



Heterogeneous Subgraph Features for Information Networks

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Learning and Predicting in Heterogeneous Networks

Many information networks are heterogeneous

- ▶ Scientific publication networks
- ▶ Knowledge bases
- ▶ Metabolic networks
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- ▶ With features, of course

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How do you learn in heterogeneous networks?

- ▶ With features, of course
- ▶ But how do you get the features?

Problems of Established Feature Extraction Approaches

Classic features:

- ▶ Require domain knowledge
- ▶ Are time-consuming to engineer
- ▶ Require metadata that may not be available

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Alternative idea: use labeled subgraph counts as features

Heterogeneous Subgraph Features

Motivation: Heterogeneous Subgraph Features

Labeled subgraphs around a node:

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Conjecture:

The subgraph neighbourhood of a node is representative of its function and label.

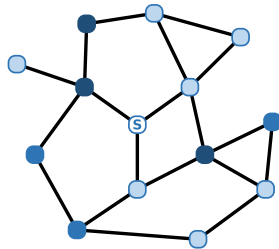
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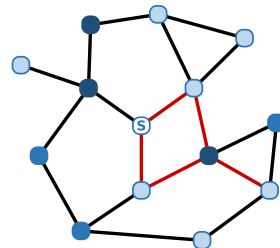
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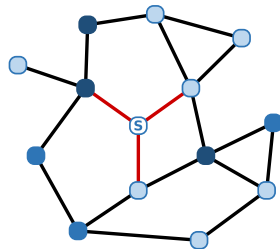
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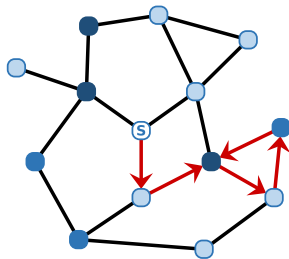
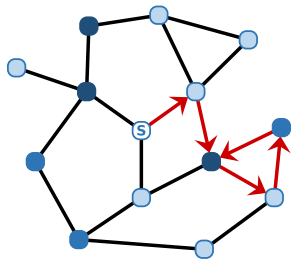


$$\text{count}(\textcircled{S}, \text{subgraph}) = 1$$

$$\text{count}(\textcircled{S}, \text{subgraph}) = 2$$



Isomorphism of Subgraphs



Problem: depending on the iteration order, the nodes of structurally identical subgraphs may be visited in different order.

Heterogeneous Subgraph Encoding

Core approach:

- ▶ Explore the local neighbourhood around each node
- ▶ Represent subgraphs by their characteristic string
- ▶ Count subgraphs by hashing the characteristic string
- ▶ Use the counts of subgraphs as node features

Heterogeneous Subgraph Encoding

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Characteristic string construction:

- ▶ Encode each node as a block
- ▶ Blocks start with the node label
- ▶ Subsequent entries denote neighbours of all given labels
- ▶ Blocks are sorted lexicographically

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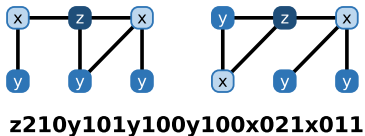


encoding scheme

Encoding Collisions

Heterogeneous degree sequences:

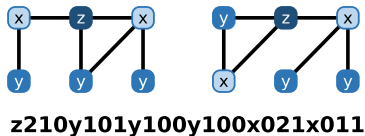
- ▶ Are a **pseudo**-canonical encoding
- ▶ May result in colliding encodings



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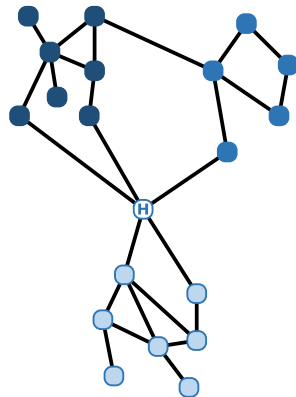
Encoding collisions:

- ▶ Can only be enumerated (no closed formula)
- ▶ Depend on the network structure and the labels
- ▶ Have negligible frequency in practice

Heuristic for Hub Mitigation

Real-world networks have:

- ▶ Skewed degree distributions
- ▶ Highly connected nodes (hubs)



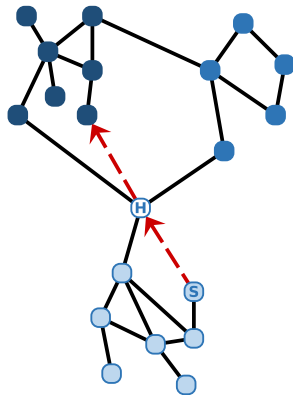
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Due to hubs:

- ▶ Feature extraction time is strongly increased
- ▶ Random walks retrieve non-local information



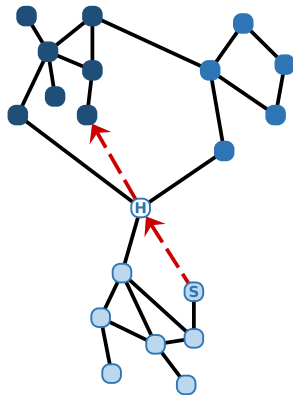
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Intuition: Do not explore beyond nodes with degree $> d_{max}$.

Evaluation: Label Prediction

Label Prediction: Task Definition

Given:

- ▶ Heterogeneous network
- ▶ Some nodes with missing labels

Predict:

- ▶ Missing node labels

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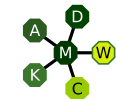
Formal approach:

- ▶ Model as a classification task using logistic regression
- ▶ Evaluate with F_1 -score

Label Prediction: Data Sets

Movie network (IMDB):

- ▶ Star-shaped structure around movies
- ▶ Low edge density



Movie Network (IMDB)

Scientific publication network (MAG):

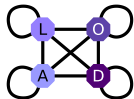
- ▶ Intermediate structure
- ▶ Papers form the core component



Microsoft Academic Graph (MAG)

Entity cooccurrence network (LOAD):

- ▶ Cooccurrences of named entities in text
- ▶ Strongly connected structure
- ▶ High edge density



Entity Co-occurrence Network (LOAD)

Feature Engineering and Extraction

Subgraph features:

- ▶ Maximum number of edges: 5
- ▶ No exploration beyond 10% of highest degree nodes
- ▶ Masked starting node label

Embedded features:

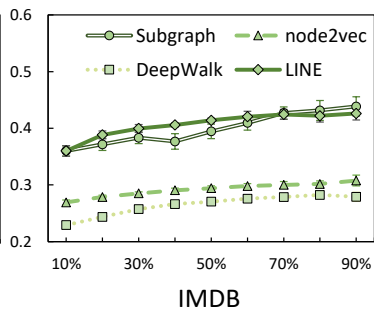
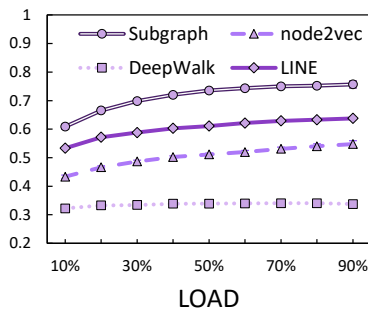
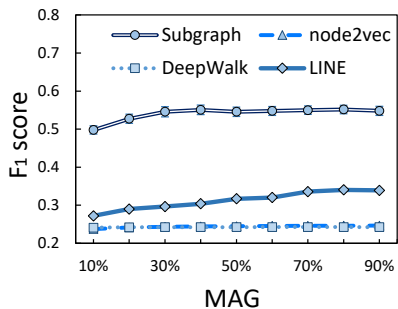
- ▶ DeepWalk
- ▶ LINE
- ▶ node2vec

Extraction Runtime Estimation (seconds per node)

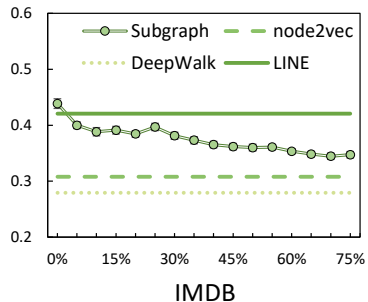
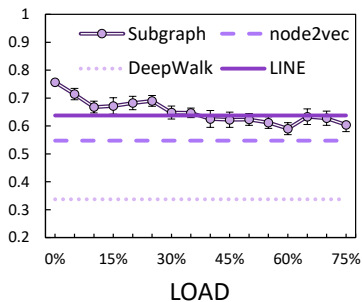
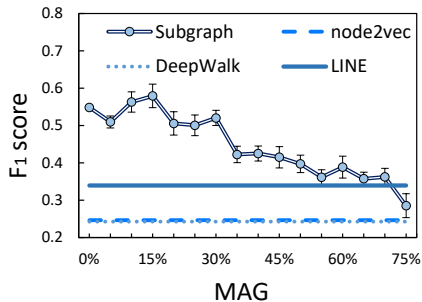
	subgraph features					node2vec	DeepWalk mean	LINE
	mean	75%	90%	95%	max			
LOAD	32.1	19.6	29.7	53.0	1046	0.19	0.11	0.66
IMDB	2.6	1.7	3.0	6.7	47	0.01	0.01	0.64
MAG	25.2	10.4	11.0	19.5	2493	0.02	0.01	0.49

Percentages denote nodes for which the extraction finished in at most the shown time.

Evaluation Results (Training Size)



Evaluation Results (Missing Labels)



Evaluation: Institution Ranking

Institution Ranking: Task Definition

Given:

- ▶ Scientific publication network
- ▶ A range of years
- ▶ A set of conferences

Predict ranking of institutions:

- ▶ For upcoming conferences
- ▶ By accepted papers
- ▶ For the next conference

KDDCup 2016. <https://kddcup2016.azurewebsites.net>

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Formal approach:

- ▶ Model as a regression task for the institution relevance score
- ▶ Evaluate with normalized discounted cumulative gain (NDCG20)

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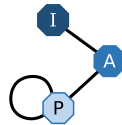
Institution Ranking: Data Set

Subset of the Microsoft Academic Graph:

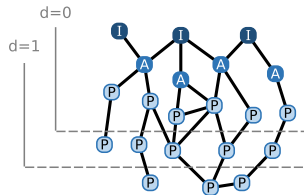
- ▶ Institutions I
- ▶ Authors A
- ▶ Papers P
- ▶ Publication data from 2011 - 2016

Data preparation:

- ▶ Focus on 5 conferences
KDD, FSE, ICML, MM, MOBICOM
- ▶ Use citations to a depth of 3



Microsoft Academic Graph
(MAG)



Feature Types and Extraction

Classic features (manually engineered):

- ▶ Previous relevance scores, publication counts, etc. (8)
- ▶ Linguistic features (32)

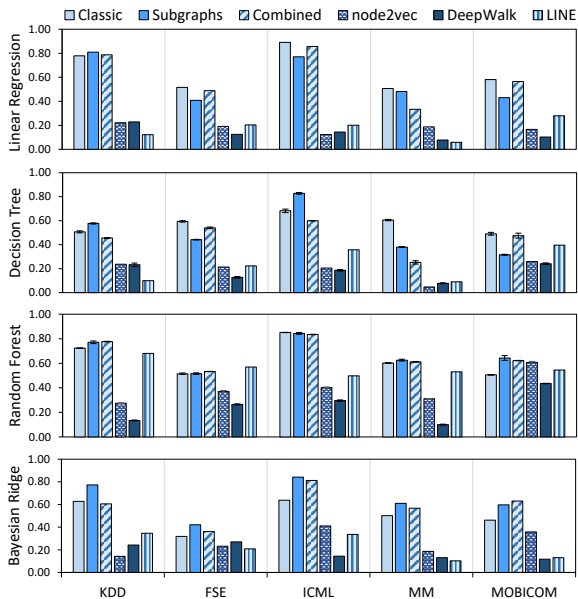
Subgraph features:

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- ▶ No maximum degree exploration limit

Embedded features:

- ▶ DeepWalk
- ▶ LINE
- ▶ node2vec

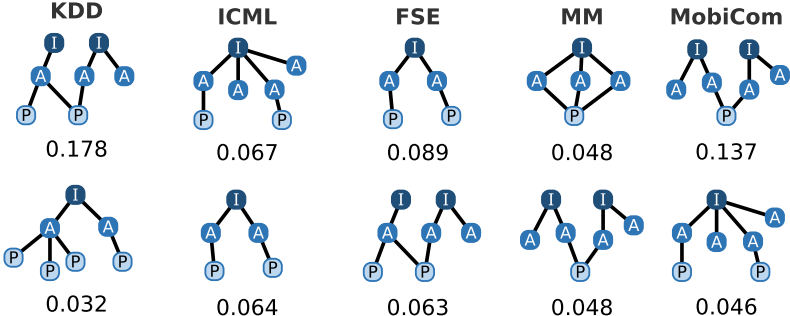
NDCG Scores for Institution Ranking



Average NDCG Scores for Institution Ranking

	LinRegr	DecTree	RanForest	BayRidge
classic	0.65	0.58	0.64	0.51
subgraph	0.58	0.51	0.68	0.65
combined	0.62	0.46	0.68	0.60
node2vec	0.18	0.19	0.39	0.27
DeepWalk	0.14	0.17	0.25	0.18
LINE	0.17	0.23	0.56	0.23

Feature Importance Analysis (Random Forest)



Summary & Resources

Heterogeneous subgraph features:

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In comparison to classic features:

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In comparison to embedded features:

- ▶ Better predictive performance
- ▶ Longer extraction time

Resources

The implementation is available online:

- ▶ C++ (core extraction routines)
- ▶ Python (wrapper)



<https://dbs.ifi.uni-heidelberg.de/resources/hsgf/>

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