

Data Mining with Graphs and Matrices

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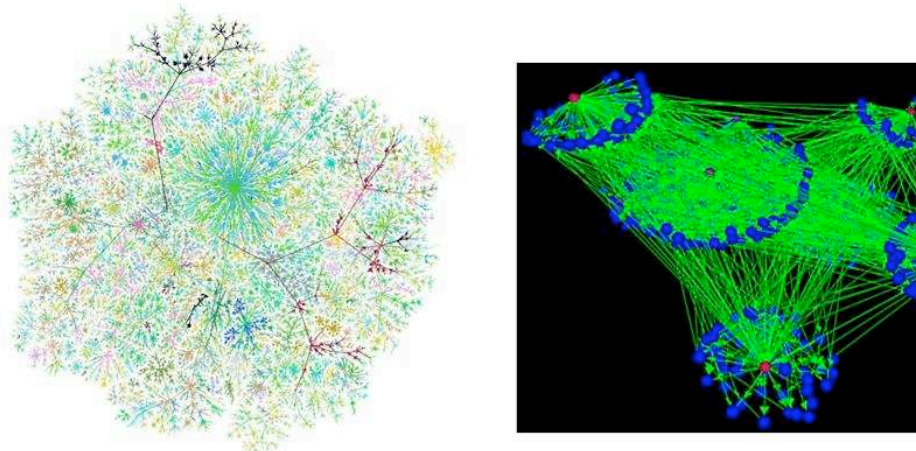
Tutorial at SDM 2009, Sparks, Nevada

<http://feiwang03.googlepages.com/sdm-tutorial>

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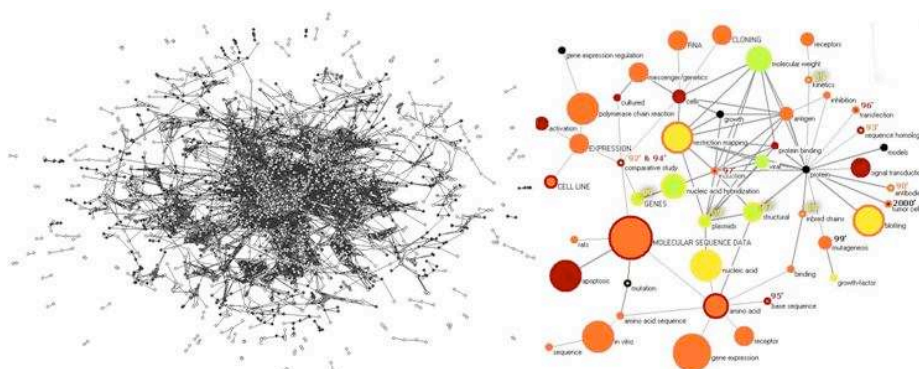
- 1 Graphs and Matrices are Everywhere
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 - Dimensionality Reduction
 - Clustering
 - Co-Clustering
- 3 Semi-supervised Learning with Graphs & Matrices
 - Semi-supervised Learning with Partially Labeled Data
 - Semi-supervised Learning Using Side-Information
- 4 Future Research Directions

Internet Graph



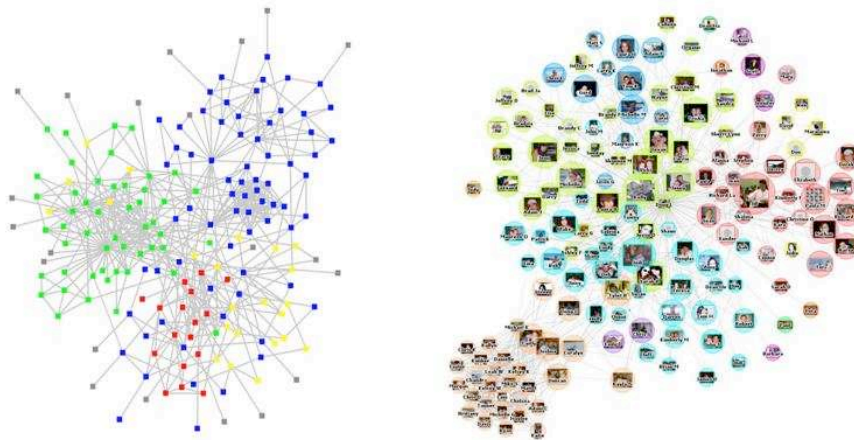
The images are downloaded from
<http://www.maths.bris.ac.uk/~maarw/graphs/graph.html>
and <http://www.netdimes.org/new/?q=node/17>

Citation Graph



The images are downloaded from
<http://www.emeraldinsight.com/fig/2780600403005.png>
and www.bordalierinstitute.com/target1.html

Friendship Graph



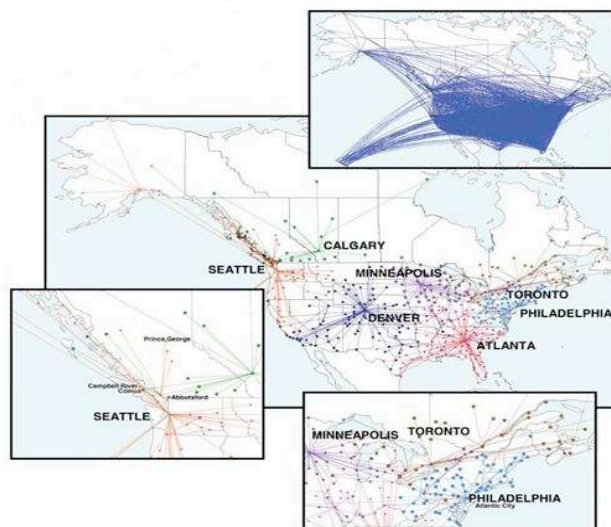
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<http://www.thenetworkthinker.com/>
and [http://myweb20list.com/blog/2008/03/23/
new-amazing-facebook-photo-mapper/my-facebook-friend-graph/](http://myweb20list.com/blog/2008/03/23/new-amazing-facebook-photo-mapper/my-facebook-friend-graph/)

Navigation icons: back, forward, search, etc.

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Airline Graph



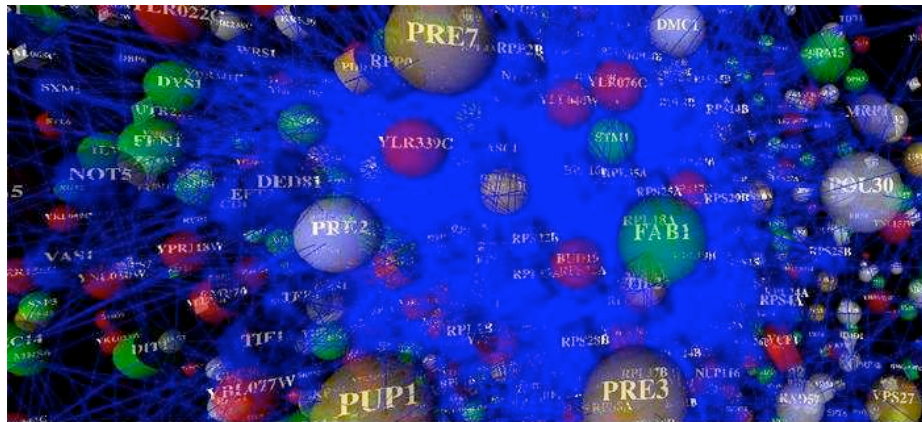
Copied from Brendan J. Frey and Delbert Dueck, University of Toronto
Clustering by Passing Messages Between Data Points. Science 315, 972-976

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Protein Interaction Graph



The images are downloaded from
<http://bioinformatics.icmb.utexas.edu/lgl/Images/rsomZoom.jpg>

Social Network Analysis

- Email network
- Represents the email communications between users
 - Cluster users
 - Identify communities

				...	
	0	5	4	...	0
	6	0	3	...	2
⋮	⋮	⋮	⋮	⋮	⋮
	0	5	10	...	0

Document-Term Matrices

- A collection of documents is represented by an $n\text{Doc-by-}n\text{Term}$ matrix (bag-of-words model).
 - Cluster or classify documents
 - Find a subset of terms that (accurately) clusters or classifies documents

	image	Bayes	matrix	...	rock
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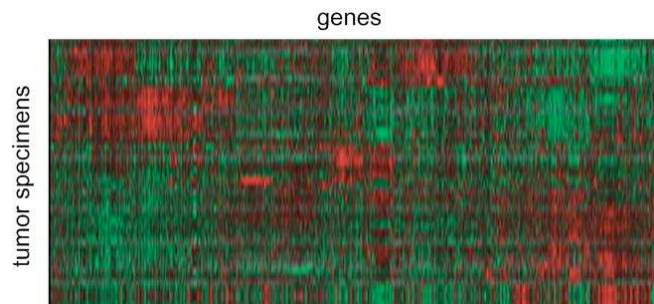
Recommendation Systems

- Collaborative filtering
 - Given the users' historical data, predict the ratings of a specific user to a new movie

				...	
	5	1	4	...	0
	1	5	3	...	2
⋮	⋮	⋮	⋮	⋮	⋮
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Bioinformatics

- Gene expression data
 - Pick a subset of genes (if it exists) that suffices in order to identify the “cancer type” of a patient



Some Notations & Preliminaries

- The data matrix $\mathbf{X} = [\mathbf{x}_1, \mathbf{x}_2, \dots, \mathbf{x}_n] \in \mathbb{R}^{d \times n}$
- Generally, a graph $\mathcal{G} = \langle \mathcal{V}, \mathcal{E} \rangle$ can be described as a matrix
 - The columns and rows are indexed by \mathcal{V}
 - The elements are the strengths on the corresponding edges in \mathcal{E}
- Analyzing graphs is usually equivalent to perform analysis on matrices

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Singular Value Decomposition

$$\begin{bmatrix} \mathbf{x}_1 & \mathbf{x}_2 & \dots & \mathbf{x}_n \end{bmatrix} = \begin{bmatrix} \mathbf{u}_1 & \dots & \mathbf{u}_k \end{bmatrix} \begin{bmatrix} \mathbf{s}_1 & \dots & \mathbf{s}_k \end{bmatrix} \begin{bmatrix} \mathbf{v}_1^T \\ \vdots \\ \mathbf{v}_k^T \end{bmatrix}$$

- Best rank-k approximation in Frobenius norm
- Exact computation of SVD takes $O(\min(dn^2, d^2n))$ time.
- The top k left/right singular vectors/values can be computed faster using Lanczos/Arnoldi methods.

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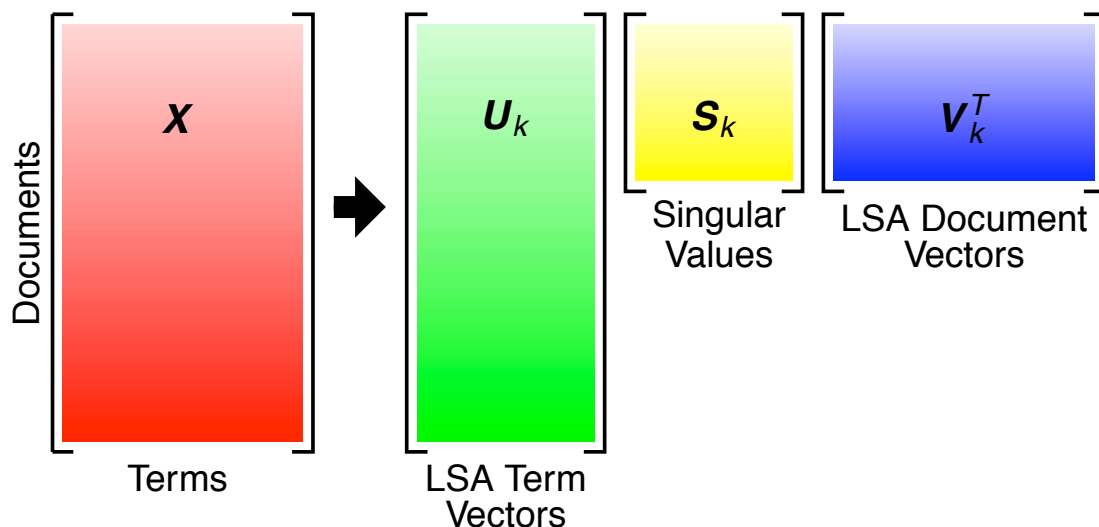
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Latent Semantic Analysis

- k-dimensional semantic structure
- Similarity on reduced-space: D-D, D-T, T-T
- Folding-in queries: $\hat{\mathbf{q}} = \mathbf{S}_k^{-1} \mathbf{V}_k^T \mathbf{q}$



Principal Component Analysis

- Find a projection vector $\mathbf{u} \in \mathbb{R}^{d \times 1}$, such that the projected data points $\mathbf{Y} = \mathbf{u}^T \mathbf{X}$ own the largest variance, i.e., we should solve the following optimization problem

$$\begin{aligned} \max_{\mathbf{u}} \quad & \mathbf{u}^T \frac{1}{n} \left(\sum_{i=1}^n (\mathbf{x}_i - \mathbf{m})(\mathbf{x}_i - \mathbf{m})^T \right) \mathbf{u} \\ \text{s.t.} \quad & \|\mathbf{u}\|^2 = 1 \end{aligned} \quad (1)$$

- From the standard theorem of Rayleigh-Ritz, we know that the optimal \mathbf{u} is the eigenvector of the data covariance matrix \mathbf{C} corresponding to its largest eigenvalue.

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PCA & SVD

- If \mathbf{X} is centralized, then the covariance matrix $\mathbf{C} = \frac{1}{n}\mathbf{XX}^T$
- Eigenvalue decomposition $\mathbf{C} = \mathbf{U}\mathbf{\Sigma}\mathbf{U}^T = \frac{1}{n}\mathbf{XX}^T$
- SVD of \mathbf{X} : $\mathbf{X} = \mathbf{USV}^T$
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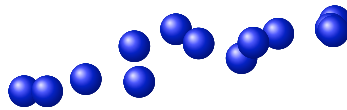
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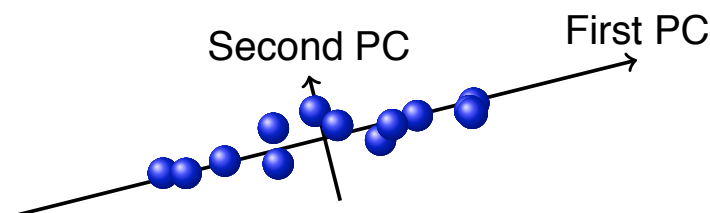
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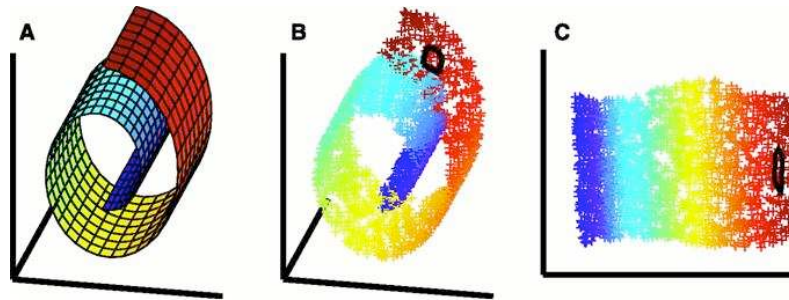
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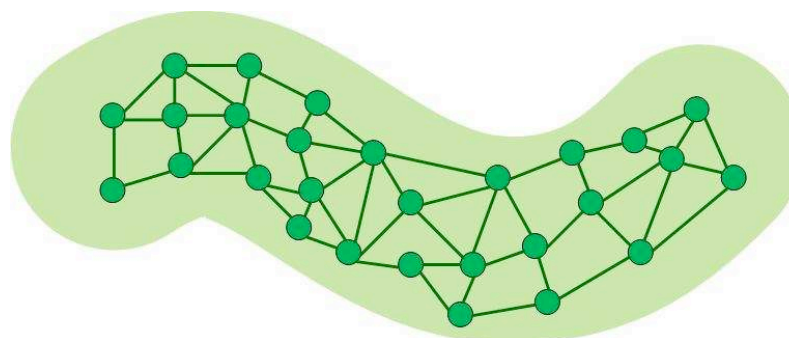
Nonlinear Embedding

- PCA is a linear method to project the data points
- What should we do if the data are nonlinearly distributed?



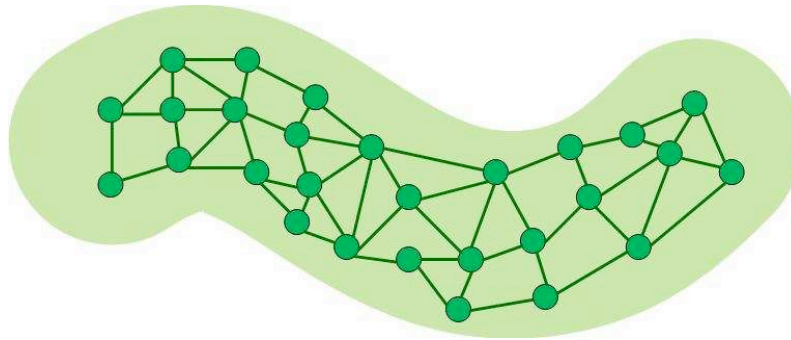
Manifold & Graph

- We usually assume that the high-dimensional data points reside (nearly) on a low-dimensional nonlinear manifold
- Find the low-dimensional embeddings of the data which preserve the graph structure



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Local Linear Embedding (LLE)

- Assume each data point can be linearly reconstructed from its neighborhood, *i.e.*, for each \mathbf{x}_i , we minimize

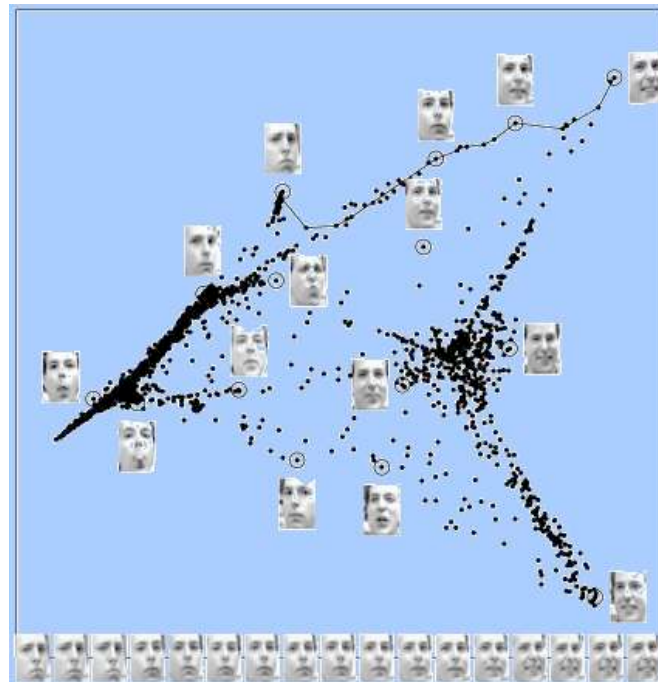
$$\begin{aligned} \varepsilon_i &= \sum_{\mathbf{x}_j \in \mathcal{N}_i} \|\mathbf{x}_i - w_{ij} \mathbf{x}_j\|^2 \\ \text{s.t. } &\sum_j w_{ij} = 1 \end{aligned} \quad (2)$$

- Then we use all $\{w_{ij}\}$ to recover the low-dimensional embedding of the data points \mathbf{Y} by solving

$$\begin{aligned} \mathcal{J} &= \sum_{i=1}^n \|\mathbf{y}_i - \sum_{\mathbf{y}_j \in \mathcal{N}_i} w_{ij} \mathbf{y}_j\|^2 \\ \text{s.t. } &\mathbf{Y}^T \mathbf{Y} = \mathbf{I} \end{aligned} \quad (3)$$

- $\mathbf{Y} = [\mathbf{y}_1, \dots, \mathbf{y}_n]$ is the low-dimensional embedded data matrix

An Example of LLE



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Data Mining with Graphs & Matrices

Laplacian Eigenmaps (LE)

- The embedded data should be sufficiently smooth with respect to the intrinsic data manifold.
- We minimize

$$\begin{aligned} \min_{\mathbf{Y}} \quad & \sum_{i \sim j} w_{ij} \|\mathbf{y}_i - \mathbf{y}_j\|^2 \\ \text{s.t.} \quad & \mathbf{Y}^T \mathbf{Y} = \mathbf{I} \end{aligned} \quad (4)$$

- w_{ij} represents the similarity between \mathbf{x}_i and \mathbf{x}_j
- Writing in matrix form $\sum_{i \sim j} w_{ij} \|\mathbf{y}_i - \mathbf{y}_j\|^2 = \text{tr}(\mathbf{Y}(\mathbf{D} - \mathbf{W})\mathbf{Y}^T)$
 - $\mathbf{W}(i, j) = w_{ij}$ is the similarity matrix
 - $\mathbf{D} = \text{diag}(\sum_j w_{1j}, \dots, \sum_j w_{2j})$
- We call $\mathbf{L} = \mathbf{D} - \mathbf{W}$ the *Laplacian matrix*

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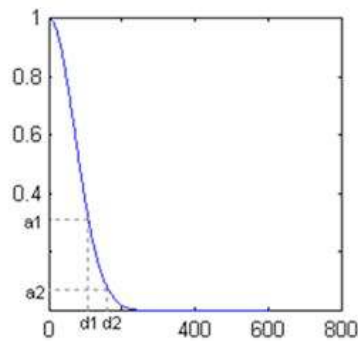
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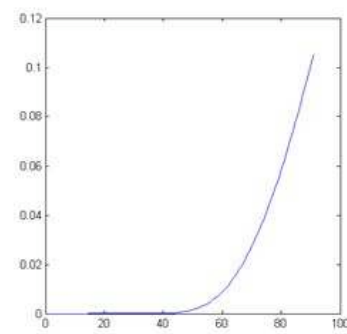
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Graph Similarities

- Node similarities: $s_{ij} = \exp\left(-\frac{\|\mathbf{x}_i - \mathbf{x}_j\|^2}{2\sigma^2}\right)$



"Closer" nodes will get larger similarity



Weight as a function of σ

Locality Preserving Projections (LPP)

- Linear version of Laplacian embedding
- Let \mathbf{P} be the projection matrix, then the goal of LPP is just to solve the following problem

$$\begin{aligned} \min_{\mathbf{P}} \quad & \text{tr}(\mathbf{P}^T \mathbf{X} \mathbf{L} \mathbf{X}^T \mathbf{P}) \\ \text{s.t.} \quad & \mathbf{P}^T \mathbf{P} = \mathbf{I} \end{aligned} \quad (5)$$

- Locality Preserving Indexing
- Laplacianface
- ...

Graph Embedding: A General Framework

- A general graph embedding framework:

$$\begin{aligned} \min_{\mathbf{y}} \quad & \sum_{i \sim j} p_{ij} \|\mathbf{y}_i - \mathbf{y}_j\|^2 \\ \text{s.t.} \quad & \mathbf{y}^T \mathbf{A} \mathbf{y} = c \end{aligned} \quad (6)$$

- $i \sim j$ denotes that there is an edge connecting \mathbf{x}_i and \mathbf{x}_j
- c is a constant

- Linearization:

$$\begin{aligned} \min_{\mathbf{p}} \quad & \sum_{i \sim j} p_{ij} \|\mathbf{p}^T \mathbf{x}_i - \mathbf{p}^T \mathbf{x}_j\|^2 \\ \text{s.t.} \quad & \mathbf{p}^T \mathbf{X} \mathbf{A} \mathbf{X}^T \mathbf{p} = c \end{aligned} \quad (7)$$

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Summarization of Different Methods from a GE Perspective (Shuicheng Yan et al. CVPR'05)

Algorithm	P	A
PCA	$p_{ij} = 1/n, \forall i \neq j$	A = I
LDA	$p_{ij} = \delta_{l_i, l_j} / n_{l_i}$	A = I - ee^T
LLE	P = W + W^T - W^TW	A = I
LPP	$p_{ij} = \exp(-\ \mathbf{x}_i - \mathbf{x}_j\ ^2 / (2\sigma^2))$	A = D

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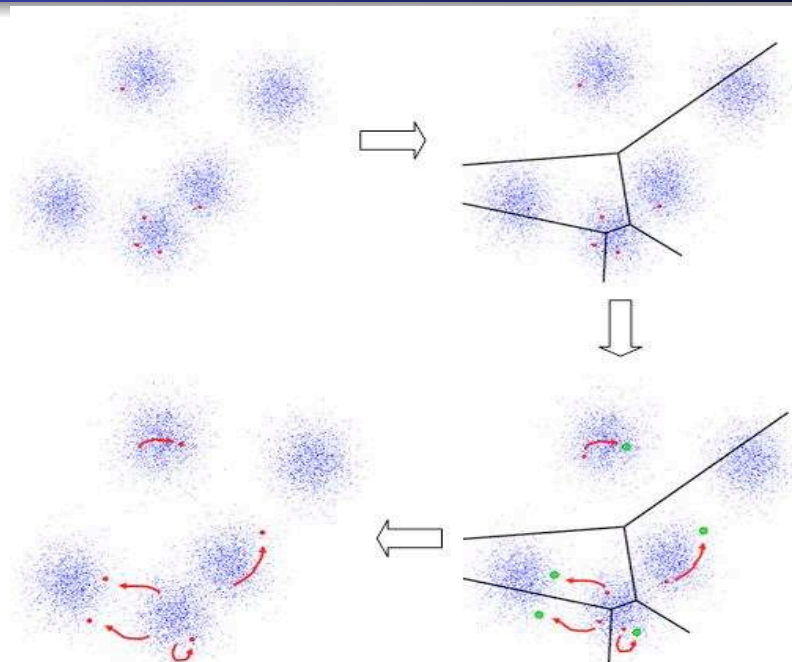
K-means

- The data points \mathbf{X} comes from C clusters. We aim to find the cluster centers $\{\mathbf{f}_i\}_{i=1}^C$ together with the clusters such that the following criterion is minimized

$$\min \sum_{i=1}^C \sum_{\mathbf{x}_j \in \pi_i} \|\mathbf{x}_j - \mathbf{f}_i\|^2 \quad (8)$$

- π_i denotes the i -th cluster
- We can resort to iterative procedures to solve the problem.

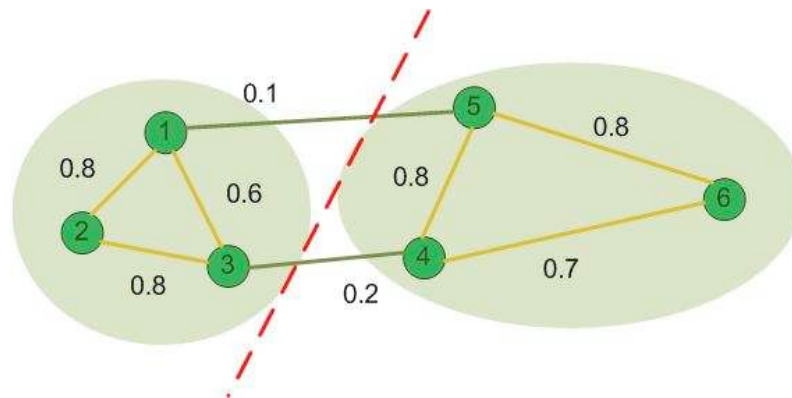
K-means Procedure



The figures come from

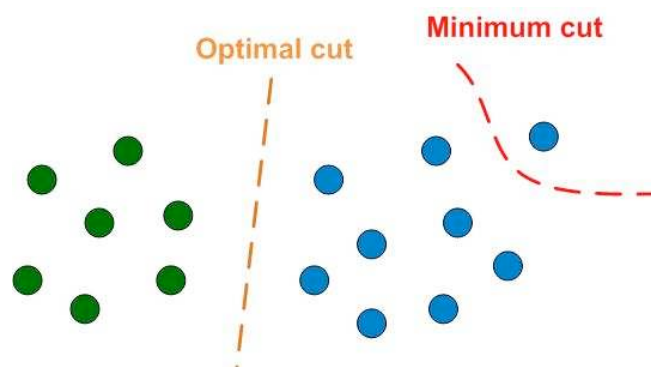
Graph Clustering

- Partition the nodes \mathcal{V} in graph \mathcal{G} into disjoint clusters
- Cut: Set of edges with points belonging to different clusters
- Association: Set of edges with points belonging to the same cluster



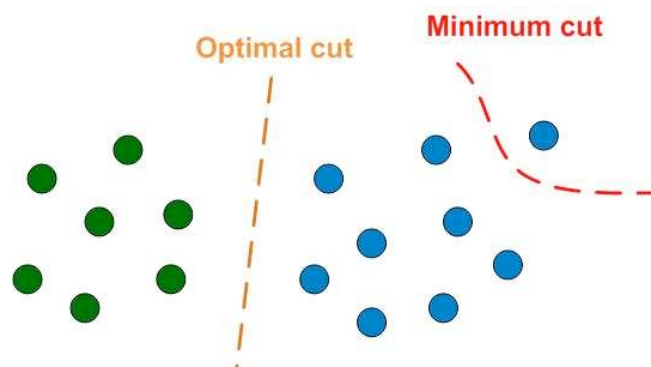
Graph Cut Criteria

- **MinCut**: Minimize the association between groups
 $\min \text{cut}(\mathcal{A}, \mathcal{B})$
- *Normalized graph cut criteria*:
 - RatioAssociation: $\max \frac{\text{asso}(\mathcal{A}, \mathcal{A})}{|\mathcal{A}|} + \frac{\text{asso}(\mathcal{B}, \mathcal{B})}{|\mathcal{B}|}$
 - RatioCut: $\min \frac{\text{cut}(\mathcal{A}, \mathcal{B})}{|\mathcal{A}|} + \frac{\text{cut}(\mathcal{B}, \mathcal{A})}{|\mathcal{B}|}$
 - NormalizedCut: $\min \frac{\text{cut}(\mathcal{A}, \mathcal{B})}{\text{vol}(\mathcal{A})} + \frac{\text{cut}(\mathcal{B}, \mathcal{A})}{\text{vol}(\mathcal{B})}$



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Some Definitions on Graphs

- **Weight Matrix \mathbf{W}** : \mathbf{W}_{ij} is the weight on the edge e_{ij}
- **Degree Matrix \mathbf{D}** : $\mathbf{D}_{ii} = \sum_j \mathbf{W}_{ij}$
- **Partition Matrix \mathbf{P}** : $\mathbf{P}_{ij} = 1$ if \mathbf{x}_i belongs to partition j ;
 Otherwise $\mathbf{P}_{ij} = 0$
- **Scaled Partition Matrix $\tilde{\mathbf{P}}$** : $\tilde{\mathbf{P}}_{ij} = 1/\sqrt{n_j}$ if \mathbf{x}_i belongs to partition j , n_j is the size of the j -th cluster; Otherwise $\tilde{\mathbf{P}}_{ij} = 0$
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Spectral Clustering

- The solutions of the above optimization problems can be finally obtained by spectral analysis of some matrices
- Ratio association: Do eigenvalue decomposition to \mathbf{W}
- Ratio cut: Do eigenvalue decomposition to $\mathbf{L} = \mathbf{D} - \mathbf{W}$
- Normalized cut: Do eigenvalue decomposition to $\hat{\mathbf{L}} = \mathbf{I} - \mathbf{D}^{-1/2}\mathbf{W}\mathbf{D}^{-1/2}$

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Spectral Clustering II

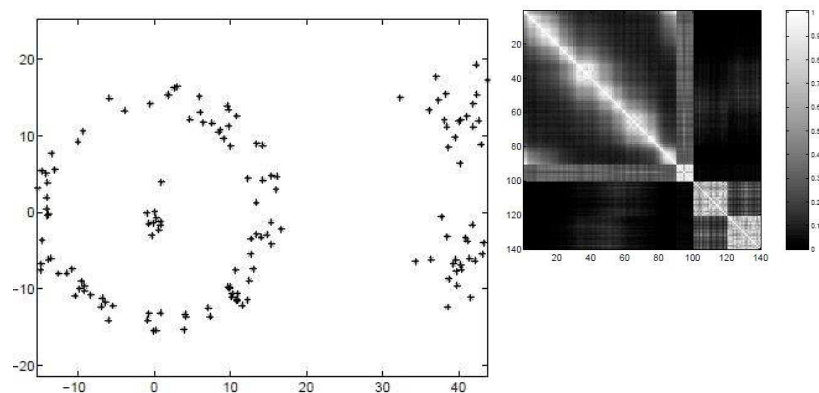
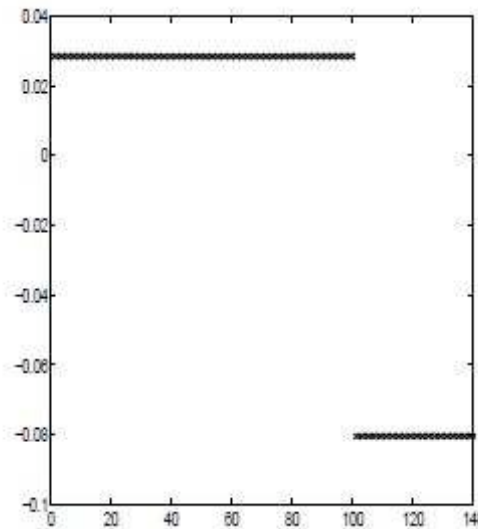


Figure from Shi & Malik. PAMI 2000.

The Eigenvectors of The Normalized Laplacian Matrix



Nonnegative Matrix Factorization

- Analyzing nonnegative matrices (document-word matrix, image matrix...)
- For a nonnegative matrix \mathbf{X} , we decompose it into two nonnegative matrices

$$\min_{\mathbf{F} \geq 0, \mathbf{G} \geq 0} \|\mathbf{X} - \mathbf{F}\mathbf{G}^T\|^2 \quad (9)$$

- Multiplicative update rule to solve the problem

$$\mathbf{F}_{ij} \leftarrow \mathbf{F}_{ij} \frac{(\mathbf{X}\mathbf{G})_{ij}}{(\mathbf{F}\mathbf{G}^T\mathbf{G})_{ij}}, \quad \mathbf{G}_{ij} \leftarrow \mathbf{G}_{ij} \frac{(\mathbf{F}^T\mathbf{X})_{ij}}{(\mathbf{F}^T\mathbf{F}\mathbf{G}^T)_{ij}}$$

- Parts-based representation

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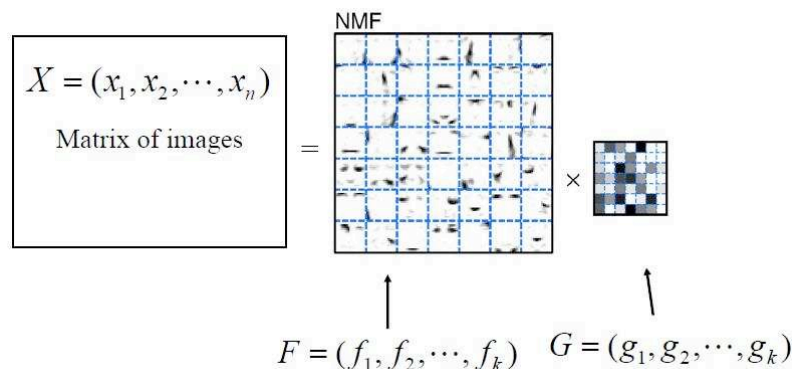
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- Parts-based representation

NMF: An Illustrative Example



Clustering Results on TDT Data

Performance comparisons using TDT2 corpus

k	Mutual Information				Accuracy			
	AA	NC	NMF	NMF-NCW	AA	NC	NMF	NMF-NCW
2	0.834	0.954	0.854	0.972	0.934	0.990	0.946	0.993
3	0.754	0.890	0.790	0.931	0.863	0.951	0.899	0.981
4	0.743	0.846	0.786	0.909	0.830	0.918	0.866	0.953
5	0.696	0.802	0.740	0.874	0.758	0.857	0.812	0.925
6	0.663	0.761	0.701	0.823	0.712	0.802	0.773	0.880
7	0.679	0.756	0.704	0.816	0.707	0.783	0.750	0.857
8	0.624	0.695	0.651	0.782	0.641	0.717	0.697	0.824
9	0.663	0.741	0.683	0.804	0.664	0.754	0.708	0.837
10	0.656	0.736	0.681	0.812	0.638	0.729	0.685	0.835
average	0.701	0.798	0.732	0.858	0.750	0.833	0.793	0.898

From Xu, Liu & Gong. SIGIR'03.

Navigation icons: back, forward, search, etc.

Clustering Results on Reuters Data

Performance comparisons using Reuters corpus

k	Mutual Information				Accuracy			
	AA	NC	NMF	NMF-NCW	AA	NC	NMF	NMF-NCW
2	0.399	0.484	0.437	0.494	0.784	0.821	0.824	0.837
3	0.482	0.536	0.489	0.574	0.709	0.765	0.731	0.803
4	0.480	0.581	0.487	0.604	0.629	0.734	0.655	0.758
5	0.565	0.590	0.587	0.600	0.655	0.695	0.686	0.722
6	0.537	0.627	0.559	0.650	0.611	0.678	0.650	0.728
7	0.560	0.599	0.575	0.624	0.584	0.654	0.624	0.696
8	0.559	0.592	0.578	0.606	0.581	0.613	0.618	0.651
9	0.603	0.633	0.614	0.659	0.599	0.640	0.634	0.692
10	0.607	0.647	0.626	0.661	0.600	0.634	0.634	0.677
average	0.532	0.588	0.550	0.608	0.639	0.693	0.673	0.729

See Xu, Liu & Gong. SIGIR'03.

Navigation icons: back, forward, search, etc.

NMF Variants

- If the data matrix \mathbf{X} has mixed signs, then
- Singular Value Decomposition: $\mathbf{X}_{\pm} \approx \mathbf{F}_{\pm} \mathbf{G}_{\pm}^T$
- Semi-NMF: $\mathbf{X}_{\pm} \approx \mathbf{F}_{\pm} \mathbf{G}_{+}^T$
- Convex-NMF: $\mathbf{X}_{\pm} \approx \mathbf{X}_{\pm} \mathbf{W}_{+} \mathbf{G}_{+}^T$
- Kernel-NMF: $\phi(\mathbf{X}_{\pm}) \approx \phi(\mathbf{X}_{\pm}) \mathbf{W}_{+} \mathbf{G}_{+}^T$

The Relationships Between NMF and K-means

- *K-means* objective:

$$\begin{aligned}
 J_{km} &= \sum_c \sum_{\mathbf{x}_i \in \pi_c} \|\mathbf{x}_i - \mathbf{f}_c\|^2 = \sum_{i=1}^n \sum_{c=1}^c g_{ic} \|\mathbf{x}_i - \mathbf{f}_c\|^2 \\
 &= \left\| \mathbf{X} - \mathbf{F} \mathbf{G}^T \right\|_F^2
 \end{aligned}$$

- Cluster center matrix: $\mathbf{F} = [\mathbf{f}_1, \mathbf{f}_2, \dots, \mathbf{f}_c] \in \mathbb{R}^{n \times C}$
- $\mathbf{G} \in \mathbb{R}^{n \times C}$ with $\mathbf{G}_{ij} = g_{ij}$, such that $g_{ij} = 1$, if $\mathbf{x}_i \in \pi_j$; $\mathbf{G}_{ij} = 0$, otherwise.
- K-means and NMF: the same objective, only different constraint
 - NMF: $\mathbf{F} \geq 0$, $\mathbf{G} \geq 0$
 - K-means: $\mathbf{G}_{ij} \in \{0, 1\}$, $\mathbf{G} \mathbf{1} = \mathbf{1}$

The Relationships Between K-means and PCA

- $\varepsilon_k = \sum_{i=1}^{n_k} \|\mathbf{x}_i^{(k)} - \mathbf{m}_k\|^2 = \|\mathbf{X}_k - \mathbf{m}_k \mathbf{e}^T\|^2$
- $\varepsilon_k = \text{trace}(\mathbf{X}_k(\mathbf{I}_{n_k} - \mathbf{e}\mathbf{e}^T/n_k)\mathbf{X}_k^T)$
- Finally,

$$\varepsilon = \sum_{k=1}^C \varepsilon_k = \sum_{k=1}^C \left(\text{trace}(\mathbf{X}_k^T \mathbf{X}_k) - \left(\frac{\mathbf{e}^T}{\sqrt{n_k}} \right) \mathbf{X}_k^T \mathbf{X}_k \left(\frac{\mathbf{e}^T}{\sqrt{n_k}} \right) \right)$$
- Let $\tilde{\mathbf{P}} = \text{diag}(\frac{\mathbf{e}_{n_1}}{\sqrt{n_1}}, \dots, \frac{\mathbf{e}_{n_C}}{\sqrt{n_C}})$
- Then $\varepsilon = \text{trace}(\mathbf{X}^T \mathbf{X}) - \text{trace}(\tilde{\mathbf{P}}^T \mathbf{X}^T \mathbf{X} \tilde{\mathbf{P}})$ subject to $\tilde{\mathbf{P}}^T \tilde{\mathbf{P}} = \mathbf{I}$
- Therefore we need to maximize $\text{trace}(\tilde{\mathbf{P}}^T \mathbf{X}^T \mathbf{X} \tilde{\mathbf{P}})$ and get $\tilde{\mathbf{P}}$.
- According to the Ky Fan theorem, $\tilde{\mathbf{P}}$ is composed of the eigenvectors of $\mathbf{X}^T \mathbf{X}$ corresponding to its largest C eigenvalues
- If \mathbf{X} is centralized, then it is equivalent to PCA

The Relationships Between K-means and Spectral Clustering

- From last slide we can see that the relaxed solution of kmeans is equivalent to analyze the eigenstructure of $\mathbf{A} = \mathbf{X}^T \mathbf{X}$
- If we define the similarity matrix $\mathbf{W} = \mathbf{A}$, then kmeans is equivalent to ratio association
- Define the weighted kmeans criterion

$$\tilde{\varepsilon} = \sum_{k=1}^C \sum_{\mathbf{x}_i \in \pi_k} w_i \|\mathbf{x}_i - \mathbf{m}_k\|^2$$
- Using similar derivation procedure, we can derive that optimizing the above criterion is equivalent to solve

$$\max_{\tilde{\mathbf{P}}} \text{trace}(\tilde{\mathbf{P}}^T \mathbf{D}^{1/2} \mathbf{W} \mathbf{D}^{1/2} \tilde{\mathbf{P}}) \quad (10)$$

The Relationships Between NMF and Spectral Clustering

- Let the normalized similarity matrix be $\tilde{\mathbf{W}} = \mathbf{D}^{-1/2} \mathbf{W} \mathbf{D}^{-1/2}$
- Then we have the following theorem

Theorem

Normalized Cut using similarity $\tilde{\mathbf{W}}$ is equivalent to the following symmetric nonnegative matrix factorization

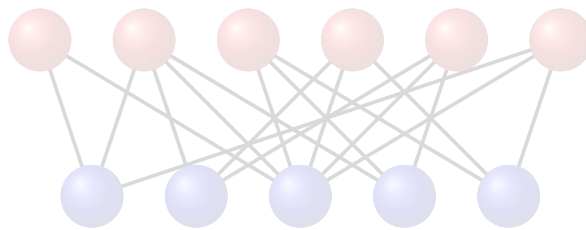
$$\min_{\tilde{\mathbf{P}} \geq 0} \mathcal{J} = \|\tilde{\mathbf{W}} - \tilde{\mathbf{P}} \tilde{\mathbf{P}}^T\|^2 \quad (11)$$

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- 1 Graphs and Matrices are Everywhere
- 2 Unsupervised Learning with Graphs & Matrices
 - Dimensionality Reduction
 - Clustering
 - Co-Clustering
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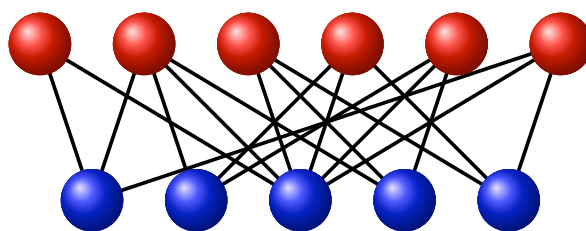
The Problem

- Usually the data we face with are relational, *i.e.*, there are multiple type of data interrelated with each other
- How to cluster those relational data simultaneously?



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A Spectral Approach

- Define the similarity matrix on the bi-partite graph

$$\mathbf{A} = \begin{bmatrix} \mathbf{0} & \mathbf{R} \\ \mathbf{R}^T & \mathbf{0} \end{bmatrix}$$

- Also the concatenated cluster membership vector $\mathbf{x} = [\mathbf{x}_I^T, \mathbf{x}_{II}^T]^T$
- Then the co-clustering problem becomes a graph-cut problem on the bi-partite graph, *i.e.*, we should solve the following generalized eigenvalue decomposition problem

$$\mathbf{L}\mathbf{x} = \lambda\mathbf{D}\mathbf{x} \quad (12)$$

- where $\mathbf{D} = \text{diag}(\sum_j A_{1j}, \dots, \sum_j A_{n_j})$, $\mathbf{L} = \mathbf{D} - \mathbf{A}$

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Nonnegative Matrix Tri-Factorization

- Factorize the user-movie rating matrix \mathbf{X} into three matrices \mathbf{F} , \mathbf{S} , \mathbf{G} , such that
 - \mathbf{F} represents the cluster memberships on the user side
 - \mathbf{G} represents the cluster memberships on the movie side
- By relaxing the integer constraints on \mathbf{F} , \mathbf{G} , we need to solve the following optimization problem

$$\min_{\mathbf{F} \geq 0, \mathbf{S} \geq 0, \mathbf{G} \geq 0} \|\mathbf{X} - \mathbf{F}\mathbf{S}\mathbf{G}^T\|^2, \quad s.t. \mathbf{F}^T\mathbf{F} = \mathbf{I}, \mathbf{G}\mathbf{G}^T = \mathbf{I} \quad (13)$$

- We can derive some multiplicative update rules to solve for the optimal \mathbf{F} , \mathbf{S} , \mathbf{G}

An Example of NMTF

Datasets	BiOR-NM3F			K-means		
	Purity	Entropy	ARI	Purity	Entropy	ARI
CSTR	0.754	0.402	0.436	0.712	0.412	0.189
WebKB4	0.583	0.372	0.428	0.534	0.442	0.418
Reuters	0.558	0.976	0.510	0.545	0.726	0.506
WebAce	0.541	0.889	0.449	0.546	0.868	0.452
Newsgroups	0.507	1.233	0.179	0.330	1.488	0.149

Performance Comparisons of clustering algorithms.
 Each entry is the corresponding performance value of the algorithm on the row dataset.

Other Types of Co-Clustering Methods

- Information-Theoretic Co-clustering (Dhillon et al. KDD'03)
- Bayesian Co-Clustering (Shan & Banerjee. ICDM'08)
- Tensor Method (Banerjee et al. SDM'07)
- Collective Factorization on Related Matrices (Long et al. ICML'06)
- Multiple Latent Semantic Analysis (Wang et al. SIGIR'06)

Why Semi-supervised Learning

- Traditional learning problems
 - Supervised learning: learning with labeled data set
 - Unsupervised learning: learning with unlabeled data set
- Problems
 - Supervised learning: requires much human effort, expensive and time consuming
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The Similarity Between SSL and Ranking

		Classes						Queries			
		1	2	...	C			1	2	...	C
Data	1	f_{11}	f_{12}	...	f_{1C}	Data	1	r_{11}	r_{12}	...	r_{1C}
	2	f_{21}	f_{22}	...	f_{2C}		2	r_{21}	r_{22}	...	r_{2C}
	...	\vdots	\vdots	\vdots	\vdots		...	\vdots	\vdots	\vdots	\vdots
	n	f_{n1}	f_{n2}	...	f_{nC}		n	r_{n1}	r_{n2}	...	r_{nC}

The Similarity Between SSL and Collaborative Filtering

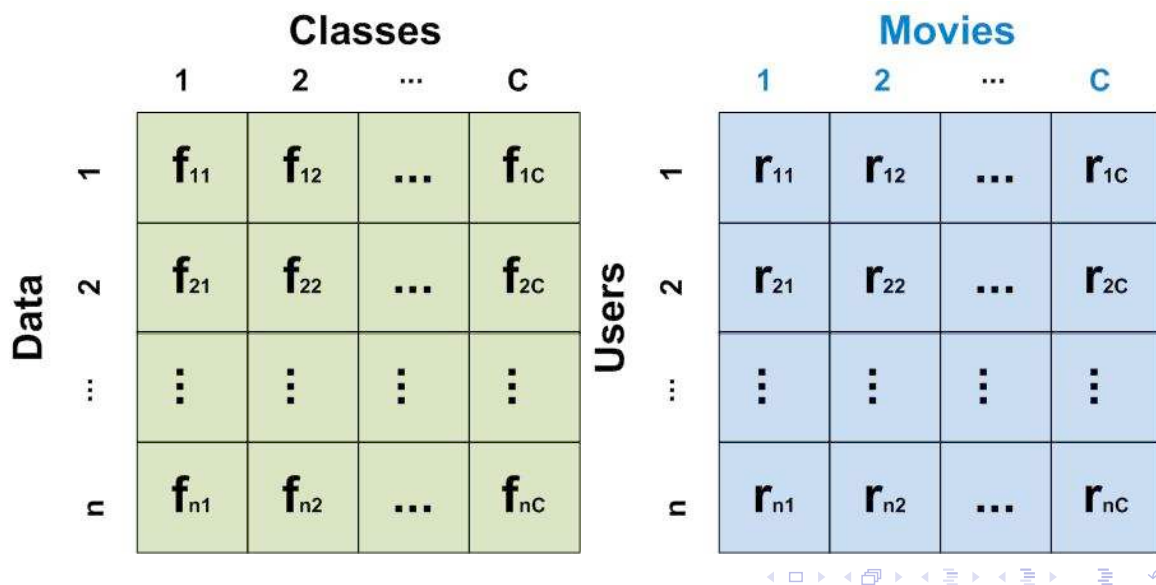


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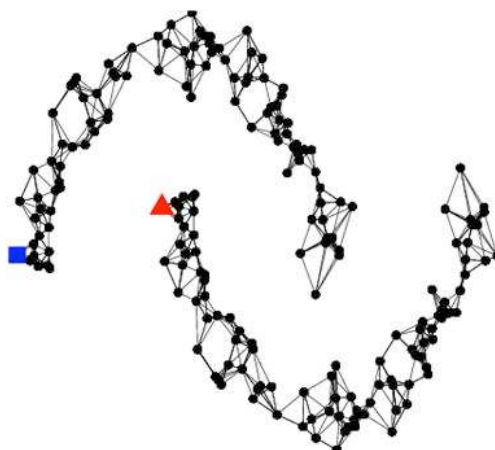
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Semi-supervised Assumption

- *Smoothness Assumption*: If two points $\mathbf{x}_1, \mathbf{x}_2$ in a high-density region are close, then so should be the corresponding outputs y_1, y_2
- *Cluster Assumption*: If points are in the same cluster, they are likely to be of the same class
- *Manifold Assumption*: The (high-dimensional) data lie (roughly) on a low-dimensional manifold

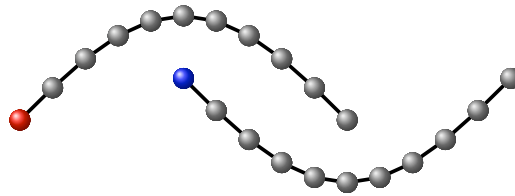
Label Propagation

- Connect the data points that are close to each other (Nearest Neighbor Graph)
- Propagate the class labels over the connected graph



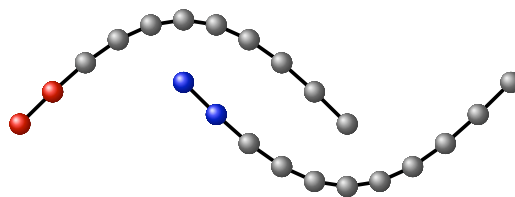
Propagation Rules

- Initial label vector: $\mathbf{y} \in \mathbb{R}^{n \times 1}$
 - $y_i = t_i$ if \mathbf{x}_i is labeled as t_i ; $y_i = 0$ if \mathbf{x}_i is unlabeled
- $f_i^{(1)} = y_i$ if \mathbf{x}_i is labeled; $f_i^{(1)} = \alpha \sum_{\mathbf{x}_j \in \mathcal{N}_i} \mathbf{P}_{ij} y_j$ otherwise
 - $\mathbf{P} \in \mathbb{R}^{n \times n}$ is the propagation matrix
 - Matrix form: $\mathbf{f}^{(1)} = \mathbf{y} + \alpha \mathbf{P} \mathbf{y}$
- $\mathbf{f}^{(2)} = \mathbf{f}^{(1)} + \alpha \mathbf{P} \mathbf{f}^{(1)} = (\mathbf{I} + \alpha \mathbf{P} + \alpha^2 \mathbf{P}^2) \mathbf{y}$
- Finally $\mathbf{f}^{(\infty)} = \sum_{i=0}^{\infty} \alpha^i \mathbf{P}^i \mathbf{y} = (\mathbf{I} - \alpha \mathbf{P})^{-1} \mathbf{y}$



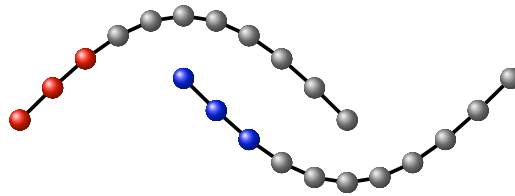
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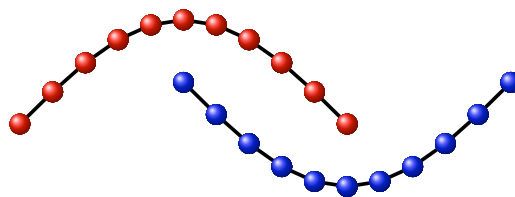
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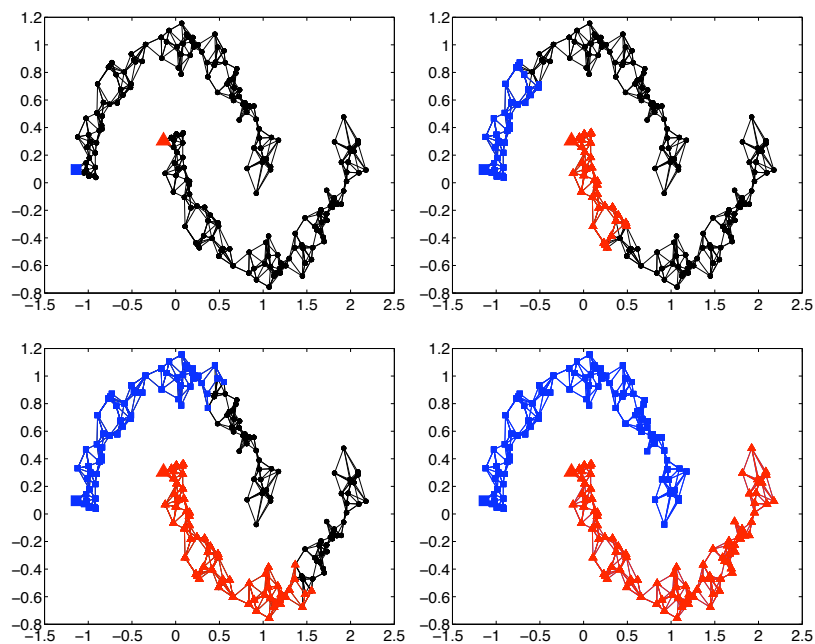


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An Example



Navigation icons: back, forward, search, etc.

Fei Wang, Tao Li, Chris Ding

Data Mining with Graphs & Matrices

The Calculation of \mathbf{P}

- Asymmetrically Normalized Similarity Matrix:

$$\mathbf{P} = \mathbf{D}^{-1}\mathbf{W}$$

- Symmetrically Normalized Similarity Matrix:

$$\mathbf{P} = \mathbf{D}^{-1/2}\mathbf{W}\mathbf{D}^{-1/2}$$

- How to determine the optimal σ when computing \mathbf{W}_{ij} ?
- Linear Neighborhood Similarity

$$\min_{\mathbf{W}_{ij}} \|\mathbf{x}_i - \sum_{\mathbf{x}_j \in \mathcal{N}_i} \mathbf{W}_{ij} \mathbf{x}_j\|^2$$

$$s.t. \sum_j \mathbf{W}_{ij} = 1, \mathbf{W}_{ij} \geq 0$$

Navigation icons: back, forward, search, etc.

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$$\begin{aligned} \min_{\mathbf{W}_{ij}} \quad & \|\mathbf{x}_i - \sum_{\mathbf{x}_j \in \mathcal{N}_i} \mathbf{W}_{ij} \mathbf{x}_j\|^2 \\ \text{s.t.} \quad & \sum_j \mathbf{W}_{ij} = 1, \quad \mathbf{W}_{ij} \geq 0 \end{aligned}$$

Navigation icons: back, forward, search, etc.

The Calculation of \mathbf{P}

- Asymmetrically Normalized Similarity Matrix:

$$\mathbf{P} = \mathbf{D}^{-1}\mathbf{W}$$

- Symmetrically Normalized Similarity Matrix:

$$\mathbf{P} = \mathbf{D}^{-1/2}\mathbf{W}\mathbf{D}^{-1/2}$$

- How to determine the optimal σ when computing \mathbf{W}_{ij} ?
- Linear Neighborhood Similarity

$$\begin{aligned} \min_{\mathbf{W}_{ij}} \quad & \|\mathbf{x}_i - \sum_{\mathbf{x}_j \in \mathcal{N}_i} \mathbf{W}_{ij} \mathbf{x}_j\|^2 \\ \text{s.t.} \quad & \sum_j \mathbf{W}_{ij} = 1, \quad \mathbf{W}_{ij} \geq 0 \end{aligned}$$

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A Regularization Framework

- Label consistency: the predicted labels should be sufficiently close to the initial labels on the labeled data points
- Label smoothness: the predicted labels should be sufficiently smooth with respect to the data manifold (graph)

$$\min_{\mathbf{f}} \sum_{i=1}^l (f_i - t_i)^2 + \sum_{i=l+1}^n f_i^2 + \mu \sum_{i \sim j} w_{ij} (f_i - f_j)^2$$

- The first term reflects label consistency
- The second term guarantees the predicted label values should fall in a reasonable range for numerical stability
- The third term reflects label smoothness
- $\mathbf{f} = (\mathbf{I} + \mu \mathbf{L})^{-1} \mathbf{y}$

A Regularization Framework

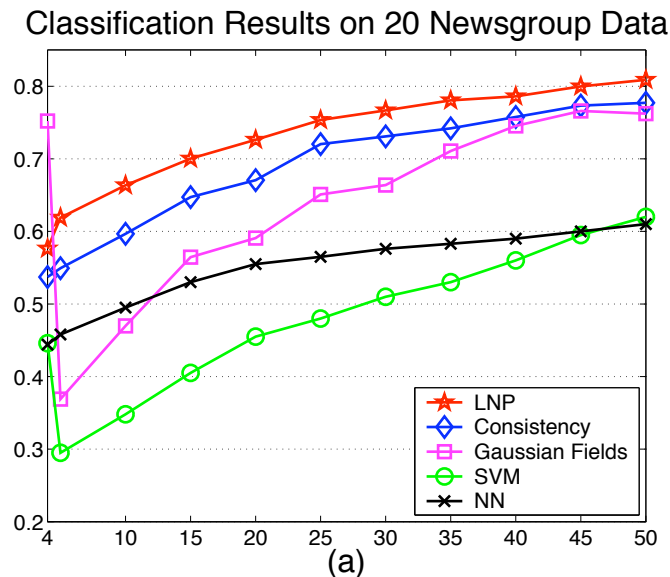
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Experimental Results on 20Newsgroup Data

autos, motorcycles, baseball, and hockey under rec



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Data Mining with Graphs & Matrices

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 - Semi-supervised Learning Using Side-Information
- 4 Future Research Directions

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Data Mining with Graphs & Matrices

What is Side-Information

- Types of side-information
 - Must-link: a pair of points should belong to the same class
 - Cannot-link: a pair of points should not appear in the same class
- Side-information is a type of prior knowledge weaker than partial labeling
 - Knowing the partial labeling, we can transform it into side-information
 - But not vice versa

Pairwise Constrained K-means Clustering

- *K-means* objective: $J_{km} = \sum_c \sum_{\mathbf{x}_i \in \pi_c} \|\mathbf{x}_i - \mathbf{f}_c\|^2$
- Matrix form: $J_{km} = \left\| \mathbf{X} - \mathbf{F}\mathbf{G}^T \right\|_F^2$
 - Cluster center matrix: $\mathbf{F} = [\mathbf{f}_1, \mathbf{f}_2, \dots, \mathbf{f}_C] \in \mathbb{R}^{n \times C}$
 - $\mathbf{G} \in \mathbb{R}^{n \times C}$ with $\mathbf{G}_{ij} = 1$, if $\mathbf{x}_i \in \pi_j$; $\mathbf{G}_{ij} = 0$, otherwise.
- The objective of PCKM

$$J(\pi) = \sum_c \sum_{\mathbf{x}_i \in \pi_c} \|\mathbf{x}_i - \mathbf{f}_c\|^2 + \sum_{\substack{\mathbf{x}_i, \mathbf{x}_j \in \mathcal{M} \\ \text{s.t. } l_i \neq l_j}} \theta_{ij} + \sum_{\substack{\mathbf{x}_i, \mathbf{x}_j \in \mathcal{C} \\ \text{s.t. } l_i = l_j}} \tilde{\theta}_{ij},$$

- $\{\theta_{ij} \geq 0\}$: penalties for violating the must-link constraints
- $\{\tilde{\theta}_{ij} \geq 0\}$: penalties for violating the cannot-link constraints

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Penalized Matrix Factorization

- Changing the penalties of violations in the constraints in \mathcal{M} into the *awards* as

$$\begin{aligned} J(\pi) &= \sum_c \sum_{\mathbf{x}_i \in \pi_c} \|\mathbf{x}_i - \mathbf{f}_c\|^2 - \sum_{\substack{\mathbf{x}_i, \mathbf{x}_j \in \mathcal{M} \\ \text{s.t. } l_i = l_j}} \theta_{ij} + \sum_{\substack{\mathbf{x}_i, \mathbf{x}_j \in \mathcal{C} \\ \text{s.t. } l_i = l_j}} \tilde{\theta}_{ij} \\ &= \sum_c \sum_{\mathbf{x}_i} \mathbf{G}_{ic} \|\mathbf{x}_i - \mathbf{f}_c\|^2 + \sum_c \sum_{i,j} \mathbf{G}_{ic} \mathbf{G}_{jc} \Theta_{ij} \end{aligned}$$

- $\Theta_{ij} = \begin{cases} \tilde{\theta}_{ij}, & (\mathbf{x}_i, \mathbf{x}_j) \in \mathcal{C} \\ -\theta_{ij}, & (\mathbf{x}_i, \mathbf{x}_j) \in \mathcal{M} \\ 0, & \text{otherwise} \end{cases}$

- Penalized matrix factorization objective

$$\begin{aligned} \min_{\mathbf{F}, \mathbf{G}} \quad & J(\pi) = \left\| \mathbf{X} - \mathbf{F}\mathbf{G}^T \right\|_F^2 + \text{tr}(\mathbf{G}^T \mathbf{\Theta} \mathbf{G}) \\ \text{s.t.} \quad & \mathbf{G} \geq 0 \end{aligned} \quad (14)$$

Penalized Matrix Factorization

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Updating Rules for PMF

Table: Penalized Matrix Factorization for Constrained Clustering

Inputs: Data matrix \mathbf{X} , Constraints matrix Θ .

Outputs: \mathbf{F} , \mathbf{G} .

1. Initialize \mathbf{G} ;

2. Repeat the following steps until convergence:

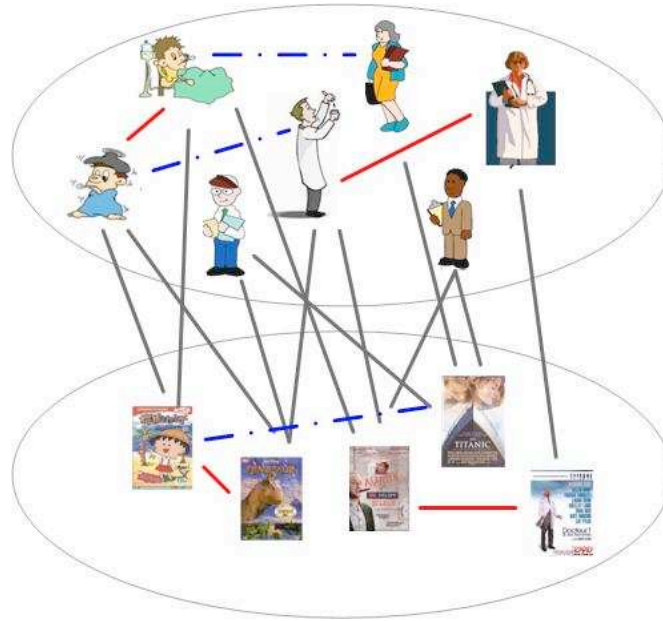
(a). Fixing \mathbf{G} , updating \mathbf{F} by $\mathbf{F} = \mathbf{X}\mathbf{G}(\mathbf{G}^T\mathbf{G})^{-1}$;

(b). Fixing \mathbf{F} , updating \mathbf{G} by

$$\mathbf{G}_{ij} \leftarrow \mathbf{G}_{ij} \sqrt{\frac{(\mathbf{X}^T \mathbf{F})_{ij}^+ + [\mathbf{G}(\mathbf{F}^T \mathbf{F})^-]_{ij} + (\Theta^- \mathbf{G})_{ij}}{(\mathbf{X}^T \mathbf{F})_{ij}^- + [\mathbf{G}(\mathbf{F}^T \mathbf{F})^+]_{ij} + (\Theta^+ \mathbf{G})_{ij}}}$$

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Side-Information on Bi-partite Graph



Navigation icons: back, forward, search, etc.

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PMF on Bi-partite Graph

$$\min_{\mathbf{G}_1 \geq 0, \mathbf{G}_2 \geq 0} J = \|\mathbf{R}_{12} - \mathbf{G}_1 \mathbf{S} \mathbf{G}_2^T\|^2 + tr(\mathbf{G}_1^T \Theta_1 \mathbf{G}_1) + tr(\mathbf{G}_2^T \Theta_2 \mathbf{G}_2)$$

Table: PMF on Bi-partite Graph

Inputs: Relation matrix \mathbf{R}_{12} , Constraints matrices Θ_1, Θ_2 .

Outputs: $\mathbf{G}_1, \mathbf{S}, \mathbf{G}_2$.

1. Initialize $\mathbf{G}_1, \mathbf{G}_2$;
2. Repeat the following steps until convergence:

(a). Fixing $\mathbf{G}_1, \mathbf{G}_2$, updating \mathbf{S} using

$$\mathbf{S} \leftarrow (\mathbf{G}_1^T \mathbf{G}_1)^{-1} \mathbf{G}_1^T \mathbf{R}_{12} \mathbf{G}_2 (\mathbf{G}_2^T \mathbf{G}_2)^{-1};$$

(b). Fixing \mathbf{S}, \mathbf{G}_2 , updating \mathbf{G}_1 using

$$\mathbf{G}_{1ij} \leftarrow \mathbf{G}_{1ij} \sqrt{\frac{(\mathbf{R}_{12} \mathbf{G}_2 \mathbf{S}^T)_{ij}^+ + [\mathbf{G}_1 (\mathbf{S}^T \mathbf{G}_2^T \mathbf{G}_2 \mathbf{S})^-]_{ij} + (\Theta_1^- \mathbf{G}_1)_{ij}}{(\mathbf{R}_{12} \mathbf{G}_2 \mathbf{S}^T)_{ij}^- + [\mathbf{G}_1 (\mathbf{S}^T \mathbf{G}_2^T \mathbf{G}_2 \mathbf{S})^+]_{ij} + (\Theta_1^+ \mathbf{G}_1)_{ij}}};$$

(c). Fixing \mathbf{G}_1, \mathbf{S} , updating \mathbf{G}_2 using

$$\mathbf{G}_{2ij} \leftarrow \mathbf{G}_{2ij} \sqrt{\frac{(\mathbf{R}_{12}^T \mathbf{G}_1 \mathbf{S})_{ij}^+ + [\mathbf{G}_2 (\mathbf{S} \mathbf{G}_1^T \mathbf{G}_1 \mathbf{S}^T)^-]_{ij} + (\Theta_2^- \mathbf{G}_2)_{ij}}{(\mathbf{R}_{12}^T \mathbf{G}_1 \mathbf{S})_{ij}^- + [\mathbf{G}_2 (\mathbf{S} \mathbf{G}_1^T \mathbf{G}_1 \mathbf{S}^T)^+]_{ij} + (\Theta_2^+ \mathbf{G}_2)_{ij}}}.$$

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Table: The F measure of three algorithms on the BBS data set

Data Sets	Algorithm	$d = 3$	$d = 4$	$d = 5$	$d = 6$
1	MLSA	0.7019	0.7079	0.7549	0.7541
1	SRC	0.7281	0.6878	0.6183	0.6183
1	Tri-SPMF	0.7948	0.8011	0.8021	0.7993
2	MLSA	0.7651	0.7429	0.7581	0.7309
2	SRC	0.7627	0.7226	0.7280	0.6965
2	Tri-SPMF	0.8007	0.7984	0.7938	0.7896
3	MLSA	0.6689	0.6511	0.6987	0.7301
3	SRC	0.7556	0.7666	0.7472	0.7125
3	Tri-SPMF	0.8095	0.8034	0.7993	0.7874

Tensor & Hypergraph Based Methods

- In knowledge & information management, we usually face with multi-relational data
 - Graph based methods can capture the pairwise relationships
 - Matrix is also only composed of two dimensions
- Hypergraph is more efficient in describing the multiple-wise relationships
- Tensor is also a structure that can capture multiple-wise relationships

Efficient & Large Scale Methods

- Matrix & Graph based methods usually involve high computational cost
 - eigenvalue decomposition
 - solving large scale linear equation systems
 - constrained optimization
- How to make the algorithm more efficient?
 - Exploring the sparsity
- How to improve scalability?
 - Smart sampling

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Probabilistic Interpretations

- Potential problems of describing the data with matrices
 - Too large
 - Too complicated
 - Missing entries
 - Noisy entries
 -
- Probabilistic interpretations & graphical models
 - Discover latent structures
 - Relationships with matrix based methods?









Knowledge Transfer Across Different Domains

- The multi-relational data contain data points from different domains
 - We may easily get some prior knowledge on some domains
- How to transfer the knowledge from one domain to another?
 - What knowledge to transfer?
 - How?
 - Is it really helps?

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