Fast and Accurate Low Rank Approximation of Massive Graphs

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IPAM Aug 25, 2010

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Outline

• Some Problems in Network Analysis

- Link prediction problem
- Link prediction with multiple sources of information
- Affiliation recommendation problem

Tools and Methods

- Path based methods for link prediction
- Low rank approximations
- Graph clustering
- Clustered low rank approximation
- Experimental Results
- Summary and Conclusions

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Networks in Applications

- Web graphs
- Collaboration and citation networks
- Social networks (Facebook, MySpace, LiveJournal, ...)
- Call graph networks (SKT, AT&T)
- Networks in Bioinformatics

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Graphs

- Graph $G = (\mathcal{V}, \mathcal{E})$, \mathcal{V} is a set of vertices, and \mathcal{E} is a set of edges between vertices.
- The adjacency matrix $A = [a_{ij}]$ of G is given by

 $a_{ij} = w_{ij}$ if there is an edge between vertex *i* and *j* $a_{ij} = 0$ otherwise

- Undirected graph then A is symmetric
- Directed graph then A is non-symmetric

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Link Prediction Problem

Consider a social network that evolves with time,

$$\cdots \longrightarrow A^{(t-2)} \longrightarrow A^{(t-1)} \longrightarrow A^{(t)} \xrightarrow{?} A^{t+1}$$



Q: Can we predict links that will form at time step t + 1? A: Many models exist, e.g. common neighbors, the Katz measure, etc.

Link prediction with multiple sources of information

In most cases, we have a social network between users



But also additional sources of information

- Other types of links between users, e.g. family ties, affiliations
- User profiles, demographic information
- Blog postings by users, movie ratings, etc

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Affiliation recommendation/prediction

Consider a users \times affiliations network



Affiliation recommendation

We want to suggest groups/affiliations to users



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Affiliation recommendation given a social network

Suppose we additionally have a social network:



Can the social network help to improve affiliation recommendations?

Challenges

- Huge number of users and/or affiliations, e.g. Facebook, MySpace, Orkut, LiveJournal
- Multiple sources of information
- Need scalable algorithms and "accurate" predictions

Tools and Methods

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Path based methods for link prediction

• No. of common neighbors can be computed as:

$$P_{\rm cn} = A^2$$

Yields no. of paths of length 2 between any two vertices

• Katz measure and truncated Katz measure

$$P_{\text{katz}} = \beta A + \beta^2 A^2 + \beta^3 A^3 + \dots = \sum_{i=1}^{\infty} \beta^i A^i = (I - \beta A)^{-1} - I$$
$$P_{\text{t-katz}} = \beta A + \beta^2 A^2 + \dots + \beta^k A^k = \sum_{i=1}^k \beta^i A^i$$

- A^3 gives no. of paths of length 3, A^4 is no. of paths of length 4, & so on
- Small β penalizes paths with larger lengths
- Large β amplifies paths with larger lengths

A social network and its adjacency matrix



Link prediction based on common neighbors

- No. of common neighbors is given by A^2
- Carol: common neighbor predicts links to Bob, Dave and Eve (in red).



Link prediction based on Katz measure

$$K(A,\beta) = \beta A + \beta^2 A^2 + \beta^3 A^3 + \dots = (I - \beta A)^{-1} - I$$

- With $\beta = 0.4$
- Top two predictions for Carol are to Bob and Dave (in red)
- Katz score between Carol & Eve is smaller than other scores (in green)



After a few time steps....





Common Neighbors

- All possible predictions in red, based on common neighbors.
- Possible recommendation: top two highest scores



Katz measure

$$\mathit{Katz}(A,\beta) = \sum_{i=1}^{\infty} \beta^i A^i = (I - \beta A)^{-1} - I, \qquad \beta < |\lambda_i| \quad \forall \ i$$

• With $\beta = 1/3$ top three Katz scores are the X's



Fast and Accurate Low Rank Approximation of Massive Graphs

Importance of low rank approximations

- Enables scalability
- Can filter out noise
- Introduces interpretable features...
- For example, with the spectral approximation $A \approx V \Lambda V^{\mathsf{T}}$,

$$A^{k} \approx (VDV^{\mathsf{T}})^{k} = (VDV^{\mathsf{T}})(VDV^{\mathsf{T}})\cdots(VDV^{\mathsf{T}}) = VD^{k}V^{\mathsf{T}}$$

Link predictors with low rank approximations

• With spectral approximation,

$$A \approx V \Lambda V^{\mathsf{T}}$$

• Common neighbor,

$$P_{\rm cn} = A^2, \qquad P_{\rm cn-lr} = V \Lambda^2 V^{\rm T}$$

Katz measure,

$$P_{\text{katz}} = (I - \beta A)^{-1} - I = \sum_{i=1}^{\infty} \beta^{i} A^{i} \qquad P_{\text{t-katz}} = \sum_{i=1}^{k} \beta^{i} A^{i}$$
$$P_{\text{katz-Ir}} = V \left((I - \beta \Lambda)^{-1} - I \right) V^{\mathsf{T}} \qquad P_{\text{t-katz-Ir}} = \sum_{i=1}^{k} \beta^{i} V \Lambda^{i} V^{\mathsf{T}}$$

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Generalized Katz, evolving graphs and model learning

Replace β in truncated Katz with $\alpha_1, \ldots, \alpha_k$

$$P_{t-katz} = \sum_{i=1}^{k} \beta^{i} A^{i} \quad \Rightarrow \quad P_{gt-katz} = \sum_{i=1}^{k} \alpha_{i} A^{i}$$

Social network graphs are evolving....

- A adjacency matrix at time step t₁
- B adjacency matrix at time step $t_2 > t_1$
- Usually $B = A + \Delta$

Learn α_i from snapshots A and B

$$\min_{\alpha_i} \left\| \sum_{i=1}^k \alpha_i A^i - B \right\|_F \quad \text{or rather} \quad \min_{\alpha_i} \left\| \left(\sum_{i=1}^k \alpha_i A^i - B \right) \cdot M \right\|_F$$

where $M_{ij} = 0$ if $A_{ij} = 1$ and $B_{ij} = 1$, otherwise $M_{ij} = 1$

Link prediction with multiple sources(networks)

• Paths with edges in A:

$$i \xrightarrow{A} j \xrightarrow{A} k, \qquad A^2$$

• Paths with edges in *B*:

$$i \xrightarrow{B} j \xrightarrow{B} k, \qquad B^2$$

• Hybrid paths with edges in A and B:

$$i \xrightarrow{B} j \xrightarrow{A} k, \qquad BA$$



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Link prediction with multiple sources(networks)

 In general, utilizing single source and hybrid source paths of maximum length l_{max} involves terms from

$$(I + A + B + C)^{I_{\max}}$$

- Compare with truncated Katz
 - Linear combination in terms of $\{A, A^2, \cdots, A^{l_{max}}\}$
 - Linear combination in terms of

 $\{A, B, C, A^2, B^2, C^2, AB, AC, BA, BC, CA, CB\}$ $I_{max} = 2$

- Weights learned using "Hierarchical sparsity regularization"
- Utilizing multiple sources can improve link prediction
- Experiments with Arxiv and CiteSeer data
- Sources include:
 - $\textcircled{1} \quad \text{author} \ \times \ \text{author collaboration network}$
 - 2 paper \times paper citation network
 - \bigcirc author \times paper network
 - author × author networks based on similarities of abstracts, titles and keywords.

Affiliation recommendation



A B > A B >

Affiliation recommendation given a social network

A is the affiliation network, S is the social network

- Method 1: Low rank approximation of A
- Method 2: Low rank approximations of the combined matrix

$$C = \begin{bmatrix} \lambda S & A \\ A^{T} & 0 \end{bmatrix} \approx \begin{bmatrix} V_1 \\ V_2 \end{bmatrix} \wedge \begin{bmatrix} V_1^{T} & V_2^{T} \end{bmatrix},$$

where λ controls amount of influence of the social network.

• Predictions based on $V_1 \Lambda V_2^T$

Affiliation recommendation given a social network

• Method 3: Katz or truncated Katz measure on the combined matrix

$$P_{\mathsf{katz}} = \beta \mathcal{C} + \beta^2 \mathcal{C}^2 + \cdots$$

$$P_{\text{t-katz}} = \beta C + \beta^2 C^2 + \dots + \beta^I C^I$$

Predictions are based on the (1,2) block (corresponding to A in C), e.g.

$$P_{t-katz}^{(1,2)} = \beta A + \beta^2 \lambda S A + \beta^3 \lambda^2 (S^2 A + A A^T A)$$

We can use both low rank approach and Katz measure approach.

• Method 4: Common subspace to approximate A and S

$$A \approx Q D_A V^{\mathsf{T}}, \qquad S \approx Q D_S Q^{\mathsf{T}}$$

Q spans dominant subspaces of both A and S

Graph Clustering/Community Detection

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Graph Partitioning/Clustering

• In many applications, goal is to partition/cluster nodes of a graph:



High School Friendship Network

Graph Partitioning/Clustering

• In many applications, goal is to partition/cluster nodes of a graph:



The Internet

[The Internet Mapping Project, Hal Burch and Bill Cheswick, Lumeta Corp, 1999]

Graph clustering

• Cluster vertices \mathcal{V} into c disjoint sets \mathcal{V}_i ,

$$\mathcal{V} = \cup_{i=1}^{c} \mathcal{V}_{i}$$
 and $\mathcal{V}_{i} \cap \mathcal{V}_{j} = \emptyset$ $i \neq j$

• Objective functions for clustering

$$\begin{aligned} \mathsf{RCut} &= \min_{\mathcal{V}_1, \dots, \mathcal{V}_c} \sum_{i=1}^c \frac{\mathsf{links}(\mathcal{V}_i, \mathcal{V}n\mathcal{V}_i)}{|\mathcal{V}_i|} \quad \text{(Chan et al. 1994)} \\ \mathsf{NCut} &= \min_{\mathcal{V}_1, \dots, \mathcal{V}_c} \sum_{i=1}^c \frac{\mathsf{links}(\mathcal{V}_i, \mathcal{V}n\mathcal{V}_i)}{\mathsf{degree}(\mathcal{V}_i)} \quad \text{(Shi and Malik 2000)} \\ \mathsf{KLObj} &= \min_{\mathcal{V}_1, \dots, \mathcal{V}_c} \sum_{i=1}^c \frac{\mathsf{links}(\mathcal{V}_i, \mathcal{V}n\mathcal{V}_i)}{|\mathcal{V}_i|} \quad \mathsf{s.t.} \quad |\mathcal{V}_i| = |\mathcal{V}_j| \quad \text{(Kernighan and Lin 1970)} \end{aligned}$$

- Spectral clustering can be expensive for massive graphs
- Fast clustering algorithms without eigenvector computations
 - GRACLUS (Dhillon et al. 2007) and METIS (Karypis and Kumar 1999)

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Clustering example: arXiv data graph condMat



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Motivation: main idea through an example

$$A = \begin{bmatrix} A_{11} & 0 \\ 0 & A_{22} \end{bmatrix}$$

Let $\sigma_1(A_{22}) < \sigma_k(A_{11})$ and $\bar{U}_k \bar{\Sigma}_k \bar{V}_k^\mathsf{T} \approx A_{11}$

$$A pprox U_k \Sigma_k V_k^{\mathsf{T}} = egin{bmatrix} ar{U}_k ar{\Sigma}_k ar{V}_k^{\mathsf{T}} & 0 \ 0 & 0 \end{bmatrix}$$

No information from A_{22} is extracted. Approximate each block: $\overline{U}_k \overline{\Sigma}_k \overline{V}_k^{\mathsf{T}} \approx A_{11}$ and $\hat{U}_k \hat{\Sigma}_k \hat{V}_k^{\mathsf{T}} \approx A_{22}$

$$A \approx \begin{bmatrix} \bar{U}_k & 0\\ 0 & \hat{U}_k \end{bmatrix} \begin{bmatrix} \bar{\Sigma}_k & 0\\ 0 & \hat{\Sigma}_k \end{bmatrix} \begin{bmatrix} \bar{V}_k & 0\\ 0 & \hat{V}_k \end{bmatrix}^{\mathsf{T}},$$

Main idea continued

$$A = \begin{bmatrix} A_{11} & A_{12} \\ A_{21} & A_{22} \end{bmatrix}$$

Compute a low rank approximation of each diagonal block

 $U_i S_{ii} V_i^{\mathsf{T}} \approx A_{ii} \qquad U_i, \ V_i \text{ orthonormal}$

Approximate now

where

$$A = \begin{bmatrix} A_{11} & A_{12} \\ A_{21} & A_{22} \end{bmatrix} \approx \begin{bmatrix} U_1 & 0 \\ 0 & U_2 \end{bmatrix} \begin{bmatrix} S_{11} & S_{12} \\ S_{21} & S_{22} \end{bmatrix} \begin{bmatrix} V_1 & 0 \\ 0 & V_2 \end{bmatrix}^{\mathsf{T}}$$
$$S_{ij} = U_i^{\mathsf{T}} A_{ij} V_j$$

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Low rank vs clustered low-rank





- Observe diag (U_1, U_2, \cdots, U_c) and has the same memory usage as U
- Experiments show that most of U is contained in diag (U_1, U_2, \cdots, U_c)
- Similarly of V and diag (V_1, V_2, \cdots, V_c)

Algorithm: Clustered low rank approximation

Input: An $m \times m$ adjacency matrix A of a graph, number of clusters c**Output:** Clustered low rank approximation of A

- 1: Cluster the graph into c clusters
- 2: Compute a low rank approximation of each cluster

$$U_i S_i V_i \approx A_{ii}$$

3: Extend the cluster-wise approximations, into an approximation for the entire matrix \boldsymbol{A}



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Different low rank approximations

- Deterministic methods truncated SVD using ARPACK, PROPACK, SVDPACK.
- Stochastic methods

$$Y = A\Omega$$
 or $Y = (AA^T)^q A\Omega$

where q is small (1,2 or 3), and Ω is a random matrix (standard Gaussian). An approximation is obtained with

$$A \approx \hat{A} = P_Y A = Y(Y^T Y)^{-1} Y^T A$$

where P_Y is an orthogonal projection onto the range space of Y

Deterministic error bound—preliminaries

For any partitioning

$$A = \begin{bmatrix} A_{11} & \cdots & A_{1c} \\ \vdots & \ddots & \vdots \\ A_{c1} & \cdots & A_{cc} \end{bmatrix}$$

and any $Y^{(i)}$ form

$$Y = \begin{bmatrix} Y^{(1)} & & \\ & \ddots & \\ & & Y^{(c)} \end{bmatrix} \qquad P_Y = \begin{bmatrix} P_{Y^{(1)}} & & \\ & \ddots & \\ & & & P_{Y^{(c)}} \end{bmatrix}$$

 P_Y and each $P_{Y^{(i)}}$ are orthogonal projectors

Deterministic clustered error bound

The approximation error is given by

$$||A - \hat{A}|| = ||A - P_Y A|| = ||(I - P_Y)A||$$

Theorem

$$\|(I - P_Y)A\|_F^2 \le \sum_{i,j=1}^c \|(I - P_{Y^{(i)}})A_{ij}\|_F^2$$

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Introduce variables

Assume we have c clusters

$$A = \begin{bmatrix} A_{11} & \cdots & A_{1c} \\ \vdots & \ddots & \vdots \\ A_{c1} & \cdots & A_{cc} \end{bmatrix}$$

Generate

$$Y^{(i)} = A_{ii}\Omega^{(i)}$$
$$Y^{(i)} = (A_{ii}A_{ii}^{\mathsf{T}})^{q}A_{ii}\Omega^{(i)}$$

using random $\Omega^{(i)}$

$$Y = \begin{bmatrix} Y^{(1)} & & \\ & \ddots & \\ & & Y^{(c)} \end{bmatrix} \qquad P_Y = \begin{bmatrix} P_{Y^{(1)}} & & \\ & \ddots & \\ & & P_{Y^{(c)}} \end{bmatrix}$$

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Theorem

$$\begin{split} \mathbb{E}\|(I-P_Y)A\|_F &\leq \sum_{i=1}^c \left(1+\frac{k_i}{p_i+1}\right)^{1/2} \|\Sigma_2^{(i)}\|_F + \sum_{i,j=1, i\neq j}^c \|A_{ij}\|_F^2 \\ \mathbb{E}\|(I-P_Y)A\|_2 &\leq \sum_{i=1}^c \left(\left(1+\frac{\sqrt{k_i}}{\sqrt{p_i-1}}\right) \|\Sigma_2^{(i)}\|_2 + \frac{e\sqrt{k_i+p_i}}{p_i} \|\Sigma_2^{(i)}\|_F \right) \\ &+ \sum_{i,j=1, i\neq j}^c \|A_{ij}\|_2^2 \end{split}$$

$$A_{ii} pprox U^{(i)} \Sigma^{(i)} (V^{(i)})^{\mathsf{T}} = U^{(i)} \begin{bmatrix} \Sigma_1^{(i)} & 0 \\ 0 & \Sigma_2^{(i)} \end{bmatrix} \begin{bmatrix} V_1^{(i)} & V_2^{(i)} \end{bmatrix}^{\mathsf{T}}$$

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Experimental Results

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Google web matrix—performance comparison

- 434,818 vertices; 3,419,124 edges
- Edges within clusters: 98.2%, 97.8%, 97.6%; graph is highly clusterable
- "Ranks" are *k* = 20, 50, 100, 150, 200.



LiveJournal graph

- 3,828,682 vertices; 65,825,429 edges
- Edges within clusters: 76.9%, 69.3%, 66.3%; graph not highly clusterable
- "Ranks" are k = 20, 50, 100, 150, 200.



Image segmentation graph

Here we use the normalized adjacency matrix:

- 10,000 vertices; 1,091,910 edges
- Edges within clusters: 77.5%, 70.4%; graph not highly clusterable



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Network	Date	# nodes	# links	# added links	% added links
Flickr	4/14/2007	1,990,149	41,302,536	_	_
	4/25/2007	1,990,149	42,056,754	754,218	1.8%
	5/6/2007	1,990,149	42,879,714	822,960	1.9%
LiveJournal	02/16/2009	1,770,961	83,663,478	_	_
	03/4/2009	1,770,961	84,413,542	750,064	0.8%
	04/03/2009	1,770,961	85,713,766	1,300,224	1.5%
MySpace	12/11/2008	2,137,264	90,333,122	_	_
	1/11/2009	2,137,264	90,979,264	646,142	0.7%
	2/14/2009	2,137,264	91,648,716	669,452	0.7%

	# clusters	avg size	% intra links	% inter links
Flickr	18	110,563	71.8%	28.2%
LiveJournal	17	106,241	72.5%	27.5%
MySpace	17	125,721	51.9%	48.1%

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Introduce the sets

 $\begin{aligned} \mathcal{E} &= \{(i,j) \mid A_{ij} = 1\}, & \text{``old links''} \\ \mathcal{N} &= \{(i,j) \mid A_{ij} = 0 \& B_{ij} = 1\}, & \text{newly formed links} \\ \mathcal{Z} &= \{(i,j) \mid A_{ij} = 0 \& B_{ij} = 0\}, & \text{no links between vertices } i \text{ and } j \end{aligned}$ Concrete example (MySpace): A is 2.1M × 2.1M matrix with

 $|\mathcal{E}|\approx 0.0020\%, \quad |\mathcal{N}|\approx 1.46\cdot 10^{-5}\%, \quad |\mathcal{Z}|\approx 99.998\%$

Training Randomly sample 100,000 links from ${\cal N}$ and 500,000 links from ${\cal Z},$ true ratio 1 to 6.8M

Testing Randomly sample testing subsets from \mathcal{N} and \mathcal{Z} , compute corresponding scores, and predict links on highest scores.

Predictions Generic predictor in factored form

$$P = \bar{V}\bar{D}\bar{V}^{\mathsf{T}}$$

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we can compute P_{ij} for any ij

Performance of link predictors

- Ompute scores for 100k positive & 500k negative links (600k total)
- Sort the scores
- For a given threshold consider all scores above this threshold as predictions of friendships
- Plot false positive rate (FPR) vs false negative rate (FNR) for a range of threshold values

 $FPR = \frac{\#of \text{ incorrectly predicted friend links}}{\#of \text{ non-friend pairs}}$ $FNR = \frac{\#of \text{ missed friend links}}{\#of \text{ new friend links}}$

Sech threshold value gives one point in the plot

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Link prediction results on LiveJournal

Lower-left better; "-c" indicates clustering is involved



Clustering improves both Katz measures and Common neighbors method

Link prediction results on Flickr

Lower-left better; "-c" indicates clustering is involved



Best method "SL-c" Spectral learning with clustering (not in this talk)

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Affiliation recommendation on Youtube data

Upper-left is better



Clear improvement in performance by utilizing the social network (for both truncated Katz and latent factors model (LFM)).

Affiliation recommendation on Youtube data

Upper-left is better



Best two methods: truncated Katz measure using Common Subspaces and truncated Katz measure using latent factors model and clustering. Clustering gives a substantial boost in performance (compare "pink" with "red square")

Summary and Conclusions

- Clustered low rank approximation
 - Improved quality of approximation with identical memory consumption faster than state-of-the-art (PROPACK, SVDPACK, ARPACK). Note: clustering time included.
- Prediction methods
 - Katz and CN using graph embedding
 - Generalized truncated Katz
- Utilizing multiple sources improves link prediction
- Utilizing social network improves affiliation recommendation
- Improved and scalable computation of proximity measures & link predictions with clustered low rank approximation
- Fruitful to combine clustering structure with low rank approximation framework

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