network *learning*

introduction to *network science in Python* (NetPy)

Lovro Šubelj University of Ljubljana 3rd October 2024

learning tasks

modern machine learning with network data

— node-level tasks

- node classification (e.g. finding hoaxes on Wikipedia)
- node ranking (e.g. finding top influencers on Instagram)
- network clustering (e.g. research areas of scientific papers)

— edge-level tasks

- link prediction (e.g. product recommendation on Amazon)
- strength of ties (e.g. close friends/acquaintances on Facebook)

— graph-level tasks

- graph classification (e.g. playing strategy in football)
- graph generation (e.g. good candidates for new drugs)
- etc.

learning *since* ~2000

use network analysis techniques directly

- node ranking tasks
 node centrality, link analysis, graphlets, egonets etc.
- link prediction tasks
 link bridging, prediction indices, matrix factorization etc.
- network clustering tasks
 community detection, (stochastic) blockmodeling etc.







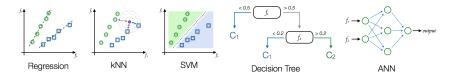


— etc.

learning *until* \sim 2010

use *network analysis* techniques for *features*

- 1. generate node/link/graph features from network structure
- 2. feed generated features into machine learning method



but features are task dependent & redesigned every time!

for survey see [ZPS+16]

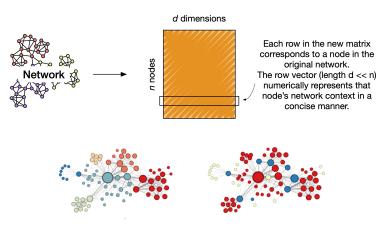
learning modern

use machine learning methods for embeddings/directly

- dimensionality reduction/matrix factorization (e.g. NMF) decomposition of adjacency matrix A or graph Laplacian L
- 2. random walks on network (e.g. node2vec [GL16], struct2vec [FRS17]) similar nodes have similar embeddings independently of task
- graph neural networks (e.g. GCN [KW17], GAT, GraphSAGE [HYL17]) node/edge/graph representations are learned for specific task

for *survey* see [MKNŠ21]

learning node2vec

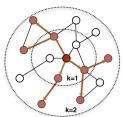


for *paper* see [GL16]

learning GraphSAGE

$$h_i^0 = x_i$$

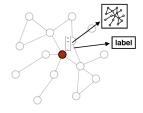
$$h_i^k = \sigma\left(\frac{W_k \cdot \text{CONCAT}(h_i^{k-1}, \text{AGGREGATE}_k(\{h_j^{k-1} \mid j \in \Gamma_i\}))}{} \right)$$



1. Sample neighborhood



2. Aggregate feature information from neighbors



Predict graph context and label using aggregated information

for *paper* see [HYL17]

learning references



Daniel R. Figueiredo, Leonardo F. R. Ribeiro, and Pedro H. P. Saverese.

struc2vec: Learning node representations from structural identity.

In Proceedings of the ACM SIGKDD International Conference on Knowledge Discovery and Data Mining, pages 1–9, 2017.



Aditya Grover and Jure Leskovec.

node2vec: Scalable feature learning for networks.

In Proceedings of the ACM SIGKDD International Conference on Knowledge Discovery and Data Mining, pages 855–864, 2016.



Will Hamilton, Zhitao Ying, and Jure Leskovec.

Inductive representation learning on large graphs.

In I. Guyon, U. V. Luxburg, S. Bengio, H. Wallach, R. Fergus, S. Vishwanathan, and R. Garnett, editors, Advances in Neural Information Processing Systems, volume 30. Curran Associates, Inc., 2017.



Thomas N. Kipf and Max Welling.

Semi-Supervised Classification with Graph Convolutional Networks.

In Proceedings of the 5th International Conference on Learning Representations, ICLR '17, 2017.



I. Makarov, D. Kiselev, N Nikitinsky, and L. Šubelj.

Survey on graph embeddings and their applications to machine learning problems on graphs. PeerJ Comput. Sci., 7:e357, 2021.



M. Zanin, D. Papo, P. A. Sousa, E. Menasalvas, A. Nicchi, E. Kubik, and S. Boccaletti.
Combining complex networks and data mining: Why and how.

Phys. Rep., 635:1–44, 2016.