can be converted to a singular value decomposition (SVD) problem.

#### Related Work: Information Theoretic Co-Clustering (KDD 2003)

- $C_X : \{x_1, ..., x_m\} \to \{\hat{x}_1, ..., \hat{x}_r\}$  $C_Y : \{y_1, ..., y_n\} \to \{\hat{y}_1, ..., \hat{y}_s\}$
- An optimal co-clustering minimizes  $I(X,Y) - I(\hat{X},\hat{Y})$ subject to the constraints on the number of row and column clusters.

It can be proved that  $I(X,Y) - I(\hat{X},\hat{Y}) = D(p(X,Y) \parallel q(X,Y))$ where D(,) denotes the KL divergence, and q(X,Y) is a distribution of the form  $q(x,y) = p(\hat{x},\hat{y}) p(x \mid \hat{x}) p(y \mid \hat{y})$ 

[Step 1] Set i = 1. Start with  $(R_i, C_i)$ , Compute  $q_{[i,i]}$ . [Step 2] For every row x, assign it to the cluster  $\hat{x}$  that minimizes  $KL(p(y|x) || q_{[i,i]}(y|\hat{x}))$ [Step 3] We have  $(R_{i+1}, C_i)$ . Compute  $q_{[i+1,i]}$ . [Step 4] For every column y, assign it to the cluster  $\hat{y}$  that minimizes  $KL(p(x|y) || q_{[i+1,i]}(x|\hat{y}))$ [Step 5] We have  $(R_{i+1}, C_{i+1})$ . Compute  $q_{[i+1,i+i]}$ . Iterate 2-5.

#### Going Beyond...

- Modeling the relationships
  - Unified Relationship Matrix
  - Tensor
  - Collective bipartite graphs
- Designing effective data mining algorithms
  - High-order Heterogeneous Coclustering
  - High-order Heterogeneous Coranking

#### **Unified Relationship Matrix**

- Integrate pairwise relationship matrices into a unified matrix
  - L'<sub>M</sub>: intra-type adjacency matrix
  - L'<sub>NM</sub>: inter-type adjacency matrix

$$L = \begin{vmatrix} \lambda_{11}L_1 & \lambda_{12}L_{12} & \cdots & \lambda_{1N}L_{1N} \\ \lambda_{21}L_{21} & \lambda_{22}L_2 & \cdots & \lambda_{2N}L_{2N} \\ \vdots & \vdots & \ddots & \vdots \\ \lambda_{N1}L_{N1} & \lambda_{N2}L_{N2} & \cdots & \lambda_{NN}L_N \end{vmatrix} \qquad \qquad L_{urm} = D^{-1}L$$

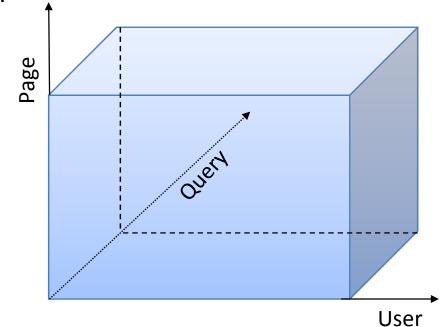
Combination coefficients can be manually set or learned from labeled data

- Representative Work
  - Wensi Xi, et al, Link Fusion: A Unified Link Analysis Framework for Multi-Type Interrelated Data Objects. WWW 2004.
  - Zaiqing Nie, et al, Object-Level Ranking: Bringing Order to Web Objects. **WWW 2005**.
  - Wensi Xi, et al, SimFusion: Measuring Similarity using Unified Relationship Matrix, SIGIR 2005.
  - Xuanhui Wang, et al, Latent Semantic Analysis for Multiple-Type Interrelated Data Objects, *SIGIR 2006*.

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#### Tensor

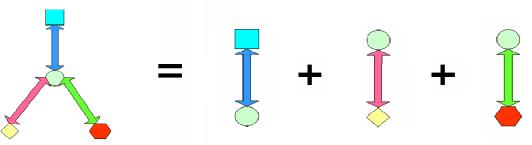
• Use multi-linear algebra to represent heterogeneous relationship.



- Representative Work
  - Jian-Tao Sun, et al, CubeSVD: A Novel Approach to Personalized Web Search, WWW 2005.

#### Collective Bi-partite Graphs

 Decompose heterogeneous relationship into a collections of pairwise relationships.



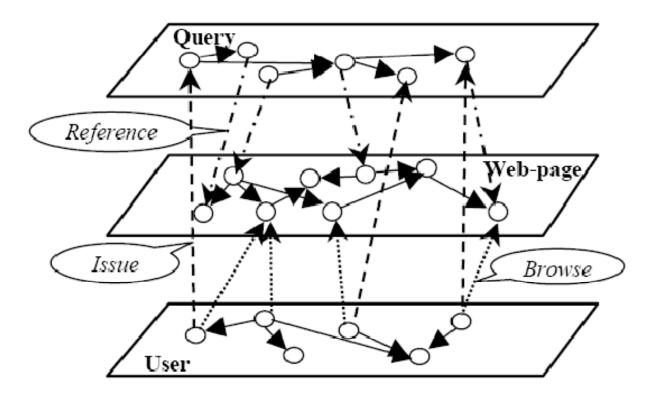
- Representative Work
  - Bin Gao, Tie-Yan Liu, et al, Hierarchical Taxonomy Preparation for Text Categorization Using Consistent Bipartite Spectral Graph Co-partitioning, *IEEE TKDE*.
  - Bin Gao, Tie-Yan Liu, et al, Consistent Bipartite Graph Co-Partitioning for Star-Structured High-Order Heterogeneous Data Co-Clustering, *KDD 2005*.
  - Bin Gao, Tie-Yan Liu, et al, Star-Structured High-Order Heterogeneous Data Co-clustering based on Consistent Information Theory, *ICDM 2006*.
  - Bo Long, Zhongfei Zhang, et al, Spectral Clustering for Multi-type Relational Data, *ICML 2006*.

# Algorithms

- Unified Relationship Matrix
  - LinkFusion (WWW 2004)
  - Object-level Ranking (WWW 2005)
  - SimFusion (SIGIR 2005)
  - Multi-type LSA (SIGIR 2006)
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# Link Fusion

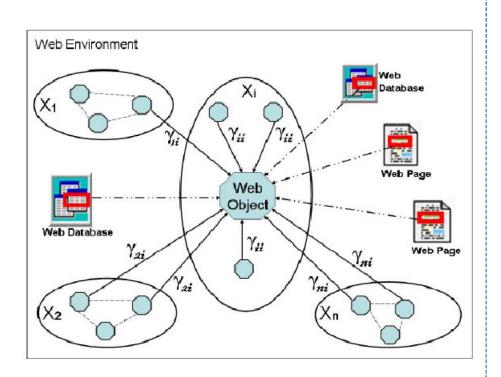
• High-order heterogeneous version of PageRank



## Random Walk on Heterogeneous Graph

- Construct the URM by merging pair-wise PageRank matrices with manually-set combination coefficients.
- Imagine a Markov random walk over the heterogeneous graph represented by the URM.
- Ranking over heterogeneous data will correspond to the principle eigenvector of the URM:  $w = L_{urm}^{T}w$ , and the convergence can be proven.

#### **Object-Level Ranking**



Conf./  
Journal 
$$\gamma_1$$
 Paper  $\gamma_2$  Author  
 $\gamma_3$ 

$$R_X = \varepsilon R_{EX} + (1 - \varepsilon) \sum_{\forall Y} \gamma_{YX} M_{YX}^T R_Y$$

- Use similar URM formulation to LinkFusion
- Learn the combination coefficients with a training set.

## Learning the Coefficients

#### **Subgraph Selection**

Starting with the labeling data objects, and including all other objects with less than *k*-step links from them.

Algorithm DiameterEstimator( $\delta$ :stopping threshold) for (each object type X)  $n \leftarrow \text{total number of different object types related}$ to objects of type X; for (each related object type Y)  $\gamma_{YX} \leftarrow \frac{1}{n}$ ; end for compute the *PopRank* scores over the entire graph;  $R \leftarrow$  the ranking vector of the training objects;  $R' \leftarrow E$ ;  $k \leftarrow 0;$ while( $||R - R'||_1 > \delta$ ) k + +;compute the PopRank scores over the k diameter subgraph:  $R' \leftarrow$  the ranking vector of the training objects; end while return k: End DiameterEstimator;

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#### Parameter Search

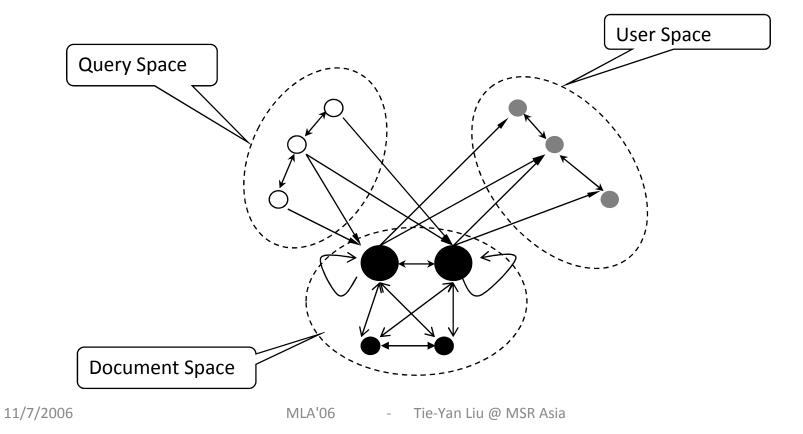
Using simulated annealing based method to search the best parameter in the selected subgraph.

```
Algorithm SAFA (timeout: stopping condition)
   for (each object type X)
     n \leftarrow \text{total number of different object types related}
           to objects of type X;
     for (each related object type Y) \gamma_{YX} \leftarrow \frac{1}{n};
   end for
   t \leftarrow a large number:
   do
     for (each object type X)
        for (each object type Y)
           repeat
             repeat
                randomly select \gamma'_{YX} in Neighbor(\gamma_{YX})
                diff \leftarrow f(\gamma_{YX}) - f(\gamma'_{YX});
               if diff > 0 then \gamma_{YX} \leftarrow \gamma'_{YX};
                else generate random x in (0,1)
                    if x < exp(-diff/t) then \gamma_{YX} \leftarrow \gamma'_{YX};
             until iteration count =
                        max_number_iteration;
             t \leftarrow 0.9t;
           until iteration count =
                       max_number_iteration;
        end for
     end for
   until timeout;
   return the best combination of \gamma_{YXs};
End SAFA;
```

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### SimFusion

The similarity of two data objects in one data type can be reinforced by the similarity value of other data objects they are related to.



## Mathematical Formulation

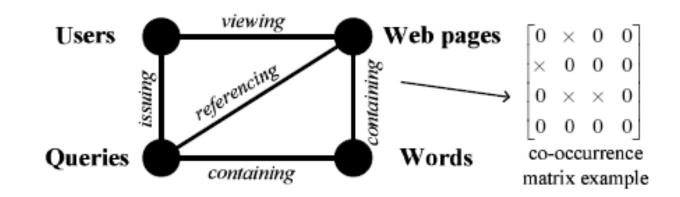
• The similarity reinforcement assumption can be represented as:

$$- S^{new} = L_{urm} S^{original} L_{urm}^{T}$$
$$- S^{n} = L_{urm} S^{n-1} L_{urm}^{T} = L_{urm}^{n} S^{0} (L_{urm}^{n})^{T}$$

- Convergence can be proven.
- The so-calculated similarity can be used for many applications such as object clustering and information retrieval.

## Multi-type LSA

- The Mutual Reinforcement Principle of LSA
  - On a multiple-type graph G with N vertices and a number of pairwise co-occurrence relationships, *important* objects of a type co-occur with *important objects* of other types.



## Low Rank Approximation

- Conduct EVD on the URM
- Apply similar ideas to principal component analysis, we can regard top k eigenvectors as representing the top k important concepts, and use them to span a k-dimensional semantic space to represent all the objects.
- Use the low-rank approximation of the URM to capture latent semantics, just as classical LSA does.

## **Discussions on URM**

#### • Pros

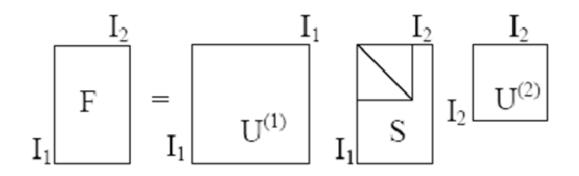
- By building URM, traditional methods for homogeneous data can be easily used.
- Linear algebra might be the most mature mathematical tool in data mining.
- Cons
  - Basic assumption in these approaches is questionable: is it really reasonable that heterogeneous relationship can become homogeneous with linear scaling?

# Algorithms

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  - LinkFusion (WWW 2004)
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- Tensor
  - CubeSVD (WWW 2005)
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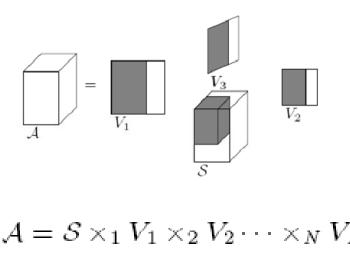
## CubeSVD

- Matrix Singular Value Decomposition (SVD)
  - Latent Semantic Indexing (LSI)
    - Apply SVD on document-term matrix
  - In Recommender System
    - Apply SVD on user-item preference matrix



# CubeSVD (cont.)

- Tensor Singular Value Decomposition (High-order SVD)
  - Higher-Order SVD might also capture the latent factors that govern the relations among multi-type objects.
  - These semantic relationships can be used to get better clustering.



$$\mathfrak{A} = \mathcal{S} \times_1 V_1 \times_2 V_2 \cdots \times_N V_N$$

1. Construct tensor  $\mathcal{A}$  from the clickthrough data. Suppose the numbers of user, query and Web page are m, n, k respectively, then  $\mathcal{A} \in \mathbb{R}^{m \times n \times k}$ . Each tensor element measures the preference of a (user, query) pair on a Web page.

2. Calculate the matrix unfolding  $A_u$ ,  $A_g$  and  $A_p$  from tensor  $\mathcal{A}$ .  $A_u$  is calculated by varying user index of tensor  $\mathcal{A}$  while keeping query and page index fixed.  $A_q$  and  $A_p$  are computed in a similar way. Thus  $A_u$ ,  $A_q$ ,  $A_p$  is a matrix of  $m \times nk$ ,  $n \times mk$ ,  $k \times mn$  respectively.

3. Compute SVD on  $A_u$ ,  $A_q$  and  $A_p$ , set  $V_u$ ,  $V_q$  and  $V_p$ to be the left matrix of the SVD respectively.

4. Select  $m_0 \in [1, m], n_0 \in [1, n]$  and  $k_0 \in [1, k]$ . Remove the right-most  $m - m_0$ ,  $n - n_0$  and  $k - k_0$  columns from  $V_u, V_q$  and  $V_p$ , then denote the reduced left matrix by  $W_u, W_q$  and  $W_p$  respectively. Calculate the core tensor as follows:

$$\mathcal{S} = \mathcal{A} \times_1 W_u^T \times_2 W_q^T \times_3 W_p^T$$

5. Reconstruct the original tensor by:

$$\hat{\mathcal{A}} = \mathcal{S} \times_1 V_u \times_2 V_q \times_3 V_p$$

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## **Discussions on Tensor**

- Pros
  - Using tensor to represent heterogeneous data objects is more natural than URM
- Cons
  - Multi-linear algebra is in its initial stage, and many basic operations for tensor have not been reasonably define.
    - Tensors cannot always be "diagonalized"
    - k successive rank-1 approximations to tensors do not necessarily result in the best rank-k approximation
    - Eight factors about tensor
  - Complexity of tensor operator is very high, thus tensor based methods are difficult to scale up.

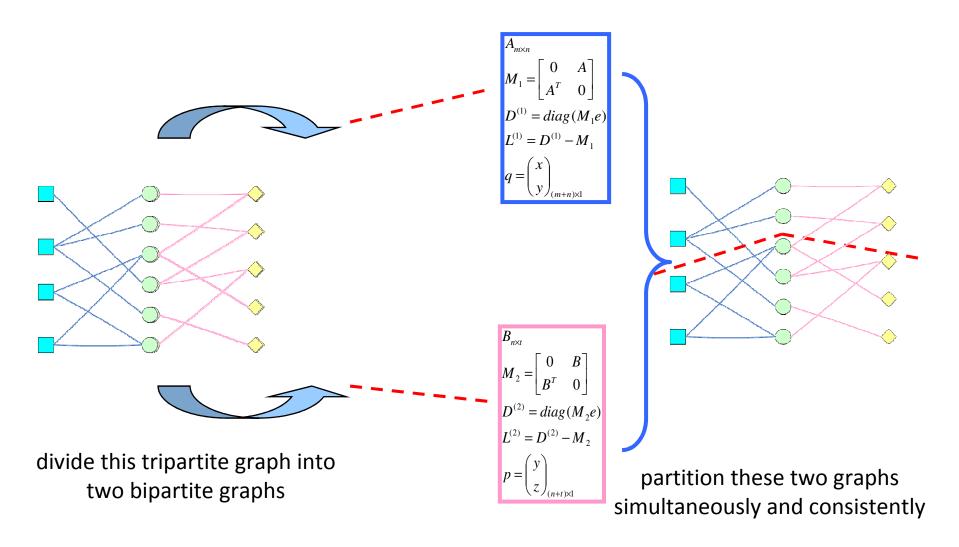
# Algorithms

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#### **Consistent Bipartite Graph Copartitioning**

- User graphs to represent the heterogeneous relationship.
- Divide the heterogeneous graph into a collection of bipartite graphs.
- Conduct spectral co-clustering on each bipartite graph, provided that the partitioning of the shared part of two bipartite graphs should be the same or almost the same.
- Develop an SDP-based solution to get the consistent partitioning results.

### **Consistent Partitioning**



#### Formulating the Optimization Problem

- Minimize the cuts of the two bipartite graphs, with the constraints that their partitioning results on the central type of objects are the same.
- Objective Function:

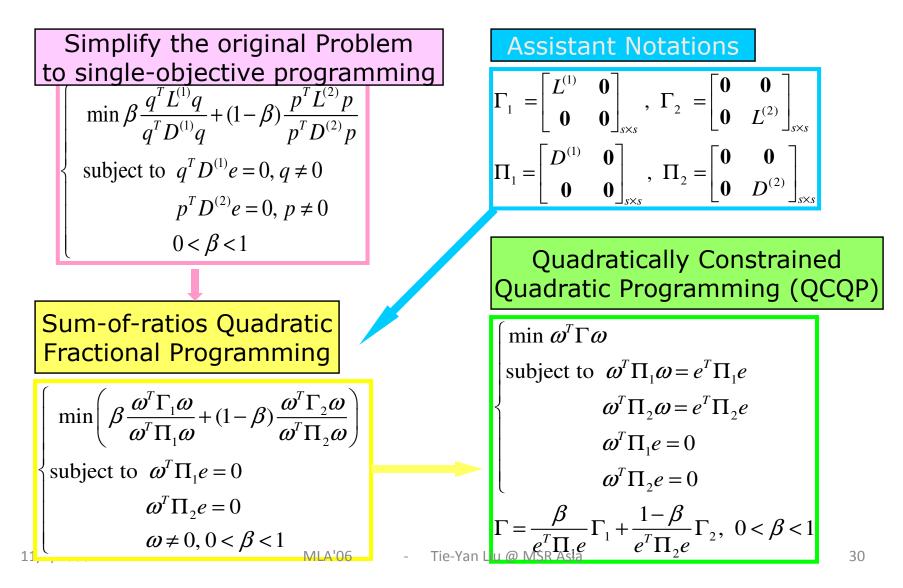
$$\min \quad \frac{q^T L^{(1)} q}{q^T D^{(1)} q}$$

$$\min \quad \frac{p^T L^{(2)} p}{p^T D^{(2)} p} \qquad \qquad q = \begin{pmatrix} x \\ y \end{pmatrix}_{(m+n) \times 1}$$
subject to  $q^T D^{(1)} e = 0, q \neq 0$ 

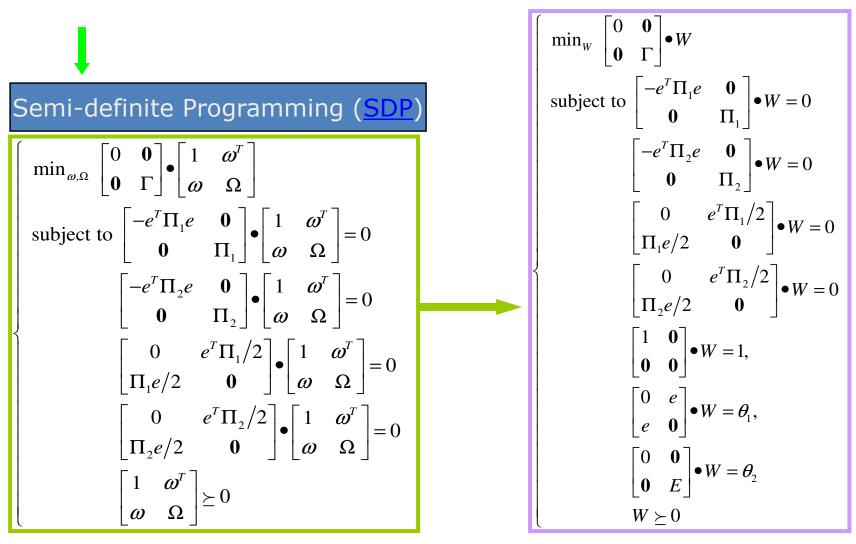
$$p^T D^{(2)} e = 0, p \neq 0$$

$$0 < \beta < 1 \qquad \qquad p = \begin{pmatrix} y \\ z \end{pmatrix}_{(n+t) \times 1}$$

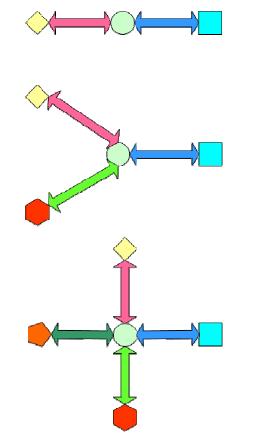
#### How to Solve the Optimization Problem #1: Convert it to a QCQP Problem



#### How to Solve the Optimization Problem #2: Convert QCQP to SDP

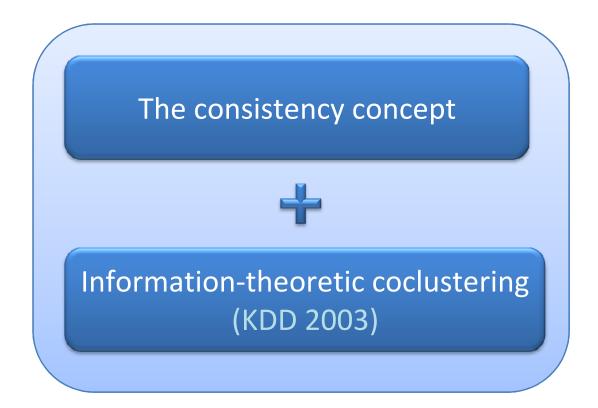


#### Extension to More Complex Heterogeneous Graphs



$$\begin{cases} \min \sum_{i=1}^{k-1} \beta_i \frac{q_i^T L^{(i)} q_i}{q_i^T D^{(i)} q_i} \\ \text{subject to } q_i^T D^{(i)} e = 0, q_i \neq 0, i = 1, \dots, k-1 \\ \\ \sum_{i=1}^{k-1} \beta_i = 1, \ 0 < \beta_i < 1 \end{cases}$$

#### Consistent Information-theoretic Co-clustering

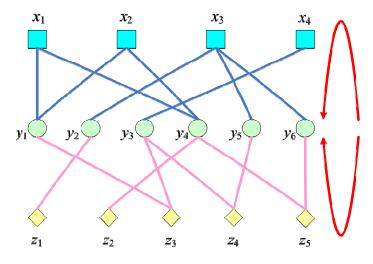


#### **Mathematical Formulation**

• Co-clustering

 $C_X : \{x_1, ..., x_m\} \to \{\hat{x}_1, ..., \hat{x}_r\}$  $C_Y : \{y_1, ..., y_n\} \to \{\hat{y}_1, ..., \hat{y}_s\}$  $C_Z : \{z_1, ..., z_l\} \to \{\hat{z}_1, ..., \hat{z}_t\}$ 

• A consistent co-clustering minimizes the following objective functions



(i)  $F(X,Y,Z) = \alpha D(p_1(X,Y) || q_1(X,Y)) + (1-\alpha)D(p_2(Y,Z) || q_2(Y,Z)),$ where  $0 < \alpha < 1$ 

(*ii*)  $F(X,Y,Z) = \min_{X,Y,Z} \left\{ \max \left\{ D(p_1(X,Y) \| q_1(X,Y)), D(p_2(Y,Z) \| q_2(Y,Z)) \right\} \right\}$ 

• Similar iterative method can be used to optimize *F(X,Y,Z)*, and the convergence can be proved.

#### Generalized SVD for Co-clustering

- Rather than integrating heterogeneous relationship in a unified matrix or using tensor, we try to connect heterogeneous relationships using generalized SVD.
- While SVD corresponds to the optimal embedding of bipartite graph, GSVD might correspond to tripartite graph.

**Theorem 1** If we have  $\hat{A} \in \mathbb{R}^{m \times n}$  and  $\hat{B} \in \mathbb{R}^{n \times t}$ ,  $m \le n \le t$ , then there exists unitary matrices  $U \in \mathbb{R}^{m \times m}$ ,  $V \in \mathbb{R}^{p \times t}$  and reversible matrix  $X \in \mathbb{R}^{n \times n}$  such that:  $\begin{cases} \hat{A} = UCX^T \\ \hat{B} = XSV^T \end{cases}$ , (11) where  $C = diag(c_1, c_2, ..., c_m)$ ,  $c_i \ge 0$  and  $S = diag(s_1, s_2, ..., s_n)$ ,  $s_i \ge 0$ .

#### Generalized SVD for Co-clustering

- 1. Given A and B, form  $P_1$ ,  $P_2$ ,  $R_1$ ,  $R_2$ , and  $\hat{A}$ ,  $\hat{B}$ .
- 2. Compute GSVD of  $\hat{A}$ ,  $\hat{B}$  to get U, X, V, C, and S.
- 3. Form  $H = CX^T XS$  and compute SVD of it to get  $U_H, V_H$ .
- 4. Form  $U^* = UU_H, V^* = VV_H$  and take the second column vectors of them,  $u_2$  and  $v_2$ , to form the normalized embedding vector

$$\omega_2 = [P_1^{-1/2} u_2 \ R_2^{-1/2} v_2]^T.$$

5. Cluster on the one-dimensional data  $P_1^{-1/2}u_2$  and  $R_2^{-1/2}v_2$  to obtain the desired bipartition of categories and terms, respectively.

# No mathematical proof yet, since generalized SVD has no explicit objective function.

## Spectral Clustering for Multi-type Relational Data

Handling both pairwise relations and features

$$\begin{split} L &= \sum_{1 \leq i < j \leq m} w_a^{(ij)} ||R^{(ij)} - C^{(i)} A^{(ij)} (C^{(j)})^T ||^2 + \sum_{1 \leq i \leq m} w_b^{(i)} ||F^{(i)} - C^{(i)} B^{(i)} ||^2 \\ & & \downarrow \\ \max_{\substack{\{(C^{(i)})^T C^{(i)}\} \\ \equiv I_{k_i}\}_{1 \leq i \leq m}} \sum_{1 \leq i \leq m} w_b^{(i)} tr((C^{(i)})^T F^{(i)} (F^{(i)})^T C^{(i)}) + \sum_{1 \leq i < j \leq m} w_a^{(ij)} tr((C^{(i)})^T R^{(ij)} C^{(j)} (C^{(j)})^T (R^{(ij)})^T C^{(i)}) \\ & & \downarrow \\ & & \downarrow \\ & & (C^{(p)})^T C^{(p)} = I_{k_p} tr((C^{(p)})^T M^{(p)} C^{(p)}) \\ M^{(p)} &= w_b^{(p)} (F^{(p)} (F^{(p)})^T) + \sum_{p < j \leq m} w_a^{(pj)} (R^{(pj)} C^{(j)} (C^{(j)})^T (R^{(pj)^T})) + \sum_{1 \leq j < p} w_a^{(jp)} ((R^{(jp)})^T C^{(j)} (C^{(j)})^T (R^{(jp)})). \end{split}$$

## **Optimization Steps**

- It can be proved the final equivalent optimization problem has close-form solution.
- The following algorithm is used to approximate this solution.

Algorithm 1 Spectral Relational Clustering Input: Relation matrices  $\{R^{(ij)} \in \mathbb{R}^{n_i \times n_j}\}_{1 \le i < j \le m}$ , feature matrices  $\{F^{(i)} \in \mathbb{R}^{n_i \times f_i}\}_{1 \le i \le m}$ , numbers of clusters  $\{k_i\}_{1 \le i \le m}$ , weights  $\{w_a^{(ij)}, w_b^{(i)} \in R_-\}_{1 \le i < j \le m}$ . Output: Cluster indicator matrices  $\{C^{(p)}\}_{1 \le p \le m}$ . Method: 1: Initialize  $\{C^{(p)}\}_{1 \le p \le m}$  with othonormal matrices.

- 2: repeat
- 3: for p = 1 to m do
- 4: Compute the matrix  $M^{(p)}$  as in Eq. (9).
- Update C<sup>(p)</sup> by the leading k<sub>p</sub> eigenvectors of M<sup>(p)</sup>.
- 6: end for
- 7: until convergence
- 8: for p = 1 to m do
- transform C<sup>(p)</sup> into a cluster indicator matrix by the k-means.
- 10: **end for**

# **Discussions on Collective Graphs**

#### • Pros

- It is more natural to decompose heterogeneous relationships into homogenous relationships, than to combine homogeneous relationships to heterogeneous relationships.
- Cons
  - Complexity of graph processing is relatively high than power method.
  - Graph fusion has not been well studied yet.

## Summary

	URM	Tensor	Consistent Bipartite Graph
Clustering Cu	SimFusion Multi-type LSA	CubeSVD Cons	Consistent Bipartite Graph Copartitioning Consistent Information- Theoretic Coclustering istent Rank? I Data
Ranking	LinkFusion Object-level Ranking	Ş	Ş

## Future Work

- Modeling the heterogeneous relationship more effectively.
  - Matrix, tensor, graphs, ...
  - What is the next?
- Develop more efficient algorithms for high-order heterogeneous data mining.
  - Scalability is an issue for most of the algorithms mentioned in this talk.
  - Large-scale (multi-)linear algebra and large scale optimization
  - Supervised or semi-supervised learning for high-order heterogeneous data (i.i.d is not a reasonable assumption).

## **Further Discussions**

- Although data objects are heterogeneous, they can be regarded as sampled from the same probability space.
  - The heterogeneity just comes from different views of the space.
- Can we recover the unified probability space and solve this problem from the root?
  - Reference paper
    - Ying Liu, Tao Qin, Tie-Yan Liu, et al, Similarity Space Projection: A Novel Framework for Web Image Search and Annotation. MIR 2005.



# Thanks!

tyliu@microsoft.com

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