

# Learning Relation Networks for Relational Retrieval

Thesis Proposal, Ni Lao

Mar 2, 2011

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# Outline



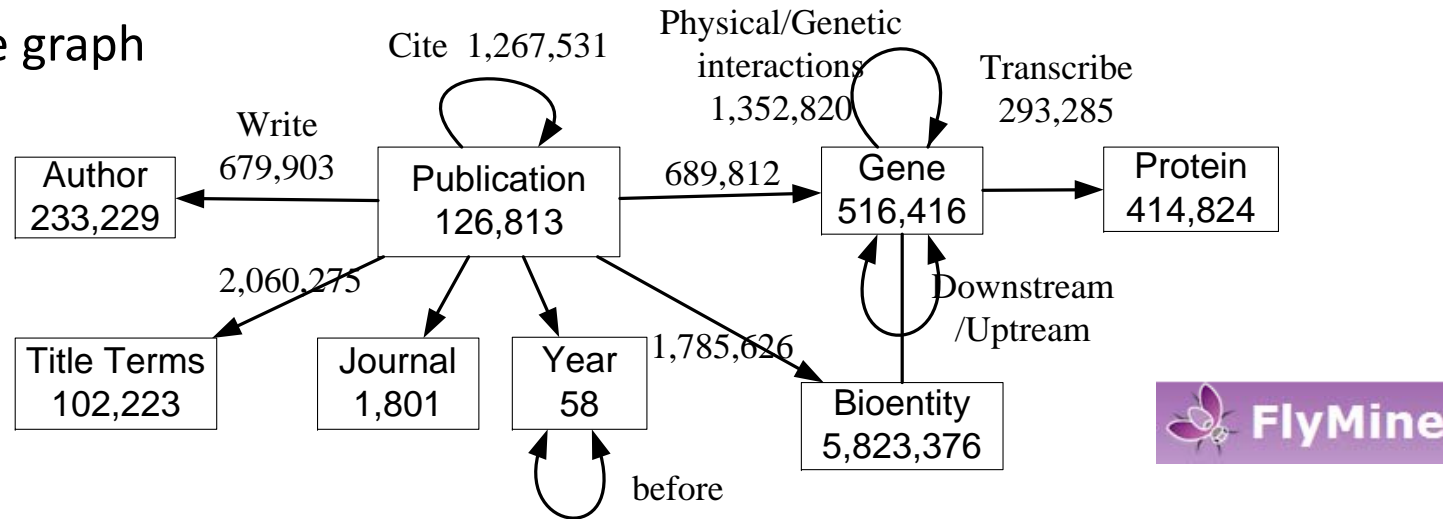
- Introduction
  - Tasks & motivation
  - Thesis goal & expected contributions
  - Compare to existing approaches
- Our Prior Work
  - Path Ranking Algorithm (Lao & Cohen, ECML 2010)
  - Efficient inference (Lao & Cohen, KDD 2010)
- Proposed Model Efficiency Extensions
  - Sparse gradient estimation
  - Cost sensitive parameter regularization
- Proposed Model Complexity Extensions
  - Virtual Relations
  - Path concatenation
  - Graph structure learning
  - Relation networks
- Work in Progress
  - Reading recommendation (Lao & Cohen, ISMB)
  - Link prediction with an ontology (Lao et al., EMNLP)

# Relational Retrieval Problems

- Data of many retrieval/recommendation tasks can be represented as **labeled directed graphs**, e.g. scientific literature
  - Typed nodes: documents, terms, metadata
  - Labeled edges: citation, authorOf, datePublished
- Can support a family of *typed proximity queries*
  - ad hoc retrieval: terms → documents
  - Citation recommendation: paper → papers
- Which **combination of these relations** is important in answering the queries?

# Biology Literature Data

- Flymine graph



- Tasks

- Gene recommendation:
- Reference recommendation:
- Venue recommendation:
- Expert-finding:
- Reading recommendation:

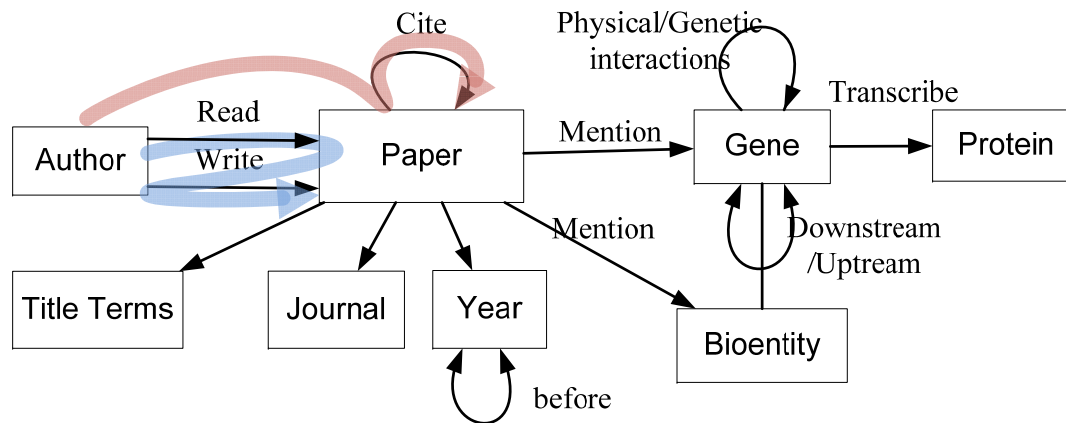
user, year → gene  
 title words, year → paper  
 genes, title words → journal  
 title words, genes → author  
 user → paper

# Biology Literature Data

- Example strategies for reading recommendation

$author \xrightarrow{Write} paper^1 \xrightarrow{CitedBy} paper^2$

$author^1 \xrightarrow{Read} paper^1 \xrightarrow{WrittenBy} author^2 \xrightarrow{Write} paper^2$



- Random walk with restart can be used for inference
- How to discover and combine different retrieval strategies?

# Knowledgebase Data

- Graph representation of a knowledgebase
  - entities and concepts as nodes, and relations among them as edges
  - NELL@CMU (Never-Ending Language Learner) has over 242K beliefs
  - e.g. AthletePlaysSport(agassi,tennis), Generalizations(redmond,city)
- Expand knowledgebase by link prediction
  - given a node X and an relation type R, what are the nodes in the graph which should have relation R with X?
  - e.g. ?Y: AthletePlaysSport(agassi,Y)

$athlete^1 \xrightarrow{PlaysFor} team \xrightarrow{Plays} sport$

$athlete^1 \xrightarrow{PlaysFor} team \xrightarrow{PlaysFor^{-1}} athlete^2 \xrightarrow{Plays} sport$

- Random walk with restart can be used for inference
- How to **discover and combine** different retrieval strategies?

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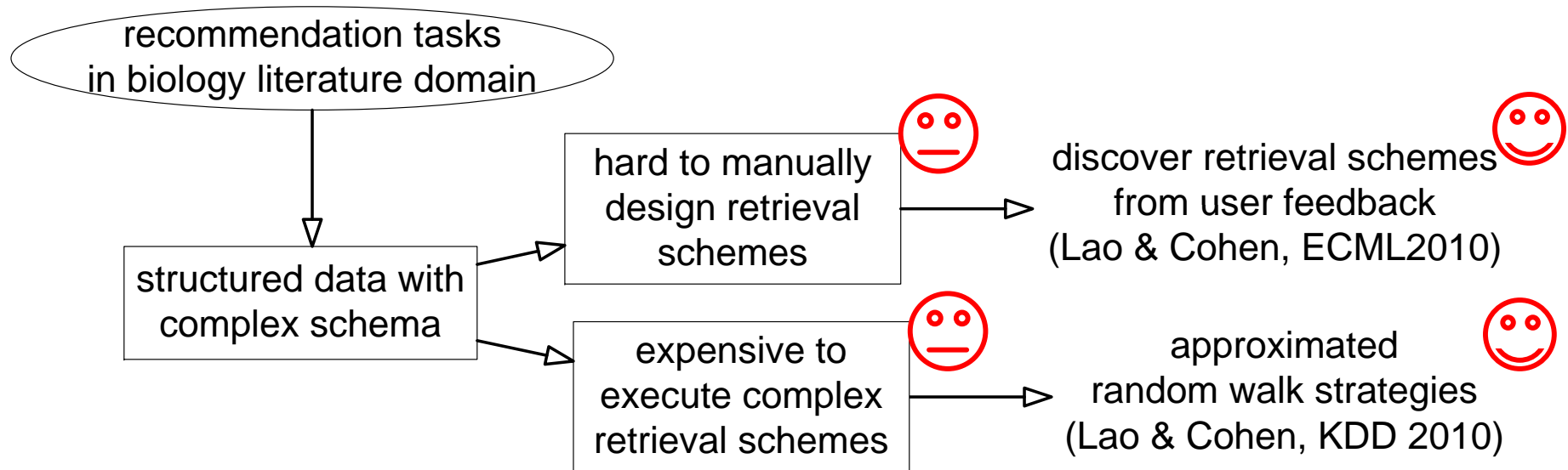


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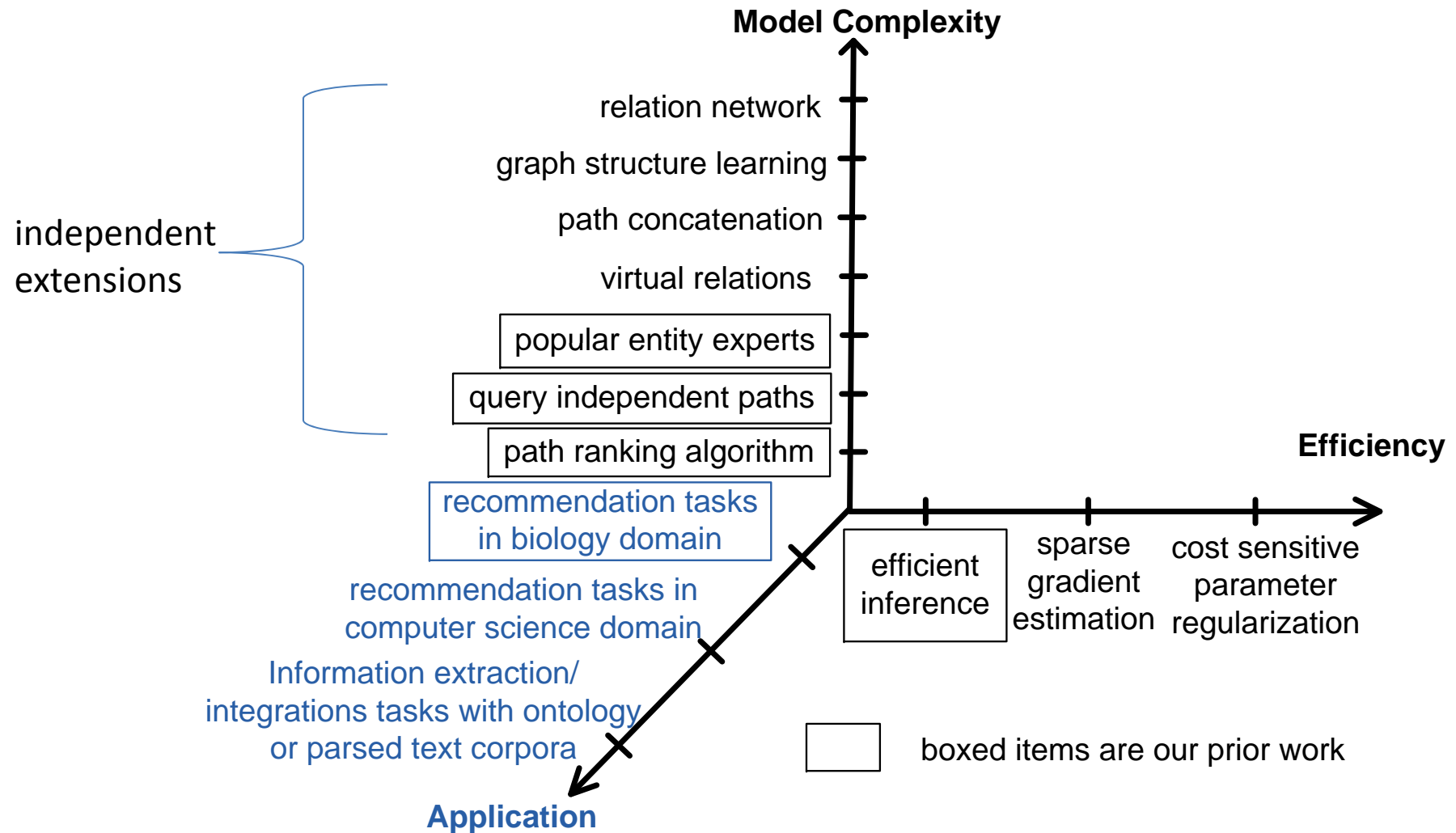
# Thesis Goal

- Explore different ways of constructing the random walk models so that **complex retrieval strategies** on **graph** can be encoded
- We also develop algorithms that can **efficiently discover and execute** these strategies

# Our Prior Work



# Expected Contributions



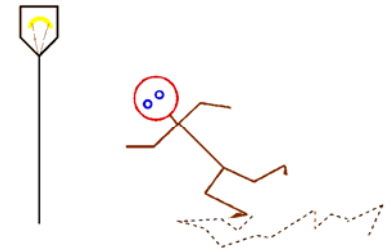
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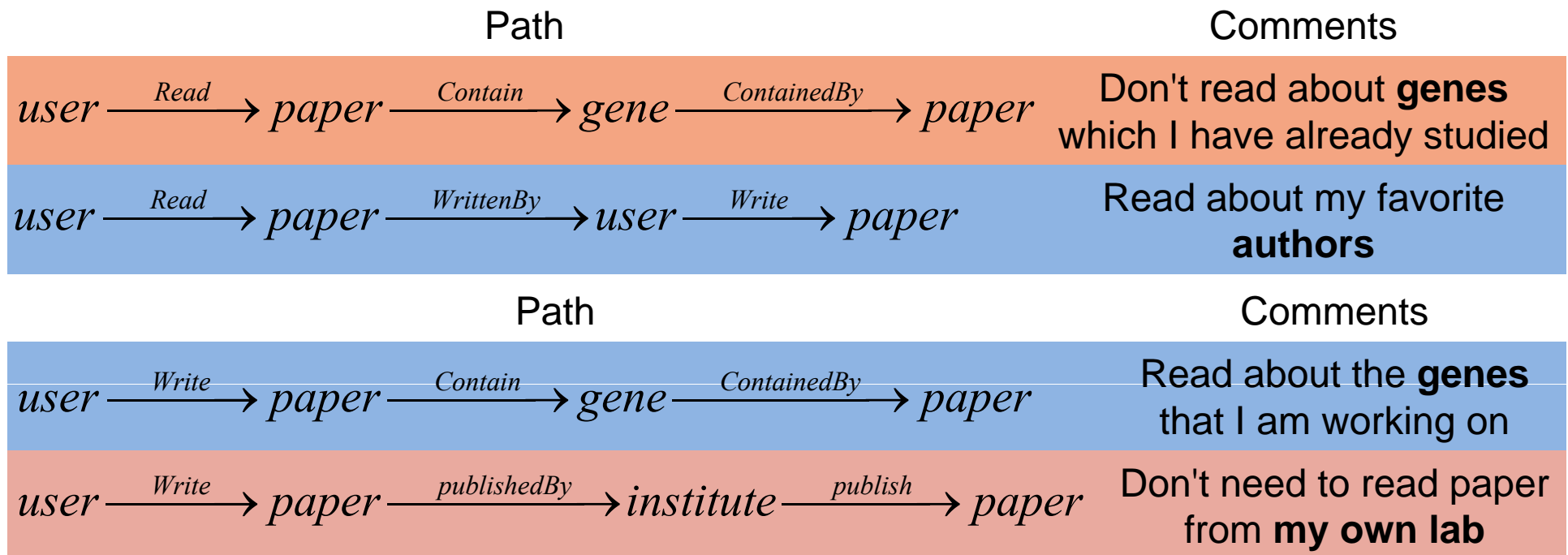
# Random Walks with Restart (RWR)

- RWR is a commonly used similarity measure for proximity between query and target nodes
  - topic-sensitive Pagerank (Haveliwala, 2002)
  - personalized Pagerank (Jeh & Widom, 2003)
  - ObjectRank (Balmin et al., 2004),
  - personal information management (Minkov & Cohen, 2007)
- RWR can be improved by supervised learning of edge weights
  - quadratic programming (Tsoi et al., 2003),
  - simulated annealing (Nie et al., 2005),
  - back-propagation (Diligenti et al., 2005; Minkov & Cohen, 2007),
  - limited memory Newton method (Agarwal et al., 2006)
- Document embedding and recommendation by
  - combining random walks with multiple sub-graphs which are generated from different relations (Zhou et. al, WWW2008)



# The Limitation of RWR

- **One-parameter-per-edge label** is limited because a same edge can appear in both **positive** and **negative** paths
  - **paths** instead of **edges** encode the semantics of a retrieval strategy



# Relational Learning Approaches

- To answer the query  $?Y: AthletePlaysSport(agassi, Y)$
- Horn clause rules
  - $AthletePlaysForTeam(X, B) \& TeamPlaysSport(B, Y) \rightarrow AthletePlaysSport(X, Y)$
- Path constrained random walk
  - $athlete^1 \xrightarrow{PlaysFor} team \xrightarrow{Plays} sport$

	softly combine rules	fast inference
First Order Inductive Learner (FOIL) (Quinlan & Cameron-Jones, 1993)	no	no
Markov Logic Network (MLN) (Richardson & Domingos, 2006)	yes	no
Path Ranking Algorithm (PRA) (Lao & Cohen, 2010 ECML)	yes	yes

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# Path Constrained Random Walk

(Lao & Cohen, ECML 2010)

- A *Relation path*  $P=(R_1, \dots, R_n)$  is a sequence of relations

– E.g.  $year \xrightarrow{PublishedIn^{-1}} paper$   
 $year \xrightarrow{PublishedIn^{-1}} paper \xrightarrow{Cite} paper$

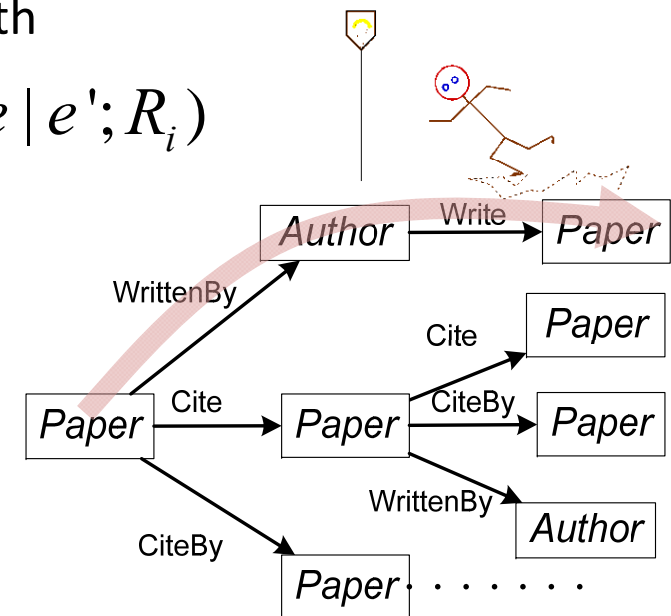
- *Path Constrained Random Walk*

– Recursively define a distribution for each path

$$h_{\mathbf{E}_s, R_1 \dots R_{i+1}}(e) = \sum_{e' \in range(R_i)} h_{\mathbf{E}_s, R_1 \dots R_i}(e') P(e | e'; R_i)$$

$$P(e | e'; R_i) = \begin{cases} 1 / \deg(e', R_i) & e' \xrightarrow{R_i} e \\ 0 & otherwise \end{cases}$$

$$h_{\mathbf{E}_s, \langle empty \rangle}(e) = \begin{cases} 1 / |\mathbf{E}_s| & e \in \mathbf{E}_s \\ 0 & otherwise \end{cases}$$



# Path Ranking Algorithm (PRA)

(Lao & Cohen, ECML 2010)

- Given a set of seed nodes  $\mathbf{E}_q$ , and a target type  $T_q$ , a PRA model can rank target entities by **linearly combine** the distributions of different paths

$$score(e; \theta) = \sum_{P \in \mathbf{P}(q, L)} h_P(e, \mathbf{E}_q) \theta_P$$

- where  $\mathbf{P}(q, L) = \{P\}$  is the set of all relation paths with range  $T_q$  and length  $\leq L$
- or in matrix form  $s = A\theta$ ,
  - $A$  is the feature matrix, each column of which is a sparse distribution produced by one of the relation paths

# Parameter Estimation

- Given a set of training data  $D = \{(A^{(m)}, y^{(m)})\}$ 
  - $A^{(m)}$  is the m-th feature matrix
  - $y^{(m)}$  is a binary vector representing relevance judgments
- Parameter  $\theta$  can be optimized by maximizing a regularized log-likelihood

$$O(\theta) = \sum_{m=1..M} o_m(\theta) - \lambda_1 \|\theta\|_1 - \lambda_2 \|\theta\|_2 / 2$$

- per-query objective function

$$o_m(\theta) = |P_m|^{-1} \sum_{i \in P_m} \ln p_i^{(m)} + |N_m|^{-1} \sum_{i \in N_m} \ln(1 - p_i^{(m)})$$

- predicted relevance

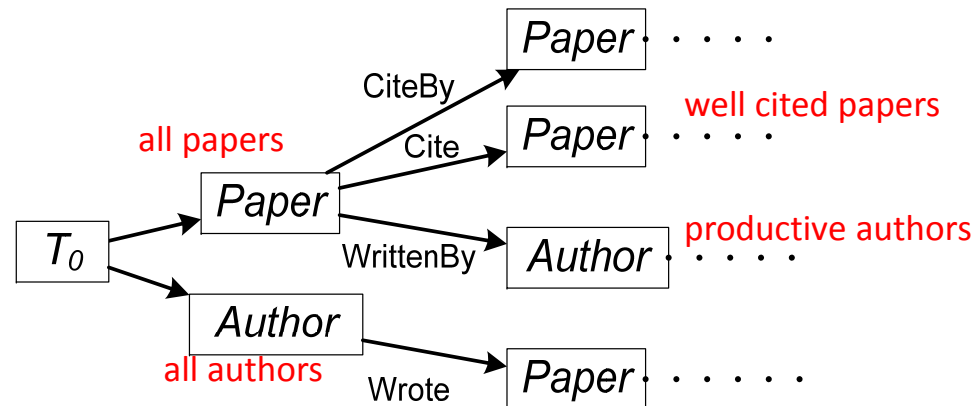
$$p_i^{(m)} = p(y_i^{(m)} = 1 | q^{(m)}; \theta) = \frac{\exp(\theta^T A_i^{(m)})}{1 + \exp(\theta^T A_i^{(m)})}$$

- $P_m$  is the index set of relevant entities
- $N_m$  is the index set of irrelevant entities (sub-sampled)

# Ext 1: Query Independent Paths

- Motivated by PageRank
  - assign a (query independent) **importance score** to each web page
  - later combined with a (query dependent) **relevance score**
- Generalize to **heterogeneous graph**
  - we include to each query a special entity  $e_0$  of special type  $T_0$
  - $T_0$  has relation to all other entity types, and  $e_0$  has links to all entities
  - therefore, we have a set of **query independent paths** (random walks on which can be calculate offline)

- Example



# Ext.2: Popular Entity Biases

- There are **entity specific** characteristics which cannot be captured by a general model
  - **in query log mining**, documents with lower rank to a query may be interesting to the users because of features not captured in the data
  - **in personalized search**, the same query may represent different information needs for different users
- A simple approach of adding bias terms
  - Introduce a bias  $\theta_e$  for each target entity  $e$
  - Introduce a bias  $\theta_{e',e}$  for each query-target entity pair  $(e',e)$

$$s(e; \theta) = \sum_{P.T_{last}=T_q} h_P^T(e) \theta_P + \theta_e + \sum_{e' \in \mathcal{E}_q} \theta_{e',e}$$

- Efficiency consideration
  - Only add to the model top  $J$  parameters (measured by  $|dO(\theta)/d\theta_e|$ ) at each LBFGS iteration

# Experiment Setup

- Data sources for bio-informatics
  - [Saccharomyces Genome Database \(SGD\)](#) a database for yeast
  - [Flymine](#) a database for fruit flies
  - [PubMed](#) on-line archive of over 18 million biological abstracts
  - [PubMed Central \(PMC\)](#) full-text copies of over 1 million of these papers
- Tasks
  - Gene recommendation: author, year → gene
  - Venue recommendation: genes, title words → journal
  - Reference recommendation: title words, year → paper
  - Expert-finding: title words, genes → author
- Data split
  - automatically generated labels
  - 2000 training, 2000 tuning, 2000 test queries
- Time variant graph (for training)
  - each edge is tagged with a time stamp (year)
  - only consider edges that are earlier than the query during random walk

# Example Features

ID	Weight	Feature	
1	272.4	$word \rightarrow paper \xrightarrow{Cite^{-1}} paper \xrightarrow{Cite} paper$	1) Papers co-cited with the on-topic papers
2	156.7	$word \rightarrow paper \xrightarrow{Cite} paper$	2) Aggregated citations of the on-topic papers
3	100.5	$gene \rightarrow paper \xrightarrow{Cite^{-1}} paper \xrightarrow{Cite} paper$	
4	83.7	$word \rightarrow paper \xrightarrow{Cite^{-1}} paper$	
5	50.2	$gene \rightarrow paper \xrightarrow{Cite} paper$	
6	41.4	$word \rightarrow paper$	6) Resembles an ad-hoc retrieval system
7	29.3	$year \rightarrow paper \xrightarrow{Cite} paper$	
8	13.0	$year \xrightarrow{Before^{-1}} year \rightarrow paper \xrightarrow{Cite} paper$	7,8) Papers cited during the past two years
...			
9	3.7	$T^* \rightarrow paper \xrightarrow{Cite} paper$	9) Well cited papers
10	2.9	GAL4>Nature. 1988. GAL4-VP16 is an unusually potent transcriptional activator.	
11	2.1	CYC1>Cell. 1979. Sequence of the gene for iso-1-cytochrome c in Saccharomyces cerevisiae.	
...			10,11) (Important) early papers about specific query terms
12	-5.4	$year \xrightarrow{Before^{-1}} year \rightarrow paper$	
13	-39.1	$year \rightarrow paper$	
14	-49.0	$T^* \rightarrow year \rightarrow paper$	

# Evaluations

- Compare the MAP of PRA to
  - Random walk with restart model(RWR)
  - Query independent paths (qip)
  - Popular entity biases (pop)

PRA can improve over RWR based models

Corpus	Task	RWR	PRA+qip+pop
yeast	Venue Rec.	44.2	49.3 (+11.5)
yeast	Reference Rec.	16.0	19.8 (+23.8)
yeast	Expert Rec.	11.1	12.9 (+16.2)
yeast	Gene Rec.	14.4	15.3 (+6.3)
fly	Venue Rec.	48.3	51.7 (+7.0)
fly	Reference Rec.	20.5	21.7 (+5.9)
fly	Expert Rec.	7.2	8.5 (+18.1)
fly	Gene Rec.	19.2	21.0 (+9.4)

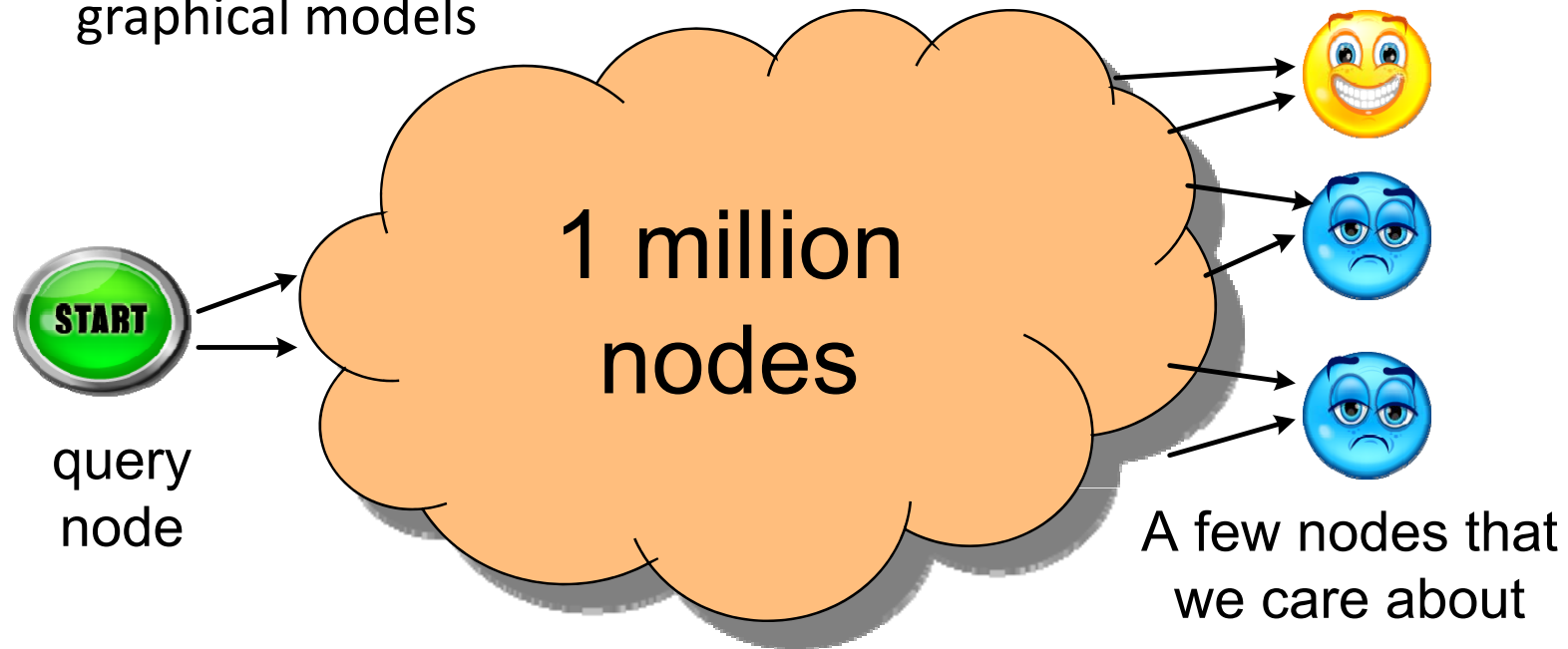
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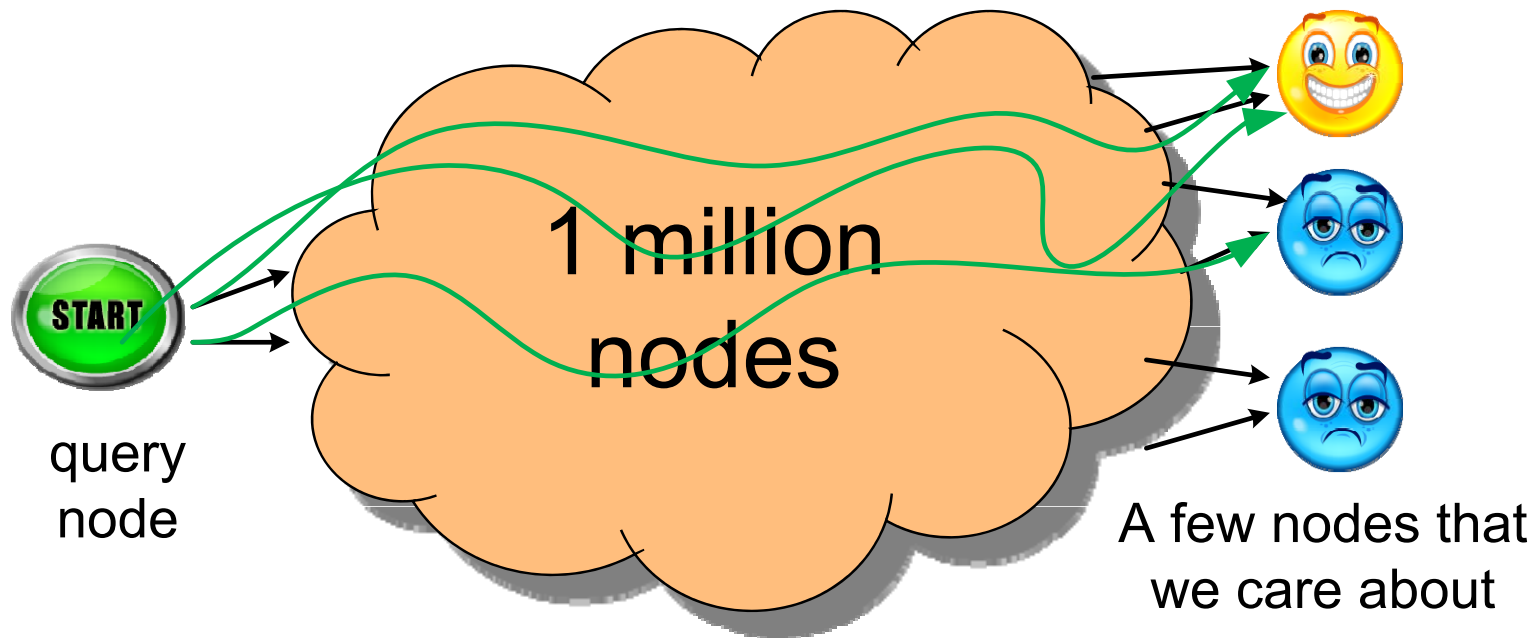
# Efficient Inference

- Exact random walk results in probability to many internal nodes on the graph
  - Computation should be focused on the nodes we care about
  - e.g. Query-Specific Inference (Chechetka & Guestrin, 2010) on graphical models



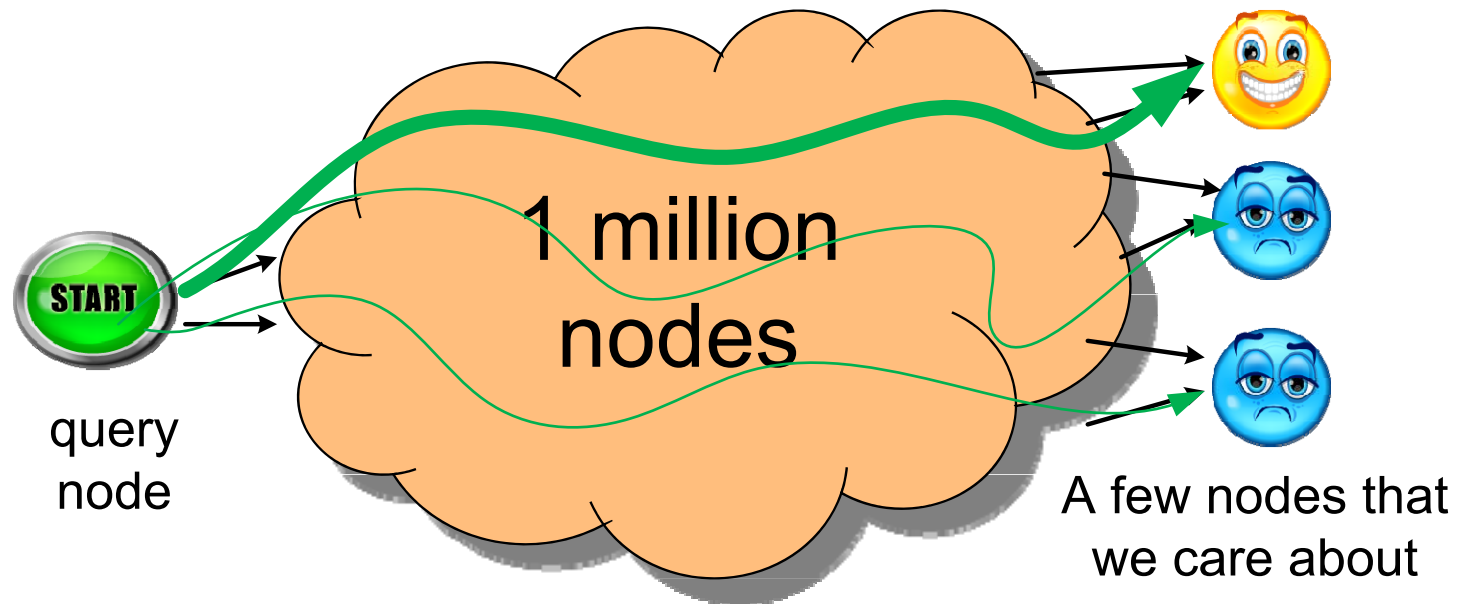
# Efficient Inference

- Rational for sampling
  - a few random walkers are enough to distinguish good target nodes from bad target nodes



# Efficient Inference

- Rational for truncation
  - large number of internal nodes which have small probabilities are not influential to the target nodes
  - we can safely drop them



# Four Strategies for Efficient Random Walks

- Ways to keep the distribution  $h(e)$  sparse at each step of random walk.
- Fixed Truncation (Chakrabarti, 2007)
  - Truncate by fixed value

$$h_{i+1}(e) = \max(0, h_i(e) - \varepsilon)$$

- Beam Truncation
  - Keep top  $W$  probable entities

$$h_{i+1}(e) = \max(0, h_i(e) - \varepsilon W)$$

- Fingerprinting (sampling) (Fogaras, 2004)
  - Simulate a large number of random walkers

$$h_{i+1}(e) = \frac{\# \text{times the walkers visit } e}{\# \text{walkers}}$$

- Weighted Particle Filtering (Lao & Cohen, KDD 2010)
  - A combination of exact inference and sampling

# Weighted Particle Filtering

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## Algorithm 1 Weighted Particle Filtering

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**Input:** distribution  $h_i(e)$ , relation  $R$ , threshold  $\varepsilon_{min}$

**Output:**  $h_{i+1}(e)$

**Set**  $h_{i+1}(e) = 0$  (should not take any time)

**for** each  $e$  with  $h_i(e) \neq 0$  **do**

$size_{new} = h_i(e) / |R(e)|$

**if**  $size_{new} > \varepsilon_{min}$  **then**     ← Start with exact inference

**for** each  $e' \in R(e)$  **do**

$h_{i+1}(e') + = size_{new}$

**end for**

**else**     ← switch to sampling when the branching is high

**for**  $k=1..floor(h_i(e)/\varepsilon_{min})$  **do**

            randomly pick  $e' \in R(e)$

$h_{i+1}(e') + = \varepsilon_{min}$

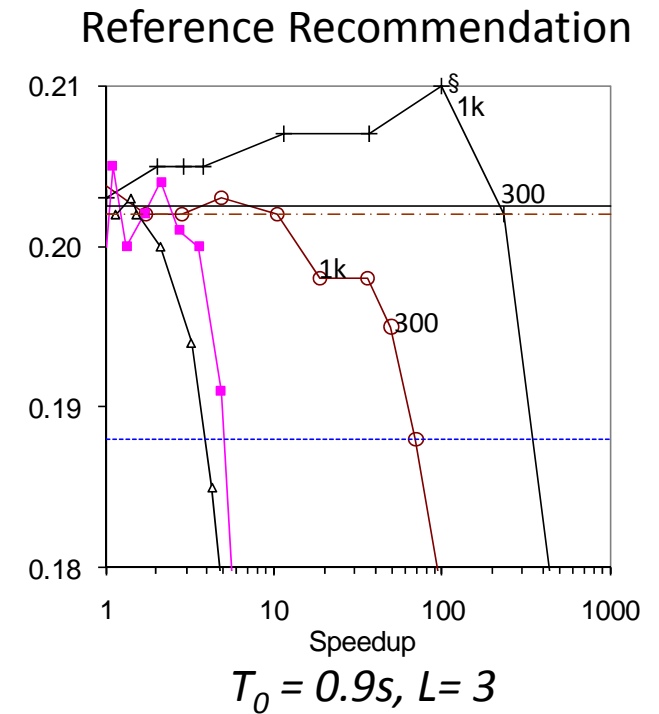
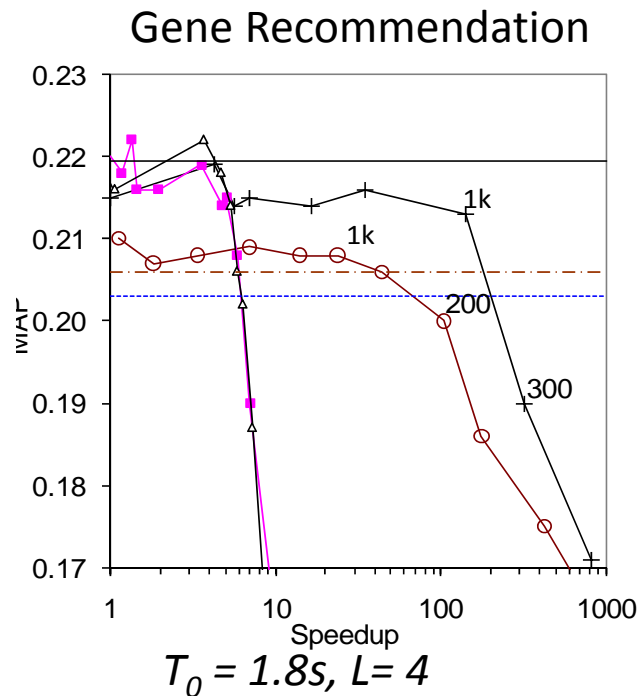
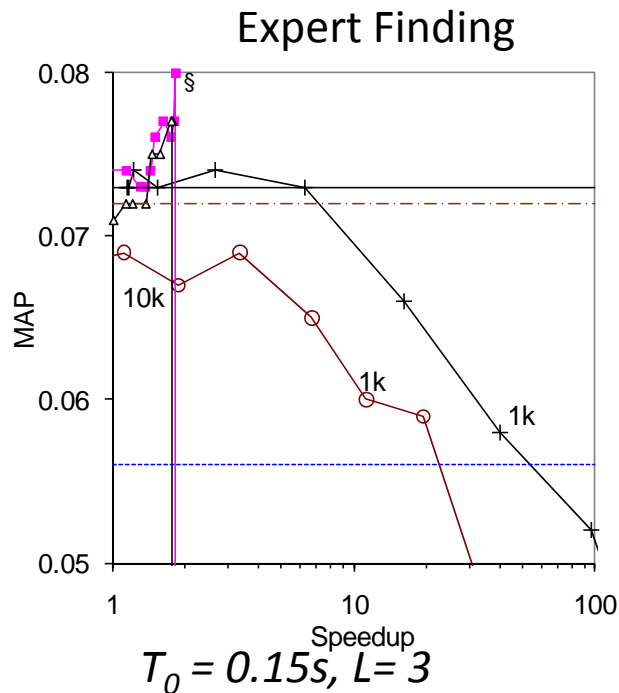
**end for**

**end if**

**end for**

# Results on The Fly Data

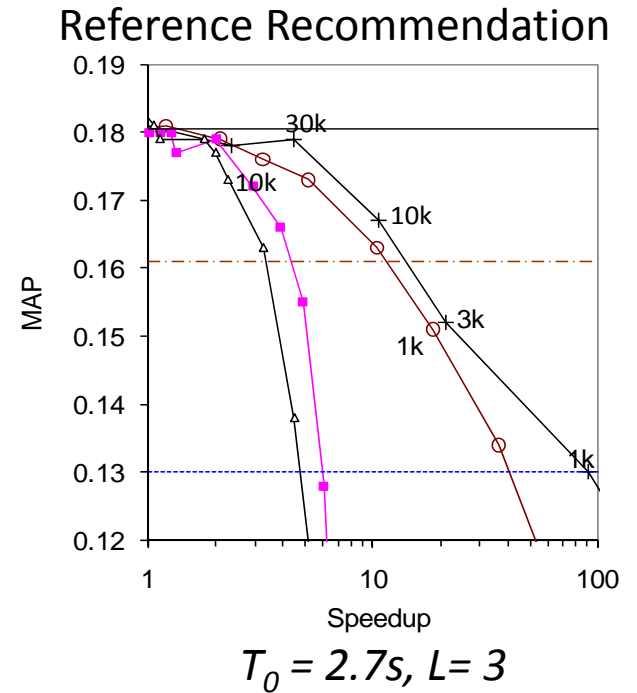
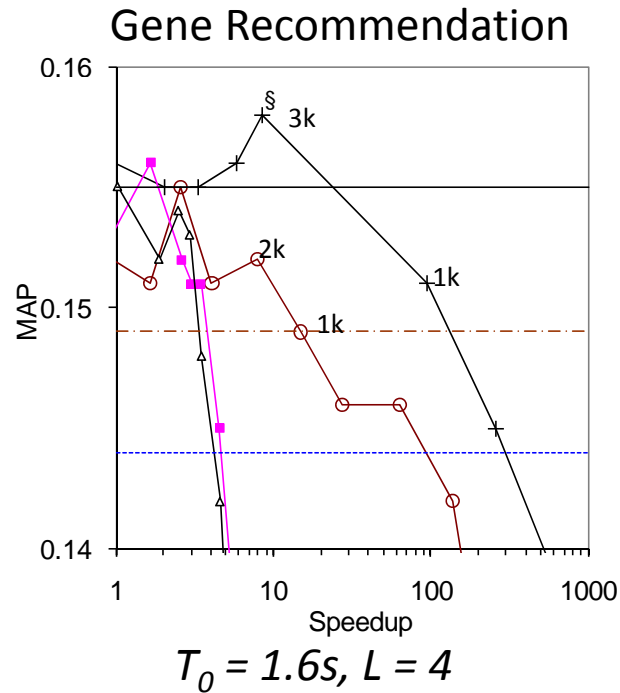
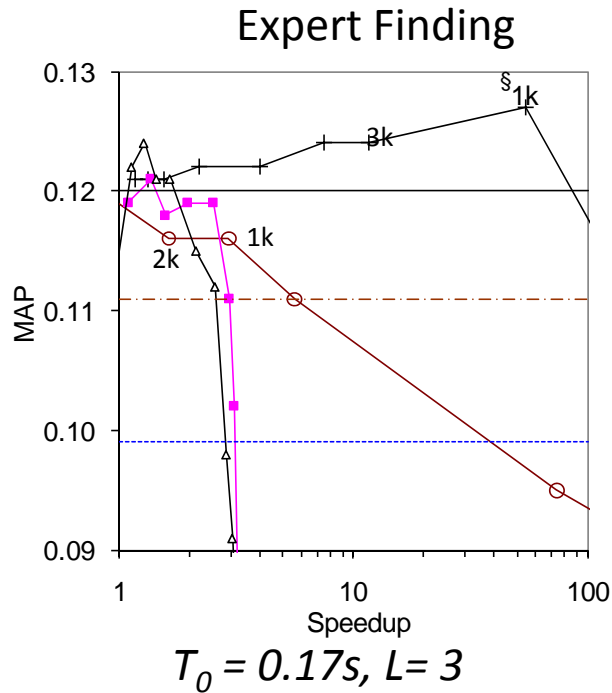
Up to 100x speedup with particle filtering



- Fingerprinting
- +— Particle Filtering
- Fixed Truncation
- △— Beam Truncation
- - - PCRW-exact
- · - · RWR-exact
- · - · RWR-exact (No Training)


# Results on The Yeast Data

Up to 100x speedup with particle filtering



- Fingerprinting
- + Particle Filtering
- Fixed Truncation
- △ Beam Truncation
- PCRW-exact
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# Sparse Gradient Estimation

- How to efficiently find useful features from many?
- Observations on [the decomposition of gradients](#)
  - the gradient of a feature  $x_i$  can be approximated by considering its gradients on a subset of training examples

$$\begin{aligned} \frac{dL(\theta)}{d\theta_i} &= \sum_{m=1..M} (y_i^{(m)} - p_i^{(m)}) x_i^{(m)} \\ &= \sum_{m=1..M} (y_i^{(m)} - p_i^{(m)}) (x_i^{(m)} - \bar{x}_i) \end{aligned}$$

assuming that there is a bias feature  $x_0$ , and its gradient is zero

$$\approx \sum_{\substack{m: |y_i^{(m)} - p_i^{(m)}| > \epsilon_1, |x_i^{(m)} - \bar{x}_i| > \epsilon_2 \\ \text{or sample } m \text{ with } p \propto |y_i^{(m)} - p_i^{(m)}| |x_i^{(m)} - \bar{x}_i|}} (y_i^{(m)} - p_i^{(m)}) (x_i^{(m)} - \bar{x}_i)$$

- a sparse gradient estimation of all the features is useful for our model complexity extensions
  - Path concatenation, Graph structure learning, Relation networks

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# Cost Sensitive Parameter Regularization

- We augment the objective function by the **estimated cost of random walk** on training data

$$O(\theta) = \sum_i o_i(\theta) - \mu \sum_j c_j(\pi) - \lambda |\theta|_2 / 2$$

- $\pi$  indicates whether or not each node on the relation tree is enabled
- $c_j(\pi)$  is the cost of random walk on the  $j$ -th relation tree node
  - measured by time or number of RW operations
- A coordinate ascent optimization
  - $\theta$  step: optimize  $\theta$  with LBFGS
    - For those nodes with  $\pi_i=0$ , their weights are fixed to 0
  - $\pi$  step:
    - For any node with  $\pi_i=0$ , if  $\delta_i - \mu c_i > 0$ , then set  $\pi_i=1$
    - For any node with  $\pi_i=1$ , if  $\delta_i + \mu c_i > 0$ , then set  $\pi_i=0$
    - $\delta_i$  is the estimated change of  $O(\theta)$  as a result of adding or removing the  $i$ -th node from the model

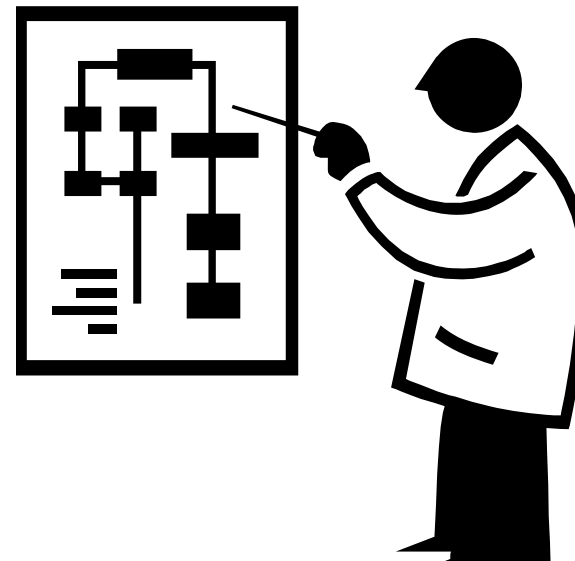
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# Virtual Relation

- In order to integrate other algorithms into a random walk based model, we propose to generalize the concept of a **relation** to any **function** that projects a distribution on the graph to another distribution on the graph
  - infinite steps of random walk with restart
  - a query expansion algorithm
  - a classifier
  - a word stemmer
  - etc.



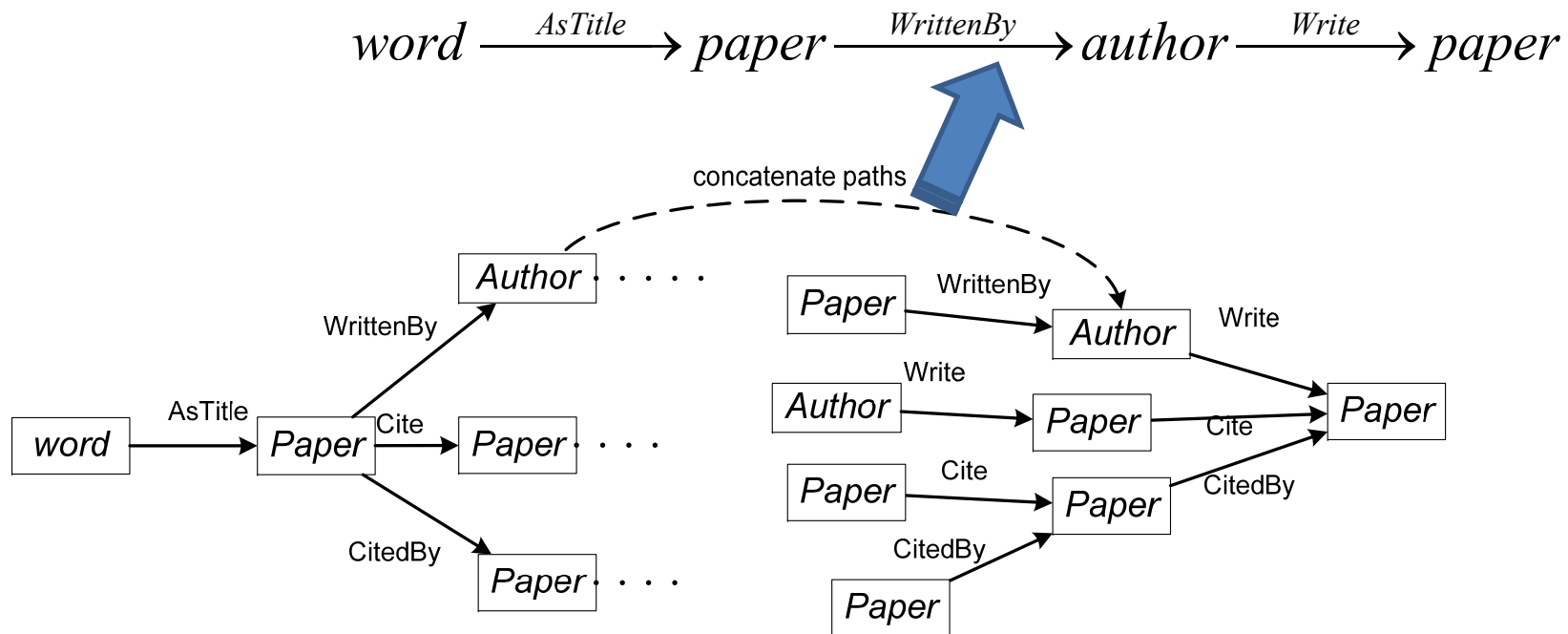
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# Path Concatenation

- We can efficiently explore large strategy space by combining existing paths
  - candidate paths' gradients can be estimated by combining **forward random walk** and **backward propagation of gradients**



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  - Efficient inference (Lao & Cohen, KDD 2010)
- Proposed Model Efficiency Extensions
  - Sparse gradient estimation
  - Cost sensitive parameter regularization
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  - Virtual Relations
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# Relation networks

- Express conjunctions
  - e.g., we may want the retrieved document to be relevant to both the query words and the user who sent the query
- Switch strategies between queries
  - e.g. depending on whether a user has reading (or publication) history, the optimal weighting of paths might be different.
  - e.g. if the text query cannot retrieve satisfactory results, the relative weighting of other query expansion strategies might need to be adjusted.

# Relation networks

- Introduce two hyper-edges that might be useful for retrieval tasks
  - AND operator

$$h_{A \cap B}(e) = h_A(e)h_B(e)$$

- IF-NOT operator

$$h_{A \rightarrow B}(e) = \begin{cases} h_A(e) & h_B(e') = 0 \text{ for every } e' \\ 0 & \textit{else} \end{cases}$$

- Further assume that these hyper nodes cannot be the parent to any other nodes
  - The number of potential IF-NOT nodes is  $O(nm)$
  - The number of potential AND nodes is  $O(m)$
  - where  $n$  is the number of nodes in  $G$ , and  $m$  is the number of nodes in  $G$  with the query target type

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# Reading Recommendation

(Lao & Cohen, ISMB)

- Goal
  - a reading recommendation system based on users' past **reading** and **publication** history
- Data
  - yeast graph
  - 22 years' reading history of biologist Dr. John L. Woolford
- Experiment
  - predict for each year what Dr. Woolford is going to read

# Evaluation

- Compare the MAP of PRA to
  - Random walk with restart model(RWR)
  - Query independent paths (qip)

PRA can improve over RWR based models

Tree depth	Rank by Citations	RWR (no train)	RWR	PRA	PRA+qip (L=3)
	0.080				
L=2		0.189	0.204	0.218	<b>0.319</b>
L=3		0.210	0.251	0.304	0.306
L=4		0.192	0.202	0.296	0.315

Leverage user's reading and publication history and combine with other meta-data

# Model

ID	Weight	Feature	Comments
1	1712.4	$year \xrightarrow{In^{-1}} paper$	Prefer papers from the query year
2	1099.6	$author \xrightarrow{Read} paper \xrightarrow{HasMajorMQ} topic \xrightarrow{HasMajorMQ^{-1}} paper$	Prefer papers with similar mesh qualifier to what I read before
3	767.0	$author \xrightarrow{Read} paper \xrightarrow{HasTitle} word \xrightarrow{HasTitle^{-1}} paper$	Prefer papers with similar <i>titles</i> to what I have read
4	672.2	$author \xrightarrow{Read} paper \xrightarrow{Write^{-1}} author \xrightarrow{Write} paper$	Prefer paper written by my favorite <i>authors</i>
5	441.2	$author \xrightarrow{Read} paper \xrightarrow{Cite} paper \xrightarrow{Cite^{-1}} paper$	Prefer papers which <i>share references</i> with what I generally read
6	337.9	$author \xrightarrow{Write} paper \xrightarrow{HasMajorMQ} topic \xrightarrow{HasMajorMQ^{-1}} paper$	Prefer papers with the same major <i>Mesh qualifier</i> as my papers
...			
7	131.3	$author \xrightarrow{Write} paper \xrightarrow{HasGene} gene \xrightarrow{HasGene^{-1}} paper$	Prefer the <i>genes</i> that I have been working on
8	71.4	$author \xrightarrow{Write} paper \xrightarrow{Cite^{-1}} paper \xrightarrow{Cite^{-1}} paper$	Prefer <i>follow up papers</i> to my own paper
9	37.2	$author \xrightarrow{Write} paper \xrightarrow{Cite^{-1}} paper \xrightarrow{Cite} paper$	Prefer papers <i>co-cited</i> with my papers
10	26.7	$year \xrightarrow{After} year \xrightarrow{Read} paper \xrightarrow{Cite^{-1}} paper$	Prefer <i>follow up papers</i> to my readings last year
11	25.6	$author \xrightarrow{Write} paper$	Prefer my own papers
...			
12	-285.1	$e^* \xrightarrow{AnyInstitute} institute \xrightarrow{Affiliation^{-1}} paper$	Disfavor papers published by less established institutes
13	-325.6	$author \xrightarrow{Read} paper \xrightarrow{HasGene} gene \xrightarrow{HasGene^{-1}} paper$	Disfavor <i>genes</i> which I have already read about
14	-334.2	$e^* \xrightarrow{AnyJournal} journal \xrightarrow{In^{-1}} paper$	Disfavor papers published by less popular journals
15	-399.9	$author \xrightarrow{Write} paper \xrightarrow{Affiliation} institute \xrightarrow{Affiliation^{-1}} paper$	Disfavor paper from <i>my own lab</i>

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# Link Prediction on NELL

(Lao et al., EMNLP)

- Pick the top 50 common relations, create two tasks for each relation:
  - ?Y: AthletePlaysSport(Y,tennis)
  - ?Y: AthletePlaysSport(agassi,Y)
- A query is generated for each entity (e.g. tennis) which have such relation. Its actual links are used as relevance judgment

weight	path	comments
28.6	$athlete^1 \xrightarrow{Generalize} concept \xrightarrow{Degeneralize} athelete^2 \xrightarrow{Plays} paper$	popular sports
24.2	$athlete \xrightarrow{PlaysIn} league \xrightarrow{SubOrganization} team \xrightarrow{Plays} sport$	sports played by <b>other teams</b> in my league
14.2	$athlete^1 \xrightarrow{PlaysIn} league \xrightarrow{PlaysIn^{-1}} athlete^2 \xrightarrow{Plays} sport$	sports played by <b>other players</b> in my league
	...	

# Link Prediction on NELL

- Result with 5-fold cross validation

	#Query	MRR	RW Time (sec)	Training Time (sec)
<a href="#">citylocatedinstate</a>	1126	<b>0.622</b>	31	201
<a href="#">_citylocatedinstate</a>	85	<b>0.884</b>	5	126
<a href="#">citylocatedincountry</a>	688	<b>0.459</b>	16	66
<a href="#">_citylocatedincountry</a>	295	<b>0.916</b>	5	208
<a href="#">hasofficeincity</a>	398	<b>0.791</b>	27	443
<a href="#">_hasofficeincity</a>	489	<b>0.785</b>	16	80
<a href="#">athleteplayssport</a>	1119	<b>0.906</b>	6	21
...				

Reasonably good  
accuracy

Learning and inference  
are very efficient

# Tentative Schedule

Year	Month	Research Activity
2011	Feb-Mar	Explore recommendation tasks on other data sets, and explore other information extraction/integration tasks
	Apr	Experiment with the path concatenation algorithm
	May	Experiment with the structure learning algorithm
	Jun-Jul	Experiment with the relation network algorithm
	Aug	Experiment with cost sensitive parameter regularization
	Sep	Experiment with virtual edges
	Oct-Dec	Path concatenation and structure learning for relation networks
2012	Jan-Apr	Write thesis
	May	Defend thesis

# Conclusion

- We proposed to extent our prior work in three directions
- We hypothesis that more **complex** models can give better accuracy, and the **efficiency** algorithms can significantly improve speed
- Thank you for your comments

