EvalNE: A Framework for Evaluating Network Embeddings on Link Prediction

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Outline

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2. Objectives
3. Network Embedding (NE)
4. Link Prediction (LP)
5. Evaluating NE on LP
6. EvalNE frameworks
7. Experiments

Motivation

Difficulty of comparing new network embedding methods against the sota.

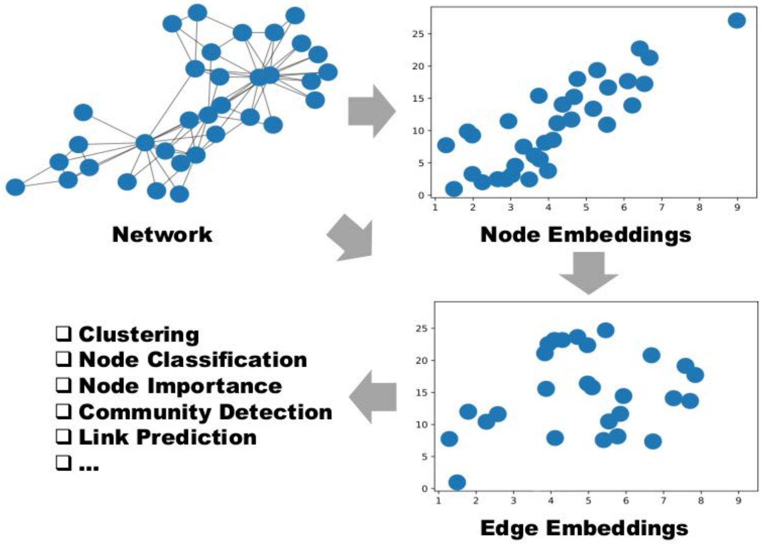
- Non-standard evaluations → *incomparable results*
  - Networks
  - Methods
  - Method implementations
  - Hyperparameter tuning
  - Evaluation metrics
- LP a complex task → *evaluation prone to errors, many evaluation choices*
- Current NE frameworks → *limited LP evaluation capabilities, very restricted*
  - OpenNE
  - GEM

Objectives

- Address the reproducibility crisis in the field of Network Embedding (NE) for Link Prediction (LP)
- Simplify evaluation of NE methods and comparison with sota
- Provide a unified benchmarking framework
  - Flexible enough to adapt to existing evaluation settings
  - Flexible to incorporate any method and data
  - Minimize the likelihood of evaluation errors
  - With justified recommendations of the most adequate evaluation pipelines

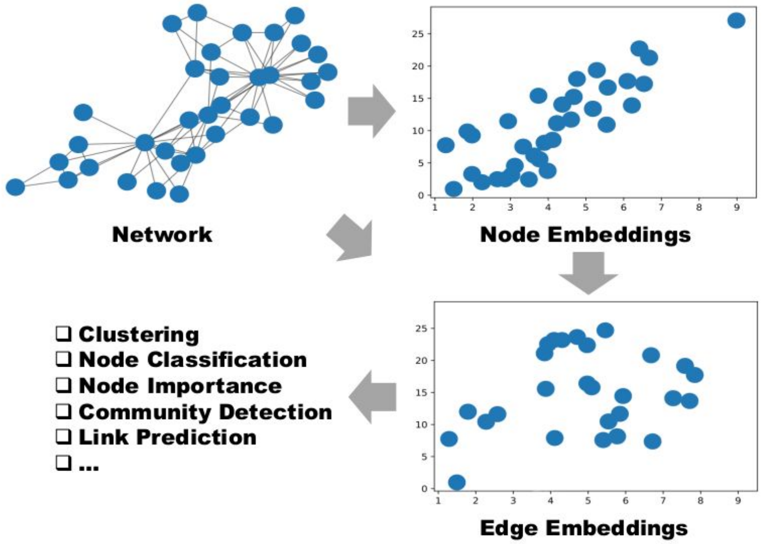
Network Embedding (NE)

- A mapping of network nodes to d-dimensional vector representations
- The representation learned can be used as features for a variety of standard ML tasks (e.g. clustering, classification, etc.)
- Constitute a way of bringing all the power of standard ML to graphs
- Node embeddings and/or edge embeddings



Network Embedding (NE)

- Formally, a network embedding is a mapping Φ : V→ $R^{|V|\times d}$ where d << |V|. This mapping Φ defines the latent representation (or embedding) of each node v ∈ V.
- Categories of NE methods
  - Matrix factorization (e.g. LapEig, MatFact)
  - Random walks (e.g. DeepWalk, Node2vec)
  - Deep learning (e.g. SDNE, BINE)
- Learning embeddings:
  1. Proximity measure defined on the graph
  2. Similarity in the embedding space
  3. Cost function



Network Embedding Evaluation

The quality of the embeddings provided by NE methods is generally assessed through the following tasks:

- Multi-label classification
- Clustering
- Visualization
- Link prediction

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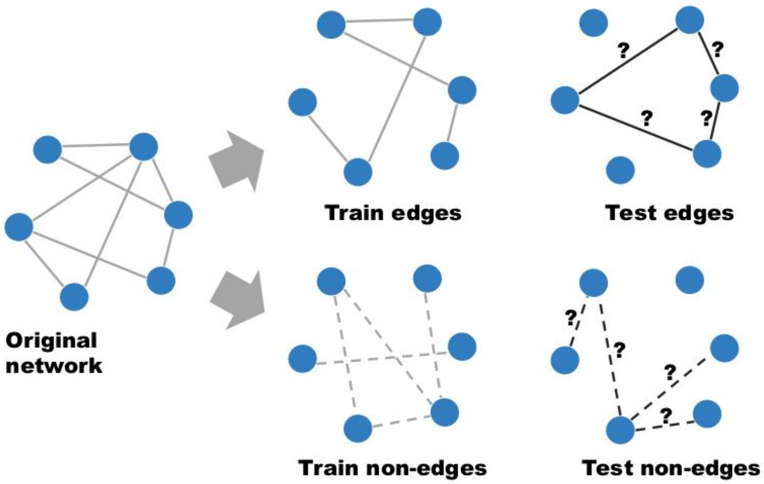
Only node embedding , embed complete network and evaluate

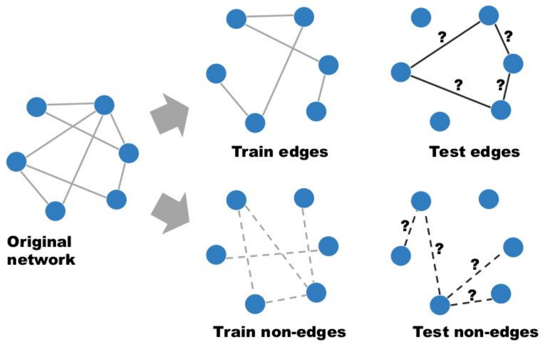
Edge embedding, evaluation requires embedding of a subgraph of the original network or snapshot of the network in time

Link Prediction (LP)

- Estimate the likelihood of the existence of edges between pairs of nodes
- Binary classification with positive and negative examples (both true edges and non-edges required for evaluation)
  - Split the network edges in a set of train edges and a set of test edges (snapshots of the network in time can be used for train/test)
  - Generate sets of *false* edges or non-edges
  - Train the binary classifier with a set of train edges and train non-edges
  - Evaluate performance on the test edges



Evaluating NE methods on LP



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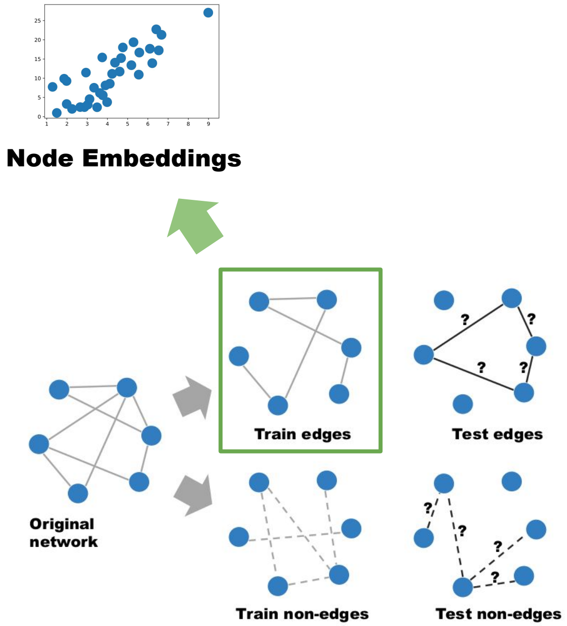

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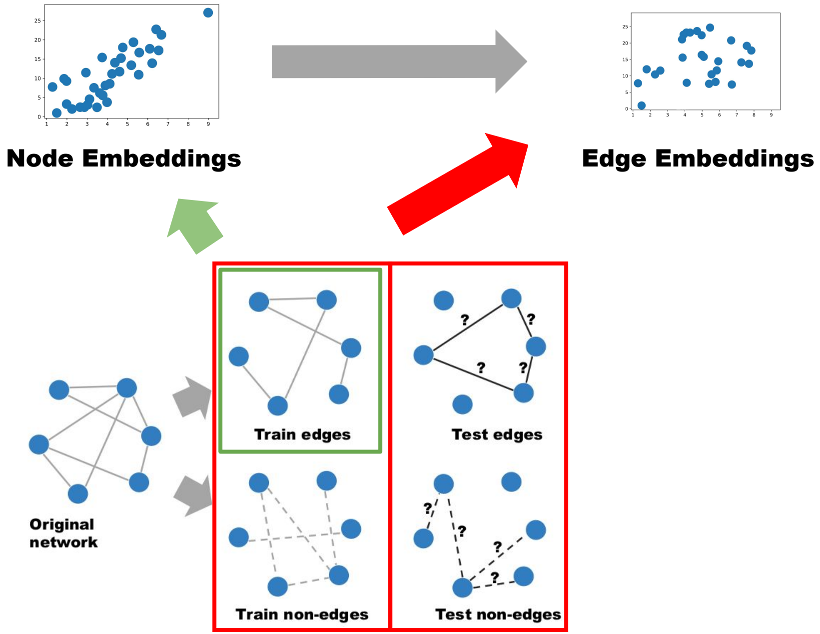
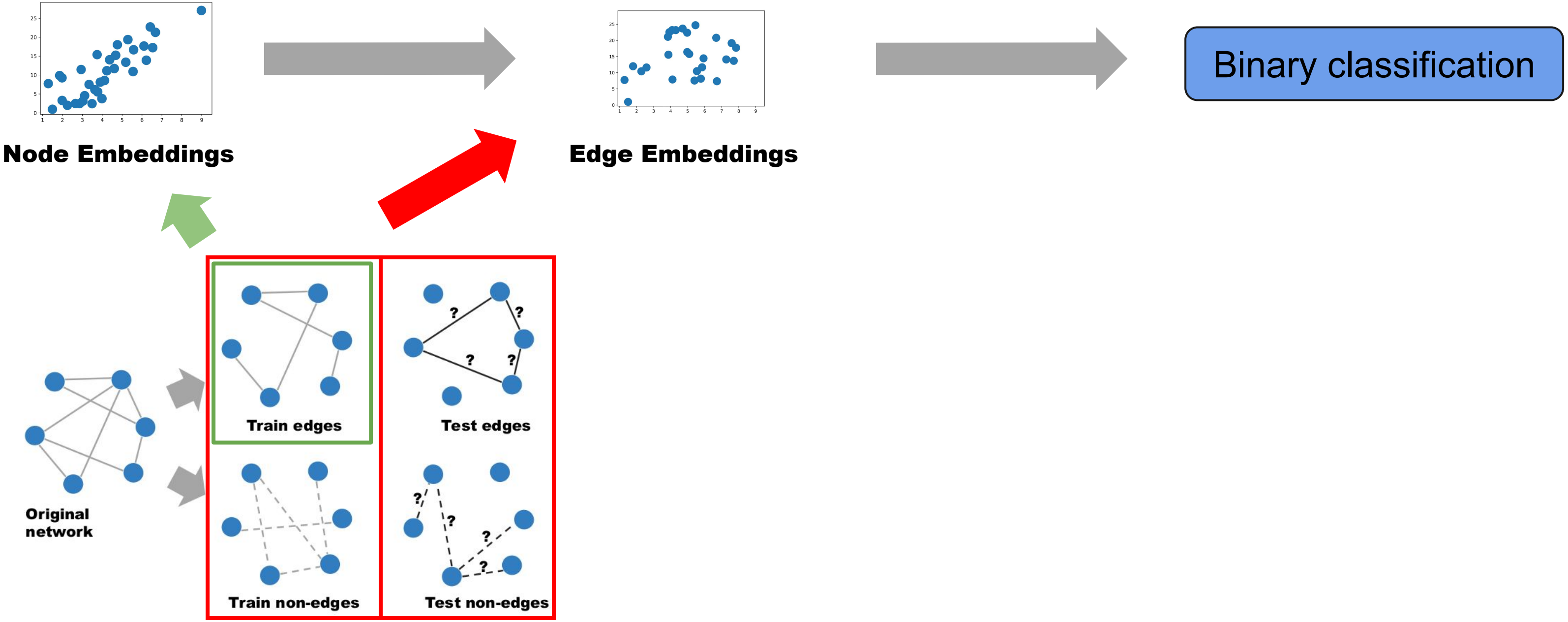
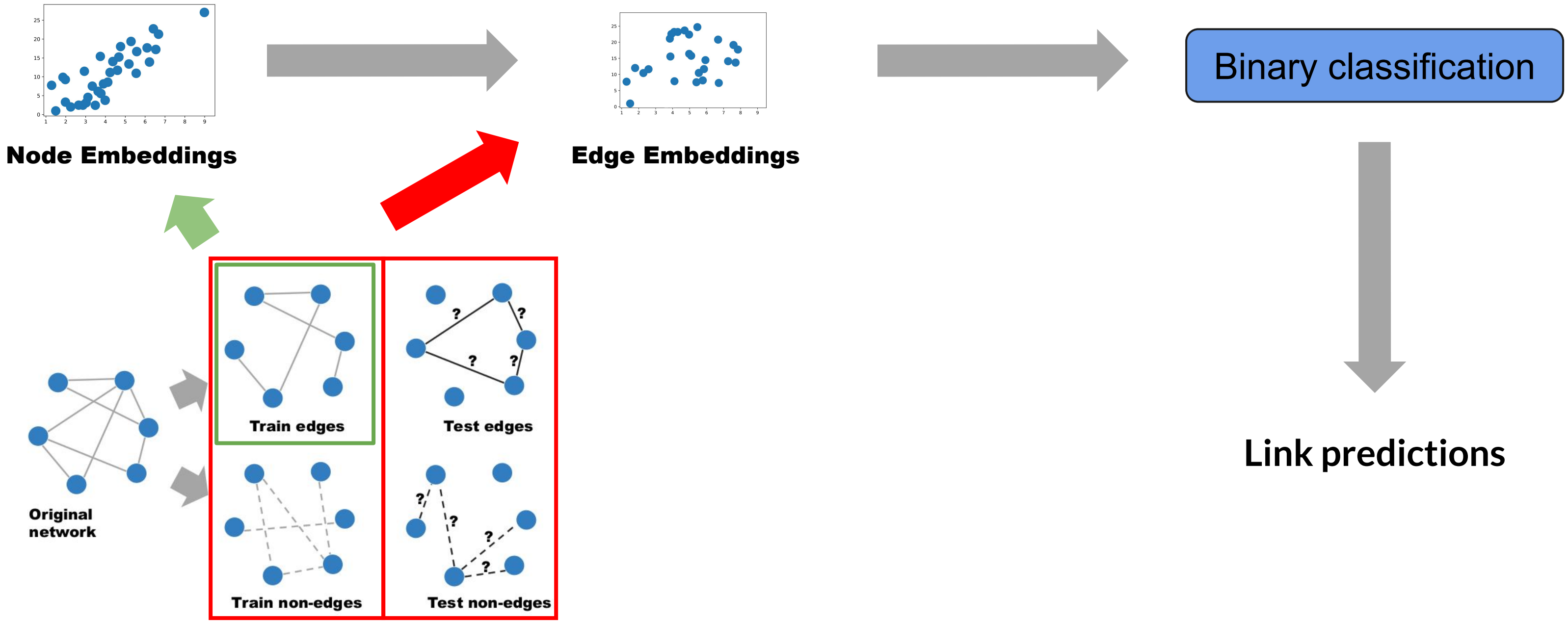


Evaluating NE methods on LP



Evaluating NE methods on LP



Evaluating NE methods on LP

Evaluation choices:

- Network preprocessing
  - Restrict graph to main cc
  - Relabel nodes
- Train/test fraction
  - Common values 30-90
- Non-edge sampling
  - Open-world
  - Closed-world
- Train/Test edge selection
  - Naive slow approaches

Evaluating NE methods on LP

Evaluation choices:

- Node to edge embedding
- LP heuristics
- Binary classifiers
- Evaluation metrics
    - Commonly AUROC, prec@k, prec-recall

Average (Avg.):

$$x_u \oplus x_v \equiv \frac{x_{u,i} + x_{v,i}}{2}$$

Hadamard (Had.):

$$x_u \odot x_v \equiv x_{u,i} * x_{v,i}$$

Weighted L_1:

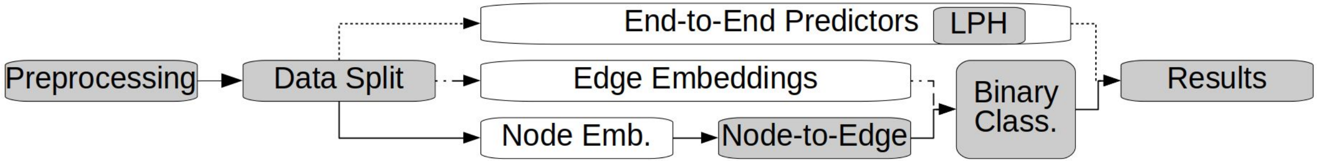
$$||x_u \cdot x_v||_{\bar{1}} \equiv |x_{u,i} - x_{v,i}|$$

Weighted L_2:

$$||x_u \cdot x_v||_{\bar{2}} \equiv |x_{u,i} - x_{v,i}|^2$$

EvalNE

- CLI tool and API
- Open-source (https://github.com/Dru-Mara/EvalNE)
- Cross-platform
- Complete documentation (https://evalne.readthedocs.io/en/latest/)
- Easy to use (no coding required)



Main Features

- Highly **flexible evaluation** pipelines (described in **conf. files**)
- Automated method evaluation
- Automated **hyper-parameter tuning**
- Simple addition of new methods
- Language-independent evaluation
- **Efficient train/test edge split algorithm**
- Many evaluation criteria
- Main node-to-edge embedding methods

Alg. 1: Train/Test edge selection

1. Obtain a uniform spanning tree ST of G
2. Initialize the set of training edges E_{train} to all edges in ST
3. Select edges uniformly at random without replacement from the remaining edges $E \setminus E_{train}$.

We select a spanning tree uniformly at random from the set of all possible ones using Broder's algorithm [2]:

1. Select a random vertex s of G and start a random walk on the graph until every vertex is visited. For each vertex $i \in V \setminus \{s\}$ collect the edge $e = (j, i)$ that corresponds to the first entrance to vertex i. Let T be this collection of edges.
2. Output the set T.

Toolbox Use

Through CLI:

- Fill configuration file
- Run:
    - `foo@bar:~$ python evalne conf.ini`

```
[GENERAL]
EDGE_EMBEDDING_METHODS = average hadamard
LP_MODEL = LogisticRegression
EXP_REPEATS = 10
EMBED_DIM = 128
VERBOSE = True

[NETWORKS]
NAMES = Facebook PPI ArXiv
INPATHS = ../data/Facebook/facebook_combined.txt
          ../data/PPI/ppi.edgelist
          ../data/Astro-PH/CA-AstroPh.txt
OUTPATHS = ../output/Facebook/
           ../output/PPI/
           ../output/Astro-Ph/
DIRECTED = False False False
SEPARATORS = '\s' ',' '\t'
COMMENTS = '#' '#' ';'
```

```
[PREPROCESSING]
RELABEL = True
DEL_SELFLOOPS = True
PREP_NW_NAME = prep_graph.edgelist
WRITE_STATS = True
DELIMITER = ','

[TRAINTEST]
TRAIN_FRAC = 0.5
FAST_SPLIT = True
OWA = True
NUM_FE_TRAIN = None
NUM_FE_TEST = None
TRAINTEST_PATH = train_test_splits/

[REPORT]
MAXIMIZE = auroc
SCORES = %(maximize)s
CURVES = roc
PRECATK_VALS = 2 10 100 200 500 800 1000
```

Toolbox Use

Through CLI:

```
[BASELINES]
LP_BASELINES = common_neighbours
               jaccard_coefficient
               adamic_adar_index
               preferential_attachment
NEIGHBOURHOOD = in out

[OPENNE METHODS]
NAMES_OPNE = node2vec deepWalk line
METHODS_OPNE = python -m openne --method node2vec --epochs 100
               python -m openne --method deepWalk --epochs 100
               python -m openne --method line --epochs 100
TUNE_PARAMS_OPNE = --p 0.25 0.5 1 2 4 --q 0.25 0.5 1 2 4
```

```
[OTHER METHODS]
NAMES_OTHER = prune
EMBTYPE_OTHER = ne
METHODS_OTHER = python ../methods/PRUNE/src/main.py --inputgraph {} --output {} --dimension {}
#                ../methods/metapath2vec/metapath2vec -train {} -output {} -size {}
TUNE_PARAMS_OTHER = -negative 1 5 10
INPUT_DELIM_OTHER = '\s'
OUTPUT_DELIM_OTHER = ','
```

Toolbox Use

As an API:

```
from evalne.evaluation import evaluator
from evalne.preprocessing import preprocess as pp

# Load and preprocess the network
G = pp.load_graph('../evalne/tests/data/network.edgelist')
G, _ = pp.prep_graph(G)

# Create an evaluator and generate train/test edge split
nee = evaluator.Evaluator()
_ = nee.traintest_split.compute_splits(G)
```

```
# Set the baselines
methods = ['random_prediction', 'common_neighbours', 'jaccard_coefficient']

# Evaluate baselines
nee.evaluate_baseline(methods=methods)
```

Toolbox Use

```
try:
    # Check if OpenNE is installed
    import openne

    # Set embedding methods from OpenNE
    methods = ['node2vec', 'deepwalk', 'GraRep']
    commands = [
        'python -m openne --method node2vec --graph-format edgelist --p 1 --q 1',
        'python -m openne --method deepWalk --graph-format edgelist --number-walks 40',
        'python -m openne --method grarep --graph-format edgelist --epochs 10']
    edge_emb = ['average', 'hadamard']

    # Evaluate embedding methods
    for i in range(len(methods)):
        command = commands[i] + " --input {} --output {} --representation-size {}"
        nee.evaluate_cmd(method_name=methods[i], method_type='ne', command=command,
                         edge_embedding_methods=edge_emb, input_delim=' ', output_delim=' ')
```

```
# Get output
results = nee.get_results()
for result in results:
    result.pretty_print()
```

Experimental Results

Replicating the Node2vec [1] LP evaluation:

- Table presents original values for LP.
- In parenthesis (our - original) results.

Issues:

- Missing details in experimental setup
- Class probabilities vs class labels
- Method implementations used

		Facebook	PPI	arXiv
	CN	0.81 (+0.14)	0.71 (+0.06)	0.82 (+0.13)
	JC	0.88 (+0.04)	0.70 (+0.04)	0.81 (+0.12)
	AA	0.83 (+0.13)	0.71 (+0.06)	0.83 (+0.12)
	PA	0.71 (+0.04)	0.67 (+0.13)	0.70 (+0.08)
Avg.	DeepWalk	0.72 (−0.01)	0.69 (+0.08)	0.71 (+0.01)
	LINE	0.70 (−0.03)	0.63 (+0.12)	0.65 (+0.14)
	node2vec	0.73 (−0.01)	0.75 (−0.01)	0.72 (−0.02)
Had.	DeepWalk	0.97 (−0.03)	**0.74 (−0.2)**	0.93 (−0.12)
	LINE	0.95 (−0.06)	0.72 (−0.01)	0.89 (+0.05)
	node2vec	0.97 (0.0)	**0.77 (−0.17)**	0.94 (−0.05)
W L_1	DeepWalk	0.96 (−0.01)	0.60 (+0.14)	0.83 (+0.09)
	LINE	**0.95 (−0.33)**	0.70 (−0.01)	**0.88 (−0.28)**
	node2vec	0.96 (−0.01)	0.63 (−0.03)	0.85 (+0.03)
W L_2	DeepWalk	0.96 (−0.01)	0.61 (+0.14)	0.83 (+0.09)
	LINE	**0.95 (−0.33)**	0.71 (−0.02)	**0.89 (−0.27)**
	node2vec	0.96 (0.0)	0.62 (−0.02)	0.85 (+0.03)

Experimental Results

Replicating the CNE [2] LP evaluation:

Issues:

- Performance degradation from parallelization (Metapath2vec)

	Facebook	PPI	arXiv	BlogCatalog	wikipedia	studentdb
CN	0.97 (+0.01)	0.77 (0.0)	0.94 (+0.01)	0.92 (+0.01)	0.84 (0.0)	0.42 (−0.01)
JS	0.97 (+0.01)	0.76 (0.0)	0.94 (+0.01)	0.78 (0.0)	0.50 (−0.01)	0.42 (−0.01)
AA	0.98 (0.0)	0.77 (+0.01)	0.94 (+0.01)	0.93 (0.0)	0.86 (+0.01)	0.42 (−0.01)
PA	0.83 (+0.01)	0.89 (+0.01)	0.86 (+0.01)	0.95 (0.0)	0.91 (+0.01)	0.91 (+0.01)
DeepWalk	0.98 (0.0)	0.64 (+0.01)	0.92 (+0.01)	0.61 (−0.01)	0.56 (0.0)	0.76 (+0.03)
LINE	0.95 (0.0)	0.75 (+0.01)	0.98 (0.0)	0.76 (+0.01)	0.71 (0.0)	0.86 (−0.02)
Node2vec	0.99 (0.0)	0.68 (+0.02)	0.97 (0.0)	0.73 (−0.05)	0.67 (−0.08)	0.83 (0.0)
Metapath	**0.74 (+0.17)**	0.85 (0.0)	0.83 (+0.02)	0.91 (0.0)	0.83 (+0.02)	0.92 (−0.01)
CNE(unif.)	0.99 (0.0)	0.89 (+0.01)	0.99 (0.0)	0.92 (+0.01)	0.84 (0.0)	0.93 (0.0)
CNE(deg.)	0.99 (0.0)	0.91 (0.0)	0.99 (0.0)	0.96 (0.0)	0.92 (−0.01)	0.94 (0.0)

Experimental Results

Replicating the PRUNE [3] LP evaluation:

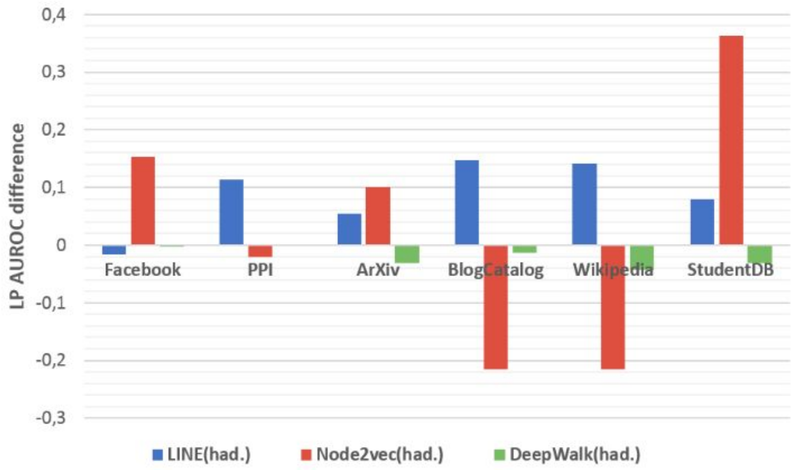
Issues:

- Missing details in experimental setup
- No open-source implementation of one of the baselines (NRCL)

	DeepWalk	LINE	Node2vec	SDNE	PRUNE
Hep-Ph	0.80 (−0.05)	0.80 (−0.09)	0.81 (−0.05)	0.75 (−0.04)	0.86 (−0.03)
FB-wallpost	0.83 (+0.01)	0.78 (+0.09)	0.85 (−0.09)	0.86 (−0.02)	0.88 (−0.01)

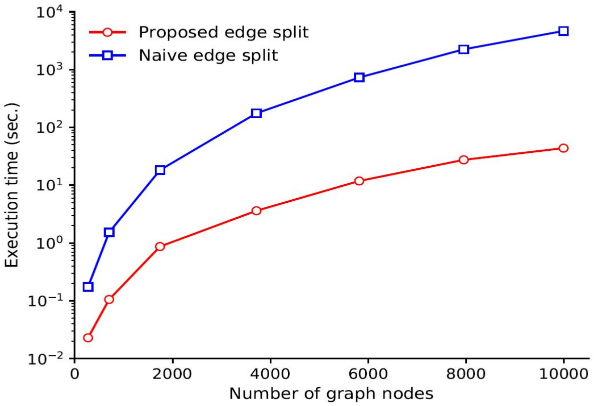
Experimental Results

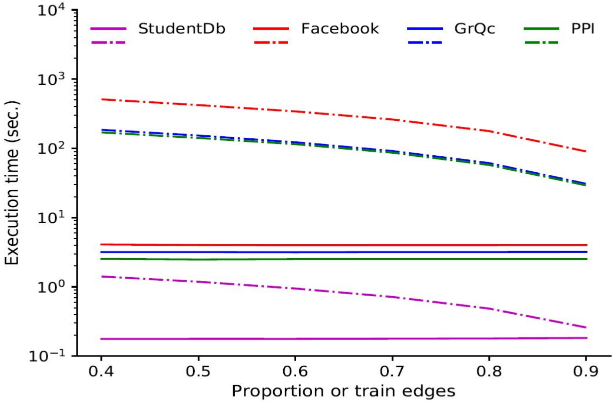
Difference in performance between two popular implementations of NE methods (OpenNE and original)



Experimental Results

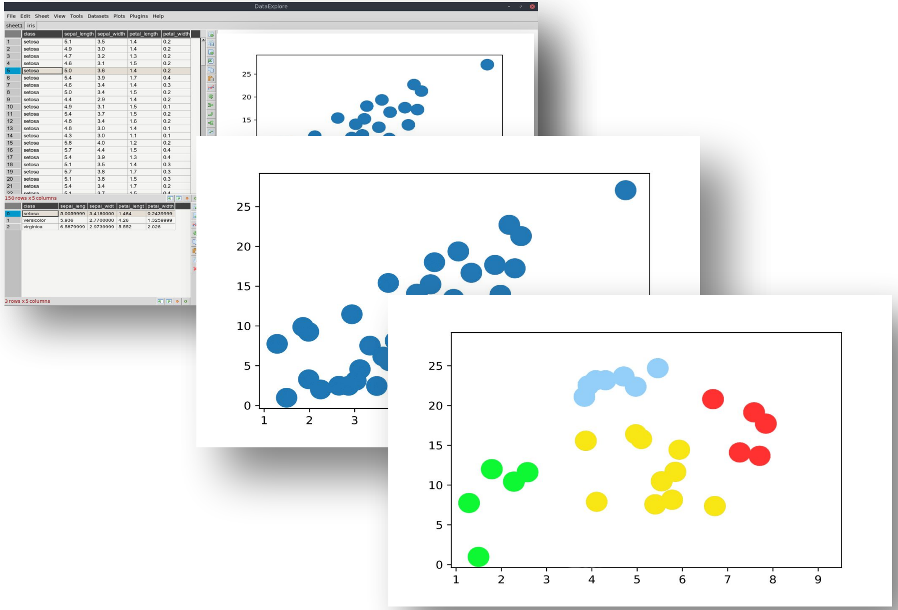
Scalability of the edge set selection method and comparison with the naive approach:





Future Work

- Integrate **embedding visualization.**
- Include **multi-label classification** evaluation.
- Design a flexible **GUI** capable of auto-generating configuration files.
- Include **Wilson's loop-erased random walk** algorithm for selecting a spanning tree uniformly at random.



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Thanks!

Questions

Experimental Results

Replicating the SDNE [4] LP evaluation:

Issues:

- Missing details in experimental setup
- The authors used all graph non-edges to compute prec@k. We approximated this values.

	prec@100	prec@200	prec@300	prec@500	prec@800	prec@1000	prec@10000
SDNE	1 (−0.00)	1 (−0.00)	1 (+0.01)	0.99 (−0.00)	0.97 (+0.03)	0.91 (+0.09)	0.25 (−0.12)
LINE	1 (−0.00)	1 (−0.00)	0.99 (+0.01)	0.93 (+0.06)	0.74 (+0.26)	0.79 (+0.11)	0.21 (−0.13)
DeepWalk	**0.6 (+0.40)**	**0.55 (+0.45)**	**0.44 (+0.56)**	**0.34 (+0.65)**	**0.29 (+0.70)**	**0.29 (+0.71)**	0.15 (+0.01)
GraRep	**0.04 (+0.96)**	**0.03 (+0.97)**	**0.03 (+0.97)**	**0.04 (+0.96)**	**0.03 (+0.97)**	**0.03 (+0.97)**	**0.19 (+0.16)**
CN	1 (−0.00)	0.96 (+0.03)	0.96 (+0.03)	0.98 (−0.00)	0.87 (+0.05)	0.79 (+0.09)	0.19 (−0.00)
LapEig	0.93 (+0.07)	0.85 (+0.15)	**0.82 (+0.17)**	**0.66 (+0.34)**	**0.46 (+0.53)**	**0.39 (+0.48)**	0.05 (+0.15)