Bipartite Edge Prediction via Transductive Learning over Product Graphs

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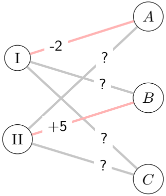
July 8, 2015

Outline

Problem Description

- Many applications involve predicting the edges of a bipartite graph.



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2. Host-Pathogen Interaction
3. Question-Answering Mapping
4. Citation Network . . .

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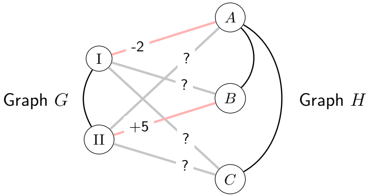

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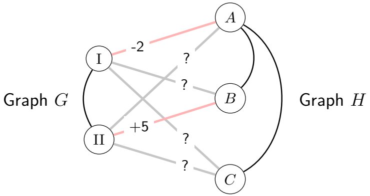

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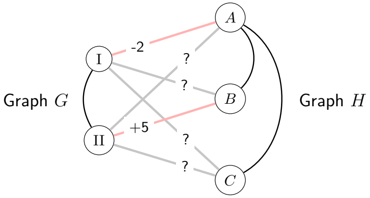

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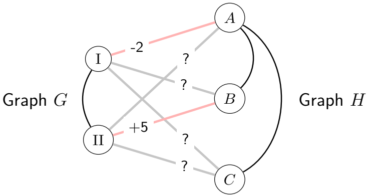
- Heterogeneous info: $G + H +$ partial observations
- Combine them to make better edge predictions?

The Proposed Framework



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  1. Labeled edges (red) are highly sparse
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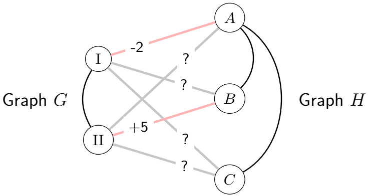

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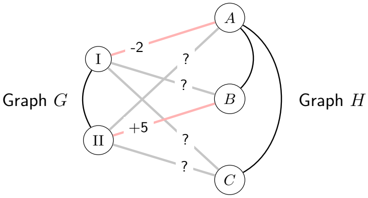

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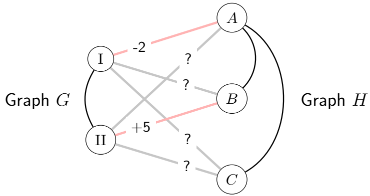

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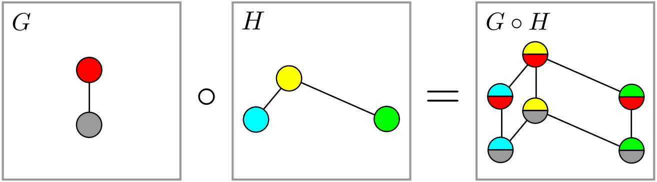
- Prerequisite: a similarity measure among the edges, i.e. a "Graph of Edges" (not directly provided)
- Can be induced from G and H via Graph Product!

The Proposed Framework

The "Graph of Edges" can be induced by taking the product of G and H



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  - Each Vertex $\sim$ edge (in the original bipartite graph)
  - Each Edge $\sim$ edge-edge similarity

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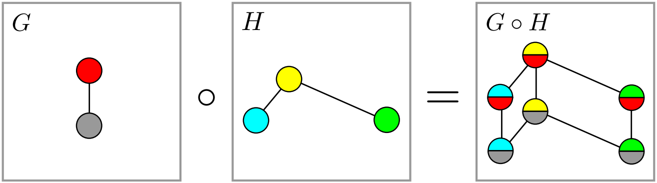

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  - Each Vertex $\sim$ edge (in the original bipartite graph)
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- The adjacency matrix of the product graph is defined by “$\circ$” (to be discussed later).

The Proposed Framework

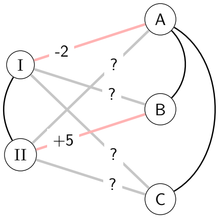
Problem Mapping

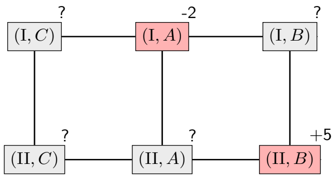
Edge Prediction (Original Problem)

Given G, H and labeled edges, predict the unlabeled edges

Vertex Prediction (Equivalent Problem)

Given $G \circ H$ and labeled vertices, predict the unlabeled vertices





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Product Graph Construction

Q: When should vertex $(i, j) \sim (i', j')$ in the product graph?

Tensor GP $i \sim i'$ in G AND $j \sim j'$ in H

Cartesian GP $(i \sim i'$ in G AND $j = j')$ OR $(i = i'$ AND $j \sim j'$ in $H)$

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To compute the adjacency matrices of PG

- $G \circ_{Tensor} H = \underbrace{G \otimes H}_{\text{Kronecker (a.k.a. Tensor) Product}}$
- $G \circ_{Cartesian} H = G \otimes I + I \otimes H = \underbrace{G \oplus H}_{\text{Kronecker Sum}}$

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Both GPs can be written in the form of spectral decomposition

$$G \circ_{Tensor} H = \sum_{i,j} (\lambda_i \times \mu_j)(u_i \otimes v_j)(u_i \otimes v_j)^\top \tag{1}$$

$$G \circ_{Cartesian} H = \sum_{i,j} (\lambda_i + \mu_j)(u_i \otimes v_j)(u_i \otimes v_j)^\top \tag{2}$$

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Generalization: Spectral Graph Product

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Commutative Property: $G \circ H$ and $H \circ G$ are isomorphic.

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Learning Objective

$$\min_f \quad \underbrace{\ell(f)}_{\text{Loss Function}} + \underbrace{\lambda f^\top A^{-1} f}_{\text{Graph Regularization}} \tag{4}$$

f_i system-predicted value for vertex i in A

$\ell(f)$ quantifies the gap between f and partially observed labels.

$\lambda f^\top A^{-1} f$ quantifies the smoothness over graph

- Underlying assumption: $f \sim \mathcal{N}(0, A)$

Graph-based Transductive Learning

The enhanced learning objective

$$\min_{f} \quad \underbrace{\ell(f)}_{\text{Loss Function}} + \underbrace{\lambda f^\top \kappa(A)^{-1} f}_{\text{Graph Regularization}} \tag{5}$$

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- k-step Random Walk $\kappa(A) = A^k$
- Regularized Laplacian $\kappa(A) = (\epsilon I - A)^{-1} = I + A + A^2 + A^3 + \ldots$
- Diffusion Process $\kappa(A) = \exp(A) \equiv I + A + \frac{1}{2!}A^2 + \frac{1}{3!}A^3 + \cdots$

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All can be viewed as to transform the spectrum of $A := \sum_i \theta_i u_i u_i^\top$

$$A^k = \sum_i \theta_i^k u_i u_i^\top \quad (\epsilon I - A)^{-1} = \sum_i \frac{1}{\epsilon - \theta_i} u_i u_i^\top \quad \exp(A) = \sum_i e^{\theta_i} u_i u_i^\top$$

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  Can be performed much more efficiently

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$$\underbrace{(X \otimes Y)f}_{O(m^2n^2)\text{ time/space}} = (X \otimes Y)vec(F) \equiv \underbrace{vec(XFY^\top)}_{O(mn(m+n))\text{ time, }O((m+n)^2)\text{ space}} \tag{7}$$

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  - An interesting observation: $rank(\Sigma)$ is usually a small constant!
  - Example: Diffusion process over the Cartesian PG

$$\Sigma = \begin{bmatrix} e^{-(\lambda_1+\mu_1)} & \dots & e^{-(\lambda_1+\mu_n)} \\ \vdots & \ddots & \vdots \\ e^{-(\lambda_m+\mu_1)} & \dots & e^{-(\lambda_m+\mu_n)} \end{bmatrix} = \begin{bmatrix} e^{-\lambda_1} \\ \vdots \\ e^{-\lambda_m} \end{bmatrix} \begin{bmatrix} e^{-\mu_1} & \dots & e^{-\mu_n} \end{bmatrix}$$

$\implies rank(\Sigma) = 1$

Outline

Datasets and Baselines

Datasets

Dataset	G	H
Movielens-100K	Users	Movies
Cora	Publications	Publications
Courses	Courses	Prerequisite Courses

Baselines

MC Matrix Completion.
- Ignores the info of G and H.

TK Tensor Kernel.
- Implicitly construct PG, no transduction

GRMC Graph Regularized Matrix Completion.
- Transduction over G and H, no PG constructed

Results

Performance of several interesting combinations of $\circ$ and κ

Dataset	Graph Transduction	Graph Product	MAP	AUC	ndcg@3
Courses	Random Walk	Tensor	0.488	0.827	0.461
	Diffusion	Cartesian	**0.518**	**0.872**	**0.500**
	von-Neumann	Tensor	0.472	0.861	0.449
	von-Neumann	Cartesian	0.366	0.531	0.359
	Sigmoid	Cartesian	0.443	0.617	0.431
Cora	Random Walk	Tensor	0.222	0.764	0.205
	Diffusion	Cartesian	**0.256**	**0.884**	**0.232**
	von-Neumann	Tensor	0.230	0.853	0.211
	von-Neumann	Cartesian	0.218	0.633	0.212
	Sigmoid	Cartesian	0.192	0.443	0.188
MovieLens	Random Walk	Tensor	-	-	0.7695
	Diffusion	Cartesian	-	-	0.7702
	von-Neumann	Tensor	-	-	**0.7720**
	von-Neumann	Cartesian	-	-	0.7624
	Sigmoid	Cartesian	-	-	0.7650

Results

Proposed method (Diff + Cartesian GP) v.s. Baselines

Dataset	Method	MAP	AUC	ndcg@3
Courses	MC	0.319	0.758	0.294
	GRMC	0.366	0.777	0.343
	TK	0.449	0.810	0.446
	Proposed	**0.490**	**0.838**	**0.473**
Cora	MC	0.101	0.697	0.086
	GRMC	0.115	0.702	0.101
	TK	0.248	0.872	0.231
	Proposed	**0.268**	**0.894**	**0.243**
MovieLens	MC	-	-	0.748
	GRMC	-	-	0.752
	TK	-	-	0.718
	Proposed	-	-	**0.765**

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On-going Work

- Extend to k Graphs $(k > 2)$
  - Bipartite Graph $\rightarrow$ k-partite Graph
  - Edge $\rightarrow$ Hyperedge
- Determine the “optimal” graph product for any given problem.

Thanks!

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