

Modeling polypharmacy side effects with graph convolutional networks

Visualization & Metrics

Henrik Wenck, Simon Witzke

01

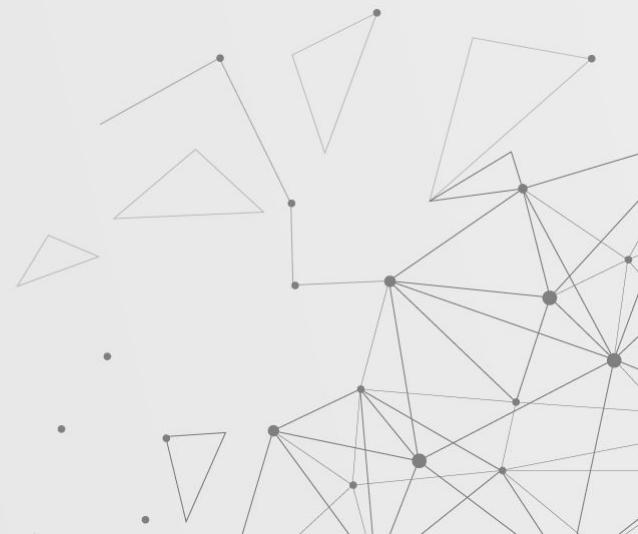
Our Dataset



Datasets from “*Modeling polypharmacy side effects with graph convolutional networks*”

1. Protein-protein interaction network

2. Drug-target protein associations
3. Drug-target protein associations culled from several curated databases
4. Polypharmacy side effects in the form of (drug A, side effect type, drug B) triples
5. Side effects of individual drugs in the form of (drug A, side effect type) tuples
6. Side effect categories

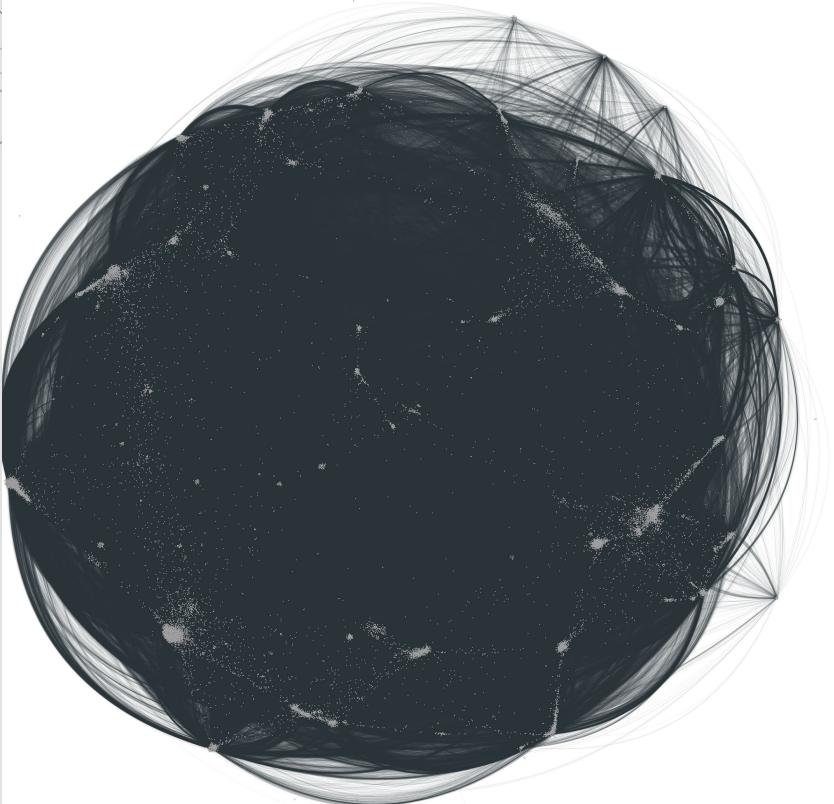


02

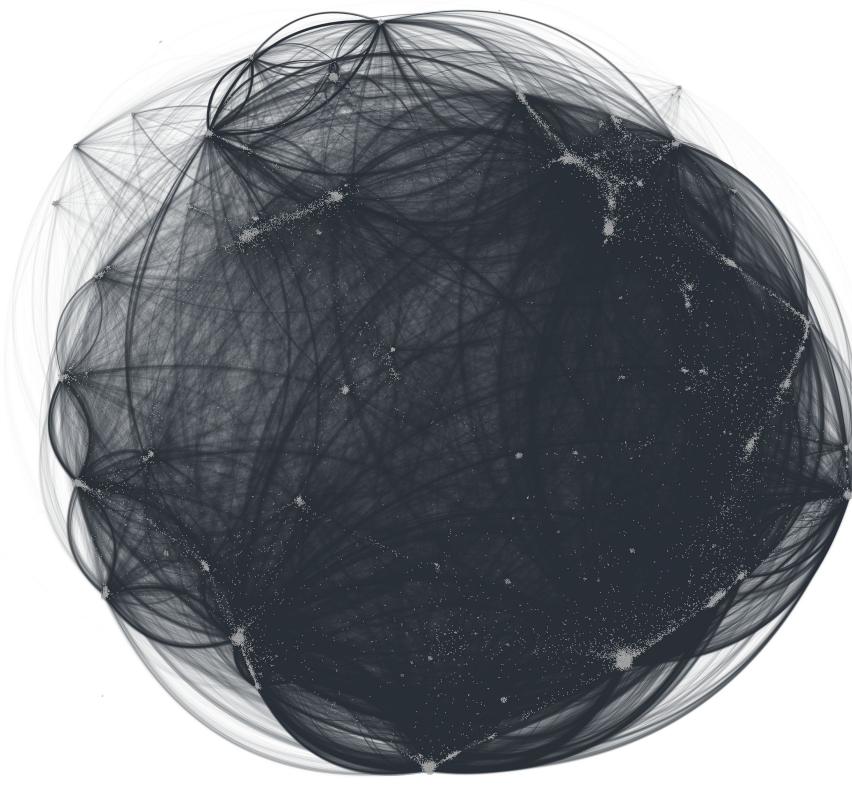
Our Graph



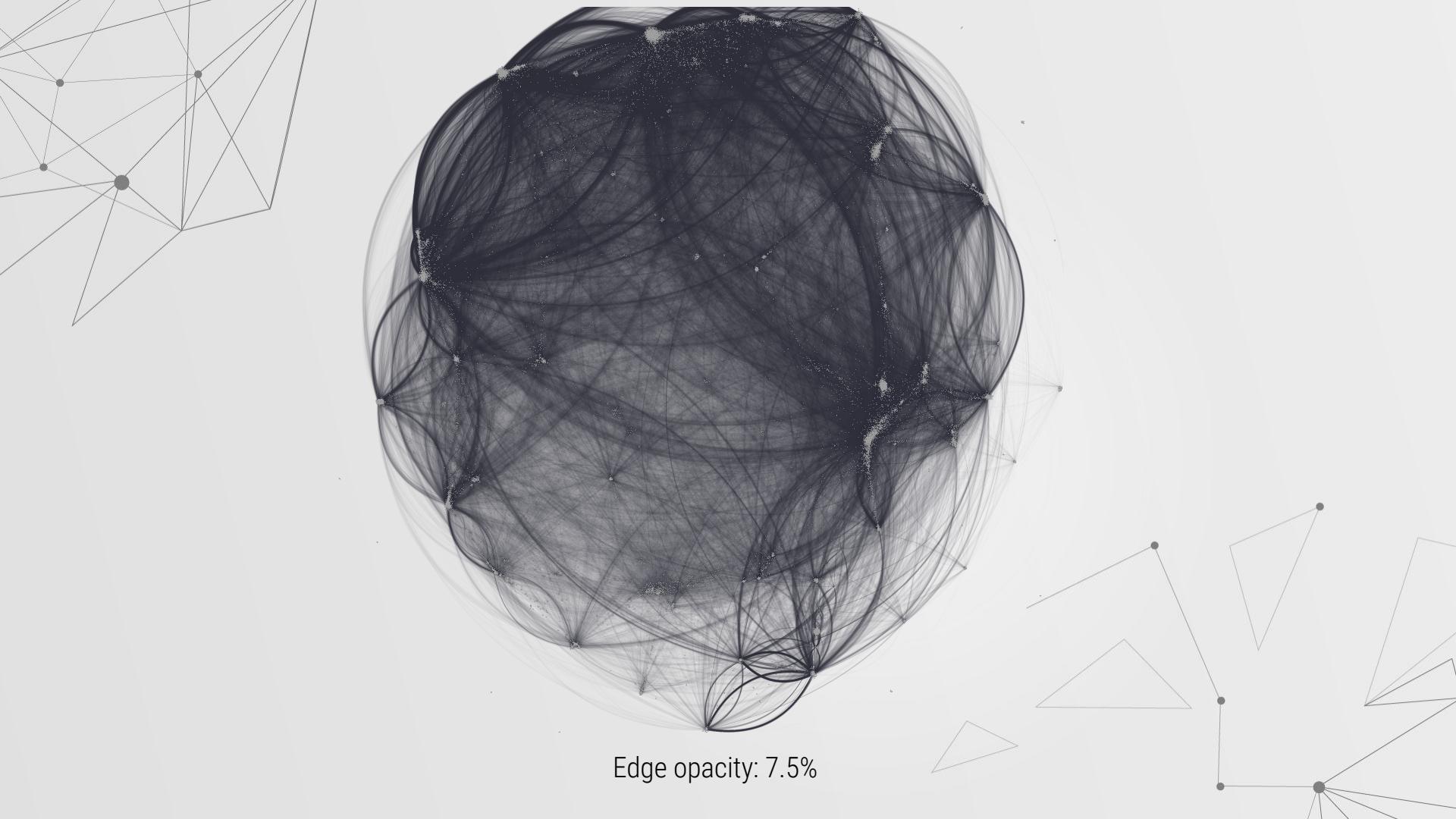
Igraph plots



Edge opacity: 50%



Edge opacity: 15%



A faint, abstract network graph is visible in the background, consisting of numerous small, dark gray dots connected by thin gray lines, forming a complex web of triangles and polygons.

03

Network-level metrics

OUR NUMBERS

274.5

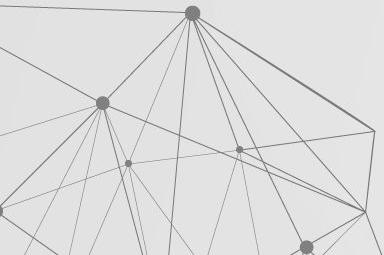
Average node degree

0.234

Average clustering

0

Node connectivity



04

Node-level metrics



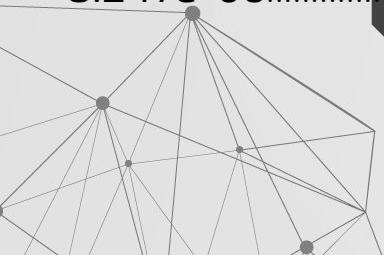
OUR NUMBERS

Assortativity Coefficient

-0.01

1.298e-47 Eigenvector centrality 0.077 , 0.078, 0.08

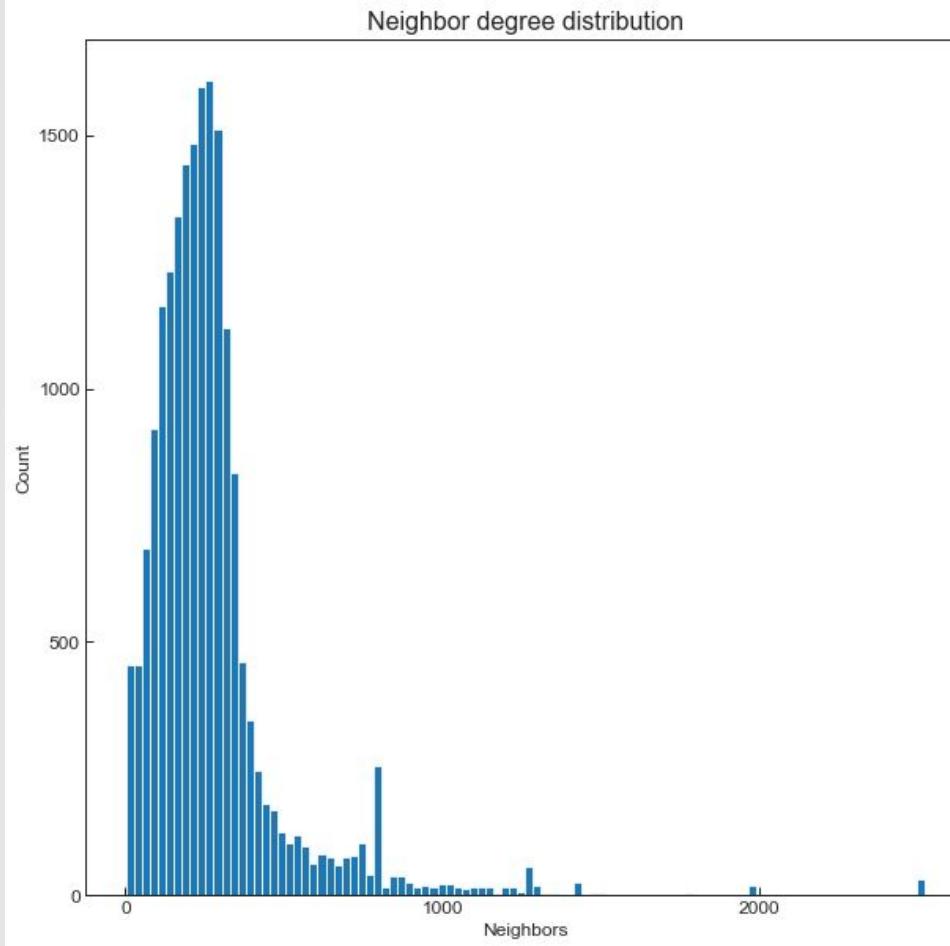
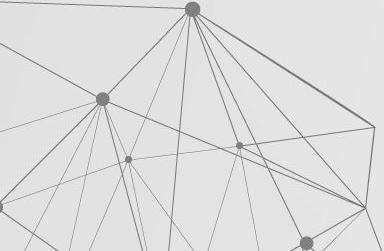
8.247e-06 Page Rank 0.0013, 0.0017, 0.0022

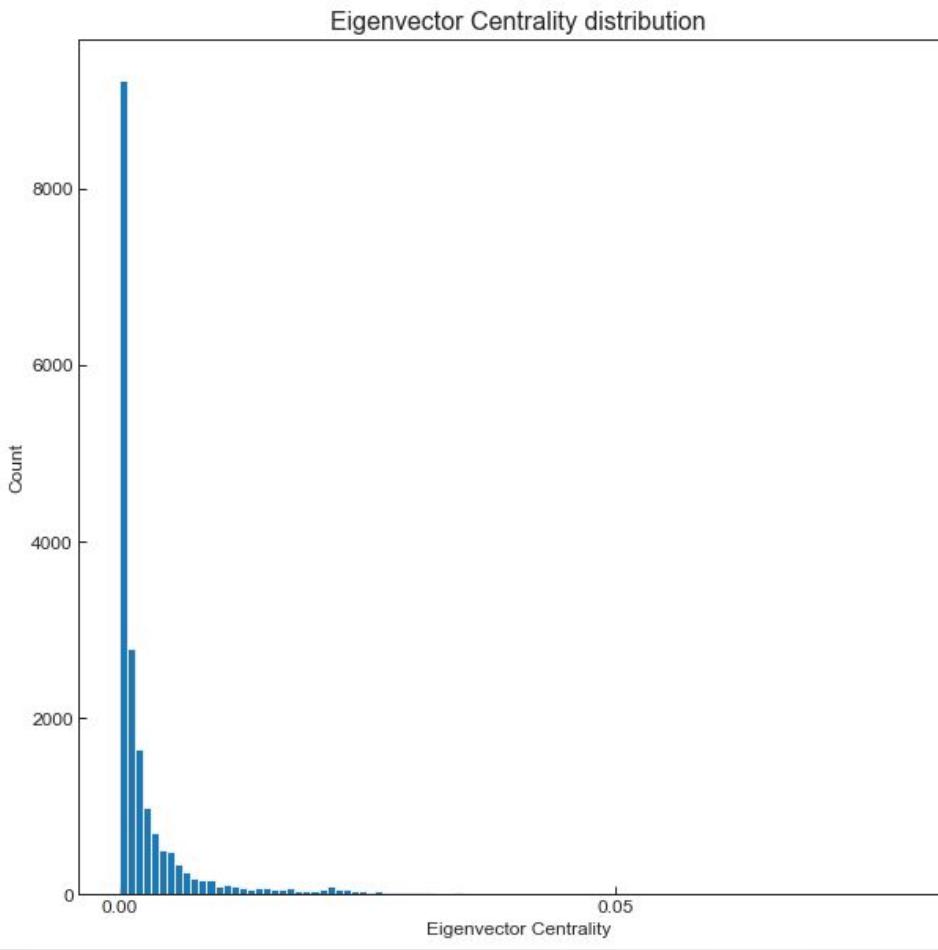
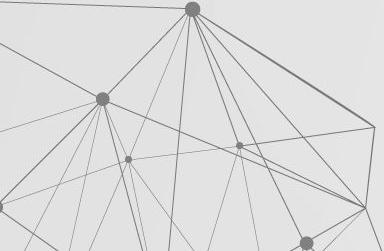


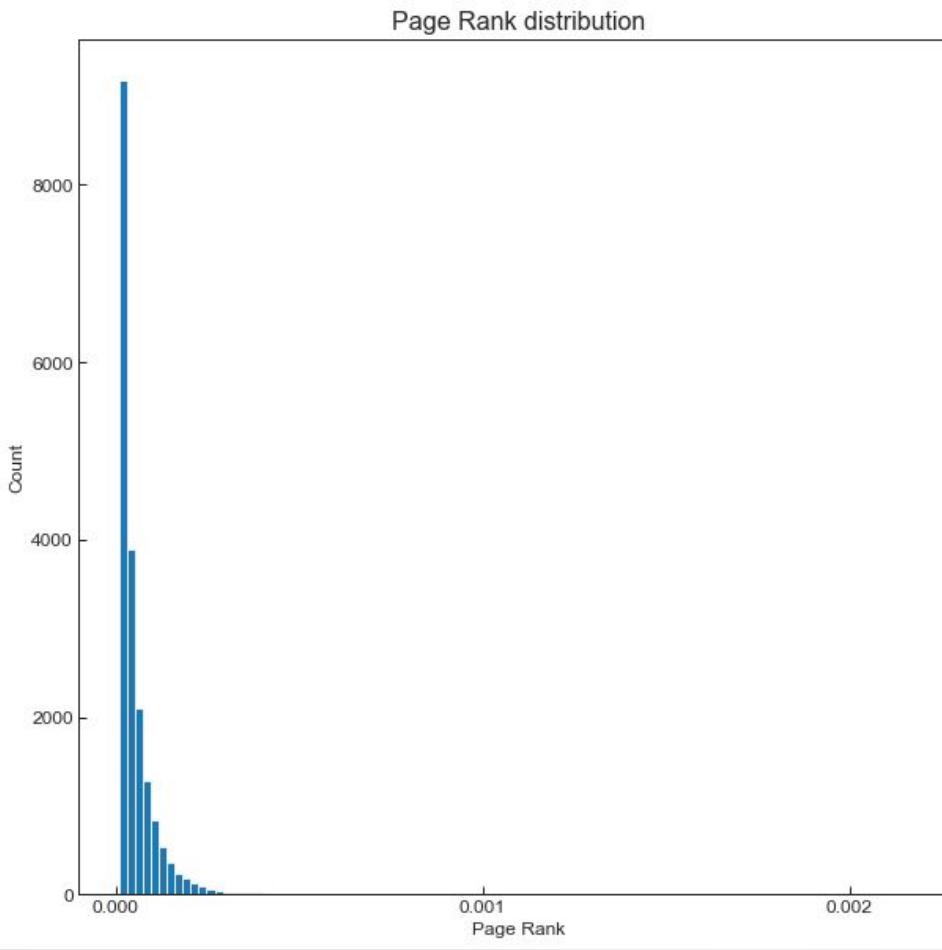
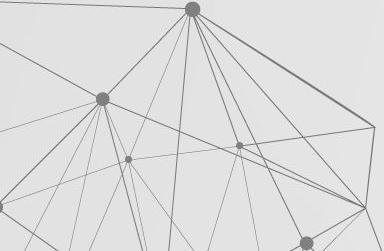
The background features a complex network graph on the left side, composed of numerous small, thin gray lines connecting dark gray circular nodes of varying sizes. To the right of the graph, several larger, thin gray triangles are scattered across the white space, some containing small dark gray dots.

05

Distributions







06

Related Work

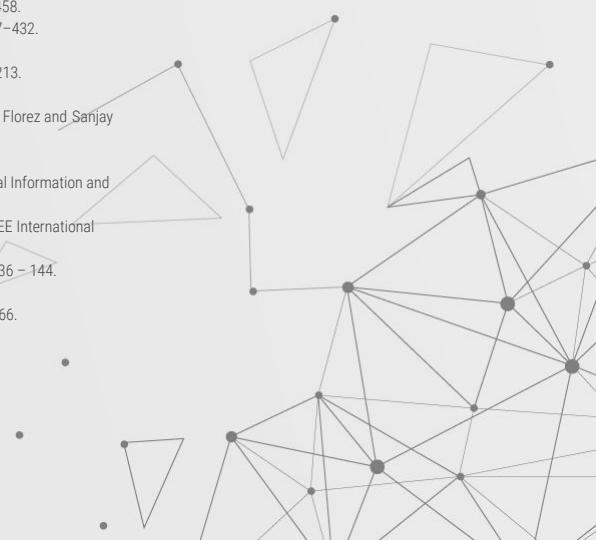
RESOURCES

Paper

1. Andreea Deac, Yu-Hsiang Huang, Petar Veličković, Pietro Liò, and Jian Tang. 2019. Drug-Drug Adverse Effect Prediction with Graph Co-Attention. arXiv:1905.00534 [stat.ML]
2. Giovanna Maria Dimitri and Pietro Liò. 2017. DrugClust: A machine learning approach for drugs side effects prediction. Computational Biology and Chemistry 68 (June 2017), 204–210. <https://doi.org/10.1016/j.combiolchem.2017.03.008>
3. Elizabeth D. Kantor, Colin D. Rehm, Jennifer S. Haas, Andrew T. Chan, and Edward L. Giovannucci. 2015. Trends in Prescription Drug Use Among Adults in the United States From 1999-2012. JAMA 314, 17 (Nov. 2015), 1818. <https://doi.org/10.1001/jama.2015.13766>
4. Simon Kocabek, Primoz Kocabek, Andraz Stozer, Tina Zupanic, Tudor Groza, and Gregor Stiglic. 2018. Building interpretable models for polypharmacy prediction in older chronic patients based on drug prescription records. PeerJ 6 (Oct. 2018), e5765. <https://doi.org/10.7717/peerj.5765>
5. Brandon Malone, Alberto García-Durán, and Mathias Niepert. 2018. Knowledge Graph Completion to Predict Polypharmacy Side Effects. In Lecture Notes in Computer Science. Springer International Publishing, 144–149. https://doi.org/10.1007/978-3-030-06016-9_14
6. S. Mizutani, E. Pauwels, V. Stoven, S. Goto, and Y. Yamanishi. 2012. Relating drug-protein interaction network with drug side effects. Bioinformatics 28, 18 (Sept. 2012), i522–i528. <https://doi.org/10.1093/bioinformatics/bts383>
7. Vít Nováček and Sameh K. Mohamed. 2020. Predicting Polypharmacy Side-effects Using Knowledge Graph Embeddings. AMIA Jt Summits Transl Sci Proc 2020(2020), 449–458.
8. B. Reason, M. Terner, A. Moses McKeag, B. Tipper, and G. Webster. 2012. The impact of polypharmacy on the health of Canadian seniors. Family Practice 29, 4 (Jan. 2012), 427–432. <https://doi.org/10.1093/fampra/cmr124>
9. Itay Shaked, Matthew A. Oberhardt, Nir Atias, Roded Sharan, and Eytan Ruppin. 2016. Metabolic Network Prediction of Drug Side Effects. Cell Systems 2, 3 (March 2016), 209–213. <https://doi.org/10.1016/j.cels.2016.03.001>
10. Ruiyi Wang, Tong Li, Zhen Yang, and Haiyang Yu. 2020. Predicting Polypharmacy Side Effects Based on an Enhanced Domain Knowledge Graph. In Applied Informatics, Hector Florez and Sanjay Misra (Eds.). Springer International Publishing, Cham, 89–103.
11. Hao Xu, Shengqi Sang, and Haiping Lu. 2020. Tri-graph Information Propagation for Polypharmacy Side Effect Prediction. arXiv:2001.10516 [cs.LG]
12. Yoshihiro Yamanishi, Edouard Pauwels, and Masaaki Kotera. 2012. Drug Side-Effect Prediction Based on the Integration of Chemical and Biological Spaces. Journal of Chemical Information and Modeling 52, 12 (Dec. 2012), 3284–3292. <https://doi.org/10.1021/ci2005548>
13. Wen Zhang, Yanlin Chen, Shikui Tu, Feng Liu, and Qianlong Qu. 2016. Drug side effect prediction through linear neighborhoods and multiple data source integration. In 2016 IEEE International Conference on Bioinformatics and Biomedicine (BIBM). IEEE. <https://doi.org/10.1109/bibm.2016.7822555>
14. Xian Zhao, Lei Chen, and Jing Lu. 2018. A similarity-based method for prediction of drug side effects with heterogeneous information. Mathematical Biosciences 306 (2018), 136 – 144. <https://doi.org/10.1016/j.mbs.2018.09.010>
15. Marinka Zitnik, Monica Agrawal, and Jure Leskovec. 2018. Modeling polypharmacy side effects with graph convolutional networks. Bioinformatics 34, 13 (June 2018), i457–i466. <https://doi.org/10.1093/bioinformatics/bty2943>

Books

16. Roy J. Vaz and Thomas Klabunde (2008). Antitargets: Prediction and Prevention of Drug Side Effects. John Wiley & Sons.





04

Other metrics



OUR NUMBERS

500

new clients last semester

ongoing projects

500

