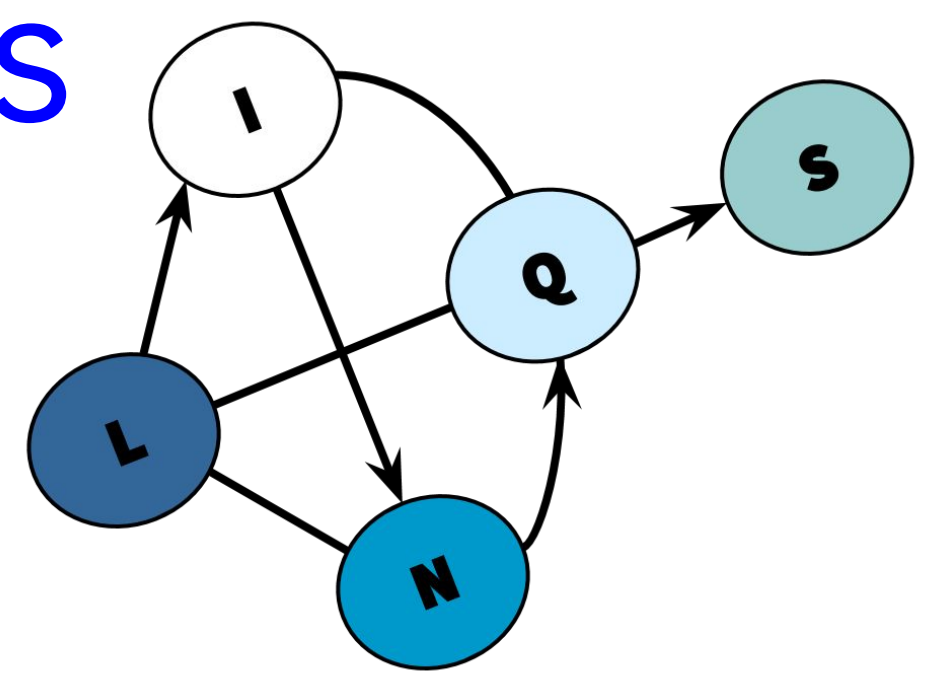


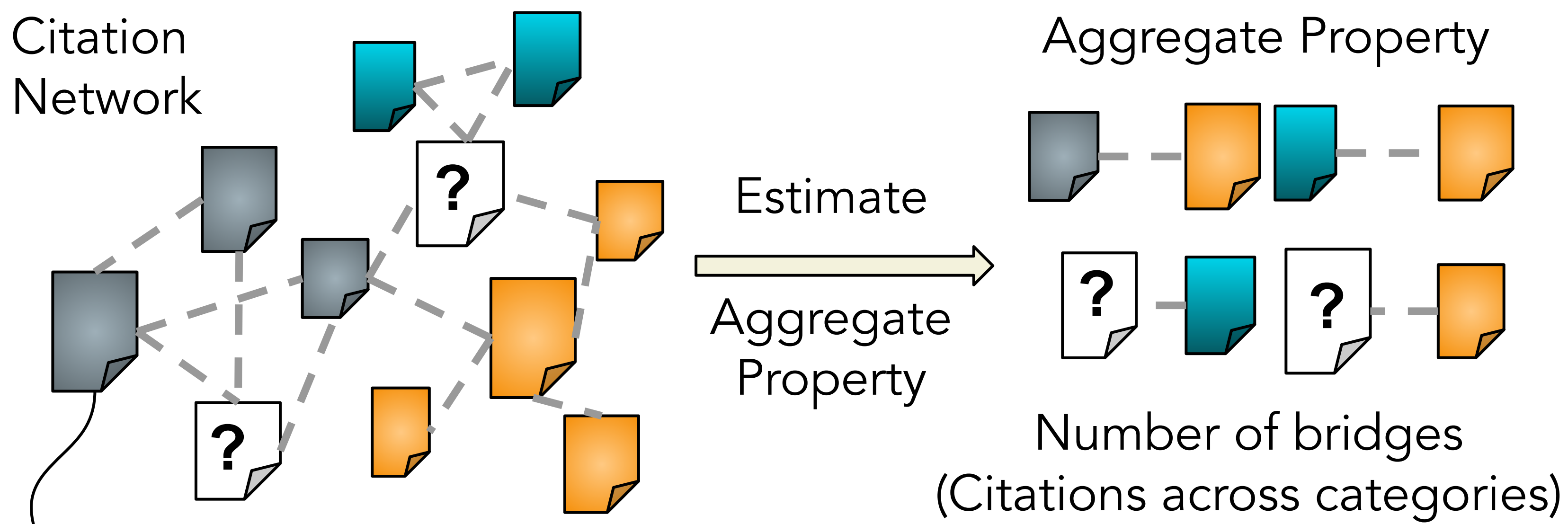


Estimating Aggregate Properties In Relational Networks With Unobserved Data



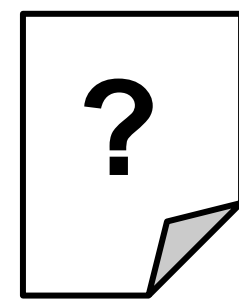
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University of California, Santa Cruz
^{*}Equal Contribution

Goal



Challenge

- Estimating aggregate properties when network is not fully observed (E.g. missing node labels)

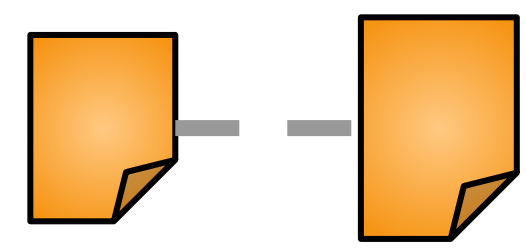


Aggregate properties

- Aggregate property (Q):** Aggregate function computed on a set of subgraphs that satisfy given conditions (Q: graph → R)
 - Properties involving multiple nodes, edges and labels

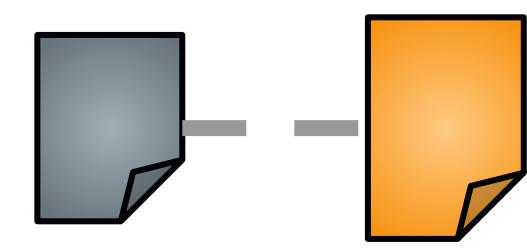
Q1: Category cohesion:

of links across documents that belong to same category



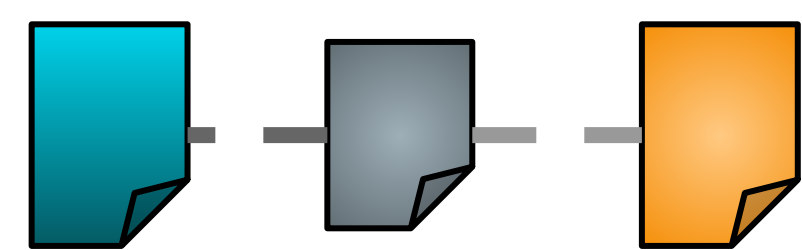
Q2: Category separation:

of links across documents that belong to different category



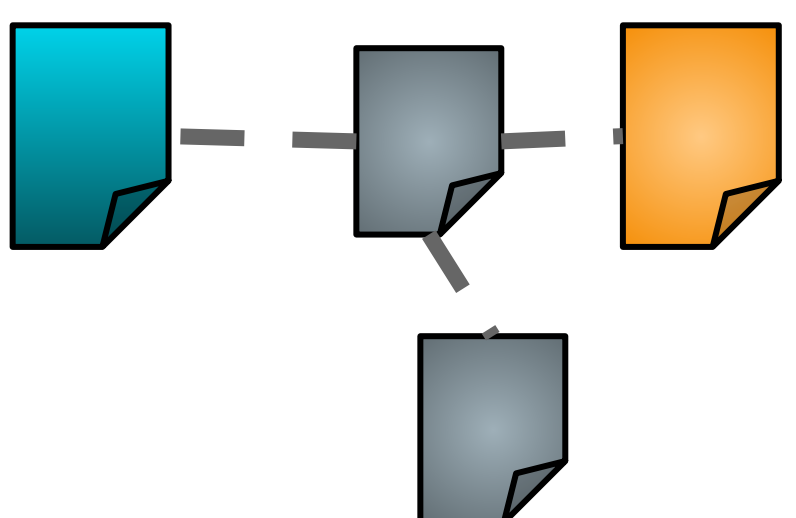
Q3: Diversity of influence:

of nodes linked to at least half of all categories



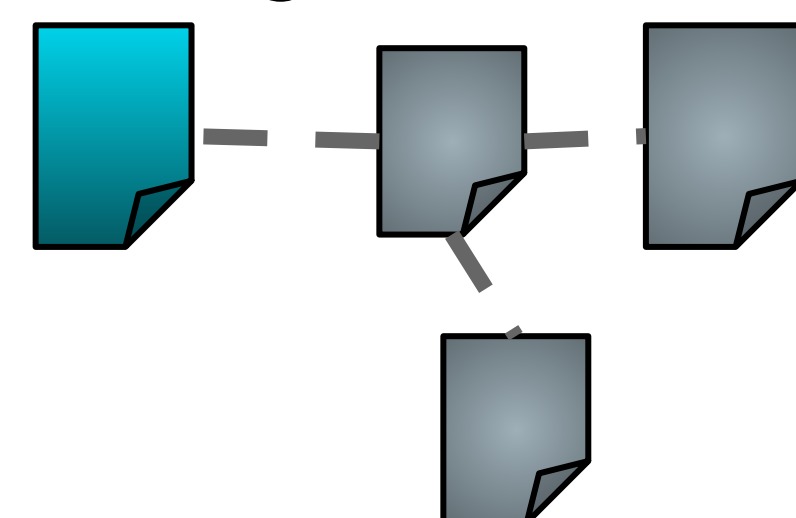
Q4: Exterior documents

of nodes where half the neighbors belong to different categories



Q5: Interior documents

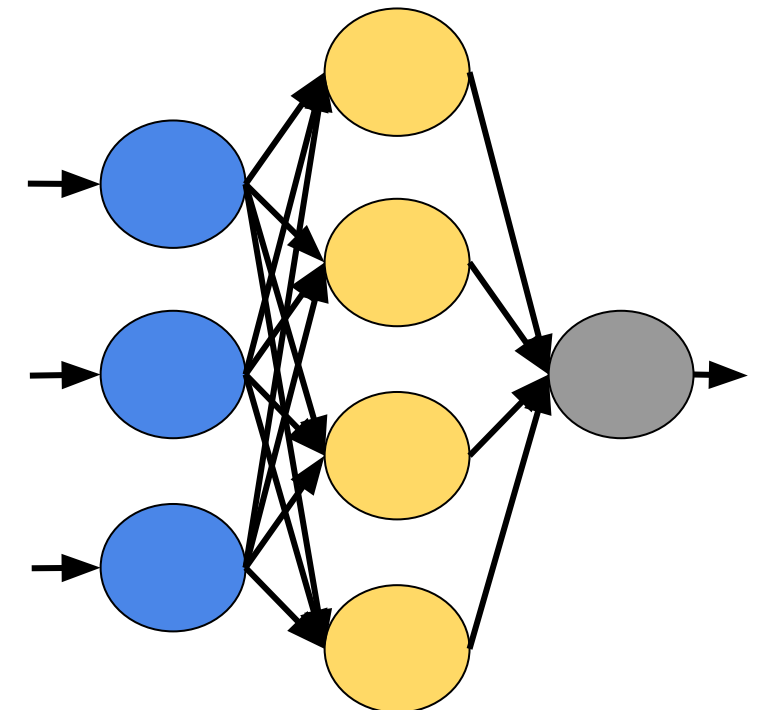
of nodes where half the neighbors belong to same categories



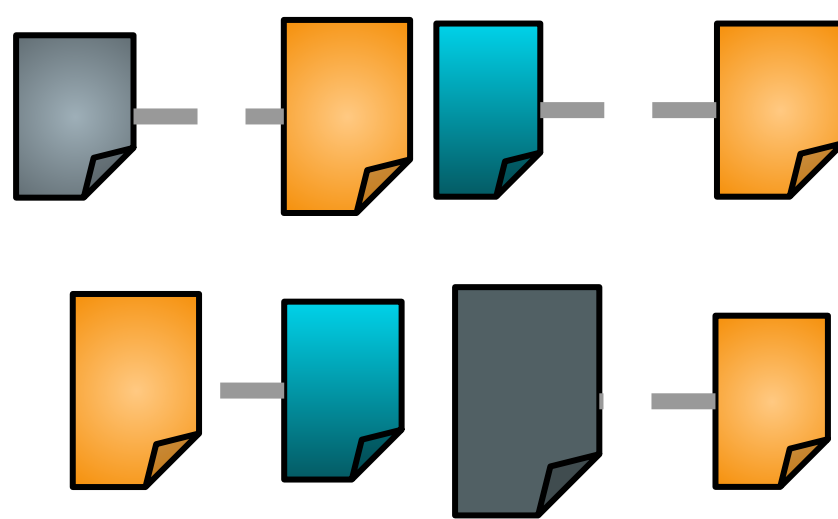
Estimating aggregate properties

Point estimate approach

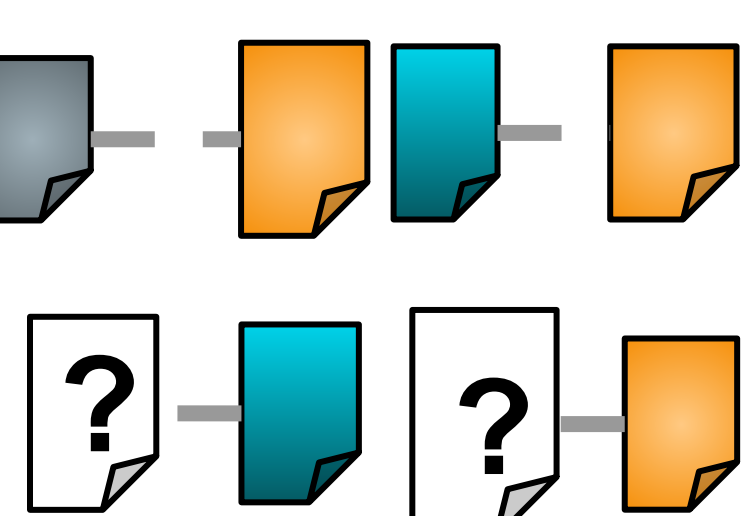
GNN model



Infer missing values



Property (Q)



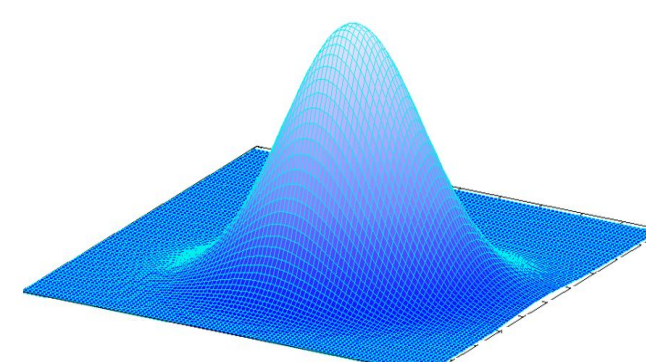
Q(Graph)

Expected aggregate approach

SRL model

```
5: link(x,y) & hascat(x,c)
  -> hascat(x,c)
5: LR(x,c) -> hascat(x,c)
```

Expectation



Infer joint probability distribution

Tractable expectation computation for PSL

- Probabilistic Soft Logic^[1] is a state-of-the-art SRL framework
- Computing expectation is intractable due to integration
- Monte Carlo approximation using samples from Gibbs sampler

Challenge 1

High rule weight → Correlated RVs → Slow convergence

- Identify **association blocks** from rules using
 - Rule weights
 - Feasible region
- Block sample RV in associated blocks

Challenge 2

Conditional distribution for Gibbs sampler

$$p(y_i | X, Y_{-i}) \propto \exp\left\{-\sum_{r=1}^{N_i} w_r \phi_r(y_i, X, Y_{-i})\right\}$$

Hard to sample from

- Single step of **Metropolis sampler inside gibbs** sampler

$$\alpha = \frac{\exp\left\{-\sum_{r=1}^{N_i} w_r \phi_r(y'_i, X, Y_{1:i-1}^{(t+1)}, Y_{i:n}^{(t)})\right\}}{\exp\left\{-\sum_{r=1}^{N_i} w_r \phi_r(y_i, X, Y_{1:i-1}^{(t+1)}, Y_{i:n}^{(t)})\right\}}$$

Acceptance ratio

[1] <http://psl.linqs.org>

Experimental evaluation

Data: Cora, Pubmed and Citeseer

Graph Neural Networks: Graph Convolutional Networks (GCN), Graph Attention Network (GAT), Graph Markov Neural Networks (GMNN)
Statistical Relational Learning: Markov Logic Networks (MLN), Probabilistic Soft Logic (PSL)

Metric: Relative error

Aggregate property estimation:

Methods	Q1	Q2	Q3	Q4	Q5	Average
PSL-MAP	0.13	0.528	0.396	0.714	0.121	0.377
MLN-MAP	0.109	0.491	0.281	0.570	0.102	0.310
PSL-MEAN	0.117	0.474	0.348	0.685	0.115	0.347
MLN-MEAN	0.064	0.261	0.113	0.362	0.053	0.170
GCN	0.089	0.361	0.169	0.626	0.102	0.269
GAT	0.129	0.526	0.293	0.709	0.119	0.355
GMNN	0.156	0.513	0.299	0.679	0.119	0.353
PSL-SAMPLES	0.108	0.441	0.312	0.618	0.105	0.316
MLN-SAMPLES	0.060	0.210	0.119	0.391	0.061	0.168

Methods	Q1	Q2	Q3	Q4	Q5	Average
PSL-MAP	0.175	0.527	0.673	0.57	0.272	0.443
MLN-MAP	0.207	0.648	0.594	0.794	0.392	0.527
PSL-MEAN	0.134	0.403	0.544	0.551	0.253	0.377
MLN-MEAN	0.137	0.731	0.792	0.691	0.315	0.554
GCN	0.211	0.637	0.712	0.813	0.396	0.553
GAT	0.248	0.747	0.9	0.887	0.416	0.639
GMNN	0.257	0.774	0.881	0.906	0.447	0.653
PSL-SAMPLES	0.137	0.413	0.539	0.499	0.236	0.364
MLN-SAMPLES	0.244	0.736	0.793	0.691	0.315	0.555

Pubmed

Methods	Q1	Q2	Q3	Q4	Q5	Average
PSL-MAP	0.047	0.205	0.165	0.1	0.062	0.115
MLN-MAP	0.032	0.046	0.412	0.436	0.242	0.234
PSL-MEAN	0.021	0.090	0.027	0.054	0.041	0.047
MLN-MEAN	0.038	0.163	0.009	0.174	0.068	0.090
GCN	0.048	0.207	0.137	0.671	0.34	0.28
GAT	0.073	0.313	0.376	0.697	0.355	0.362
GMNN	0.071	0.306	0.174	0.711	0.352	0.322
PSL-SAMPLES	0.014	0.061	0.050	0.053	0.031	0.041
MLN-SAMPLES	0.045	0.161	0.042	0.173	0.068	0.097

Cora

Citeseer

Predictive accuracy

Methods	Cora Acc (%)	Pubmed Acc (%)	Citeseer Acc (%)
PSL-MAP	85.34	83.6	72.25
MLN-MAP	77.9	76.75	71.7
PSL-MEAN	84.13	83.16	71.7
MLN-MEAN	82.35	75.14	71.25
GCN	81.96	77.73	68.78
GAT	81.43	76.87	70.41
GMNN	83.26	81.07	70.15
PSL-SAMPLES	83.01	81.88	71.29
MLN-SAMPLES	82.25	73.48	71.11

Runtime

Methods	Cora Time (sec)	Pubmed Time (sec)	Citeseer Time (sec)
PSL-MAP	14	124	37
PSL-MEAN	105	638	124
MLN-MEAN	270	1947	166
MLN-MAP	65	368	36
GCN	24	59	29
GAT	142	138	122
GMNN	30	17	8
PSL-SAMPLES	105	638	124
MLN-SAMPLES	270	1947	166

Conclusion

- Defined a suite of practical aggregate properties
- Proposed a novel sampling framework for PSL
- Extensive evaluation shows SRL approaches outperform GNNs when estimating aggregate properties