

References

- Abadi M, Barham P, Chen J, Chen Z, Davis A, Dean J, Devin M, Ghemawat S, Irving G, Isard M, et al (2016) Tensorflow: A system for large-scale machine learning. In: 12th {USENIX} Symposium on Operating Systems Design and Implementation ({OSDI} 16), pp 265–283
- Abbe E (2017) Community detection and stochastic block models: recent developments. *Journal of Machine Learning Research* 18(1):6446–6531
- Abbe E, Sandon C (2015) Community detection in general stochastic block models: Fundamental limits and efficient algorithms for recovery. In: IEEE 56th Annual Symposium on Foundations of Computer Science, pp 670–688
- Abboud R, Ceylan ii, Grohe M, Lukasiewicz T (2020) The surprising power of graph neural networks with random node initialization. *CoRR* abs/2010.01179
- Abdelaziz I, Dolby J, McCusker JP, Srinivas K (2020) Graph4Code: A machine interpretable knowledge graph for code. *arXiv preprint arXiv:200209440*
- Abdollahpouri H, Adomavicius G, Burke R, Guy I, Jannach D, Kamishima T, Krasnodebski J, Pizzato L (2020) Multistakeholder recommendation: Survey and research directions. *User Modeling and User-Adapted Interaction* 30(1):127–158
- Abid NJ, Dragan N, Collard ML, Maletic JI (2015) Using stereotypes in the automatic generation of natural language summaries for c++ methods. In: 2015 IEEE International Conference on Software Maintenance and Evolution (IC-SME), IEEE, pp 561–565
- Abney S (2007) *Semisupervised learning for computational linguistics*. CRC Press
- Adamic LA, Adar E (2003) Friends and neighbors on the web. *Social networks* 25(3):211–230
- Adams RP, Zemel RS (2011) Ranking via sinkhorn propagation. *arXiv preprint arXiv:11061925*
- Aghamohammadi A, Izadi M, Heydarnoori A (2020) Generating summaries for methods of event-driven programs: An android case study. *Journal of Systems and Software* 170:110,800

- Ahmad MA, Eckert C, Teredesai A (2018) Interpretable machine learning in health-care. In: Proceedings of the 2018 ACM international conference on bioinformatics, computational biology, and health informatics, pp 559–560
- Ahmad WU, Chakraborty S, Ray B, Chang KW (2020) A transformer-based approach for source code summarization. arXiv preprint arXiv:200500653
- Ahmed A, Shervashidze N, Narayanamurthy S, Josifovski V, Smola AJ (2013) Distributed large-scale natural graph factorization. In: Proceedings of the 22nd international conference on World Wide Web, pp 37–48
- Aho AV, Lam MS, Sethi R, Ulman JD (2006) Compilers: principles, techniques and tools. Pearson Education
- Ain QU, Butt WH, Anwar MW, Azam F, Maqbool B (2019) A systematic review on code clone detection. *IEEE Access* 7:86,121–86,144
- Airoldi EM, Blei DM, Fienberg SE, Xing EP (2008) Mixed membership stochastic blockmodels. *Journal of Machine Learning Research* 9(Sep):1981–2014
- Akoglu L, Tong H, Koutra D (2015) Graph based anomaly detection and description: a survey. *Data mining and knowledge discovery* 29(3):626–688
- Al Hasan M, Zaki MJ (2011) A survey of link prediction in social networks. In: *Social network data analytics*, Springer, pp 243–275
- Albert R, Barabási AL (2002) Statistical mechanics of complex networks. *Reviews of modern physics* 74(1):47
- Albooyeh M, Goel R, Kazemi SM (2020) Out-of-sample representation learning for knowledge graphs. In: *Empirical Methods in Natural Language Processing: Findings*, pp 2657–2666
- Ali H, Tran SN, Benetos E, Garcez ASd (2018) Speaker recognition with hybrid features from a deep belief network. *Neural Computing and Applications* 29(6):13–19
- Allamanis M (2019) The adverse effects of code duplication in machine learning models of code. In: Proceedings of the 2019 ACM SIGPLAN International Symposium on New Ideas, New Paradigms, and Reflections on Programming and Software, pp 143–153
- Allamanis M, Barr ET, Devanbu P, Sutton C (2018a) A survey of machine learning for big code and naturalness. *ACM Computing Surveys (CSUR)* 51(4):1–37
- Allamanis M, Brockschmidt M, Khademi M (2018b) Learning to represent programs with graphs. In: *International Conference on Learning Representations (ICLR)*
- Allamanis M, Barr ET, Ducousso S, Gao Z (2020) Typilus: neural type hints. In: *Proceedings of the 41st ACM SIGPLAN Conference on Programming Language Design and Implementation*, pp 91–105
- Alon U, Brody S, Levy O, Yahav E (2019a) code2seq: Generating sequences from structured representations of code. *International Conference on Learning Representations*
- Alon U, Zilberstein M, Levy O, Yahav E (2019b) code2vec: Learning distributed representations of code. *Proceedings of the ACM on Programming Languages* 3(POPL):1–29

- Amidi A, Amidi S, Vlachakis D, et al (2018) EnzyNet: enzyme classification using 3d convolutional neural networks on spatial representation. *PeerJ* 6:e4750
- Amizadeh S, Matuskevych S, Weimer M (2018) Learning to solve circuit-sat: An unsupervised differentiable approach. In: *International Conference on Learning Representations*
- Anand N, Huang PS (2018) Generative modeling for protein structures. In: *Proceedings of the 32nd International Conference on Neural Information Processing Systems*, pp 7505–7516
- Arjovsky M, Chintala S, Bottou L (2017) Wasserstein generative adversarial networks. In: *International Conference on Machine Learning*, pp 214–223
- Arora S (2020) A survey on graph neural networks for knowledge graph completion. *arXiv preprint arXiv:2007.12374*
- Arvind V, Köbler J, Rattan G, Verbitsky O (2015) On the power of color refinement. In: *International Symposium on Fundamentals of Computation Theory*, pp 339–350
- Arvind V, Fuhlbrück F, Köbler J, Verbitsky O (2019) On weisfeiler-leman invariance: subgraph counts and related graph properties. In: *International Symposium on Fundamentals of Computation Theory*, Springer, pp 111–125
- Ashburner M, Ball CA, Blake JA, Botstein D, Butler H, Cherry JM, Davis AP, Dolinski K, Dwight SS, Eppig JT, et al (2000) Gene ontology: tool for the unification of biology. *Nature genetics* 25(1):25–29
- Aynaz Taheri TBW Kevin Gimpel (2018) Learning graph representations with recurrent neural network autoencoders. In: *KDD'18 Deep Learning Day*
- Azizian W, Lelarge M (2020) Characterizing the expressive power of invariant and equivariant graph neural networks. *arXiv preprint arXiv:2006.15646*
- Babai L (2016) Graph isomorphism in quasipolynomial time. In: *Proceedings of the Forty-Eighth Annual ACM Symposium on Theory of Computing*, pp 684–697
- Babai L, Kucera L (1979) Canonical labelling of graphs in linear average time. In: *Foundations of Computer Science, 1979., 20th Annual Symposium on*, IEEE, pp 39–46
- Bach S, Binder A, Montavon G, Klauschen F, Müller KR, Samek W (2015) On pixel-wise explanations for non-linear classifier decisions by layer-wise relevance propagation. *PloS one* 10(7):e0130140
- Badihi S, Heydarnoori A (2017) Crowdsummarizer: Automated generation of code summaries for java programs through crowdsourcing. *IEEE Software* 34(2):71–80
- Bahdanau D, Cho K, Bengio Y (2015) Neural machine translation by jointly learning to align and translate. In: *3rd International Conference on Learning Representations*
- Bai L, Yao L, Kanhere SS, Wang X, Liu W, Yang Z (2019a) Spatio-temporal graph convolutional and recurrent networks for citywide passenger demand prediction. In: *Proceedings of the 28th ACM International Conference on Information and Knowledge Management, Association for Computing Machinery, CIKM '19*, p 2293–2296, DOI 10.1145/3357384.3358097

- Bai X, Zhu L, Liang C, Li J, Nie X, Chang X (2020a) Multi-view feature selection via nonnegative structured graph learning. *Neurocomputing* 387:110–122
- Bai Y, Ding H, Sun Y, Wang W (2018) Convolutional set matching for graph similarity. In: *NeurIPS 2018 Relational Representation Learning Workshop*
- Bai Y, Ding H, Bian S, Chen T, Sun Y, Wang W (2019b) Simgnn: A neural network approach to fast graph similarity computation. In: *Proceedings of the Twelfth ACM International Conference on Web Search and Data Mining*, pp 384–392
- Bai Y, Ding H, Qiao Y, Marinovic A, Gu K, Chen T, Sun Y, Wang W (2019c) Unsupervised inductive graph-level representation learning via graph-graph proximity. *arXiv preprint arXiv:190401098*
- Bai Y, Ding H, Gu K, Sun Y, Wang W (2020b) Learning-based efficient graph similarity computation via multi-scale convolutional set matching. In: *Proceedings of the AAAI Conference on Artificial Intelligence*, pp 3219–3226
- Bai Y, Xu D, Wang A, Gu K, Wu X, Marinovic A, Ro C, Sun Y, Wang W (2020c) Fast detection of maximum common subgraph via deep q-learning. *arXiv preprint arXiv:200203129*
- Bajaj M, Wang L, Sigal L (2019) G3raphground: Graph-based language grounding. In: *Proceedings of the IEEE/CVF International Conference on Computer Vision*, pp 4281–4290
- Baker B, Gupta O, Naik N, Raskar R (2016) Designing neural network architectures using reinforcement learning. *arXiv preprint arXiv:161102167*
- Baker CF, Ellsworth M (2017) Graph methods for multilingual framenets. In: *Proceedings of TextGraphs-11: the Workshop on Graph-based Methods for Natural Language Processing*, pp 45–50
- Balcilar M, Renton G, Héroux P, Gaüzère B, Adam S, Honeine P (2021) Analyzing the expressive power of graph neural networks in a spectral perspective. In: *International Conference on Learning Representations*
- Baldassarre F, Azizpour H (2019) Explainability techniques for graph convolutional networks. *arXiv preprint arXiv:190513686*
- Balinsky H, Balinsky A, Simske S (2011) Document sentences as a small world. In: *2011 IEEE International Conference on Systems, Man, and Cybernetics*, IEEE, pp 2583–2588
- Banarescu L, Bonial C, Cai S, Georgescu M, Griffitt K, Hermjakob U, Knight K, Koehn P, Palmer M, Schneider N (2013) Abstract meaning representation for sembanking. In: *Proceedings of the 7th linguistic annotation workshop and interoperability with discourse*, pp 178–186
- Bao H, Zhou X, Zhang Y, Li Y, Xie Y (2020) Covid-gan: Estimating human mobility responses to covid-19 pandemic through spatio-temporal conditional generative adversarial networks. In: *Proceedings of the 28th International Conference on Advances in Geographic Information Systems*, pp 273–282
- Barabási AL (2013) Network science. *Philosophical Transactions of the Royal Society A: Mathematical, Physical and Engineering Sciences* 371(1987):20120,375
- Barabási AL, Albert R (1999) Emergence of scaling in random networks. *science* 286(5439):509–512

- Barabasi AL, Oltvai ZN (2004) Network biology: Understanding the cell's functional organization. *Nature Reviews Genetics* 5(2):101–113
- Barber D (2004) Probabilistic modelling and reasoning: The junction tree algorithm. Course Notes
- Barceló P, Kostylev EV, Monet M, Pérez J, Reutter J, Silva JP (2019) The logical expressiveness of graph neural networks. In: *International Conference on Learning Representations*
- Bastian FB, Roux J, Niknejad A, Comte A, Fonseca Costa SS, De Farias TM, Moretti S, Parmentier G, De Laval VR, Rosikiewicz M, et al (2021) The bgee suite: integrated curated expression atlas and comparative transcriptomics in animals. *Nucleic Acids Research* 49(D1):D831–D847
- Bastings J, Titov I, Aziz W, Marcheggiani D, Sima'an K (2017) Graph convolutional encoders for syntax-aware neural machine translation. *arXiv preprint arXiv:1704.04675*
- Batagelj V, Zaversnik M (2003) An $o(m)$ algorithm for cores decomposition of networks. *arXiv preprint cs/0310049*
- Battaglia P, Pascanu R, Lai M, Rezende DJ, Kavukcuoglu K (2016) Interaction networks for learning about objects, relations and physics. In: *Proceedings of the 30th International Conference on Neural Information Processing Systems*, pp 4509–4517
- Battaglia PW, Hamrick JB, Bapst V, Sanchez-Gonzalez A, Zambaldi V, Malinowski M, Tacchetti A, Raposo D, Santoro A, Faulkner R, et al (2018) Relational inductive biases, deep learning, and graph networks. *arXiv preprint arXiv:1806.01261*
- Beaini D, Passaro S, Létourneau V, Hamilton WL, Corso G, Liò P (2020) Directional graph networks. *CoRR abs/2010.02863*
- Beck D, Haffari G, Cohn T (2018) Graph-to-sequence learning using gated graph neural networks. *arXiv preprint arXiv:1806.09835*
- Belghazi MI, Baratin A, Rajeswar S, Ozair S, Bengio Y, Hjelm RD, Courville AC (2018) Mutual information neural estimation. In: Dy JG, Krause A (eds) *Proceedings of the 35th International Conference on Machine Learning, ICML 2018, Stockholmsmässan, Stockholm, Sweden, July 10–15, 2018*, PMLR, *Proceedings of Machine Learning Research*, vol 80, pp 530–539
- Belkin M, Niyogi P (2002) Laplacian eigenmaps and spectral techniques for embedding and clustering. In: *Advances in neural information processing systems*, pp 585–591
- Bengio Y (2008) Neural net language models. *Scholarpedia* 3(1):3881
- Bengio Y, Senécal JS (2008) Adaptive importance sampling to accelerate training of a neural probabilistic language model. *IEEE Transactions on Neural Networks* 19(4):713–722
- Bennett J, Lanning S, et al (2007) The netflix prize. In: *Proceedings of KDD cup and workshop*, New York, vol 2007, p 35
- van den Berg R, Kipf TN, Welling M (2018) Graph convolutional matrix completion. *KDD18 Deep Learning Day*
- Berg Rvd, Kipf TN, Welling M (2017) Graph convolutional matrix completion. *arXiv preprint arXiv:1706.02263*

- Berger P, Hannak G, Matz G (2020) Efficient graph learning from noisy and incomplete data. *IEEE Trans Signal Inf Process over Networks* 6:105–119
- Berggård T, Linse S, James P (2007) Methods for the detection and analysis of protein–protein interactions. *PROTEOMICS* 7(16):2833–2842
- Berline N, Getzler E, Vergne M (2003) Heat kernels and Dirac operators. Springer Science & Business Media
- Bian R, Koh YS, Dobbie G, Divoli A (2019) Network embedding and change modeling in dynamic heterogeneous networks. In: *Proceedings of the 42nd International ACM SIGIR Conference on Research and Development in Information Retrieval*, pp 861–864
- Bianchi FM, Grattarola D, Alippi C (2020) Spectral clustering with graph neural networks for graph pooling. In: *International Conference on Machine Learning*, ACM, pp 2729–2738
- Bielik P, Raychev V, Vechev M (2017) Learning a static analyzer from data. In: *International Conference on Computer Aided Verification*, Springer, pp 233–253
- Biggs N, Lloyd EK, Wilson RJ (1986) *Graph Theory*, 1736–1936. Oxford University Press
- Bingel J, Sjøgaard A (2017) Identifying beneficial task relations for multi-task learning in deep neural networks. In: *Proceedings of the 15th Conference of the European Chapter of the Association for Computational Linguistics: Volume 2, Short Papers*, pp 164–169
- Bishop CM (2006) *Pattern recognition and machine learning*. springer
- Bizer C, Lehmann J, Kobilarov G, Auer S, Becker C, Cyganiak R, Hellmann S (2009) Dbpedia-a crystallization point for the web of data. *Journal of web semantics* 7(3):154–165
- Blitzer J, McDonald R, Pereira F (2006) Domain adaptation with structural correspondence learning. In: *Proceedings of the 2006 conference on empirical methods in natural language processing*, pp 120–128
- Bodenreider O (2004) The unified medical language system (umls): integrating biomedical terminology. *Nucleic acids research* 32(suppl_1):D267–D270
- Bojchevski A, Günnemann S (2019) Adversarial attacks on node embeddings via graph poisoning. In: *International Conference on Machine Learning*, PMLR, pp 695–704
- Bojchevski A, Günnemann S (2019) Certifiable robustness to graph perturbations. In: Wallach H, Larochelle H, Beygelzimer A, d'Alché-Buc F, Fox E, Garnett R (eds) *Advances in Neural Information Processing Systems*, Curran Associates, Inc., vol 32
- Bojchevski A, Matkovic Y, Günnemann S (2017) Robust spectral clustering for noisy data: Modeling sparse corruptions improves latent embeddings. In: *Proceedings of the 23rd ACM SIGKDD International Conference on Knowledge Discovery and Data Mining*, pp 737–746
- Bojchevski A, Shchur O, Zügner D, Günnemann S (2018) Netgan: Generating graphs via random walks. *arXiv preprint arXiv:180300816*

- Bojchevski A, Klicpera J, Günnemann S (2020a) Efficient robustness certificates for discrete data: Sparsity-aware randomized smoothing for graphs, images and more. In: International Conference on Machine Learning, PMLR, pp 1003–1013
- Bojchevski A, Klicpera J, Perozzi B, Kapoor A, Blais M, Rószemberczki B, Lukasik M, Günnemann S (2020b) Scaling graph neural networks with approximate pagerank. In: Proceedings of the 26th ACM SIGKDD International Conference on Knowledge Discovery & Data Mining, pp 2464–2473
- Bollacker K, Tufts P, Pierce T, Cook R (2007) A platform for scalable, collaborative, structured information integration. In: Intl. Workshop on Information Integration on the Web (IIWeb'07), pp 22–27
- Bollobás B (2013) Modern graph theory, vol 184. Springer Science & Business Media
- Bollobás B, Béla B (2001) Random graphs. 73, Cambridge university press
- Bollobás B, Janson S, Riordan O (2007) The phase transition in inhomogeneous random graphs. *Random Structures & Algorithms* 31(1):3–122
- Bordes A, Usunier N, Garcia-Duran A, Weston J, Yakhnenko O (2013) Translating embeddings for modeling multi-relational data. In: Neural Information Processing Systems, pp 1–9
- Bordes A, Glorot X, Weston J, Bengio Y (2014) A semantic matching energy function for learning with multi-relational data. *Machine Learning* 94(2):233–259
- Borgwardt KM, Ong CS, Schönauer S, Vishwanathan SVN, Smola AJ, Kriegel HP (2005) Protein function prediction via graph kernels. *Bioinformatics* 21(Supplement 1):i47–i56
- Borgwardt KM, Ghisu ME, Llinares-López F, O'Bray L, Rieck B (2020) Graph kernels: State-of-the-art and future challenges. *Found Trends Mach Learn* 13(5–6)
- Bose A, Hamilton W (2019) Compositional fairness constraints for graph embeddings. In: International Conference on Machine Learning, PMLR, pp 715–724
- Bottou L (1998) Online learning and stochastic approximations. *On-line learning in neural networks* 17(9):142
- Bourgain J (1985) On lipschitz embedding of finite metric spaces in hilbert space. *Israel Journal of Mathematics* 52(1–2):46–52
- Bourigault S, Lagnier C, Lamprier S, Denoyer L, Gallinari P (2014) Learning social network embeddings for predicting information diffusion. In: Proceedings of the 7th ACM international conference on Web search and data mining, pp 393–402
- Bouritsas G, Frasca F, Zafeiriou S, Bronstein MM (2020) Improving graph neural network expressivity via subgraph isomorphism counting. CoRR abs/2006.09252, [2006.09252](https://arxiv.org/abs/2006.09252)
- Boyd S, Boyd SP, Vandenberghe L (2004) Convex optimization. Cambridge university press
- Braschi B, Denny P, Gray K, Jones T, Seal R, Tweedie S, Yates B, Bruford E (2017) Genenames. org: the hgnc and vgc resources in
- Brauckmann A, Goens A, Ertel S, Castrillon J (2020) Compiler-based graph representations for deep learning models of code. In: Proceedings of the 29th International Conference on Compiler Construction, pp 201–211

- Braude EJ, Bernstein ME (2016) Software engineering: modern approaches. Wave-land Press
- Brin S, Page L (1998) The anatomy of a large-scale hypertextual web search engine. *Computer networks and ISDN systems* 30(1-7):107–117
- Brin S, Page L (2012) Reprint of: The anatomy of a large-scale hypertextual web search engine. *Computer networks* 56(18):3825–3833
- Brockschmidt M (2020) GNN-FiLM: Graph neural networks with feature-wise linear modulation. In: III HD, Singh A (eds) *Proceedings of the 37th International Conference on Machine Learning*, PMLR, Virtual, *Proceedings of Machine Learning Research*, vol 119, pp 1144–1152
- Bronstein MM, Bruna J, LeCun Y, Szlam A, Vandergheynst P (2017) Geometric deep learning: going beyond euclidean data. *IEEE Signal Processing Magazine* 34(4):18–42
- Browne F, Wang H, Zheng H, et al (2007) Supervised statistical and machine learning approaches to inferring pairwise and module-based protein interaction networks. In: 2007 IEEE 7th International Symposium on BioInformatics and Bio-Engineering, pp 1365–1369, DOI 10.1109/BIBE.2007.4375748
- Bruna J, Zaremba W, Szlam A, LeCun Y (2014) Spectral networks and deep locally connected networks on graphs. In: 2nd International Conference on Learning Representations, ICLR 2014
- Bui TN, Chaudhuri S, Leighton FT, Sipser M (1987) Graph bisection algorithms with good average case behavior. *Combinatorica* 7(2):171–191
- Bunke H (1997) On a relation between graph edit distance and maximum common subgraph. *Pattern Recognition Letters* 18(8):689–694
- Burt RS (2004) Structural holes and good ideas. *American journal of sociology* 110(2):349–399
- Byron O, Vestergaard B (2015) Protein–protein interactions: a supra-structural phenomenon demanding trans-disciplinary biophysical approaches. *Current Opinion in Structural Biology* 35:76 – 86, catalysis and regulation • Protein-protein interactions
- Cai D, Lam W (2020) Graph transformer for graph-to-sequence learning. In: *Proceedings of the AAAI Conference on Artificial Intelligence*, vol 34, pp 7464–7471
- Cai H, Chen T, Zhang W, Yu Y, Wang J (2018a) Efficient architecture search by network transformation. In: *Proceedings of the AAAI Conference on Artificial Intelligence*, vol 32
- Cai H, Zheng VW, Chang KCC (2018b) A comprehensive survey of graph embedding: Problems, techniques, and applications. *IEEE Transactions on Knowledge and Data Engineering* 30(9):1616–1637
- Cai H, Gan C, Wang T, Zhang Z, Han S (2020a) Once for all: Train one network and specialize it for efficient deployment. In: *ICLR*
- Cai H, Gan C, Zhu L, Han S (2020b) Tinytl: Reduce memory, not parameters for efficient on-device learning. *Advances in Neural Information Processing Systems* 33

- Cai JY, Fürer M, Immerman N (1992) An optimal lower bound on the number of variables for graph identification. *Combinatorica* 12(4):389–410
- Cai L, Ji S (2020) A multi-scale approach for graph link prediction. In: *Proceedings of the AAAI Conference on Artificial Intelligence*, vol 34, pp 3308–3315
- Cai L, Yan B, Mai G, Janowicz K, Zhu R (2019) Transgcnn: Coupling transformation assumptions with graph convolutional networks for link prediction. In: *Proceedings of the 10th International Conference on Knowledge Capture*, pp 131–138
- Cai L, Li J, Wang J, Ji S (2020c) Line graph neural networks for link prediction. *arXiv preprint arXiv:201010046*
- Cai T, Luo S, Xu K, He D, Liu Ty, Wang L (2020d) Graphnorm: A principled approach to accelerating graph neural network training. *arXiv preprint arXiv:200903294*
- Cai X, Han J, Yang L (2018c) Generative adversarial network based heterogeneous bibliographic network representation for personalized citation recommendation. In: *Proceedings of the AAAI Conference on Artificial Intelligence*, vol 32
- Cai Z, Wen L, Lei Z, Vasconcelos N, Li SZ (2014) Robust deformable and occluded object tracking with dynamic graph. *IEEE Transactions on Image Processing* 23(12):5497–5509
- Cairong Z, Xinran Z, Cheng Z, Li Z (2016) A novel dbn feature fusion model for cross-corpus speech emotion recognition. *Journal of Electrical and Computer Engineering* 2016
- Cangea C, Velickovic P, Jovanovic N, Kipf T, Liò P (2018) Towards sparse hierarchical graph classifiers. *CoRR* abs/1811.01287
- Cao S, Lu W, Xu Q (2015) Grarep: Learning graph representations with global structural information. In: *Proceedings of the 24th ACM international on conference on information and knowledge management*, pp 891–900
- Cao Y, Peng H, Philip SY (2020) Multi-information source hin for medical concept embedding. In: *Pacific-Asia Conference on Knowledge Discovery and Data Mining*, Springer, pp 396–408
- Cao Z, Simon T, Wei SE, Sheikh Y (2017) Realtime multi-person 2d pose estimation using part affinity fields. In: *Proceedings of the IEEE conference on computer vision and pattern recognition*, pp 7291–7299
- Cao Z, Hidalgo G, Simon T, Wei SE, Sheikh Y (2019) Openpose: realtime multi-person 2d pose estimation using part affinity fields. *IEEE transactions on pattern analysis and machine intelligence* 43(1):172–186
- Cappart Q, Chételat D, Khalil E, Lodi A, Morris C, Veličković P (2021) Combinatorial optimization and reasoning with graph neural networks. *CoRR* abs/2102.09544
- Carlini N, Wagner D (2017) Towards Evaluating the Robustness of Neural Networks. *IEEE Symposium on Security and Privacy* pp 39–57, DOI 10.1109/SP.2017.49
- Caron M, Bojanowski P, Joulin A, Douze M (2018) Deep clustering for unsupervised learning of visual features. In: *Proceedings of the European Conference on Computer Vision (ECCV)*, pp 132–149

- Carreira J, Zisserman A (2017) Quo vadis, action recognition? a new model and the kinetics dataset. In: proceedings of the IEEE Conference on Computer Vision and Pattern Recognition, pp 6299–6308
- Cartwright D, Harary F (1956) Structural balance: a generalization of heider's theory. *Psychological review* 63(5):277
- Cen Y, Zou X, Zhang J, Yang H, Zhou J, Tang J (2019) Representation learning for attributed multiplex heterogeneous network. In: Proceedings of the 25th ACM SIGKDD International Conference on Knowledge Discovery & Data Mining, pp 1358–1368
- Cetoli A, Bragaglia S, O'Harney A, Sloan M (2017) Graph convolutional networks for named entity recognition. In: Proceedings of the 16th International Workshop on Treebanks and Linguistic Theories, pp 37–45
- Chakrabarti D, Faloutsos C (2006) Graph mining: Laws, generators, and algorithms. *ACM computing surveys (CSUR)* 38(1)
- Chami I, Ying Z, Ré C, Leskovec J (2019) Hyperbolic graph convolutional neural networks. In: Advances in neural information processing systems, pp 4868–4879
- Chami I, Abu-El-Haija S, Perozzi B, Ré C, Murphy K (2020) Machine learning on graphs: A model and comprehensive taxonomy. *CoRR* abs/2005.03675
- Chang B, Jang G, Kim S, Kang J (2020a) Learning graph-based geographical latent representation for point-of-interest recommendation. In: Proceedings of the 29th ACM International Conference on Information & Knowledge Management, pp 135–144
- Chang H, Rong Y, Xu T, Huang W, Zhang H, Cui P, Zhu W, Huang J (2020b) A Restricted Black-Box Adversarial Framework Towards Attacking Graph Embedding Models. In: AAAI Conference on Artificial Intelligence, vol 34, pp 3389–3396, DOI 10.1609/aaai.v34i04.5741
- Chang J, Scherer S (2017) Learning representations of emotional speech with deep convolutional generative adversarial networks. In: 2017 IEEE International Conference on Acoustics, Speech and Signal Processing (ICASSP), IEEE, pp 2746–2750
- Chang S (2018) Scaling knowledge access and retrieval at airbnb. *Airbnb Engineering and Data Science*
- Chang S, Han W, Tang J, Qi GJ, Aggarwal CC, Huang TS (2015) Heterogeneous network embedding via deep architectures. In: Proceedings of the 21th ACM SIGKDD international conference on knowledge discovery and data mining, pp 119–128
- Chao YW, Vijayanarasimhan S, Seybold B, Ross DA, Deng J, Sukthankar R (2018) Rethinking the faster r-cnn architecture for temporal action localization. In: Proceedings of the IEEE Conference on Computer Vision and Pattern Recognition, pp 1130–1139
- Chen B, Sun L, Han X (2018a) Sequence-to-action: End-to-end semantic graph generation for semantic parsing. *arXiv preprint arXiv:180900773*
- Chen B, Barzilay R, Jaakkola T (2019a) Path-augmented graph transformer network. *ICML 2019 Workshop on Learning and Reasoning with Graph-Structured Data*

- Chen B, Zhang J, Zhang X, Tang X, Cai L, Chen H, Li C, Zhang P, Tang J (2020a) Coad: Contrastive pre-training with adversarial fine-tuning for zero-shot expert linking. arXiv preprint arXiv:201211336
- Chen C, Li K, Teo SG, Zou X, Wang K, Wang J, Zeng Z (2019b) Gated residual recurrent graph neural networks for traffic prediction. In: Proceedings of the AAAI Conference on Artificial Intelligence, vol 33, pp 485–492
- Chen D, Lin Y, Li L, Li XR, Zhou J, Sun X, et al (2020b) Distance-wise graph contrastive learning. arXiv preprint arXiv:201207437
- Chen D, Lin Y, Li W, Li P, Zhou J, Sun X (2020c) Measuring and relieving the over-smoothing problem for graph neural networks from the topological view. In: The Thirty-Fourth AAAI Conference on Artificial Intelligence, AAAI 2020, The Thirty-Second Innovative Applications of Artificial Intelligence Conference, IAAI 2020, The Tenth AAAI Symposium on Educational Advances in Artificial Intelligence, EAAI 2020, New York, NY, USA, February 7-12, 2020, AAAI Press, pp 3438–3445
- Chen H, Yin H, Wang W, Wang H, Nguyen QVH, Li X (2018b) Pme: projected metric embedding on heterogeneous networks for link prediction. In: Proceedings of the 24th ACM SIGKDD International Conference on Knowledge Discovery & Data Mining, pp 1177–1186
- Chen H, Xu Y, Huang F, Deng Z, Huang W, Wang S, He P, Li Z (2020d) Label-aware graph convolutional networks. In: The 29th ACM International Conference on Information and Knowledge Management, pp 1977–1980
- Chen IY, Agrawal M, Horng S, Sontag D (2020e) Robustly extracting medical knowledge from ehers: A case study of learning a health knowledge graph. In: Pac Symp Biocomput, World Scientific, pp 19–30
- Chen J, Ma T, Xiao C (2018c) Fastgcn: Fast learning with graph convolutional networks via importance sampling. In: International Conference on Learning Representations
- Chen J, Zhu J, Song L (2018d) Stochastic training of graph convolutional networks with variance reduction. In: International Conference on Machine Learning, PMLR, pp 942–950
- Chen J, Chen Y, Zheng H, Shen S, Yu S, Zhang D, Xuan Q (2020f) MGA: Momentum Gradient Attack on Network. IEEE Transactions on Computational Social Systems pp 1–10, DOI 10.1109/TCSS.2020.3031058
- Chen J, Lei B, Song Q, Ying H, Chen DZ, Wu J (2020g) A hierarchical graph network for 3d object detection on point clouds. In: Proceedings of the IEEE/CVF Conference on Computer Vision and Pattern Recognition, pp 392–401
- Chen J, Lin X, Shi Z, Liu Y (2020h) Link Prediction Adversarial Attack Via Iterative Gradient Attack. IEEE Transactions on Computational Social Systems 7(4):1081–1094, DOI 10.1109/TCSS.2020.3004059
- Chen J, Lin X, Xiong H, Wu Y, Zheng H, Xuan Q (2020i) Smoothing Adversarial Training for GNN. IEEE Transactions on Computational Social Systems pp 1–12, DOI 10.1109/TCSS.2020.3042628

- Chen J, Xu H, Wang J, Xuan Q, Zhang X (2020j) Adversarial Detection on Graph Structured Data. In: Workshop on Privacy-Preserving Machine Learning in Practice
- Chen L, Tan B, Long S, Yu K (2018e) Structured dialogue policy with graph neural networks. In: Proceedings of the 27th International Conference on Computational Linguistics, pp 1257–1268
- Chen L, Chen Z, Bruna J (2020k) On graph neural networks versus graph-augmented mlps. arXiv preprint arXiv:201015116
- Chen M, Wei Z, Huang Z, Ding B, Li Y (2020l) Simple and deep graph convolutional networks. In: International Conference on Machine Learning, PMLR, pp 1725–1735
- Chen Q, Zhou M (2018) A neural framework for retrieval and summarization of source code. In: 2018 33rd IEEE/ACM International Conference on Automated Software Engineering (ASE), IEEE, pp 826–831
- Chen T, Sun Y (2017) Task-guided and path-augmented heterogeneous network embedding for author identification. In: Proceedings of the Tenth ACM International Conference on Web Search and Data Mining, pp 295–304
- Chen T, Li M, Li Y, Lin M, Wang N, Wang M, Xiao T, Xu B, Zhang C, Zhang Z (2015) Mxnet: A flexible and efficient machine learning library for heterogeneous distributed systems. arXiv preprint arXiv:151201274
- Chen T, Bian S, Sun Y (2019c) Are powerful graph neural nets necessary? a dissection on graph classification. arXiv preprint arXiv:190504579
- Chen X, Ma H, Wan J, Li B, Xia T (2017) Multi-view 3d object detection network for autonomous driving. In: Proceedings of the IEEE conference on Computer Vision and Pattern Recognition, pp 1907–1915
- Chen XW, Liu M (2005) Prediction of protein–protein interactions using random decision forest framework. *Bioinformatics* 21(24):4394–4400
- Chen Y, Rohrbach M, Yan Z, Shuicheng Y, Feng J, Kalantidis Y (2019d) Graph-based global reasoning networks. In: Proceedings of the IEEE/CVF Conference on Computer Vision and Pattern Recognition, pp 433–442
- Chen Y, Wu L, Zaki M (2020m) Iterative deep graph learning for graph neural networks: Better and robust node embeddings. *Advances in Neural Information Processing Systems* 33
- Chen Y, Wu L, Zaki MJ (2020n) Graphflow: Exploiting conversation flow with graph neural networks for conversational machine comprehension. In: Proceedings of the Twenty-Ninth International Joint Conference on Artificial Intelligence, pp 1230–1236
- Chen Y, Wu L, Zaki MJ (2020o) Reinforcement learning based graph-to-sequence model for natural question generation. In: 8th International Conference on Learning Representations
- Chen Y, Wu L, Zaki MJ (2020p) Toward subgraph guided knowledge graph question generation with graph neural networks. arXiv preprint arXiv:200406015
- Chen YC, Bansal M (2018) Fast abstractive summarization with reinforce-selected sentence rewriting. arXiv preprint arXiv:180511080

- Chen YW, Song Q, Hu X (2021) Techniques for automated machine learning. *ACM SIGKDD Explorations Newsletter* 22(2):35–50
- Chen Z, Kommrusch SJ, Tufano M, Pouchet LN, Poshyvanyk D, Monperrus M (2019e) Sequencer: Sequence-to-sequence learning for end-to-end program repair. *IEEE Transactions on Software Engineering* pp 1–1, DOI 10.1109/TSE.2019.2940179
- Chen Z, Villar S, Chen L, Bruna J (2019f) On the equivalence between graph isomorphism testing and function approximation with gnns. In: *Advances in Neural Information Processing Systems*, pp 15,868–15,876
- Chen Z, Chen L, Villar S, Bruna J (2020q) Can graph neural networks count substructures? vol 33
- Chenxi Liu FSHAWHAYLFF Liang-Chieh Chen (2019) Auto-deeplab: Hierarchical neural architecture search for semantic image segmentation. *arXiv preprint arXiv:190102985*
- Chiang WL, Liu X, Si S, Li Y, Bengio S, Hsieh CJ (2019) Cluster-gcn: An efficient algorithm for training deep and large graph convolutional networks. In: *ACM SIGKDD International Conference on Knowledge Discovery and Data Mining (KDD)*, pp 257–266
- Chibotaru V, Bichsel B, Raychev V, Vechev M (2019) Scalable taint specification inference with big code. In: *Proceedings of the 40th ACM SIGPLAN Conference on Programming Language Design and Implementation*, pp 760–774
- Chidambaram M, Yang Y, Cer D, Yuan S, Sung YH, Strope B, Kurzweil R (2019) Learning cross-lingual sentence representations via a multi-task dual-encoder model. *ACL 2019* p 250
- Chien E, Peng J, Li P, Milenkovic O (2021) Adaptive universal generalized pagerank graph neural network. In: *International Conference on Learning Representations*
- Chiu PH, Hripcsak G (2017) Ehr-based phenotyping: bulk learning and evaluation. *Journal of biomedical informatics* 70:35–51
- Cho K, van Merriënboer B, Gulcehre C, Bahdanau D, Bougares F, Schwenk H, Bengio Y (2014a) Learning phrase representations using RNN encoder–decoder for statistical machine translation. In: *Proceedings of the 2014 Conference on Empirical Methods in Natural Language Processing (EMNLP)*, Association for Computational Linguistics, Doha, Qatar, pp 1724–1734, DOI 10.3115/v1/D14-1179
- Cho M, Lee J, Lee KM (2010) Reweighted random walks for graph matching. In: *European conference on Computer vision*, Springer, pp 492–505
- Cho M, Sun J, Duchenne O, Ponce J (2014b) Finding matches in a haystack: A max-pooling strategy for graph matching in the presence of outliers. In: *IEEE Conference on Computer Vision and Pattern Recognition*, pp 2083–2090
- Choi E, Xu Z, Li Y, Dusenberry M, Flores G, Xue E, Dai AM (2020) Learning the graphical structure of electronic health records with graph convolutional transformer. In: *The Thirty-Fourth AAAI Conference on Artificial Intelligence*, pp 606–613
- Choromanski K, Likhoshervstov V, Dohan D, Song X, Gane A, Sarlós T, Hawkins P, Davis J, Mohiuddin A, Kaiser L, Belanger D, Colwell L, Weller A (2021)

- Rethinking attention with performers. In: International Conference on Learning Representations
- Chorowski J, Weiss RJ, Bengio S, van den Oord A (2019) Unsupervised speech representation learning using wavenet autoencoders. *IEEE/ACM transactions on audio, speech, and language processing* 27(12):2041–2053
- Chung F (2007) The heat kernel as the pagerank of a graph. *Proceedings of the National Academy of Sciences* 104(50):19,735–19,740
- Chung J, Gulcehre C, Cho K, Bengio Y (2014) Empirical evaluation of gated recurrent neural networks on sequence modeling. *arXiv preprint arXiv:1412.3555*
- Cohen J, Rosenfeld E, Kolter Z (2019) Certified adversarial robustness via randomized smoothing. In: *International Conference on Machine Learning*, PMLR, pp 1310–1320
- Cohen N, Shashua A (2016) Convolutional rectifier networks as generalized tensor decompositions. In: *International Conference on Machine Learning*, PMLR, pp 955–963
- Collard ML, Decker MJ, Maletic JI (2011) Lightweight transformation and fact extraction with the srcml toolkit. In: *Source Code Analysis and Manipulation (SCAM)*, 2011 11th IEEE International Working Conference on, IEEE, pp 173–184
- Collobert R, Weston J, Bottou L, Karlen M, Kavukcuoglu K, Kuksa P (2011) Natural language processing (almost) from scratch. *Journal of machine learning research* 12(ARTICLE):2493–2537
- Colson B, Marcotte P, Savard G (2007) An overview of bilevel optimization. *Annals of operations research* 153(1):235–256
- mypy Contributors (2021) mypy - optional static typing for Python. <http://mypy-lang.org/>, accessed: 2021-01-30
- Corso G, Cavalleri L, ini D, Liò P, Velickovic P (2020) Principal neighbourhood aggregation for graph nets. *CoRR abs/2004.05718*
- Cortés-Coy LF, Linares-Vásquez M, Aponte J, Poshyvanyk D (2014) On automatically generating commit messages via summarization of source code changes. In: *2014 IEEE 14th International Working Conference on Source Code Analysis and Manipulation*, IEEE, pp 275–284
- Cosmo L, Kazi A, Ahmadi SA, Navab N, Bronstein M (2020) Latent patient network learning for automatic diagnosis. *arXiv preprint arXiv:2003.13620*
- Costa F, De Grave K (2010) Fast neighborhood subgraph pairwise distance kernel. In: *International Conference on Machine Learning*, Omnipress, pp 255–262
- Cotto KC, Wagner AH, Feng YY, Kiwala S, Coffman AC, Spies G, Wollam A, Spies NC, Griffith OL, Griffith M (2018) Dgidb 3.0: a redesign and expansion of the drug–gene interaction database. *Nucleic acids research* 46(D1):D1068–D1073
- Cozzetto D, Minneci F, Currant H, et al (2016) FFPred 3: feature-based function prediction for all gene ontology domains. *Scientific Reports* 6(1)
- Cucurull G, Taslakian P, Vazquez D (2019) Context-aware visual compatibility prediction. In: *Proceedings of the IEEE/CVF Conference on Computer Vision and Pattern Recognition*, pp 12,617–12,626

- Cui J, Kingsbury B, Ramabhadran B, Sethy A, Audhkhasi K, Cui X, Kislal E, Mangu L, Nussbaum-Thom M, Picheny M, et al (2015) Multilingual representations for low resource speech recognition and keyword search. In: 2015 IEEE Workshop on Automatic Speech Recognition and Understanding (ASRU), IEEE, pp 259–266
- Cui P, Wang X, Pei J, Zhu W (2018) A survey on network embedding. *IEEE Transactions on Knowledge and Data Engineering* 31(5):833–852
- Cui Z, Henrickson K, Ke R, Wang Y (2019) Traffic graph convolutional recurrent neural network: A deep learning framework for network-scale traffic learning and forecasting. *IEEE Transactions on Intelligent Transportation Systems* 21(11):4883–4894
- Cummins C, Fisches ZV, Ben-Nun T, Hoefler T, Leather H (2020) Programl: Graph-based deep learning for program optimization and analysis. *arXiv preprint arXiv:2003.10536*
- Cussens J (2011) Bayesian network learning with cutting planes. In: *Proceedings of the Twenty-Seventh Conference on Uncertainty in Artificial Intelligence*, pp 153–160
- Cvitkovic M, Singh B, Anandkumar A (2018) Deep learning on code with an unbounded vocabulary. In: *Machine Learning for Programming*
- Cybenko G (1989) Approximation by superpositions of a sigmoidal function. *Mathematics of control, signals and systems* 2(4):303–314
- Cygan M, Pilipczuk M, Pilipczuk M, Wojtaszczyk JO (2012) Sitting closer to friends than enemies, revisited. In: *International Symposium on Mathematical Foundations of Computer Science*, Springer, pp 296–307
- Dabkowski P, Gal Y (2017) Real time image saliency for black box classifiers. *arXiv preprint arXiv:1705.07857*
- Dahl G, Ranzato M, Mohamed Ar, Hinton GE (2010) Phone recognition with the mean-covariance restricted boltzmann machine. *Advances in neural information processing systems* 23:469–477
- Dai B, Zhang Y, Lin D (2017) Detecting visual relationships with deep relational networks. In: *Proceedings of the IEEE conference on computer vision and Pattern recognition*, pp 3076–3086
- Dai H, Dai B, Song L (2016) Discriminative embeddings of latent variable models for structured data. In: *International conference on machine learning*, PMLR, pp 2702–2711
- Dai H, Li H, Tian T, Huang X, Wang L, Zhu J, Song L (2018a) Adversarial attack on graph structured data. In: *International conference on machine learning*, PMLR, pp 1115–1124
- Dai H, Tian Y, Dai B, Skiena S, Song L (2018b) Syntax-directed variational autoencoder for structured data. *arXiv preprint arXiv:1802.08786*
- Dai Q, Li Q, Tang J, Wang D (2018c) Adversarial network embedding. In: *Proceedings of the AAAI Conference on Artificial Intelligence*, vol 32
- Dai R, Xu S, Gu Q, Ji C, Liu K (2020) Hybrid spatio-temporal graph convolutional network: Improving traffic prediction with navigation data. In: *Proceedings of the*

- 26th ACM SIGKDD International Conference on Knowledge Discovery & Data Mining, pp 3074–3082
- Daitch SI, Kelner JA, Spielman DA (2009) Fitting a graph to vector data. In: Proceedings of the 26th Annual International Conference on Machine Learning, pp 201–208
- Damonte M, Cohen SB (2019) Structural neural encoders for amr-to-text generation. arXiv preprint arXiv:1903.11410
- Dana JM, Gutmanas A, Tyagi N, et al (2018) SIFTS: updated structure integration with function, taxonomy and sequences resource allows 40-fold increase in coverage of structure-based annotations for proteins. *Nucleic Acids Research* 47(D1):D482–D489
- Das S, Lee D, Sillitoe I, et al (2015) Functional classification of CATH superfamilies: a domain-based approach for protein function annotation. *Bioinformatics* 31(21):3460–3467
- Dasgupta SS, Ray SN, Talukdar P (2018) HYTE: Hyperplane-based temporally aware knowledge graph embedding. In: Empirical Methods in Natural Language Processing, pp 2001–2011
- Davidson TR, Falorsi L, De Cao N, Kipf T, Tomczak JM (2018) Hyperspherical variational auto-encoders. In: 34th Conference on Uncertainty in Artificial Intelligence 2018, UAI 2018, Association For Uncertainty in Artificial Intelligence (AUAI), pp 856–865
- Davis AP, Grondin CJ, Johnson RJ, Sciaky D, McMorran R, Wiegers J, Wiegers TC, Mattingly CJ (2019) The comparative toxicogenomics database: update 2019. *Nucleic acids research* 47(D1):D948–D954
- De Cao N, Kipf T (2018) Molgan: An implicit generative model for small molecular graphs. arXiv preprint arXiv:1805.11973
- De Lucia A, Di Penta M, Oliveto R, Panichella A, Panichella S (2012) Using ir methods for labeling source code artifacts: Is it worthwhile? In: 2012 20th IEEE International Conference on Program Comprehension (ICPC), IEEE, pp 193–202
- Dearman D, Cox A, Fisher M (2005) Adding control-flow to a visual data-flow representation. In: 13th International Workshop on Program Comprehension (IWPC'05), IEEE, pp 297–306
- Defferrard M, X B, Vandergheynst P (2016) Convolutional neural networks on graphs with fast localized spectral filtering. In: Advances in Neural Information Processing Systems, pp 3844–3852
- Delaney JS (2004) Esol: estimating aqueous solubility directly from molecular structure. *Journal of chemical information and computer sciences* 44(3):1000–1005
- Deng C, Zhao Z, Wang Y, Zhang Z, Feng Z (2020) Graphzoom: A multi-level spectral approach for accurate and scalable graph embedding. In: International Conference on Learning Representations
- Deng Z, Dong Y, Zhu J (2019) Batch Virtual Adversarial Training for Graph Convolutional Networks. In: ICML 2019 Workshop: Learning and Reasoning with Graph-Structured Representations

- Desa U (2018) Revision of world urbanization prospects. UN Department of Economic and Social Affairs 16
- Dettmers T, Minervini P, Stenetorp P, Riedel S (2018) Convolutional 2d knowledge graph embeddings. In: Proceedings of the AAAI Conference on Artificial Intelligence, vol 32
- Devlin J, Chang MW, Lee K, Toutanova K (2019) BERT: Pre-training of deep bidirectional transformers for language understanding. In: Proceedings of the 2019 Conference of the North American Chapter of the Association for Computational Linguistics: Human Language Technologies, Volume 1 (Long and Short Papers), Association for Computational Linguistics, Minneapolis, Minnesota, pp 4171–4186, DOI 10.18653/v1/N19-1423
- Dhillon IS, Guan Y, Kulis B (2007) Weighted graph cuts without eigenvectors a multilevel approach. *IEEE Transactions on Pattern Analysis and Machine Intelligence* 29(11):1944–1957
- Diao Z, Wang X, Zhang D, Liu Y, Xie K, He S (2019) Dynamic spatial-temporal graph convolutional neural networks for traffic forecasting. In: Proceedings of the AAAI Conference on Artificial Intelligence, vol 33, pp 890–897
- Dinella E, Dai H, Li Z, Naik M, Song L, Wang K (2020) Hoppity: Learning graph transformations to detect and fix bugs in programs. In: International Conference on Learning Representations (ICLR)
- Ding M, Zhou C, Chen Q, Yang H, Tang J (2019a) Cognitive graph for multi-hop reading comprehension at scale. In: Proceedings of the 57th Annual Meeting of the Association for Computational Linguistics, pp 2694–2703
- Ding S, Qu S, Xi Y, Sangaiah AK, Wan S (2019b) Image caption generation with high-level image features. *Pattern Recognition Letters* 123:89–95
- Ding Y, Yao Q, Zhang T (2020a) Propagation model search for graph neural networks. *arXiv preprint arXiv:201003250*
- Ding Y, Zhou X, Bao H, Li Y, Hamann C, Spears S, Yuan Z (2020b) Cycling-net: A deep learning approach to predicting cyclist behaviors from geo-referenced egocentric video data. *Association for Computing Machinery, SIGSPATIAL '20*, p 337–346, DOI 10.1145/3397536.3422258
- Do K, Tran T, Venkatesh S (2019) Graph transformation policy network for chemical reaction prediction. In: Proceedings of the 25th ACM SIGKDD International Conference on Knowledge Discovery & Data Mining, pp 750–760
- Doersch C, Gupta A, Efros AA (2015) Unsupervised visual representation learning by context prediction. In: 2015 IEEE International Conference on Computer Vision, ICCV 2015, Santiago, Chile, December 7–13, 2015, IEEE Computer Society, pp 1422–1430, DOI 10.1109/ICCV.2015.167
- Dohkan S, Koike A, Takagi T (2006) Improving the performance of an svm-based method for predicting protein-protein interactions. *In Silico Biology* 6:515–529, 6
- Domingo-Fernández D, Baksi S, Schultz B, Gadiya Y, Karki R, Raschka T, Ebeling C, Hofmann-Apitius M, et al (2020) Covid-19 knowledge graph: a computable, multi-modal, cause-and-effect knowledge model of covid-19 pathophysiology. *BioRxiv*

- Donahue C, McAuley J, Puckette M (2018) Synthesizing audio with generative adversarial networks. arXiv preprint arXiv:180204208 1
- Donahue J, Anne Hendricks L, Guadarrama S, Rohrbach M, Venugopalan S, Saenko K, Darrell T (2015) Long-term recurrent convolutional networks for visual recognition and description. In: Proceedings of the IEEE conference on computer vision and pattern recognition, pp 2625–2634
- Doncheva NT, Morris JH, Gorodkin J, Jensen LJ (2018) Cytoscape StringApp: Network analysis and visualization of proteomics data. *Journal of Proteome Research* 18(2):623–632
- Dong X, Gabrilovich E, Heitz G, Horn W, Lao N, Murphy K, Strohmman T, Sun S, Zhang W (2014) Knowledge vault: A web-scale approach to probabilistic knowledge fusion. In: Proceedings of the 20th ACM SIGKDD international conference on Knowledge discovery and data mining, pp 601–610
- Dong X, Thanou D, Frossard P, Vandergheynst P (2016) Learning laplacian matrix in smooth graph signal representations. *IEEE Transactions on Signal Processing* 64(23):6160–6173
- Dong X, Thanou D, Rabbat M, Frossard P (2019) Learning graphs from data: A signal representation perspective. *IEEE Signal Processing Magazine* 36(3):44–63
- Dong Y, Chawla NV, Swami A (2017) metapath2vec: Scalable representation learning for heterogeneous networks. In: Proceedings of the 23rd ACM SIGKDD international conference on knowledge discovery and data mining, pp 135–144
- Donsker M, Varadhan S (1976) Asymptotic evaluation of certain markov process expectations for large time—iii. *Communications on Pure and Applied Mathematics* 29(4):389–461, copyright: Copyright 2016 Elsevier B.V., All rights reserved.
- Dos Santos C, Gatti M (2014) Deep convolutional neural networks for sentiment analysis of short texts. In: Proceedings of COLING 2014, the 25th International Conference on Computational Linguistics: Technical Papers, pp 69–78
- Dosovitskiy A, Springenberg JT, Riedmiller MA, Brox T (2014) Discriminative unsupervised feature learning with convolutional neural networks. In: Ghahramani Z, Welling M, Cortes C, Lawrence ND, Weinberger KQ (eds) *Advances in Neural Information Processing Systems 27: Annual Conference on Neural Information Processing Systems 2014, December 8-13 2014, Montreal, Quebec, Canada*, pp 766–774
- Dosovitskiy A, et al (2021) An image is worth 16x16 words: Transformers for image recognition at scale. *ICLR*
- Dou Y, Liu Z, Sun L, Deng Y, Peng H, Yu PS (2020) Enhancing graph neural network-based fraud detectors against camouflaged fraudsters. In: Proceedings of the 29th ACM International Conference on Information & Knowledge Management, pp 315–324
- Du M, Liu N, Yang F, Hu X (2019) Learning credible deep neural networks with rationale regularization. In: 2019 IEEE International Conference on Data Mining (ICDM), IEEE, pp 150–159
- Du M, Yang F, Zou N, Hu X (2020) Fairness in deep learning: A computational perspective. *IEEE Intelligent Systems*

- Duvenaud DK, Maclaurin D, Iparraguirre J, Bombarell R, Hirzel T, Aspuru-Guzik A, Adams RP (2015a) Convolutional networks on graphs for learning molecular fingerprints. In: *Advances in neural information processing systems*, pp 2224–2232
- Duvenaud DK, Maclaurin D, Iparraguirre J, Bombarell R, Hirzel T, Aspuru-Guzik A, Adams RP (2015b) Convolutional networks on graphs for learning molecular fingerprints. In: *Advances in Neural Information Processing Systems*, pp 2224–2232
- Dvijotham KD, Hayes J, Balle B, Kolter Z, Qin C, Gyorgy A, Xiao K, Goyal S, Kohli P (2020) A framework for robustness certification of smoothed classifiers using f-divergences. In: *International Conference on Learning Representations, ICLR*
- Dwivedi VP, Joshi CK, Laurent T, Bengio Y, Bresson X (2020) Benchmarking graph neural networks. *arXiv preprint arXiv:200300982*
- Dyer C, Ballesteros M, Ling W, Matthews A, Smith NA (2015) Transition-based dependency parsing with stack long short-term memory. *arXiv preprint arXiv:150508075*
- Easley D, Kleinberg J, et al (2012) Networks, crowds, and markets: Reasoning about a highly connected world. *Significance* 9(1):43–44
- Eksombatchai C, Jindal P, Liu JZ, Liu Y, Sharma R, Sugnet C, Ulrich M, Leskovec J (2018) Pixie: A system for recommending 3+ billion items to 200+ million users in real-time. In: *Proceedings of the 2018 world wide web conference*, pp 1775–1784
- Elinas P, Bonilla EV, Tiao L (2020) Variational inference for graph convolutional networks in the absence of graph data and adversarial settings. In: *Advances in Neural Information Processing Systems*, vol 33, pp 18,648–18,660
- Elkan C, Noto K (2008) Learning classifiers from only positive and unlabeled data. In: *Proceedings of the 14th ACM SIGKDD international conference on Knowledge discovery and data mining*, pp 213–220
- Elman JL (1990) Finding structure in time. *Cognitive Science* 14(2):179–211
- Elmsallati A, Clark C, Kalita J (2016) Global alignment of protein-protein interaction networks: A survey. *IEEE/ACM Trans Comput Biol Bioinformatics* 13(4):689–705
- Entezari N, Al-Sayouri SA, Darvishzadeh A, Papalexakis EE (2020) All you need is low (rank) defending against adversarial attacks on graphs. In: *Proceedings of the 13th International Conference on Web Search and Data Mining*, pp 169–177
- Erdős P, Rényi A (1959) On random graphs i. *Publ Math Debrecen* 6:290–297
- Erdős P, Rényi A (1960) On the evolution of random graphs. *Publ Math Inst Hung Acad Sci* 5(1):17–60
- Erkan G, Radev DR (2004) Lexrank: Graph-based lexical centrality as salience in text summarization. *Journal of artificial intelligence research* 22:457–479
- Ernst MD, Perkins JH, Guo PJ, McCamant S, Pacheco C, Tschantz MS, Xiao C (2007) The Daikon system for dynamic detection of likely invariants. *Science of computer programming* 69(1-3):35–45

- Eykholt K, Evtimov I, Fernandes E, Li B, Rahmati A, Xiao C, Prakash A, Kohno T, Song D (2018) Robust physical-world attacks on deep learning visual classification. In: IEEE Conference on Computer Vision and Pattern Recognition, CVPR, pp 1625–1634
- Faghri F, Fleet DJ, Kiros JR, Fidler S (2017) Vse++: Improving visual-semantic embeddings with hard negatives. arXiv preprint arXiv:170705612
- Fan Y, Hou S, Zhang Y, Ye Y, Abdulhayoglu M (2018) Gotcha-sly malware! scorpion a metagraph2vec based malware detection system. In: Proceedings of the 24th ACM SIGKDD International Conference on Knowledge Discovery & Data Mining, pp 253–262
- Fang Y, Sun S, Gan Z, Pillai R, Wang S, Liu J (2020) Hierarchical graph network for multi-hop question answering. In: Proceedings of the 2020 Conference on Empirical Methods in Natural Language Processing (EMNLP), pp 8823–8838
- Fatemi B, Asri LE, Kazemi SM (2021) Slaps: Self-supervision improves structure learning for graph neural networks. arXiv preprint arXiv:210205034
- Feng B, Wang Y, Wang Z, Ding Y (2021) Uncertainty-aware Attention Graph Neural Network for Defending Adversarial Attacks. In: AAAI Conference on Artificial Intelligence
- Feng F, He X, Tang J, Chua T (2019a) Graph adversarial training: Dynamically regularizing based on graph structure. TKDE pp 1–1
- Feng J, Huang M, Wang M, Zhou M, Hao Y, Zhu X (2016) Knowledge graph embedding by flexible translation. In: Proceedings of the Fifteenth International Conference on Principles of Knowledge Representation and Reasoning, pp 557–560
- Feng W, Zhang J, Dong Y, Han Y, Luan H, Xu Q, Yang Q, Kharlamov E, Tang J (2020) Graph random neural networks for semi-supervised learning on graphs. In: Advances in Neural Information Processing Systems, vol 33, pp 22,092–22,103
- Feng X, Zhang Y, Glass J (2014) Speech feature denoising and dereverberation via deep autoencoders for noisy reverberant speech recognition. In: 2014 IEEE international conference on acoustics, speech and signal processing (ICASSP), IEEE, pp 1759–1763
- Feng Y, Lv F, Shen W, Wang M, Sun F, Zhu Y, Yang K (2019b) Deep session interest network for click-through rate prediction. arXiv preprint arXiv:190506482
- Feng Y, You H, Zhang Z, Ji R, Gao Y (2019c) Hypergraph neural networks. In: Proceedings of the AAAI Conference on Artificial Intelligence, vol 33, pp 3558–3565
- Feurer M, Hutter F (2019) Hyperparameter optimization. In: Automated Machine Learning, Springer, Cham, pp 3–33
- Févotte C, Idier J (2011) Algorithms for nonnegative matrix factorization with the β -divergence. Neural computation 23(9):2421–2456
- Fey M, Lenssen JE (2019) Fast graph representation learning with PyTorch Geometric. CoRR abs/1903.02428
- Fey M, Lenssen JE, Weichert F, Müller H (2018) Splinecnn: Fast geometric deep learning with continuous b-spline kernels. In: Proceedings of the IEEE Conference on Computer Vision and Pattern Recognition, pp 869–877

- Fey M, Lenssen JE, Morris C, Masci J, Kriege NM (2020) Deep graph matching consensus. In: International Conference on Learning Representations
- Finn RD, Bateman A, Clements J, et al (2013) Pfam: the protein families database. *Nucleic Acids Research* 42(D1):D222–D230
- Foggia P, Percannella G, Vento M (2014) Graph matching and learning in pattern recognition in the last 10 years. *International Journal of Pattern Recognition and Artificial Intelligence* 28(01):1450,001
- Foltman M, Sanchez-Diaz A (2016) Studying protein–protein interactions in budding yeast using co-immunoprecipitation. In: *Yeast Cytokinesis*, Springer, pp 239–256, DOI 10.1007/978-1-4939-3145-3_17
- Fong RC, Vedaldi A (2017) Interpretable explanations of black boxes by meaningful perturbation. In: *Proceedings of the IEEE International Conference on Computer Vision*, pp 3429–3437
- Fortin S (1996) The graph isomorphism problem
- Fortunato S (2010) Community detection in graphs. *Physics reports* 486(3-5):75–174
- Fouss F, Pirotte A, Renders JM, Saeens M (2007) Random-walk computation of similarities between nodes of a graph with application to collaborative recommendation. *IEEE Transactions on knowledge and data engineering* 19(3):355–369
- Fowkes J, Chanthirasegaran P, Ranca R, Allamanis M, Lapata M, Sutton C (2017) Autofolding for source code summarization. *IEEE Transactions on Software Engineering* 43(12):1095–1109
- Franceschi L, Niepert M, Pontil M, He X (2019) Learning discrete structures for graph neural networks. In: *Proceedings of the 36th International Conference on Machine Learning*, vol 97, pp 1972–1982
- Freeman LA (2003) A refresher in data flow diagramming: an effective aid for analysts. *Commun ACM* 46(9):147–151, DOI 10.1145/903893.903930
- Freeman LC (2000) Visualizing social networks. *Journal of social structure* 1(1):4
- Fröhlich H, Wegner JK, Sieker F, Zell A (2005) Optimal assignment kernels for attributed molecular graphs. In: *International Conference on Machine Learning*, pp 225–232
- Fu R, Zhang Z, Li L (2016) Using lstm and gru neural network methods for traffic flow prediction. In: *2016 31st Youth Academic Annual Conference of Chinese Association of Automation (YAC)*, IEEE, pp 324–328
- Fu Ty, Lee WC, Lei Z (2017) Hin2vec: Explore meta-paths in heterogeneous information networks for representation learning. In: *Proceedings of the 2017 ACM on Conference on Information and Knowledge Management*, pp 1797–1806
- Fu X, Zhang J, Meng Z, King I (2020) Magnn: metapath aggregated graph neural network for heterogeneous graph embedding. In: *Proceedings of The Web Conference 2020*, pp 2331–2341
- Fu Y, Ma Y (2012) *Graph embedding for pattern analysis*. Springer Science & Business Media

- Gabrielé M, Manoel A, Luneau C, Barbier J, Macris N, Krzakala F, Zdeborová L (2019) Entropy and mutual information in models of deep neural networks. *Journal of Statistical Mechanics: Theory and Experiment* 2019(12):124,014
- Gao D, Li K, Wang R, Shan S, Chen X (2020a) Multi-modal graph neural network for joint reasoning on vision and scene text. In: *Proceedings of the IEEE/CVF Conference on Computer Vision and Pattern Recognition*, pp 12,746–12,756
- Gao H, Ji S (2019) Graph u-nets. In: *International Conference on Machine Learning*, PMLR, pp 2083–2092
- Gao H, Wang Z, Ji S (2018a) Large-scale learnable graph convolutional networks. In: *Proceedings of the 24th ACM SIGKDD International Conference on Knowledge Discovery & Data Mining*, ACM, pp 1416–1424
- Gao J, Yang Z, Nevatia R (2017) Cascaded boundary regression for temporal action detection. *arXiv preprint arXiv:170501180*
- Gao J, Li X, Xu YE, Sisman B, Dong XL, Yang J (2019a) Efficient knowledge graph accuracy evaluation. *arXiv preprint arXiv:190709657*
- Gao S, Chen C, Xing Z, Ma Y, Song W, Lin SW (2019b) A neural model for method name generation from functional description. In: *2019 IEEE 26th International Conference on Software Analysis, Evolution and Reengineering (SANER)*, IEEE, pp 414–421
- Gao X, Hu W, Qi GJ (2021) Unsupervised learning of topology transformation equivariant representations
- Gao Y, Guo X, Zhao L (2018b) Local event forecasting and synthesis using unpaired deep graph translations. In: *Proceedings of the 2nd ACM SIGSPATIAL Workshop on Analytics for Local Events and News*, pp 1–8
- Gao Y, Wu L, Homayoun H, Zhao L (2019c) Dyngraph2seq: Dynamic-graph-to-sequence interpretable learning for health stage prediction in online health forums. In: *2019 IEEE International Conference on Data Mining (ICDM)*, IEEE, pp 1042–1047
- Gao Y, Yang H, Zhang P, Zhou C, Hu Y (2020b) Graph neural architecture search. In: *International Joint Conference on Artificial Intelligence*, pp 1403–1409
- Garcia V, Bruna J (2017) Few-shot learning with graph neural networks. *arXiv preprint arXiv:171104043*
- García-Durán A, Dumančić S, Niepert M (2018) Learning sequence encoders for temporal knowledge graph completion. In: *Proceedings of the 2018 Conference on Empirical Methods in Natural Language Processing*, pp 4816–4821, DOI 10.18653/v1/D18-1516
- Garey MR (1979) A guide to the theory of np-completeness. *Computers and intractability*
- Garey MR, Johnson DS (2002) *Computers and intractability*, vol 29. wh freeman New York
- Garg V, Jegelka S, Jaakkola T (2020) Generalization and representational limits of graph neural networks. In: *International Conference on Machine Learning*, PMLR, pp 3419–3430
- Gaudelet T, Day B, Jamasb AR, Soman J, Regep C, Liu G, Hayter JBR, Vickers R, Roberts C, Tang J, Roblin D, Blundell TL, Bronstein MM, Taylor-King JP (2020)

- Utilising graph machine learning within drug discovery and development. CoRR abs/2012.05716
- Gavin AC, Bösche M, Krause R, et al (2002) Functional organization of the yeast proteome by systematic analysis of protein complexes. *Nature* 415(6868):141–147
- Geisler S, Zügner D, Günnemann S (2020) Reliable graph neural networks via robust aggregation. *Advances in Neural Information Processing Systems* 33
- Geisler S, Zügner D, Bojchevski A, Günnemann S (2021) Attacking Graph Neural Networks at Scale. In: *Deep Learning for Graphs at AAAI Conference on Artificial Intelligence*
- Gema RP, Robles G, Alexander S, Zaidman A, Germán DM, Gonzalez-Barahona JM (2020) How bugs are born: a model to identify how bugs are introduced in software components. *Empirical Software Engineering* 25(2):1294–1340
- Geng X, Li Y, Wang L, Zhang L, Yang Q, Ye J, Liu Y (2019) Spatiotemporal multi-graph convolution network for ride-hailing demand forecasting. In: *Proceedings of the AAAI conference on artificial intelligence*, vol 33, pp 3656–3663
- Ghosal D, Hazarika D, Majumder N, Roy A, Poria S, Mihalcea R (2020) Kingdom: Knowledge-guided domain adaptation for sentiment analysis. *arXiv preprint arXiv:200500791*
- Gidaris S, Singh P, Komodakis N (2018) Unsupervised representation learning by predicting image rotations. In: *6th International Conference on Learning Representations, ICLR 2018, Vancouver, BC, Canada, April 30 - May 3, 2018, Conference Track Proceedings*, OpenReview.net
- Gilbert EN (1959) Random graphs. *The Annals of Mathematical Statistics* 30(4):1141–1144
- Gilmer J, Schoenholz SS, Riley PF, Vinyals O, Dahl GE (2017) Neural message passing for quantum chemistry. In: Precup D, Teh YW (eds) *Proceedings of the 34th International Conference on Machine Learning, ICML 2017, Sydney, NSW, Australia, 6-11 August 2017*, PMLR, *Proceedings of Machine Learning Research*, vol 70, pp 1263–1272
- Girvan M, Newman ME (2002) Community structure in social and biological networks. *Proceedings of the national academy of sciences* 99(12):7821–7826
- Glorigrijevic V, Renfrew PD, Kosciulek T, Leman JK, Berenberg D, Vatanen T, Chandler C, Taylor BC, Fisk IM, Vlamakis H, et al (2020) Structure-based function prediction using graph convolutional networks. *bioRxiv* p 786236
- Goel R, Kazemi SM, Brubaker M, Poupart P (2020) Diachronic embedding for temporal knowledge graph completion. In: *Proceedings of the AAAI Conference on Artificial Intelligence*, vol 34, pp 3988–3995
- Gold S, Rangarajan A (1996) A graduated assignment algorithm for graph matching. *IEEE Transactions on pattern analysis and machine intelligence* 18(4):377–388
- Goldberg D, Nichols D, Oki BM, Terry D (1992) Using collaborative filtering to weave an information tapestry. *Communications of the ACM* 35(12):61–70

- Gong X, Chang S, Jiang Y, Wang Z (2019) Autogan: Neural architecture search for generative adversarial networks. In: Proceedings of the IEEE/CVF International Conference on Computer Vision, pp 3224–3234
- Gong Y, Jiang Z, Feng Y, Hu B, Zhao K, Liu Q, Ou W (2020) Edgerec: Recommender system on edge in mobile taobao. In: Proceedings of the 29th ACM International Conference on Information & Knowledge Management, pp 2477–2484
- Goodfellow I, Shlens J, Szegedy C (2015) Explaining and harnessing adversarial examples. In: International Conference on Learning Representations
- Goodfellow IJ, Pouget-Abadie J, Mirza M, Bing X, Bengio Y (2014a) Generative adversarial nets. MIT Press
- Goodfellow IJ, Pouget-Abadie J, Mirza M, Xu B, Warde-Farley D, Ozair S, Courville A, Bengio Y (2014b) Generative adversarial networks. arXiv preprint arXiv:1406.2661
- Goodwin T, Harabagiu SM (2013) Automatic generation of a qualified medical knowledge graph and its usage for retrieving patient cohorts from electronic medical records. In: 2013 IEEE Seventh International Conference on Semantic Computing, IEEE, pp 363–370
- Gori M, Monfardini G, Scarselli F (2005) A new model for learning in graph domains. In: IEEE International Joint Conference on Neural Networks, vol 2, pp 729–734, DOI 10.1109/IJCNN.2005.1555942
- Goyal P, Ferrara E (2018) Graph embedding techniques, applications, and performance: A survey. Knowledge-Based Systems 151:78–94
- Grattarola D, Alippi C (2020) Graph neural networks in TensorFlow and Keras with Spektral. CoRR abs/2006.12138, [2006.12138](#)
- Graves A (2013) Generating sequences with recurrent neural networks. CoRR abs/1308.0850
- Graves A, Fernández S, Schmidhuber J (2005) Bidirectional lstm networks for improved phoneme classification and recognition. In: International Conference on Artificial Neural Networks, Springer, pp 799–804
- Grbovic M, Cheng H (2018) Real-time personalization using embeddings for search ranking at airbnb. In: Proceedings of the 24th ACM SIGKDD International Conference on Knowledge Discovery & Data Mining, pp 311–320
- Greff K, Srivastava RK, Koutník J, Steunebrink BR, Schmidhuber J (2016) Lstm: A search space odyssey. IEEE transactions on neural networks and learning systems 28(10):2222–2232
- Gremse M, Chang A, Schomburg I, Grote A, Scheer M, Ebeling C, Schomburg D (2010) The brenda tissue ontology (bto): the first all-integrating ontology of all organisms for enzyme sources. Nucleic acids research 39(suppl_1):D507–D513
- Grohe M (2017) Descriptive complexity, canonisation, and definable graph structure theory, vol 47. Cambridge University Press
- Grohe M, Otto M (2015) Pebble games and linear equations. The Journal of Symbolic Logic pp 797–844
- Grover A, Leskovec J (2016) node2vec: Scalable feature learning for networks. In: Proceedings of the 22nd ACM SIGKDD international conference on Knowledge discovery and data mining, pp 855–864

- Grover A, Zweig A, Ermon S (2019) Graphite: Iterative generative modeling of graphs. In: International Conference on Machine Learning, pp 2434–2444
- Gu J, Cai J, Joty SR, Niu L, Wang G (2018) Look, imagine and match: Improving textual-visual cross-modal retrieval with generative models. In: Proceedings of the IEEE Conference on Computer Vision and Pattern Recognition, pp 7181–7189
- Gu S, Lillicrap T, Ghahramani Z, Turner RE, Levine S (2016) Q-prop: Sample-efficient policy gradient with an off-policy critic. arXiv preprint arXiv:161102247
- Guan Y, Myers CL, Hess DC, et al (2008) Predicting gene function in a hierarchical context with an ensemble of classifiers. *Genome Biology* 9(Suppl 1):S3
- Gui H, Liu J, Tao F, Jiang M, Norick B, Han J (2016) Large-scale embedding learning in heterogeneous event data. In: 2016 IEEE 16th International Conference on Data Mining (ICDM), IEEE, pp 907–912
- Gui T, Zou Y, Zhang Q, Peng M, Fu J, Wei Z, Huang XJ (2019) A lexicon-based graph neural network for chinese ner. In: Proceedings of the 2019 Conference on Empirical Methods in Natural Language Processing and the 9th International Joint Conference on Natural Language Processing (EMNLP-IJCNLP), pp 1039–1049
- Guille A, Hacid H, Favre C, Zighed DA (2013) Information diffusion in online social networks: A survey. *ACM Sigmod Record* 42(2):17–28
- Gulrajani I, Ahmed F, Arjovsky M, Dumoulin V, Courville A (2017) Improved training of wasserstein gans. arXiv preprint arXiv:170400028
- Guo G, Ouyang S, He X, Yuan F, Liu X (2019a) Dynamic item block and prediction enhancing block for sequential recommendation. In: Proceedings of the International Joint Conference on Artificial Intelligence, pp 1373–1379
- Guo H, Tang R, Ye Y, Li Z, He X (2017) Deepfm: a factorization-machine based neural network for ctr prediction. In: Proceedings of the International Joint Conference on Artificial Intelligence, pp 1725–1731
- Guo M, Chou E, Huang DA, Song S, Yeung S, Fei-Fei L (2018a) Neural graph matching networks for fewshot 3d action recognition. In: Proceedings of the European Conference on Computer Vision (ECCV), pp 653–669
- Guo S, Lin Y, Feng N, Song C, Wan H (2019b) Attention based spatial-temporal graph convolutional networks for traffic flow forecasting. In: Proceedings of the AAAI Conference on Artificial Intelligence, vol 33, pp 922–929
- Guo X, Wu L, Zhao L (2018b) Deep graph translation. arXiv preprint arXiv:180509980
- Guo X, Zhao L, Nowzari C, Rafatirad S, Homayoun H, Dinakarrao SMP (2019c) Deep multi-attributed graph translation with node-edge co-evolution. In: 2019 IEEE International Conference on Data Mining (ICDM), IEEE, pp 250–259
- Guo Y, Li M, Pu X, et al (2010) Pred_ppi: a server for predicting protein-protein interactions based on sequence data with probability assignment. *BMC Research Notes* 3(1):145
- Guo Z, Zhang Y, Lu W (2019d) Attention guided graph convolutional networks for relation extraction. In: Proceedings of the 57th Annual Meeting of the Association for Computational Linguistics, pp 241–251

- Guo Z, Zhang Y, Teng Z, Lu W (2019e) Densely connected graph convolutional networks for graph-to-sequence learning. *Transactions of the Association for Computational Linguistics* 7:297–312
- Gurwitz D (2020) Repurposing current therapeutics for treating covid-19: A vital role of prescription records data mining. *Drug development research* 81(7):777–781
- Gutmann M, Hyvärinen A (2010) Noise-contrastive estimation: A new estimation principle for unnormalized statistical models. In: *Proceedings of the International Conference on Artificial Intelligence and Statistics*
- Ha D, Dai A, Le QV (2017) Hypernetworks. In: *Proceedings of the International Conference on Learning Representations (ICLR)*
- Haghighi A, Ng AY, Manning CD (2005) Robust textual inference via graph matching. In: *Proceedings of Human Language Technology Conference and Conference on Empirical Methods in Natural Language Processing*, pp 387–394
- Haiduc S, Aponte J, Moreno L, Marcus A (2010) On the use of automated text summarization techniques for summarizing source code. In: *2010 17th Working Conference on Reverse Engineering, IEEE*, pp 35–44
- Haldar R, Wu L, Xiong J, Hockenmaier J (2020) A multi-perspective architecture for semantic code search. *arXiv preprint arXiv:200506980*
- Hamaguchi T, Oiwa H, Shimbo M, Matsumoto Y (2017) Knowledge transfer for out-of-knowledge-base entities: a graph neural network approach. In: *Proceedings of the 26th International Joint Conference on Artificial Intelligence*, pp 1802–1808
- Hamilton W, Ying Z, Leskovec J (2017a) Inductive representation learning on large graphs. In: *Advances in Neural Information Processing Systems*, vol 30
- Hamilton WL (2020) Graph representation learning. *Synthesis Lectures on Artificial Intelligence and Machine Learning* 14(3):1–159
- Hamilton WL, Ying R, Leskovec J (2017b) Inductive representation learning on large graphs. In: *Advances in Neural Information Processing Systems*, pp 1025–1035
- Hamilton WL, Ying R, Leskovec J (2017c) Representation learning on graphs: Methods and applications. *IEEE Data Engineering Bulletin* 40(3):52–74
- Hammond DK, Vandergheynst P, Gribonval R (2011) Wavelets on graphs via spectral graph theory. *Applied and Computational Harmonic Analysis* 30(2):129–150
- Han J, Luo P, Wang X (2019) Deep self-learning from noisy labels. In: *2019 IEEE/CVF International Conference on Computer Vision, ICCV 2019, Seoul, Korea (South), October 27 - November 2, 2019, IEEE*, pp 5137–5146, DOI 10.1109/ICCV.2019.00524
- Han JDJ, Dupuy D, Bertin N, et al (2005) Effect of sampling on topology predictions of protein-protein interaction networks. *Nature Biotechnology* 23(7):839–844
- Han K, Wang Y, Chen H, Chen X, Guo J, Liu Z, Tang Y, Xiao A, Xu C, Xu Y, et al (2020) A survey on visual transformer. *arXiv preprint arXiv:201212556*
- Han X, Zhu H, Yu P, Wang Z, Yao Y, Liu Z, Sun M (2018) Fewrel: A large-scale supervised few-shot relation classification dataset with state-of-the-art evaluation.

- In: Proceedings of the 2018 Conference on Empirical Methods in Natural Language Processing, pp 4803–4809
- Haque S, LeClair A, Wu L, McMillan C (2020) Improved automatic summarization of subroutines via attention to file context. *International Conference on Mining Software Repositories* p 300–310
- Hart PE, Nilsson NJ, Raphael B (1968) A formal basis for the heuristic determination of minimum cost paths. *IEEE transactions on Systems Science and Cybernetics* 4(2):100–107
- Hashemifar S, Neyshabur B, Khan AA, et al (2018) Predicting protein–protein interactions through sequence-based deep learning. *Bioinformatics* 34(17):i802–i810
- Hasibi R, Michoel T (2020) Predicting gene expression from network topology using graph neural networks. *arXiv preprint arXiv:200503961*
- Hassan AE, Xie T (2010) Software intelligence: the future of mining software engineering data. In: Proceedings of the FSE/SDP workshop on Future of software engineering research, pp 161–166
- Hassani K, Khasahmadi AH (2020) Contrastive multi-view representation learning on graphs. In: *International Conference on Machine Learning*, PMLR, pp 4116–4126
- Hastings J, Owen G, Dekker A, Ennis M, Kale N, Muthukrishnan V, Turner S, Swainston N, Mendes P, Steinbeck C (2016) Chebi in 2016: Improved services and an expanding collection of metabolites. *Nucleic acids research* 44(D1):D1214–D1219
- Haveliwala TH (2002) Topic-sensitive pagerank. In: Proceedings of the 11th international conference on World Wide Web, ACM, pp 517–526
- He K, Zhang X, Ren S, Sun J (2016a) Deep residual learning for image recognition. In: Proceedings of the IEEE conference on computer vision and pattern recognition, pp 770–778
- He K, Gkioxari G, Dollár P, Girshick R (2017a) Mask r-cnn. In: Proceedings of the IEEE international conference on computer vision, pp 2961–2969
- He Q, Chen B, Agarwal D (2016b) Building the linkedin knowledge graph. *Engineering linkedin com*
- He X, Niyogi P (2004) Locality preserving projections. *Advances in neural information processing systems* 16(16):153–160
- He X, Liao L, Zhang H, Nie L, Hu X, Chua TS (2017b) Neural collaborative filtering. In: Proceedings of the 26th international conference on world wide web, pp 173–182
- He X, Deng K, Wang X, Li Y, Zhang Y, Wang M (2020) Lightgcn: Simplifying and powering graph convolution network for recommendation. In: Proceedings of the 43rd International ACM SIGIR Conference on Research and Development in Information Retrieval, pp 639–648
- He Y, Song Y, Li J, Ji C, Peng J, Peng H (2019) Hetespaceywalk: A heterogeneous spacey random walk for heterogeneous information network embedding. In: Proceedings of the 28th ACM International Conference on Information and Knowledge Management, pp 639–648

- Hearst MA, Dumais ST, Osuna E, Platt J, Scholkopf B (1998) Support vector machines. *IEEE Intelligent Systems and their applications* 13(4):18–28
- Heimer RZ, Myrseth KOR, Schoenle RS (2019) Yolo: Mortality beliefs and household finance puzzles. *The Journal of Finance* 74(6):2957–2996
- Helfgott HA, Bajpai J, Dona D (2017) Graph isomorphisms in quasi-polynomial time. *arXiv preprint arXiv:171004574*
- Helgason S (1979) *Differential geometry, Lie groups, and symmetric spaces*. Academic press
- Hellendoorn VJ, Bird C, Barr ET, Allamanis M (2018) Deep learning type inference. In: *Proceedings of the 2018 26th ACM joint meeting on european software engineering conference and symposium on the foundations of software engineering*, pp 152–162
- Hellendoorn VJ, Devanbu PT, Polozov O, Marron M (2019a) Are my invariants valid? a learning approach. *arXiv preprint arXiv:190306089*
- Hellendoorn VJ, Sutton C, Singh R, Maniatis P, Bieber D (2019b) Global relational models of source code. In: *International Conference on Learning Representations*
- Henaff M, Bruna J, LeCun Y (2015) Deep convolutional networks on graph-structured data. *arXiv preprint arXiv:150605163*
- Henderson K, Gallagher B, Eliassi-Rad T, Tong H, Basu S, Akoglu L, Koutra D, Faloutsos C, Li L (2012) Rolx: structural role extraction & mining in large graphs. In: *the ACM SIGKDD international conference on Knowledge discovery and data mining*, pp 1231–1239
- Hensman S (2004) Construction of conceptual graph representation of texts. In: *Proceedings of the Student Research Workshop at HLT-NAACL 2004*, pp 49–54
- Hermann KM, Hill F, Green S, Wang F, Faulkner R, Soyer H, Szepesvari D, Czarnecki WM, Jaderberg M, Teplyashin D, et al (2017) Grounded language learning in a simulated 3d world. *arXiv preprint arXiv:170606551*
- Herzig R, Levi E, Xu H, Gao H, Brosh E, Wang X, Globerson A, Darrell T (2019) Spatio-temporal action graph networks. In: *2019 IEEE/CVF International Conference on Computer Vision Workshop (ICCVW)*, pp 2347–2356, DOI 10.1109/ICCVW.2019.00288
- Hidasi B, Karatzoglou A, Baltrunas L, Tikk D (2015) Session-based recommendations with recurrent neural networks. *arXiv preprint arXiv:151106939*
- Higgins I, Matthey L, Pal A, Burgess C, Glorot X, Botvinick M, Mohamed S, Lerchner A (2017) beta-vae: Learning basic visual concepts with a constrained variational framework. *ICLR*
- Himmelstein DS, Lizee A, Hessler C, Brueggeman L, Chen SL, Hadley D, Green A, Khankhanian P, Baranzini SE (2017) Systematic integration of biomedical knowledge prioritizes drugs for repurposing. *Elife* 6:e26,726
- Hinton GE, Osindero S, Teh YW (2006) A fast learning algorithm for deep belief nets. *Neural computation* 18(7):1527–1554
- Hirsch CN, Hirsch CD, Brohammer AB, et al (2016) Draft assembly of elite inbred line PH207 provides insights into genomic and transcriptome diversity in maize. *The Plant Cell* 28(11):2700–2714

- Hjelm RD, Fedorov A, Lavoie-Marchildon S, Grewal K, Bachman P, Trischler A, Bengio Y (2018) Learning deep representations by mutual information estimation and maximization. arXiv preprint arXiv:180806670
- Ho Y, Gruhler A, Heilbut A, et al (2002) Systematic identification of protein complexes in *saccharomyces cerevisiae* by mass spectrometry. *Nature* 415(6868):180–183
- Hochreiter S, Schmidhuber J (1997) Long short-term memory. *Neural computation* 9(8):1735–1780
- Hoff PD, Raftery AE, Handcock MS (2002) Latent space approaches to social network analysis. *Journal of the American Statistical Association* 97(460):1090–1098
- Hoffart J, Suchanek FM, Berberich K, Lewis-Kelham E, De Melo G, Weikum G (2011) Yago2: exploring and querying world knowledge in time, space, context, and many languages. In: *Proceedings of the 20th international conference companion on World wide web*, pp 229–232
- Hoffman MD, Blei DM, Wang C, Paisley J (2013) Stochastic variational inference. *The Journal of Machine Learning Research* 14(1):1303–1347
- Hogan A, Blomqvist E, Cochez M, d’Amato C, de Melo G, Gutierrez C, Gayo JEL, Kirrane S, Neumaier S, Polleres A, et al (2020) Knowledge graphs. arXiv preprint arXiv:200302320
- Holland PW, Laskey KB, Leinhardt S (1983) Stochastic blockmodels: First steps. *Social networks* 5(2):109–137
- Holmes R, Murphy GC (2005) Using structural context to recommend source code examples. In: *Proceedings. 27th International Conference on Software Engineering, 2005. ICSE 2005.*, IEEE, pp 117–125
- Hong D, Gao L, Yao J, Zhang B, Plaza A, Chanussot J (2020a) Graph convolutional networks for hyperspectral image classification. *IEEE Transactions on Geoscience and Remote Sensing* pp 1–13, DOI 10.1109/TGRS.2020.3015157
- Hong H, Guo H, Lin Y, Yang X, Li Z, Ye J (2020b) An attention-based graph neural network for heterogeneous structural learning. In: *Proceedings of the AAAI Conference on Artificial Intelligence*, vol 34, pp 4132–4139
- Hornik K, Stinchcombe M, White H, et al (1989) Multilayer feedforward networks are universal approximators. *Neural Networks* 2(5):359–366
- Horton T (1992) *Object-oriented analysis & design*. Englewood Cliffs (New Jersey): Prentice-Hall
- Hosseini A, Chen T, Wu W, Sun Y, Sarrafzadeh M (2018) Heteromed: Heterogeneous information network for medical diagnosis. In: *Proceedings of the 27th ACM International Conference on Information and Knowledge Management*, pp 763–772
- Hou S, Ye Y, Song Y, Abdulhayoglu M (2017) Hindroid: An intelligent android malware detection system based on structured heterogeneous information network. In: *Proceedings of the 23rd ACM SIGKDD international conference on knowledge discovery and data mining*, pp 1507–1515
- Houlsby N, Giurghi A, Jastrzebski S, Morrone B, De Laroussilhe Q, Gesmundo A, Attariyan M, Gelly S (2019) Parameter-efficient transfer learning for nlp. In: *International Conference on Machine Learning*, PMLR, pp 2790–2799

- Hsieh K, Wang Y, Chen L, Zhao Z, Savitz S, Jiang X, Tang J, Kim Y (2020) Drug repurposing for covid-19 using graph neural network with genetic, mechanistic, and epidemiological validation. arXiv preprint arXiv:200910931
- Hsu WN, Zhang Y, Glass J (2017) Unsupervised learning of disentangled and interpretable representations from sequential data. In: Proceedings of the 31st International Conference on Neural Information Processing Systems, pp 1876–1887
- Hsu WN, Zhang Y, Weiss RJ, Chung YA, Wang Y, Wu Y, Glass J (2019) Disentangling correlated speaker and noise for speech synthesis via data augmentation and adversarial factorization. In: ICASSP 2019-2019 IEEE International Conference on Acoustics, Speech and Signal Processing (ICASSP), IEEE, pp 5901–5905
- Hu B, Shi C, Zhao WX, Yu PS (2018a) Leveraging meta-path based context for top-n recommendation with a neural co-attention model. In: Proceedings of the 24th ACM SIGKDD International Conference on Knowledge Discovery & Data Mining, pp 1531–1540
- Hu B, Fang Y, Shi C (2019a) Adversarial learning on heterogeneous information networks. In: Proceedings of the 25th ACM SIGKDD International Conference on Knowledge Discovery & Data Mining, pp 120–129
- Hu B, Zhang Z, Shi C, Zhou J, Li X, Qi Y (2019b) Cash-out user detection based on attributed heterogeneous information network with a hierarchical attention mechanism. In: Proceedings of the AAAI Conference on Artificial Intelligence, vol 33, pp 946–953
- Hu L, Xu S, Li C, Yang C, Shi C, Duan N, Xie X, Zhou M (2020a) Graph neural news recommendation with unsupervised preference disentanglement. In: Proceedings of the 58th Annual Meeting of the Association for Computational Linguistics, pp 4255–4264
- Hu R, Aggarwal CC, Ma S, Huai J (2016) An embedding approach to anomaly detection. In: 2016 IEEE 32nd International Conference on Data Engineering (ICDE), IEEE, pp 385–396
- Hu W, Fey M, Zitnik M, Dong Y, Ren H, Liu B, Catasta M, Leskovec J (2020b) Open graph benchmark: Datasets for machine learning on graphs. arXiv preprint arXiv:200500687
- Hu W, Liu B, Gomes J, Zitnik M, Liang P, Pande VS, Leskovec J (2020c) Strategies for pre-training graph neural networks. In: 8th International Conference on Learning Representations, ICLR 2020, Addis Ababa, Ethiopia, April 26-30, 2020, OpenReview.net
- Hu X, Chiueh Tc, Shin KG (2009) Large-scale malware indexing using function-call graphs. In: Proceedings of the 16th ACM Conference on Computer and Communications Security (CCS), Association for Computing Machinery, New York, NY, USA, p 611–620
- Hu X, Li G, Xia X, Lo D, Jin Z (2018b) Deep code comment generation. In: Proceedings of the 26th Conference on Program Comprehension, ACM, pp 200–210
- Hu X, Li G, Xia X, Lo D, Lu S, Jin Z (2018c) Summarizing source code with transferred api knowledge. In: Proceedings of the 27th International Joint Conference on Artificial Intelligence, AAAI Press, pp 2269–2275

- Hu Z, Fan C, Chen T, Chang KW, Sun Y (2019c) Pre-training graph neural networks for generic structural feature extraction. arXiv preprint arXiv:190513728
- Hu Z, Dong Y, Wang K, Chang KW, Sun Y (2020d) Gpt-gnn: Generative pre-training of graph neural networks. In: Proceedings of the 26th ACM SIGKDD International Conference on Knowledge Discovery & Data Mining, pp 1857–1867
- Hu Z, Dong Y, Wang K, Sun Y (2020e) Heterogeneous graph transformer. In: Proceedings of The Web Conference 2020, pp 2704–2710
- Huang D, Chen P, Zeng R, Du Q, Tan M, Gan C (2020a) Location-aware graph convolutional networks for video question answering. In: The Thirty-Fourth AAAI Conference on Artificial Intelligence, AAAI Press, pp 11,021–11,028
- Huang G, Liu Z, Van Der Maaten L, Weinberger KQ (2017a) Densely connected convolutional networks. In: Proceedings of the IEEE conference on computer vision and pattern recognition, pp 4700–4708
- Huang H, Wang X, Yi Z, Ma X (2000) A character recognition based on feature extraction. *Journal of Chongqing University (Natural Science Edition)* 23:66–69
- Huang H, Alvarez S, Nusinow DA (2016a) Data on the identification of protein interactors with the evening complex and PCH1 in arabidopsis using tandem affinity purification and mass spectrometry (TAP-MS). *Data in Brief* 8:56–60
- Huang J, Li Z, Li N, Liu S, Li G (2019) Attpool: Towards hierarchical feature representation in graph convolutional networks via attention mechanism. In: IEEE/CVF International Conference on Computer Vision, pp 6479–6488
- Huang JT, Sharma A, Sun S, Xia L, Zhang D, Pronin P, Padmanabhan J, Ottaviano G, Yang L (2020b) Embedding-based retrieval in facebook search. In: Proceedings of the 26th ACM SIGKDD International Conference on Knowledge Discovery & Data Mining, pp 2553–2561
- Huang L, Ma D, Li S, Zhang X, Houfeng W (2019a) Text level graph neural network for text classification. In: Proceedings of the 2019 Conference on Empirical Methods in Natural Language Processing and the 9th International Joint Conference on Natural Language Processing (EMNLP-IJCNLP), pp 3435–3441
- Huang Q, Yamada M, Tian Y, Singh D, Yin D, Chang Y (2020c) Graphlime: Local interpretable model explanations for graph neural networks. arXiv preprint arXiv:200106216
- Huang S, Kang Z, Tsang IW, Xu Z (2019b) Auto-weighted multi-view clustering via kernelized graph learning. *Pattern Recognition* 88:174–184
- Huang W, Zhang T, Rong Y, Huang J (2018) Adaptive sampling towards fast graph representation learning. *Advances in Neural Information Processing Systems* 31:4558–4567
- Huang X, Alzantot M, Srivastava M (2019c) Neuroninspect: Detecting backdoors in neural networks via output explanations. arXiv preprint arXiv:191107399
- Huang X, Song Q, Li Y, Hu X (2019d) Graph recurrent networks with attributed random walks. In: Proceedings of the 25th ACM SIGKDD International Conference on Knowledge Discovery & Data Mining, pp 732–740

- Huang Y, Wang W, Wang L (2017b) Instance-aware image and sentence matching with selective multimodal lstm. In: Proceedings of the IEEE Conference on Computer Vision and Pattern Recognition, pp 2310–2318
- Huang Z, Mamoulis N (2017) Heterogeneous information network embedding for meta path based proximity. arXiv preprint arXiv:170105291
- Huang Z, Xu W, Yu K (2015) Bidirectional lstm-crf models for sequence tagging. arXiv preprint arXiv:150801991
- Huang Z, Zheng Y, Cheng R, Sun Y, Mamoulis N, Li X (2016b) Meta structure: Computing relevance in large heterogeneous information networks. In: Proceedings of the 22nd ACM SIGKDD International Conference on Knowledge Discovery and Data Mining, pp 1595–1604
- Hurle M, Yang L, Xie Q, Rajpal D, Sanseau P, Agarwal P (2013) Computational drug repositioning: from data to therapeutics. *Clinical Pharmacology & Therapeutics* 93(4):335–341
- Hussein R, Yang D, Cudré-Mauroux P (2018) Are meta-paths necessary? revisiting heterogeneous graph embeddings. In: Proceedings of the 27th ACM International Conference on Information and Knowledge Management, pp 437–446
- Hutchins WJ (1995) Machine translation: A brief history. In: Concise history of the language sciences, Elsevier, pp 431–445
- Ioannidis VN, Marques AG, Giannakis GB (2019) Graph neural networks for predicting protein functions. In: 2019 IEEE 8th International Workshop on Computational Advances in Multi-Sensor Adaptive Processing (CAMSAP), pp 221–225, DOI 10.1109/CAMSAP45676.2019.9022646
- Ioannidis VN, Song X, Manchanda S, Li M, Pan X, Zheng D, Ning X, Zeng X, Karypis G (2020) Drkg - drug repurposing knowledge graph for covid-19. <https://github.com/gnn4dr/DRKG/>
- Ioffe S, Szegedy C (2015) Batch normalization: Accelerating deep network training by reducing internal covariate shift. In: International Conference on Machine Learning, pp 448–456
- Irving G, Szegedy C, Alemi AA, Eén N, Chollet F, Urban J (2016) DeepMath - deep sequence models for premise selection. *Advances in neural information processing systems* 29:2235–2243
- Irwin JJ, Sterling T, Mysinger MM, Bolstad ES, Coleman RG (2012) Zinc: a free tool to discover chemistry for biology. *Journal of Chemical Information and Modeling* 52(7):1757–1768
- Issa NT, Stathias V, Schürer S, Dakshanamurthy S (2020) Machine and deep learning approaches for cancer drug repurposing. In: Seminars in cancer biology, Elsevier
- Ito T, Chiba T, Ozawa R, et al (2001) A comprehensive two-hybrid analysis to explore the yeast protein interactome. *Proceedings of the National Academy of Sciences of the United States of America* 98(8):4569–4574
- Iyer S, Konstas I, Cheung A, Zettlemoyer L (2016) Summarizing source code using a neural attention model. In: Proceedings of the 54th Annual Meeting of the Association for Computational Linguistics (Volume 1: Long Papers), pp 2073–2083

- Jaakkola T, Sontag D, Globerson A, Meila M (2010) Learning bayesian network structure using lp relaxations. In: Proceedings of the Thirteenth International Conference on Artificial Intelligence and Statistics, JMLR Workshop and Conference Proceedings, pp 358–365
- Jabri A, Owens A, Efros AA (2020) Space-time correspondence as a contrastive random walk. arXiv preprint arXiv:200614613
- Jacob Y, Denoyer L, Gallinari P (2014) Learning latent representations of nodes for classifying in heterogeneous social networks. In: Proceedings of the 7th ACM international conference on Web search and data mining, pp 373–382
- Jain A, Zamir AR, Savarese S, Saxena A (2016a) Structural-RNN: Deep learning on spatio-temporal graphs. In: IEEE Conference on Computer Vision and Pattern Recognition, pp 5308–5317
- Jain A, Zamir AR, Savarese S, Saxena A (2016b) Structural-rnn: Deep learning on spatio-temporal graphs. In: Proceedings of the ieee conference on computer vision and pattern recognition, pp 5308–5317
- Jaitly N, Hinton G (2011) Learning a better representation of speech soundwaves using restricted boltzmann machines. In: 2011 IEEE International Conference on Acoustics, Speech and Signal Processing (ICASSP), IEEE, pp 5884–5887
- Jang E, Gu S, Poole B (2017) Categorical reparameterization with gumbel-softmax. In: 5th International Conference on Learning Representations
- Jang S, Moon SE, Lee JS (2019) Brain signal classification via learning connectivity structure. arXiv preprint arXiv:190511678
- Jassal B, Matthews L, Viteri G, Gong C, Lorente P, Fabregat A, Sidiropoulos K, Cook J, Gillespie M, Haw R, et al (2020) The reactome pathway knowledgebase. *Nucleic acids research* 48(D1):D498–D503
- Jean S, Cho K, Memisevic R, Bengio Y (2014) On using very large target vocabulary for neural machine translation. arXiv preprint arXiv:14122007
- Jebara T, Wang J, Chang SF (2009) Graph construction and b-matching for semi-supervised learning. In: Proceedings of the 26th annual international conference on machine learning, pp 441–448
- Jeh G, Widom J (2002) Simrank: a measure of structural-context similarity. In: Proceedings of the eighth ACM SIGKDD international conference on Knowledge discovery and data mining, ACM, pp 538–543
- Jeh G, Widom J (2003) Scaling personalized web search. In: the International Conference on World Wide Web, pp 271–279
- Jenatton R, Le Roux N, Bordes A, Obozinski G (2012) A latent factor model for highly multi-relational data. In: Advances in Neural Information Processing Systems 25 (NIPS 2012), pp 3176–3184
- Ji G, He S, Xu L, Liu K, Zhao J (2015) Knowledge graph embedding via dynamic mapping matrix. In: Proceedings of the 53rd annual meeting of the association for computational linguistics and the 7th international joint conference on natural language processing, pp 687–696
- Ji G, Liu K, He S, Zhao J (2016) Knowledge graph completion with adaptive sparse transfer matrix. In: Proceedings of the AAAI Conference on Artificial Intelligence, vol 30

- Jia J, Wang B, Cao X, Gong NZ (2020) Certified robustness of community detection against adversarial structural perturbation via randomized smoothing. In: The Web Conference, pp 2718–2724
- Jia X, De Brabandere B, Tuytelaars T, Gool LV (2016) Dynamic filter networks. *Advances in neural information processing systems* 29:667–675
- Jiang B, Sun P, Tang J, Luo B (2019a) GLMNet: Graph learning-matching networks for feature matching. *arXiv preprint arXiv:191107681*
- Jiang B, Zhang Z, Lin D, Tang J, Luo B (2019b) Semi-supervised learning with graph learning-convolutional networks. In: *Proceedings of the IEEE Conference on Computer Vision and Pattern Recognition*, pp 11,313–11,320
- Jiang C, Coenen F, Sanderson R, Zito M (2010) Text classification using graph mining-based feature extraction. In: *Research and Development in Intelligent Systems XXVI*, Springer, pp 21–34
- Jiang S, Balaprakash P (2020) Graph neural network architecture search for molecular property prediction. *arXiv preprint arXiv:200812187*
- Jiang S, McMillan C, Santelices R (2016) Do programmers do change impact analysis in debugging? *Empirical Software Engineering* pp 1–39
- Jiang S, Armaly A, McMillan C (2017) Automatically generating commit messages from diffs using neural machine translation. In: *Proceedings of the 32nd IEEE/ACM International Conference on Automated Software Engineering*, IEEE Press, pp 135–146
- Jiménez J, Doerr S, Martínez-Rosell G, et al (2017) DeepSite: protein-binding site predictor using 3d-convolutional neural networks. *Bioinformatics* 33(19):3036–3042
- Jin H, Zhang X (2019) Latent Adversarial Training of Graph Convolution Networks. In: *ICML 2019 Workshop: Learning and Reasoning with Graph-Structured Representations*
- Jin H, Song Q, Hu X (2019a) Auto-keras: An efficient neural architecture search system. In: *Proceedings of the 25th ACM SIGKDD International Conference on Knowledge Discovery & Data Mining*, pp 1946–1956
- Jin H, Shi Z, Peruri VJSA, Zhang X (2020a) Certified robustness of graph convolution networks for graph classification under topological attacks. *Advances in Neural Information Processing Systems* 33
- Jin J, Qin J, Fang Y, Du K, Zhang W, Yu Y, Zhang Z, Smola AJ (2020b) An efficient neighborhood-based interaction model for recommendation on heterogeneous graph. In: *Proceedings of the 26th ACM SIGKDD International Conference on Knowledge Discovery & Data Mining*, pp 75–84
- Jin L, Gildea D (2020) Generalized shortest-paths encoders for amr-to-text generation. In: *Proceedings of the 28th International Conference on Computational Linguistics*, pp 2004–2013
- Jin M, Chang H, Zhu W, Sojoudi S (2019b) Power up! robust graph convolutional network against evasion attacks based on graph powering. *CoRR* abs/1905.10029, [1905.10029](https://arxiv.org/abs/1905.10029)

- Jin W, Barzilay R, Jaakkola T (2018a) Junction tree variational autoencoder for molecular graph generation. In: Proceedings of the 35th International Conference on Machine Learning, pp 2323–2332
- Jin W, Barzilay R, Jaakkola TS (2018b) Junction tree variational autoencoder for molecular graph generation. In: International Conference on Machine Learning, pp 2328–2337
- Jin W, Yang K, Barzilay R, Jaakkola T (2018c) Learning multimodal graph-to-graph translation for molecular optimization. arXiv preprint arXiv:181201070
- Jin W, Barzilay R, Jaakkola T (2020c) Composing molecules with multiple property constraints. arXiv preprint arXiv:200203244
- Jin W, Derr T, Liu H, Wang Y, Wang S, Liu Z, Tang J (2020d) Self-supervised learning on graphs: Deep insights and new direction. arXiv preprint arXiv:200610141
- Jin W, Ma Y, Liu X, Tang X, Wang S, Tang J (2020e) Graph structure learning for robust graph neural networks. In: The 26th ACM SIGKDD Conference on Knowledge Discovery and Data Mining, pp 66–74
- Jin W, Derr T, Wang Y, Ma Y, Liu Z, Tang J (2021) Node similarity preserving graph convolutional networks. In: Proceedings of the 14th ACM International Conference on Web Search and Data Mining, pp 148–156
- Johansson FD, Dubhashi D (2015) Learning with similarity functions on graphs using matchings of geometric embeddings. In: ACM SIGKDD International Conference on Knowledge Discovery and Data Mining, pp 467–476
- Johnson D, Larochelle H, Tarlow D (2020) Learning graph structure with a finite-state automaton layer. In: Larochelle H, Ranzato M, Hadsell R, Balcan MF, Lin H (eds) Advances in Neural Information Processing Systems, Curran Associates, Inc., vol 33, pp 3082–3093
- Jonas E (2019) Deep imitation learning for molecular inverse problems. Advances in Neural Information Processing Systems 32:4990–5000
- Jurafsky D (2000) Speech & language processing. Pearson Education India
- Kagdi H, Collard ML, Maletic JI (2007) A survey and taxonomy of approaches for mining software repositories in the context of software evolution. Journal of software maintenance and evolution: Research and practice 19(2):77–131
- Kahneman D (2011) Thinking, fast and slow. Macmillan
- Kalchbrenner N, Grefenstette E, Blunsom P (2014) A convolutional neural network for modelling sentences. In: Proceedings of the 52nd Annual Meeting of the Association for Computational Linguistics, Association for Computational Linguistics, pp 655–665, DOI 10.3115/v1/P14-1062
- Kalliamvakou E, Gousios G, Blincoe K, Singer L, German DM, Damian D (2014) The promises and perils of mining github. In: Proceedings of the 11th working conference on mining software repositories, pp 92–101
- Kalofolias V (2016) How to learn a graph from smooth signals. In: Artificial Intelligence and Statistics, PMLR, pp 920–929
- Kalofolias V, Perraudin N (2019) Large scale graph learning from smooth signals. In: 7th International Conference on Learning Representations
- Kaluza MCDP, Amizadeh S, Yu R (2018) A neural framework for learning dag to dag translation. In: NeurIPS'2018 Workshop

- Kampffmeyer M, Chen Y, Liang X, Wang H, Zhang Y, Xing EP (2019) Rethinking knowledge graph propagation for zero-shot learning. In: Proceedings of the IEEE/CVF Conference on Computer Vision and Pattern Recognition, pp 11,487–11,496
- Kandasamy K, Neiswanger W, Schneider J, Poczos B, Xing E (2018) Neural architecture search with bayesian optimisation and optimal transport. In: Advances in Neural Information Processing Systems
- Kanehisa M, Goto S (2000) Kegg: kyoto encyclopedia of genes and genomes. *Nucleic acids research* 28(1):27–30
- Kanehisa M, Araki M, Goto S, Hattori M, Hirakawa M, Itoh M, Katayama T, Kawashima S, Okuda S, Tokimatsu T, et al (2007) Kegg for linking genomes to life and the environment. *Nucleic acids research* 36(suppl_1):D480–D484
- Kang U, Tong H, Sun J (2012) Fast random walk graph kernel. In: SIAM International Conference on Data Mining, pp 828–838
- Kang WC, McAuley J (2018) Self-attentive sequential recommendation. In: 2018 IEEE International Conference on Data Mining (ICDM), IEEE, pp 197–206
- Kang Z, Pan H, Hoi SC, Xu Z (2019) Robust graph learning from noisy data. *IEEE transactions on cybernetics* 50(5):1833–1843
- Karampatsis RM, Sutton C (2020) How often do single-statement bugs occur? the ManySStuBs4J dataset. In: Proceedings of the 17th International Conference on Mining Software Repositories, pp 573–577
- Karamshuk D, Noulas A, Scellato S, Nicosia V, Mascolo C (2013) Geo-spotting: mining online location-based services for optimal retail store placement. In: Proceedings of the 19th ACM SIGKDD international conference on Knowledge discovery and data mining, pp 793–801
- Karita S, Watanabe S, Iwata T, Ogawa A, Delcroix M (2018) Semi-supervised end-to-end speech recognition. In: Interspeech, pp 2–6
- Karpathy A, Fei-Fei L (2015) Deep visual-semantic alignments for generating image descriptions. In: Proceedings of the IEEE conference on computer vision and pattern recognition, pp 3128–3137
- Karypis G, Kumar V (1995) Multilevel graph partitioning schemes. In: ICPP (3), pp 113–122
- Karypis G, Kumar V (1998) A fast and high quality multilevel scheme for partitioning irregular graphs. *SIAM Journal on scientific Computing* 20(1):359–392
- Katharopoulos A, Vyas A, Pappas N, Fleuret F (2020) Transformers are rnns: Fast autoregressive transformers with linear attention. In: International Conference on Machine Learning, PMLR, pp 5156–5165
- Katz L (1953) A new status index derived from sociometric analysis. *Psychometrika* 18(1):39–43
- Kawahara J, Brown CJ, Miller SP, Booth BG, Chau V, Grunau RE, Zwicker JG, Hamarneh G (2017) Brainnetcnn: Convolutional neural networks for brain networks; towards predicting neurodevelopment. *NeuroImage* 146:1038–1049
- Kazemi E, Hassani SH, Grossglauser M (2015) Growing a graph matching from a handful of seeds. *Proc VLDB Endow* 8(10):1010–1021

- Kazemi SM, Poole D (2018) Simple embedding for link prediction in knowledge graphs. In: *Neural Information Processing Systems*, p 4289–4300
- Kazemi SM, Goel R, Eghbali S, Ramanan J, Sahota J, Thakur S, Wu S, Smyth C, Poupart P, Brubaker M (2019) Time2vec: Learning a vector representation of time. *arXiv preprint arXiv:190705321*
- Kazemi SM, Goel R, Jain K, Kobzyev I, Sethi A, Forsyth P, Poupart P (2020) Representation learning for dynamic graphs: A survey. *Journal of Machine Learning Research* 21(70):1–73
- Kazi A, Cosmo L, Navab N, Bronstein M (2020) Differentiable graph module (dgm) graph convolutional networks. *arXiv preprint arXiv:200204999*
- Kearnes S, McCloskey K, Berndl M, Pande V, Riley P (2016) Molecular graph convolutions: moving beyond fingerprints. *Journal of computer-aided molecular design* 30(8):595–608
- Keriven N, Peyré G (2019) Universal invariant and equivariant graph neural networks. In: *Advances in Neural Information Processing Systems*, pp 7090–7099
- Kersting K, Kriege NM, Morris C, Mutzel P, Neumann M (2016) Benchmark data sets for graph kernels
- Khezerlou AV, Zhou X, Li L, Shafiq Z, Liu AX, Zhang F (2017) A traffic flow approach to early detection of gathering events: Comprehensive results. *ACM Transactions on Intelligent Systems and Technology (TIST)* 8(6):1–24
- Khezerlou AV, Zhou X, Tong L, Li Y, Luo J (2021) Forecasting gathering events through trajectory destination prediction: A dynamic hybrid model. *IEEE Transactions on Knowledge and Data Engineering* 33(3):991–1004, DOI 10.1109/TKDE.2019.2937082
- Khrulkov V, Novikov A, Oseledets I (2018) Expressive power of recurrent neural networks. In: *International Conference on Learning Representations*
- Kiefer S, Schweitzer P, Selman E (2015) Graphs identified by logics with counting. In: *International Symposium on Mathematical Foundations of Computer Science*, pp 319–330
- Kilicoglu H, Shin D, Fiszman M, Rosembat G, Rindfleisch TC (2012) Semmeddb: a pubmed-scale repository of biomedical semantic predications. *Bioinformatics* 28(23):3158–3160
- Kim B, Koyejo O, Khanna R, et al (2016) Examples are not enough, learn to criticize! criticism for interpretability. In: *NIPS*, pp 2280–2288
- Kim D, Oh A (2021) How to find your friendly neighborhood: Graph attention design with self-supervision. In: *International Conference on Learning Representations*
- Kim J, Kim T, Kim S, Yoo CD (2019) Edge-labeling graph neural network for few-shot learning. In: *Proceedings of the IEEE/CVF Conference on Computer Vision and Pattern Recognition*, pp 11–20
- Kingma DP, Welling M (2013) Auto-encoding variational bayes. *arXiv preprint arXiv:1312.6114*
- Kingma DP, Welling M (2014) Auto-encoding variational bayes. In: *2nd International Conference on Learning Representations*

- Kingma DP, Rezende DJ, Mohamed S, Welling M (2014) Semi-supervised learning with deep generative models. In: Proceedings of the 27th International Conference on Neural Information Processing Systems-Volume 2, pp 3581–3589
- Kingsbury PR, Palmer M (2002) From treebank to propbank. In: LREC, Citeseer, pp 1989–1993
- Kipf T, Fetaya E, Wang KC, Welling M, Zemel R (2018) Neural relational inference for interacting systems. In: International Conference on Machine Learning, pp 2688–2697
- Kipf TN, Welling M (2016) Variational graph auto-encoders. arXiv preprint arXiv:161107308
- Kipf TN, Welling M (2017a) Semi-supervised classification with graph convolutional networks. In: International Conference on Learning Representations
- Kipf TN, Welling M (2017b) Semi-supervised classification with graph convolutional networks. In: 5th International Conference on Learning Representations, ICLR 2017, Toulon, France, April 24–26, 2017, Conference Track Proceedings, OpenReview.net
- Kireev DB (1995) ChemNet: A novel neural network based method for graph/property mapping. *Journal of Chemical Information and Computer Sciences* 35(2):175–180
- Klicpera J, Bojchevski A, Günnemann S (2019a) Predict then propagate: Graph neural networks meet personalized pagerank. In: International Conference on Learning Representations
- Klicpera J, Weißenberger S, Günnemann S (2019b) Diffusion improves graph learning. In: Advances in Neural Information Processing Systems, pp 13,333–13,345
- Klicpera J, Groß J, Günnemann S (2020) Directional message passing for molecular graphs. In: International Conference on Learning Representations
- Ko AJ, Myers BA, Coblenz MJ, Aung HH (2006) An exploratory study of how developers seek, relate, and collect relevant information during software maintenance tasks. *IEEE Transactions on software engineering* 32(12):971–987
- Koch O, Kriege NM, Humbeck L (2019) Chemical similarity and substructure searches. In: Encyclopedia of Bioinformatics and Computational Biology, Academic Press, Oxford, pp 640–649
- Kohavi R, John GH (1995) Automatic parameter selection by minimizing estimated error. In: Machine Learning Proceedings 1995, Elsevier, pp 304–312
- Koivisto M, Sood K (2004) Exact bayesian structure discovery in bayesian networks. *The Journal of Machine Learning Research* 5:549–573
- Koncel-Kedziorski R, Bekal D, Luan Y, Lapata M, Hajishirzi H (2019) Text generation from knowledge graphs with graph transformers. In: Proceedings of the 2019 Conference of the North American Chapter of the Association for Computational Linguistics: Human Language Technologies, Volume 1 (Long and Short Papers), pp 2284–2293
- Koo DCE, Bonneau R (2018) Towards region-specific propagation of protein functions. *Bioinformatics* 35(10):1737–1744

- Kool W, Van Hoof H, Welling M (2019) Stochastic beams and where to find them: The gumbel-top-k trick for sampling sequences without replacement. In: International Conference on Machine Learning, PMLR, pp 3499–3508
- Koren Y (2008) Factorization meets the neighborhood: a multifaceted collaborative filtering model. In: Proceedings of the 14th ACM SIGKDD international conference on Knowledge discovery and data mining, ACM, pp 426–434
- Koren Y (2009) Collaborative filtering with temporal dynamics. In: Proceedings of the 15th ACM SIGKDD international conference on Knowledge discovery and data mining, pp 447–456
- Koren Y, Bell R, Volinsky C (2009) Matrix factorization techniques for recommender systems. *Computer* 42(8):30–37
- Korte BH, Vygen J, Korte B, Vygen J (2011) Combinatorial optimization, vol 1. Springer
- Kosugi S, Yamasaki T (2020) Unpaired image enhancement featuring reinforcement-learning-controlled image editing software. In: Proceedings of the AAAI Conference on Artificial Intelligence, vol 34, pp 11,296–11,303
- Kovács IA, Luck K, Spirohn K, et al (2019) Network-based prediction of protein interactions. *Nature Communications* 10(1)
- Kremenek T, Ng AY, Engler DR (2007) A factor graph model for software bug finding. In: IJCAI, pp 2510–2516
- Kriege N, Mutzel P (2012) Subgraph matching kernels for attributed graphs. In: Proceedings of the 29th International Conference on International Conference on Machine Learning, Omnipress, Madison, WI, USA, ICML'12, p 291–298
- Kriege NM, P-L G, Wilson RC (2016) On valid optimal assignment kernels and applications to graph classification. In: Advances in Neural Information Processing Systems, pp 1615–1623
- Kriege NM, Johansson FD, Morris C (2020) A survey on graph kernels. *Applied Network Science* 5(1):6
- Krishnan A (2018) Making search easier: How amazon's product graph is helping customers find products more easily. ed Amazon Blog
- Krishnapuram R, Medasani S, Jung SH, Choi YS, Balasubramaniam R (2004) Content-based image retrieval based on a fuzzy approach. *IEEE transactions on knowledge and data engineering* 16(10):1185–1199
- Krizhevsky A, Sutskever I, Hinton GE (2012) Imagenet classification with deep convolutional neural networks. *Advances in neural information processing systems* 25:1097–1105
- Kuhn M, Letunic I, Jensen LJ, Bork P (2016) The sider database of drugs and side effects. *Nucleic acids research* 44(D1):D1075–D1079
- Kulmanov M, Hoehndorf R (2019) DeepGOPlus: improved protein function prediction from sequence. *Bioinformatics*
- Kumar S, Spezzano F, Subrahmanian V, Faloutsos C (2016) Edge weight prediction in weighted signed networks. In: 2016 IEEE 16th International Conference on Data Mining (ICDM), IEEE, pp 221–230

- Kumar S, Ying J, de Miranda Cardoso JV, Palomar D (2019a) Structured graph learning via laplacian spectral constraints. In: *Advances in Neural Information Processing Systems*, pp 11,651–11,663
- Kumar S, Zhang X, Leskovec J (2019b) Predicting dynamic embedding trajectory in temporal interaction networks. In: *ACM SIGKDD International Conference on Knowledge Discovery & Data Mining*, pp 1269–1278
- Kumar S, Ying J, de Miranda Cardoso JV, Palomar DP (2020) A unified framework for structured graph learning via spectral constraints. *Journal of Machine Learning Research* 21(22):1–60
- Kusner MJ, Paige B, Hernández-Lobato JM (2017) Grammar variational autoencoder. In: *International Conference on Machine Learning*, pp 1945–1954
- Lacroix T, Obozinski G, Usunier N (2020) Tensor decompositions for temporal knowledge base completion. In: *International Conference on Learning Representations*
- Lake B, Tenenbaum J (2010) Discovering structure by learning sparse graphs. In: *Proceedings of the Annual Meeting of the Cognitive Science Society*, vol 32
- Lamb LC, Garcez A, Gori M, Prates M, Avelar P, Vardi M (2020) Graph neural networks meet neural-symbolic computing: A survey and perspective. In: *Proceedings of IJCAI-PRICAI 2020*
- Lan Z, Chen M, Goodman S, Gimpel K, Sharma P, Soricut R (2020) ALBERT: A lite BERT for self-supervised learning of language representations. In: *8th International Conference on Learning Representations, ICLR 2020, Addis Ababa, Ethiopia, April 26-30, 2020, OpenReview.net*
- Lanczos C (1950) An iteration method for the solution of the eigenvalue problem of linear differential and integral operators. United States Governm. Press Office Los Angeles, CA
- Landrieu L, Simonovsky M (2018) Large-scale point cloud semantic segmentation with superpoint graphs. In: *Proceedings of the IEEE Conference on Computer Vision and Pattern Recognition*, pp 4558–4567
- Latif S, Rana R, Khalifa S, Jurdak R, Epps J (2019) Direct modelling of speech emotion from raw speech. In: *Proceedings of the 20th Annual Conference of the International Speech Communication Association (INTERSPEECH 2019), International Speech Communication Association (ISCA)*, pp 3920–3924
- Lawler EL (1963) The quadratic assignment problem. *Management science* 9(4):586–599
- Le Cun Y, Boser B, Denker JS, Henderson D, Howard RE, Hubbard W, Jackel LD (1989) Handwritten digit recognition with a back-propagation network. In: *Neural Information Processing Systems*, pp 396–404
- Le-Khac PH, Healy G, Smeaton AF (2020) Contrastive representation learning: a framework and review. *IEEE Access* 8:1–28
- Leblay J, Chekol MW (2018) Deriving validity time in knowledge graph. In: *Companion Proceedings of the The Web Conference 2018*, pp 1771–1776
- LeClair A, McMillan C (2019) Recommendations for datasets for source code summarization. In: *Proceedings of the 2019 Conference of the North American Chap-*

- ter of the Association for Computational Linguistics: Human Language Technologies, Volume 1 (Long and Short Papers), pp 3931–3937
- LeClair A, Jiang S, McMillan C (2019) A neural model for generating natural language summaries of program subroutines. In: Proceedings of the 41st International Conference on Software Engineering, IEEE Press, pp 795–806
- LeClair A, Haque S, Wu L, McMillan C (2020) Improved code summarization via a graph neural network. In: 28th ACM/IEEE International Conference on Program Comprehension (ICPC'20)
- LeCun Y, Boser B, Denker JS, Henderson D, Howard RE, Hubbard W, Jackel LD (1989) Backpropagation applied to handwritten zip code recognition. *Neural computation* 1(4):541–551
- Lecuyer M, Atlidakis V, Geambasu R, Hsu D, Jana S (2019) Certified robustness to adversarial examples with differential privacy. In: IEEE Symposium on Security and Privacy, DOI 10.1109/SP.2019.00044
- Lee G, Yuan Y, Chang S, Jaakkola TS (2019a) Tight certificates of adversarial robustness for randomly smoothed classifiers. In: Wallach HM, Larochelle H, Beygelzimer A, d'Alché-Buc F, Fox EB, Garnett R (eds) *Advances in Neural Information Processing Systems 32: Annual Conference on Neural Information Processing Systems 2019, NeurIPS 2019, December 8–14, 2019, Vancouver, BC, Canada*, pp 4911–4922
- Lee J, Lee I, Kang J (2019b) Self-attention graph pooling. In: *International Conference on Machine Learning*, PMLR, pp 3734–3743
- Lee JB, Rossi RA, Kim S, Ahmed NK, Koh E (2019c) Attention models in graphs: A survey. *ACM Transactions on Knowledge Discovery from Data (TKDD)* 13(6):1–25
- Lee JB, Rossi RA, Kong X, Kim S, Koh E, Rao A (2019d) Graph convolutional networks with motif-based attention. In: 28th ACM International Conference on Information, pp 499–508
- Lee S, Park C, Yu H (2019e) Bhin2vec: Balancing the type of relation in heterogeneous information network. In: *Proceedings of the 28th ACM International Conference on Information and Knowledge Management*, pp 619–628
- Lei T, Jin W, Barzilay R, Jaakkola T (2017a) Deriving neural architectures from sequence and graph kernels. In: *Proceedings of the 34th International Conference on Machine Learning-Volume 70*, pp 2024–2033
- Lei T, Zhang Y, Wang SI, Dai H, Artzi Y (2017b) Simple recurrent units for highly parallelizable recurrence. *arXiv preprint arXiv:1709.02755*
- Leordeanu M, Hebert M (2005) A spectral technique for correspondence problems using pairwise constraints. In: *IEEE International Conference on Computer Vision*, pp 1482–1489
- Leskovec J, Grobelnik M, Milic-Frayling N (2004) Learning sub-structures of document semantic graphs for document summarization. In: *LinkKDD Workshop*, pp 133–138
- Leskovec J, Chakrabarti D, Kleinberg J, Faloutsos C, Ghahramani Z (2010) *Kroner graphs: an approach to modeling networks*. *Journal of Machine Learning Research* 11(2)

- Letovsky S (1987) Cognitive processes in program comprehension. *Journal of Systems and software* 7(4):325–339
- Levi FW (1942) Finite geometrical systems: six public lectures delivered in February, 1940, at the University of Calcutta. University of Calcutta
- Levie R, Monti F, Bresson X, Bronstein MM (2019) Cayleynets: Graph convolutional neural networks with complex rational spectral filters. *IEEE Trans Signal Process* 67(1):97–109
- Levin E, Pieraccini R, Eckert W (2000) A stochastic model of human-machine interaction for learning dialog strategies. *IEEE Transactions on speech and audio processing* 8(1):11–23
- Levy O, Goldberg Y (2014) Neural word embedding as implicit matrix factorization. In: *Advances in neural information processing systems*, pp 2177–2185
- Lewis HR, et al (1983) Michael r. garey, david s. johnson, computers and intractability. a guide to the theory of np-completeness. *Journal of Symbolic Logic* 48(2):498–500
- Lewis M, Liu Y, Goyal N, Ghazvininejad M, Mohamed A, Levy O, Stoyanov V, Zettlemoyer L (2020) BART: Denoising sequence-to-sequence pre-training for natural language generation, translation, and comprehension. In: *Proceedings of the 58th Annual Meeting of the Association for Computational Linguistics*, p 7871, DOI 10.18653/v1/2020.acl-main.703
- Li A, Qin Z, Liu R, Yang Y, Li D (2019a) Spam review detection with graph convolutional networks. In: *Proceedings of the 28th ACM International Conference on Information and Knowledge Management*, pp 2703–2711
- Li C, Ma J, Guo X, Mei Q (2017a) Deepcas: An end-to-end predictor of information cascades. In: *Proceedings of the 26th international conference on World Wide Web*, pp 577–586
- Li C, Liu Z, Wu M, Xu Y, Zhao H, Huang P, Kang G, Chen Q, Li W, Lee DL (2019b) Multi-interest network with dynamic routing for recommendation at tmall. In: *Proceedings of the 28th ACM International Conference on Information and Knowledge Management*, pp 2615–2623
- Li F, Gan C, Liu X, Bian Y, Long X, Li Y, Li Z, Zhou J, Wen S (2017b) Temporal modeling approaches for large-scale youtube-8m video understanding. *arXiv preprint arXiv:1707.04555*
- Li G, Muller M, Thabet A, Ghanem B (2019c) Deepgcns: Can gcns go as deep as cnns? In: *Proceedings of the IEEE/CVF International Conference on Computer Vision*, pp 9267–9276
- Li J, Wang Y, Lyu MR, King I (2018a) Code completion with neural attention and pointer networks. In: *Proceedings of the 27th International Joint Conference on Artificial Intelligence*, pp 4159–25
- Li J, Yang F, Tomizuka M, Choi C (2020a) Evolvegraph: Multi-agent trajectory prediction with dynamic relational reasoning. *Advances in Neural Information Processing Systems* 33
- Li L, Feng H, Zhuang W, Meng N, Ryder B (2017c) Cclearner: A deep learning-based clone detection approach. In: *2017 IEEE International Conference on Software Maintenance and Evolution (ICSME)*, IEEE, pp 249–260

- Li L, Tang S, Deng L, Zhang Y, Tian Q (2017d) Image caption with global-local attention. In: Proceedings of the AAAI Conference on Artificial Intelligence, vol 31
- Li L, Gan Z, Cheng Y, Liu J (2019d) Relation-aware graph attention network for visual question answering. In: Proceedings of the IEEE/CVF International Conference on Computer Vision, pp 10,313–10,322
- Li L, Wang P, Yan J, Wang Y, Li S, Jiang J, Sun Z, Tang B, Chang TH, Wang S, et al (2020b) Real-world data medical knowledge graph: construction and applications. *Artificial intelligence in medicine* 103:101,817
- Li L, Zhang Y, Chen L (2020c) Generate neural template explanations for recommendation. In: Proceedings of the 29th ACM International Conference on Information & Knowledge Management, pp 755–764
- Li M, Chen S, Chen X, Zhang Y, Wang Y, Tian Q (2019e) Actional-structural graph convolutional networks for skeleton-based action recognition. In: IEEE/CVF Conference on Computer Vision and Pattern Recognition, pp 3595–3603
- Li N, Yang Z, Luo L, Wang L, Zhang Y, Lin H, Wang J (2020d) Kghe: a knowledge graph for hepatocellular carcinoma. *BMC Medical Informatics and Decision Making* 20(3):1–11
- Li P, Chien I, Milenkovic O (2019f) Optimizing generalized pagerank methods for seed-expansion community detection. In: Advances in Neural Information Processing Systems, pp 11,705–11,716
- Li P, Wang Y, Wang H, Leskovec J (2020e) Distance encoding: Design provably more powerful neural networks for graph representation learning. *Advances in Neural Information Processing Systems* 33
- Li Q, Zheng Y, Xie X, Chen Y, Liu W, Ma WY (2008) Mining user similarity based on location history. In: Proceedings of the 16th ACM SIGSPATIAL international conference on Advances in geographic information systems, pp 1–10
- Li Q, Han Z, Wu XM (2018b) Deeper insights into graph convolutional networks for semi-supervised learning. In: Proceedings of the AAAI Conference on Artificial Intelligence, vol 32
- Li R, Tapaswi M, Liao R, Jia J, Urtasun R, Fidler S (2017e) Situation recognition with graph neural networks. In: Proceedings of the IEEE International Conference on Computer Vision, pp 4173–4182
- Li R, Wang S, Zhu F, Huang J (2018c) Adaptive graph convolutional neural networks. In: Proceedings of the AAAI Conference on Artificial Intelligence, vol 32
- Li S, Wu L, Feng S, Xu F, Xu F, Zhong S (2020f) Graph-to-tree neural networks for learning structured input-output translation with applications to semantic parsing and math word problem. In: Findings of the Association for Computational Linguistics: EMNLP 2020, Association for Computational Linguistics, Online, pp 2841–2852, DOI 10.18653/v1/2020.findings-emnlp.255, URL <https://www.aclweb.org/anthology/2020.findings-emnlp.255>
- Li X, Cheng Y, Cong G, Chen L (2017f) Discovering pollution sources and propagation patterns in urban area. In: Proceedings of the 23rd ACM SIGKDD International Conference on Knowledge Discovery and Data Mining, pp 1863–1872

- Li X, Kao B, Ren Z, Yin D (2019g) Spectral clustering in heterogeneous information networks. In: Proceedings of the AAAI Conference on Artificial Intelligence, vol 33, pp 4221–4228
- Li X, Wang C, Tong B, Tan J, Zeng X, Zhuang T (2020g) Deep time-aware item evolution network for click-through rate prediction. In: Proceedings of the 29th ACM International CIKM, pp 785–794
- Li Y, Gupta A (2018) Beyond grids: Learning graph representations for visual recognition. In: Proceedings of the 32nd International Conference on Neural Information Processing Systems, pp 9245–9255
- Li Y, King I (2020) Autograph: Automated graph neural network. In: International Conference on Neural Information Processing, Springer, pp 189–201
- Li Y, Tarlow D, Brockschmidt M, Zemel R (2016a) Gated graph sequence neural networks. In: International Conference on Learning Representations
- Li Y, Tarlow D, Brockschmidt M, Zemel R (2016b) Gated graph sequence neural networks. In: International Conference on Learning Representations (ICLR)
- Li Y, Vinyals O, Dyer C, Pascanu R, Battaglia P (2018d) Learning deep generative models of graphs. arXiv preprint arXiv:180303324
- Li Y, Yu R, Shahabi C, Liu Y (2018e) Diffusion convolutional recurrent neural network: Data-driven traffic forecasting. In: International Conference on Learning Representations
- Li Y, Zhang L, Liu Z (2018f) Multi-objective de novo drug design with conditional graph generative model. *Journal of cheminformatics* 10(1):1–24
- Li Y, Gu C, Dullien T, Vinyals O, Kohli P (2019h) Graph matching networks for learning the similarity of graph structured objects. In: International Conference on Machine Learning, PMLR, pp 3835–3845
- Li Y, Liu M, Yin J, Cui C, Xu XS, Nie L (2019i) Routing micro-videos via a temporal graph-guided recommendation system. In: Proceedings of the 27th ACM International Conference on Multimedia, pp 1464–1472
- Li Y, Lin Y, Madhusudan M, Sharma A, Xu W, Sapatnekar SS, Harjani R, Hu J (2020h) A customized graph neural network model for guiding analog ic placement. In: International Conference On Computer Aided Design, IEEE, pp 1–9
- Liang S, Srikant R (2017) Why deep neural networks for function approximation? In: 5th International Conference on Learning Representations, ICLR 2017
- Liang Y, Zhu KQ (2018) Automatic generation of text descriptive comments for code blocks. In: McIlraith SA, Weinberger KQ (eds) Proceedings of the Thirty-Second AAAI Conference on Artificial Intelligence (AAAI-18), AAAI Press, pp 5229–5236
- Liao L, He X, Zhang H, Chua TS (2018) Attributed social network embedding. *IEEE Transactions on Knowledge and Data Engineering* 30(12):2257–2270
- Liao R, Li Y, Song Y, Wang S, Nash C, Hamilton WL, Duvenaud D, Urtasun R, Zemel RS (2019a) Efficient graph generation with graph recurrent attention networks. arXiv preprint arXiv:191000760
- Liao R, Zhao Z, Urtasun R, Zemel RS (2019b) Lanczosnet: Multi-scale deep graph convolutional networks. arXiv preprint arXiv:190101484

- Liao R, Urtasun R, Zemel R (2021) A pac-bayesian approach to generalization bounds for graph neural networks. In: International Conference on Learning Representations
- Liben-Nowell D, Kleinberg J (2007) The link-prediction problem for social networks. *Journal of the American society for information science and technology* 58(7):1019–1031
- Licata L, Lo Surdo P, Iannuccelli M, Palma A, Micarelli E, Perfetto L, Peluso D, Calderone A, Castagnoli L, Cesareni G (2020) Signor 2.0, the signaling network open resource 2.0: 2019 update. *Nucleic acids research* 48(D1):D504–D510
- Lillicrap TP, Hunt JJ, Pritzel A, Heess N, Erez T, Tassa Y, Silver D, Wierstra D (2015) Continuous control with deep reinforcement learning. *arXiv preprint arXiv:150902971*
- Lin C, Sun GJ, Bulusu KC, Dry JR, Hernandez M (2020a) Graph neural networks including sparse interpretability. *arXiv preprint arXiv:200700119*
- Lin G, Wen S, Han QL, Zhang J, Xiang Y (2020b) Software vulnerability detection using deep neural networks: a survey. *Proceedings of the IEEE* 108(10):1825–1848
- Lin P, Sun P, Cheng G, Xie S, Li X, Shi J (2020c) Graph-guided architecture search for real-time semantic segmentation. In: *Proceedings of the IEEE/CVF Conference on Computer Vision and Pattern Recognition*, pp 4203–4212
- Lin T, Zhao X, Shou Z (2017) Single shot temporal action detection. In: *Proceedings of the 25th ACM international conference on Multimedia*, pp 988–996
- Lin W, Ji S, Li B (2020d) Adversarial Attacks on Link Prediction Algorithms Based on Graph Neural Networks. In: *ACM Asia Conference on Computer and Communications Security*
- Lin X, Chen X (2012) Heterogeneous data integration by tree-augmented naïve bayes for protein-protein interactions prediction. *PROTEOMICS* 13(2):261–268
- Lin Y, Liu Z, Sun M, Liu Y, Zhu X (2015) Learning entity and relation embeddings for knowledge graph completion. In: *Proceedings of the AAAI Conference on Artificial Intelligence*, vol 29
- Lin Y, Ren P, Chen Z, Ren Z, Yu D, Ma J, Rijke Md, Cheng X (2020e) Meta matrix factorization for federated rating predictions. In: *Proceedings of the 43rd International ACM SIGIR Conference on Research and Development in Information Retrieval*, pp 981–990
- Lin ZH, Huang SY, Wang YCF (2020f) Convolution in the cloud: Learning deformable kernels in 3d graph convolution networks for point cloud analysis. In: *Proceedings of the IEEE/CVF Conference on Computer Vision and Pattern Recognition*, pp 1800–1809
- Ling X, Ji S, Zou J, Wang J, Wu C, Li B, Wang T (2019) DEEPSEC: A uniform platform for security analysis of deep learning model. In: *2019 IEEE Symposium on Security and Privacy (S&P)*, IEEE, pp 673–690
- Ling X, Wu L, Wang S, Ma T, Xu F, Liu AX, Wu C, Ji S (2020) Multi-level graph matching networks for deep graph similarity learning. *arXiv preprint arXiv:200704395*

- Ling X, Wu L, Wang S, Pan G, Ma T, Xu F, Liu AX, Wu C, Ji S (2021) Deep graph matching and searching for semantic code retrieval. *ACM Transactions on Knowledge Discovery from Data (TKDD)*
- Linial N, London E, Rabinovich Y (1995) The geometry of graphs and some of its algorithmic applications. *Combinatorica* 15(2):215–245
- Linmei H, Yang T, Shi C, Ji H, Li X (2019) Heterogeneous graph attention networks for semi-supervised short text classification. In: *Proceedings of the 2019 Conference on Empirical Methods in Natural Language Processing and the 9th International Joint Conference on Natural Language Processing (EMNLP-IJCNLP)*, pp 4823–4832
- Liu A, Xu N, Zhang H, Nie W, Su Y, Zhang Y (2018a) Multi-level policy and reward reinforcement learning for image captioning. In: *IJCAI*, pp 821–827
- Liu B, Niu D, Lai K, Kong L, Xu Y (2017a) Growing story forest online from massive breaking news. In: *Proceedings of the 2017 ACM on Conference on Information and Knowledge Management*, pp 777–785
- Liu B, Niu D, Wei H, Lin J, He Y, Lai K, Xu Y (2019a) Matching article pairs with graphical decomposition and convolutions. In: *Proceedings of the 57th Annual Meeting of the Association for Computational Linguistics*, pp 6284–6294
- Liu B, Han FX, Niu D, Kong L, Lai K, Xu Y (2020a) Story forest: Extracting events and telling stories from breaking news. *ACM Transactions on Knowledge Discovery from Data (TKDD)* 14(3):1–28
- Liu C, Zoph B, Neumann M, Shlens J, Hua W, Li LJ, Fei-Fei L, Yuille A, Huang J, Murphy K (2018b) Progressive neural architecture search. In: *Proceedings of the European conference on computer vision*, pp 19–34
- Liu H, Simonyan K, Vinyals O, Fernando C, Kavukcuoglu K (2017b) Hierarchical representations for efficient architecture search. *arXiv preprint arXiv:1711.00436*
- Liu H, Simonyan K, Yang Y (2018c) Darts: Differentiable architecture search. *arXiv preprint arXiv:1806.09055*
- Liu J, Chi Y, Zhu C (2015) A dynamic multiagent genetic algorithm for gene regulatory network reconstruction based on fuzzy cognitive maps. *IEEE Transactions on Fuzzy Systems* 24(2):419–431
- Liu J, Kumar A, Ba J, Kiros J, Swersky K (2019b) Graph normalizing flows. *arXiv preprint arXiv:1905.13177*
- Liu L, Ma Y, Zhu X, et al (2019) Integrating sequence and network information to enhance protein-protein interaction prediction using graph convolutional networks. In: *2019 IEEE International Conference on Bioinformatics and Biomedicine (BIBM)*, pp 1762–1768, DOI 10.1109/BIBM47256.2019.8983330
- Liu L, Ouyang W, Wang X, Fieguth P, Chen J, Liu X, Pietikäinen M (2020b) Deep learning for generic object detection: A survey. *International journal of computer vision* 128(2):261–318
- Liu M, Gao H, Ji S (2020c) Towards deeper graph neural networks. In: *Proceedings of the 26th ACM SIGKDD International Conference on Knowledge Discovery & Data Mining*, pp 338–348
- Liu N, Tan Q, Li Y, Yang H, Zhou J, Hu X (2019a) Is a single vector enough? exploring node polysemy for network embedding. In: *Proceedings of the 25th ACM*

- SIGKDD International Conference on Knowledge Discovery & Data Mining, pp 932–940
- Liu N, Du M, Hu X (2020d) Adversarial machine learning: An interpretation perspective. *arXiv preprint arXiv:2004.11488*
- Liu P, Chang S, Huang X, Tang J, Cheung JCK (2019b) Contextualized non-local neural networks for sequence learning. In: *Proceedings of the AAAI Conference on Artificial Intelligence*, vol 33, pp 6762–6769
- Liu Q, Allamanis M, Brockschmidt M, Gaunt AL (2018d) Constrained graph variational autoencoders for molecule design. *arXiv preprint arXiv:1805.09076*
- Liu S, Yang N, Li M, Zhou M (2014) A recursive recurrent neural network for statistical machine translation. In: *Proceedings of the 52nd Annual Meeting of the Association for Computational Linguistics, ACL 2014, June 22–27, 2014, Baltimore, MD, USA, Volume 1: Long Papers, The Association for Computer Linguistics*, pp 1491–1500
- Liu S, Chen Y, Xie X, Siow JK, Liu Y (2021) Retrieval-augmented generation for code summarization via hybrid gnn. In: *9th International Conference on Learning Representations*
- Liu X, Si S, Zhu X, Li Y, Hsieh CJ (2019c) A Unified Framework for Data Poisoning Attack to Graph-based Semi-supervised Learning. In: *Neural Information Processing Systems, NeurIPS*
- Liu X, Pan H, He M, Song Y, Jiang X, Shang L (2020e) Neural subgraph isomorphism counting. In: *Proceedings of the 26th ACM SIGKDD International Conference on Knowledge Discovery & Data Mining*, pp 1959–1969
- Liu X, Zhang F, Hou Z, Wang Z, Mian L, Zhang J, Tang J (2020f) Self-supervised learning: Generative or contrastive. *arXiv preprint arXiv:2006.08218* 1(2)
- Liu Y, Lee J, Park M, Kim S, Yang E, Hwang SJ, Yang Y (2018e) Learning to propagate labels: Transductive propagation network for few-shot learning. *arXiv preprint arXiv:1805.10002*
- Liu Y, Wan B, Zhu X, He X (2020g) Learning cross-modal context graph for visual grounding. In: *Proceedings of the AAAI Conference on Artificial Intelligence*, vol 34, pp 11,645–11,652
- Liu Y, Zhang F, Zhang Q, Wang S, Wang Y, Yu Y (2020h) Cross-view correspondence reasoning based on bipartite graph convolutional network for mammogram mass detection. In: *Proceedings of the IEEE/CVF Conference on Computer Vision and Pattern Recognition*, pp 3812–3822
- Liu Z, Chen C, Yang X, Zhou J, Li X, Song L (2018f) Heterogeneous graph neural networks for malicious account detection. In: *Proceedings of the 27th ACM International Conference on Information and Knowledge Management*, pp 2077–2085
- Livshits B, Nori AV, Rajamani SK, Banerjee A (2009) Merlin: specification inference for explicit information flow problems. *ACM Sigplan Notices* 44(6):75–86
- Locatelli A, Sieniutycz S (2002) Optimal control: An introduction. *Appl Mech Rev* 55(3):B48–B49

- Loiola EM, de Abreu NMM, Boaventura-Netto PO, Hahn P, Querido T (2007) A survey for the quadratic assignment problem. *European journal of operational research* 176(2):657–690
- Lops P, De Gemmis M, Semeraro G (2011) Content-based recommender systems: State of the art and trends. In: *Recommender systems handbook*, Springer, pp 73–105
- Loukas A (2020) What graph neural networks cannot learn: depth vs width. In: *International Conference on Learning Representations*
- Lovász L, et al (1993) Random walks on graphs: A survey. *Combinatorics, Paul erdos is eighty* 2(1):1–46
- Lovell SC, Davis IW, Arendall WB, et al (2003) Structure validation by c geometry: , and c deviation. *Proteins: Structure, Function, and Bioinformatics* 50(3):437–450
- Loyola P, Marrese-Taylor E, Matsuo Y (2017) A neural architecture for generating natural language descriptions from source code changes. In: *Proceedings of the 55th Annual Meeting of the Association for Computational Linguistics (Volume 2: Short Papers)*, pp 287–292
- Lü L, Zhou T (2011) Link prediction in complex networks: A survey. *Physica A: statistical mechanics and its applications* 390(6):1150–1170
- Lu X, Wang B, Zheng X, Li X (2017a) Exploring models and data for remote sensing image caption generation. *IEEE Transactions on Geoscience and Remote Sensing* 56(4):2183–2195
- Lu Y, Zhao Z, Li G, Jin Z (2017b) Learning to generate comments for api-based code snippets. In: *Software Engineering and Methodology for Emerging Domains*, Springer, pp 3–14
- Lucic A, ter Hoeve M, Tolomei G, de Rijke M, Silvestri F (2021) Cf-gnnexplainer: Counterfactual explanations for graph neural networks. *arXiv preprint arXiv:210203322*
- Luo D, Cheng W, Xu D, Yu W, Zong B, Chen H, Zhang X (2020) Parameterized explainer for graph neural network. *arXiv preprint arXiv:201104573*
- Luo D, Cheng W, Yu W, Zong B, Ni J, Chen H, Zhang X (2021) Learning to Drop: Robust Graph Neural Network via Topological Denoising. In: *International Conference on Web Search and Data Mining, WSDM*
- Luo R, Liao W, Huang X, Pi Y, Philips W (2016) Feature extraction of hyperspectral images with semisupervised graph learning. *IEEE Journal of Selected Topics in Applied Earth Observations and Remote Sensing* 9(9):4389–4399
- Luo R, Tian F, Qin T, Chen EH, Liu TY (2018) Neural architecture optimization. In: *Advances in neural information processing systems*
- Luo X, You Z, Zhou M, et al (2015) A highly efficient approach to protein interactome mapping based on collaborative filtering framework. *Scientific Reports* 5(1):7702
- Luong T, Pham H, Manning CD (2015) Effective approaches to attention-based neural machine translation. In: *Proceedings of the 2015 Conference on Empirical Methods in Natural Language Processing*, Association for Computational Linguistics, Lisbon, Portugal, pp 1412–1421, DOI 10.18653/v1/D15-1166

- Ma G, Ahmed NK, Willke TL, Yu PS (2019a) Deep graph similarity learning: A survey. arXiv preprint arXiv:1912.11615
- Ma H, Bian Y, Rong Y, Huang W, Xu T, Xie W, Ye G, Huang J (2020a) Multi-view graph neural networks for molecular property prediction. arXiv e-prints pp arXiv-2005
- Ma J, Tang W, Zhu J, Mei Q (2019b) A flexible generative framework for graph-based semi-supervised learning. In: Advances in Neural Information Processing Systems, pp 3281–3290
- Ma J, Zhou C, Cui P, Yang H, Zhu W (2019c) Learning disentangled representations for recommendation. In: Wallach HM, Larochelle H, Beygelzimer A, d'Alché-Buc F, Fox EB, Garnett R (eds) Advances in Neural Information Processing Systems 32: Annual Conference on Neural Information Processing Systems 2019, NeurIPS 2019, December 8-14, 2019, Vancouver, BC, Canada, pp 5712–5723
- Ma J, Ding S, Mei Q (2020b) Towards more practical adversarial attacks on graph neural networks. In: Larochelle H, Ranzato M, Hadsell R, Balcan M, Lin H (eds) Advances in Neural Information Processing Systems 33: Annual Conference on Neural Information Processing Systems 2020, NeurIPS 2020, December 6-12, 2020, virtual
- Ma T, Chen J, Xiao C (2018) Constrained generation of semantically valid graphs via regularizing variational autoencoders. In: Advances in Neural Information Processing Systems, pp 7113–7124
- Ma Y, Wang S, Aggarwal CC, Tang J (2019d) Graph convolutional networks with eigenpooling. In: ACM SIGKDD International Conference on Knowledge Discovery & Data Mining, ACM, pp 723–731
- Maalej W, Tiarks R, Roehm T, Koschke R (2014) On the comprehension of program comprehension. ACM Transactions on Software Engineering and Methodology (TOSEM) 23(4):1–37
- Maddison C, Mnih A, Teh Y (2017) The concrete distribution: A continuous relaxation of discrete random variables. International Conference on Learning Representations
- Madry A, Makelov A, Schmidt L, Tsipras D, Vladu A (2017) Towards deep learning models resistant to adversarial attacks. arXiv preprint arXiv:1706.06083
- Maglott D, Ostell J, Pruitt KD, Tatusova T (2010) Entrez gene: gene-centered information at ncbi. Nucleic acids research 39(suppl_1):D52–D57
- Malewicz G, Austern MH, Bik AJ, Dehnert JC, Horn I, Leiser N, Czajkowski G (2010) Pregel: a system for large-scale graph processing. In: Proceedings of the 2010 ACM SIGMOD International Conference on Management of data, pp 135–146
- Malliaros FD, Vazirgiannis M (2013) Clustering and community detection in directed networks: A survey. Physics reports 533(4):95–142
- Man T, Shen H, Liu S, Jin X, Cheng X (2016) Predict anchor links across social networks via an embedding approach. In: Ijcai, vol 16, pp 1823–1829
- Manessi F, Rozza A (2020) Graph-based neural network models with multiple self-supervised auxiliary tasks. arXiv preprint arXiv: 2011.07267

- Manessi F, Rozza A, Manzo M (2020) Dynamic graph convolutional networks. *Pattern Recognition* 97:107,000
- Mangal R, Zhang X, Nori AV, Naik M (2015) A user-guided approach to program analysis. In: *Proceedings of the 2015 10th Joint Meeting on Foundations of Software Engineering*, pp 462–473
- Manning C, Schutze H (1999) *Foundations of statistical natural language processing*. MIT press
- Marcheggiani D, Titov I (2017) Encoding sentences with graph convolutional networks for semantic role labeling. In: *EMNLP 2017-Conference on Empirical Methods in Natural Language Processing, Proceedings*, pp 1506–1515
- Marcheggiani D, Bastings J, Titov I (2018) Exploiting semantics in neural machine translation with graph convolutional networks. *arXiv preprint arXiv:180408313*
- Maretic HP, Thanou D, Frossard P (2017) Graph learning under sparsity priors. In: *2017 IEEE International Conference on Acoustics, Speech and Signal Processing (ICASSP), Ieee*, pp 6523–6527
- Markovitz A, Sharir G, Friedman I, Zelnik-Manor L, Avidan S (2020) Graph embedded pose clustering for anomaly detection. In: *Proceedings of the IEEE/CVF Conference on Computer Vision and Pattern Recognition*, pp 10,539–10,547
- Maron H, Ben-Hamu H, Shamir N, Lipman Y (2018) Invariant and equivariant graph networks. In: *International Conference on Learning Representations*
- Maron H, Ben-Hamu H, Serviansky H, Lipman Y (2019a) Provably powerful graph networks. In: *Advances in Neural Information Processing Systems*, pp 2153–2164
- Maron H, Fetaya E, Segol N, Lipman Y (2019b) On the universality of invariant networks. In: *International Conference on Machine Learning*, pp 4363–4371
- Mathew B, Sikdar S, Lemmerich F, Strohmaier M (2020) The polar framework: Polar opposites enable interpretability of pre-trained word embeddings. In: *Proceedings of The Web Conference 2020*, pp 1548–1558
- Matsuno R, Murata T (2018) Mell: effective embedding method for multiplex networks. In: *Companion Proceedings of the The Web Conference 2018*, pp 1261–1268
- Matuszek C (2018) Grounded language learning: Where robotics and nlp meet (invited talk). In: *Proceedings of the 27th International Joint Conference on Artificial Intelligence*, pp 5687–5691
- Maziarka Ł, Danel T, Mucha S, Rataj K, Tabor J, Jastrzebski S (2020a) Molecule attention transformer. *arXiv preprint arXiv:200208264*
- Maziarka Ł, Pocha A, Kaczmarczyk J, Rataj K, Danel T, Warchoń M (2020b) Moleculecogan: a generative model for molecular optimization. *Journal of Cheminformatics* 12(1):1–18
- McBurney PW, McMillan C (2014) Automatic documentation generation via source code summarization of method context. In: *Proceedings of the 22nd International Conference on Program Comprehension, ACM*, pp 279–290
- McBurney PW, McMillan C (2016) Automatic source code summarization of context for java methods. *IEEE Transactions on Software Engineering* 42(2):103–119

- McBurney PW, Liu C, McMillan C (2016) Automated feature discovery via sentence selection and source code summarization. *Journal of Software: Evolution and Process* 28(2):120–145
- McMillan C, Grechanik M, Poshyvanyk D, Xie Q, Fu C (2011) Portfolio: finding relevant functions and their usage. In: *Proceedings of the 33rd International Conference on Software Engineering*, pp 111–120
- McMillan C, Poshyvanyk D, Grechanik M, Xie Q, Fu C (2013) Portfolio: Searching for relevant functions and their usages in millions of lines of code. *ACM Transactions on Software Engineering and Methodology (TOSEM)* 22(4):1–30
- McNee SM, Riedl J, Konstan JA (2006) Being accurate is not enough: how accuracy metrics have hurt recommender systems. In: *CHI'06 extended abstracts on Human factors in computing systems*, pp 1097–1101
- Mendez D, Gaulton A, Bento AP, Chambers J, De Veij M, Félix E, Magariños MP, Mosquera JF, Mutowo P, Nowotka M, et al (2019) ChEMBL: towards direct deposition of bioassay data. *Nucleic acids research* 47(D1):D930–D940
- Merkwirth C, Lengauer T (2005) Automatic generation of complementary descriptors with molecular graph networks. *Journal of Chemical Information and Modeling* 45(5):1159–1168
- Mesquita DPP, Jr AHS, Kaski S (2020) Rethinking pooling in graph neural networks. In: *Advances in Neural Information Processing Systems*
- Mihalcea R, Tarau P (2004) Textrank: Bringing order into text. In: *Proceedings of the 2004 conference on empirical methods in natural language processing*, pp 404–411
- Miikkulainen R, Liang J, Meyerson E, Rawal A, Fink D, Francon O, Raju B, Shahrzad H, Navruzyan A, Duffy N, et al (2019) Evolving deep neural networks. In: *Artificial Intelligence in the Age of Neural Networks and Brain Computing*, Elsevier, pp 293–312
- Mikolov T, Karafiát M, Burget L, Cernocký J, Khudanpur S (2010) Recurrent neural network based language model. In: Kobayashi T, Hirose K, Nakamura S (eds) *INTERSPEECH 2010, 11th Annual Conference of the International Speech Communication Association*, Makuhari, Chiba, Japan, September 26–30, 2010, ISCA, pp 1045–1048
- Mikolov T, Deoras A, Kombrink S, Burget L, Cernocký J (2011a) Empirical evaluation and combination of advanced language modeling techniques. In: *INTERSPEECH 2011, 12th Annual Conference of the International Speech Communication Association*, Florence, Italy, August 27–31, 2011, ISCA, pp 605–608
- Mikolov T, Kombrink S, Burget L, Černocký J, Khudanpur S (2011b) Extensions of recurrent neural network language model. In: *2011 IEEE international conference on acoustics, speech and signal processing (ICASSP)*, IEEE, pp 5528–5531
- Mikolov T, Chen K, Corrado G, Dean J (2013a) Efficient estimation of word representations in vector space. *arXiv preprint arXiv:13013781*
- Mikolov T, Sutskever I, Chen K, Corrado GS, Dean J (2013b) Distributed representations of words and phrases and their compositionality. In: *Advances in neural information processing systems*, pp 3111–3119

- Mikolov T, ÇGDJ Chen K (2013) Efficient estimation of word representations in vector space. In: International Conference on Learning Representations
- Miller BA, Çamurcu M, Gomez AJ, Chan K, Eliassi-Rad T (2019) Improving Robustness to Attacks Against Vertex Classification. In: Deep Learning for Graphs at AAAI Conference on Artificial Intelligence
- Miller GA (1995) Wordnet: a lexical database for english. *Communications of the ACM* 38(11):39–41
- Miller T (2019) Explanation in artificial intelligence: Insights from the social sciences. *Artificial intelligence* 267:1–38
- Milo R, Shen-Orr S, Itzkovitz S, Kashtan N, Chklovskii D, Alon U (2002) Network motifs: simple building blocks of complex networks. *Science* 298(5594):824–827
- Min S, Gao Z, Peng J, Wang L, Qin K, Fang B (????) Stgsn-a spatial-temporal graph neural network framework for time-evolving social networks. *Knowledge-Based Systems* p 106746
- Mir AM, Latoskinas E, Proksch S, Gousios G (2021) Type4Py: Deep similarity learning-based type inference for Python. *arXiv preprint arXiv:210104470*
- Mirza M, Osindero S (2014) Conditional generative adversarial nets. *arXiv preprint arXiv:14111784*
- Mnih A, Salakhutdinov RR (2008) Probabilistic matrix factorization. In: *Advances in neural information processing systems*, pp 1257–1264
- Mnih V, Kavukcuoglu K, Silver D, Rusu AA, Veness J, Bellemare MG, Graves A, Riedmiller M, Fidjeland AK, Ostrovski G, et al (2015) Human-level control through deep reinforcement learning. *Nature* 518(7540):529–533
- Mokou M, Lygirou V, Angelioudaki I, Paschalidis N, Stroggilos R, Frantzi M, Latosinska A, Bamias A, Hoffmann MJ, Mischak H, et al (2020) A novel pipeline for drug repurposing for bladder cancer based on patients' omics signatures. *Cancers* 12(12):3519
- Momtazpour M, Butler P, Hossain MS, Bozchalui MC, Ramakrishnan N, Sharma R (2012) Coordinated clustering algorithms to support charging infrastructure design for electric vehicles. In: *Proceedings of the ACM SIGKDD International Workshop on Urban Computing*, pp 126–133
- Montavon G, Samek W, Müller KR (2018) Methods for interpreting and understanding deep neural networks. *Digital Signal Processing* 73:1–15
- Monti F, Bronstein M, Bresson X (2017) Geometric matrix completion with recurrent multi-graph neural networks. In: *Advances in Neural Information Processing Systems*, pp 3700–3710
- Monti F, Frasca F, Eynard D, Mannion D, Bronstein MM (2019) Fake news detection on social media using geometric deep learning. In: *Workshop on Representation Learning on Graphs and Manifolds*
- Moreno L, Aponte J, Sridhara G, Marcus A, Pollock L, Vijay-Shanker K (2013) Automatic generation of natural language summaries for java classes. In: *2013 21st International Conference on Program Comprehension (ICPC)*, IEEE, pp 23–32
- Moreno L, Bavota G, Di Penta M, Oliveto R, Marcus A, Canfora G (2014) Automatic generation of release notes. In: *Proceedings of the 22nd ACM SIGSOFT In-*

- ternational Symposium on Foundations of Software Engineering, ACM, pp 484–495
- Morris C, Kersting K, Mutzel P (2017) Glocalized Weisfeiler-Lehman kernels: Global-local feature maps of graphs. In: IEEE International Conference on Data Mining, IEEE, pp 327–336
- Morris C, Ritzert M, Fey M, Hamilton WL, Lenssen JE, Rattan G, Grohe M (2019) Weisfeiler and leman go neural: Higher-order graph neural networks. In: the AAAI Conference on Artificial Intelligence, vol 33, pp 4602–4609
- Morris C, Kriege NM, Bause F, Kersting K, Mutzel P, Neumann M (2020a) TU-Dataset: A collection of benchmark datasets for learning with graphs. CoRR abs/2007.08663
- Morris C, Rattan G, Mutzel P (2020b) Weisfeiler and leman go sparse: Towards scalable higher-order graph embeddings. *Advances in Neural Information Processing Systems* 33
- Mueller J, Thyagarajan A (2016) Siamese recurrent architectures for learning sentence similarity. In: Proceedings of the AAAI Conference on Artificial Intelligence, vol 30
- Mungall CJ, Torniai C, Gkoutos GV, Lewis SE, Haendel MA (2012) Uberon, an integrative multi-species anatomy ontology. *Genome biology* 13(1):1–20
- Murphy R, Srinivasan B, Rao V, Ribeiro B (2019a) Relational pooling for graph representations. In: International Conference on Machine Learning, pp 4663–4673
- Murphy RL, Srinivasan B, Rao VA, Ribeiro B (2019b) Janosy pooling: Learning deep permutation-invariant functions for variable-size inputs. In: International Conference on Learning Representations
- Murphy RL, Srinivasan B, Rao VA, Ribeiro B (2019c) Relational pooling for graph representations. In: International Conference on Machine Learning, pp 4663–4673
- Nair V, Hinton GE (2010) Rectified linear units improve restricted boltzmann machines. In: Fürnkranz J, Joachims T (eds) Proceedings of the 27th International Conference on Machine Learning (ICML-10), June 21–24, 2010, Haifa, Israel, Omnipress, pp 807–814
- Nathani D, Chauhan J, Sharma C, Kaul M (2019) Learning attention-based embeddings for relation prediction in knowledge graphs. arXiv preprint arXiv:1906.01195
- Nelson CA, Butte AJ, Baranzini SE (2019) Integrating biomedical research and electronic health records to create knowledge-based biologically meaningful machine-readable embeddings. *Nature communications* 10(1):1–10
- Neville J, Jensen D (2000) Iterative classification in relational data. In: Proc. AAAI-2000 workshop on learning statistical models from relational data, pp 13–20
- Newman M (2010) *Networks: an introduction*. Oxford university press
- Newman M (2018) *Networks*. Oxford university press
- Newman ME (2006a) Finding community structure in networks using the eigenvectors of matrices. *Physical review E* 74(3):036,104
- Newman ME (2006b) Modularity and community structure in networks. *Proceedings of the national academy of sciences* 103(23):8577–8582

- Ng A (2011) Machine learning
- Nguyen DQ, Nguyen TD, Nguyen DQ, Phung D (2017) A novel embedding model for knowledge base completion based on convolutional neural network. arXiv preprint arXiv:1712.02121
- Nguyen HV, Bai L (2010) Cosine similarity metric learning for face verification. In: Asian conference on computer vision, Springer, pp 709–720
- Nickel M, Tresp V (2013) Tensor factorization for multi-relational learning. In: Joint European Conference on Machine Learning and Knowledge Discovery in Databases, Springer, pp 617–621
- Nickel M, Tresp V, Kriegel HP (2011) A three-way model for collective learning on multi-relational data. In: Proceedings of the 28th International Conference on International Conference on Machine Learning, Omnipress, Madison, WI, USA, ICML'11, p 809–816
- Nickel M, Jiang X, Tresp V (2014) Reducing the rank in relational factorization models by including observable patterns. In: Advances in Neural Information Processing Systems, pp 1179–1187
- Nickel M, Murphy K, Tresp V, Gabrilovich E (2016a) A review of relational machine learning for knowledge graphs. *Proceedings of the IEEE* 104(1):11–33
- Nickel M, Rosasco L, Poggio T (2016b) Holographic embeddings of knowledge graphs. In: Proceedings of the AAAI Conference on Artificial Intelligence, vol 30
- Nicora G, Vitali F, Dagliati A, Geifman N, Bellazzi R (2020) Integrated multi-omics analyses in oncology: a review of machine learning methods and tools. *Frontiers in oncology* 10:1030
- Nie P, Rai R, Li JJ, Khurshid S, Mooney RJ, Gligoric M (2019) A framework for writing trigger-action todo comments in executable format. In: Proceedings of the 2019 27th ACM Joint Meeting on European Software Engineering Conference and Symposium on the Foundations of Software Engineering, ACM, pp 385–396
- Nielson F, Nielson HR, Hankin C (2015) Principles of program analysis. Springer
- Niepert M, Ahmed M, Kutzkov K (2016) Learning convolutional neural networks for graphs. In: International Conference on Machine Learning, pp 2014–2023
- Nikolentzos G, Meladianos P, Vazirgiannis M (2017) Matching node embeddings for graph similarity. In: AAAI Conference on Artificial Intelligence, pp 2429–2435
- Ning X, Karypis G (2011) Slim: Sparse linear methods for top-n recommender systems. In: 2011 IEEE 11th International Conference on Data Mining, IEEE, pp 497–506
- Niu C, Wu F, Tang S, Hua L, Jia R, Lv C, Wu Z, Chen G (2020) Billion-scale federated learning on mobile clients: A submodel design with tunable privacy. In: Proceedings of the 26th Annual International Conference on Mobile Computing and Networking, pp 1–14
- Norcliffe-Brown W, Vafeias S, Parisot S (2018) Learning conditioned graph structures for interpretable visual question answering. In: Advances in neural information processing systems, pp 8334–8343

- Noroozi M, Favaro P (2016) Unsupervised learning of visual representations by solving jigsaw puzzles. In: European conference on computer vision, Springer, pp 69–84
- Nowozin S, Cseke B, Tomioka R (2016) f-gan: Training generative neural samplers using variational divergence minimization. In: Advances in Neural Information Processing Systems, vol 29
- Noy N, Gao Y, Jain A, Narayanan A, Patterson A, Taylor J (2019) Industry-scale knowledge graphs: lessons and challenges. *Communications of the ACM* 62(8):36–43
- NT H, Maehara T (2019) Revisiting graph neural networks: All we have is low-pass filters. arXiv preprint arXiv:190509550
- Nunes M, Pappa GL (2020) Neural architecture search in graph neural networks. In: Brazilian Conference on Intelligent Systems, Springer, pp 302–317
- Oda Y, Fudaba H, Neubig G, Hata H, Sakti S, Toda T, Nakamura S (2015) Learning to generate pseudo-code from source code using statistical machine translation (t). In: 2015 30th IEEE/ACM International Conference on Automated Software Engineering (ASE), IEEE, pp 574–584
- Ok S (2020) A graph similarity for deep learning. In: Larochelle H, Ranzato M, Hadsell R, Balcan MF, Lin H (eds) Advances in Neural Information Processing Systems, Curran Associates, Inc., vol 33, pp 1–12
- Olah C, Satyanarayan A, Johnson I, Carter S, Schubert L, Ye K, Mordvintsev A (2018) The building blocks of interpretability. Distill DOI 10.23915/distill.00010, <https://distill.pub/2018/building-blocks>
- On K, Kim E, Heo Y, Zhang B (2020) Cut-based graph learning networks to discover compositional structure of sequential video data. In: The Thirty-Fourth AAAI Conference on Artificial Intelligence, pp 5315–5322
- Oono K, Suzuki T (2020) Graph neural networks exponentially lose expressive power for node classification. In: International Conference on Learning Representations
- Oord Avd, Kalchbrenner N, Vinyals O, Espeholt L, Graves A, Kavukcuoglu K (2016) Conditional image generation with pixelcnn decoders. In: Proceedings of the 30th International Conference on Neural Information Processing Systems, pp 4797–4805
- Oord Avd, Li Y, Vinyals O (2018) Representation learning with contrastive predictive coding. arXiv preprint arXiv:180703748
- Orchard S, Ammari M, Aranda B, Breuza L, Briganti L, Broackes-Carter F, Campbell NH, Chavali G, Chen C, Del-Toro N, et al (2014) The mintact project—intact as a common curation platform for 11 molecular interaction databases. *Nucleic acids research* 42(D1):D358–D363
- Ottenstein KJ, Ottenstein LM (1984) The program dependence graph in a software development environment. *ACM Sigplan Notices* 19(5):177–184
- Ou M, Cui P, Wang F, Wang J, Zhu W (2015) Non-transitive hashing with latent similarity components. In: Proceedings of the 21th ACM SIGKDD International Conference on Knowledge Discovery and Data Mining, pp 895–904

- Ou M, Cui P, Pei J, Zhang Z, Zhu W (2016) Asymmetric transitivity preserving graph embedding. In: Proceedings of the 22nd ACM SIGKDD international conference on Knowledge discovery and data mining, pp 1105–1114
- Oyetunde T, Zhang M, Chen Y, Tang YJ, Lo C (2017) Boostgapfill: improving the fidelity of metabolic network reconstructions through integrated constraint and pattern-based methods. *Bioinformatics* 33(4):608–611
- Page L, Brin S, Motwani R, Winograd T (1999) The pagerank citation ranking: Bringing order to the web. Tech. rep., Stanford InfoLab
- Paige CC, Saunders MA (1981) Towards a generalized singular value decomposition. *SIAM Journal on Numerical Analysis* 18(3):398–405
- Pal S, Malekmohammadi S, Regol F, Zhang Y, Xu Y, Coates M (2020) Non-parametric graph learning for bayesian graph neural networks. In: Conference on Uncertainty in Artificial Intelligence, PMLR, pp 1318–1327
- Palasca O, Santos A, Stolte C, Gorodkin J, Jensen LJ (2018) Tissues 2.0: an integrative web resource on mammalian tissue expression. *Database* 2018
- Palaz D, Collobert R, et al (2015a) Analysis of cnn-based speech recognition system using raw speech as input. Tech. rep., Idiap
- Palaz D, Doss MM, Collobert R (2015b) Convolutional neural networks-based continuous speech recognition using raw speech signal. In: 2015 IEEE International Conference on Acoustics, Speech and Signal Processing (ICASSP), IEEE, pp 4295–4299
- Paliwal A, Gimeno F, Nair V, Li Y, Lubin M, Kohli P, Vinyals O (2020) Reinforced genetic algorithm learning for optimizing computation graphs. In: International Conference on Learning Representations
- Pan M, Li Y, Zhou X, Liu Z, Song R, Lu H, Luo J (2019) Dissecting the learning curve of taxi drivers: A data-driven approach. In: Proceedings of the 2019 SIAM International Conference on Data Mining, SIAM, pp 783–791
- Pan M, Huang W, Li Y, Zhou X, Liu Z, Song R, Lu H, Tian Z, Luo J (2020a) Dhpa: Dynamic human preference analytics framework: A case study on taxi drivers' learning curve analysis. *ACM Trans Intell Syst Technol* 11(1), DOI 10.1145/3360312
- Pan M, Huang W, Li Y, Zhou X, Luo J (2020b) Xgail: Explainable generative adversarial imitation learning for explainable human decision analysis. In: Proceedings of the 26th ACM SIGKDD International Conference on Knowledge Discovery and Data Mining, Association for Computing Machinery, KDD '20, p 1334–1343, DOI 10.1145/3394486.3403186
- Pan S, Wu J, Zhu X, Zhang C, Wang Y (2016) Tri-party deep network representation. In: Proceedings of the Twenty-Fifth International Joint Conference on Artificial Intelligence, pp 1895–1901
- Pan S, Hu R, Long G, Jiang J, Yao L, Zhang C (2018) Adversarially regularized graph autoencoder for graph embedding. In: Proceedings of the 27th International Joint Conference on Artificial Intelligence, pp 2609–2615
- Pan W, Su C, Chen K, Henchcliffe C, Wang F (2020c) Learning phenotypic associations for parkinson's disease with longitudinal clinical records. medRxiv

- Pandi IV, Barr ET, Gordon AD, Sutton C (2020) OptTyper: Probabilistic type inference by optimising logical and natural constraints. arXiv preprint arXiv:200400348
- Pang L, Lan Y, Guo J, Xu J, Wan S, Cheng X (2016) Text matching as image recognition. In: Proceedings of the AAAI Conference on Artificial Intelligence, vol 30
- Pang LX, Chawla S, Liu W, Zheng Y (2011) On mining anomalous patterns in road traffic streams. In: International conference on advanced data mining and applications, Springer, pp 237–251
- Panichella S, Aponte J, Di Penta M, Marcus A, Canfora G (2012) Mining source code descriptions from developer communications. In: 2012 20th IEEE International Conference on Program Comprehension (ICPC), IEEE, pp 63–72
- Paninski L (2003) Estimation of entropy and mutual information. *Neural computation* 15(6):1191–1253
- Pantziarka P, Meheus L (2018) Omics-driven drug repurposing as a source of innovative therapies in rare cancers. *Expert Opinion on Orphan Drugs* 6(9):513–517
- Park C, Kim D, Zhu Q, Han J, Yu H (2019) Task-guided pair embedding in heterogeneous network. In: Proceedings of the 28th ACM International Conference on Information and Knowledge Management, pp 489–498
- Parthasarathy S, Busso C (2017) Jointly predicting arousal, valence and dominance with multi-task learning. In: Interspeech, vol 2017, pp 1103–1107
- Pascanu R, Mikolov T, Bengio Y (2013) On the difficulty of training recurrent neural networks. In: International conference on machine learning, PMLR, pp 1310–1318
- Paszke A, Gross S, Massa F, Lerer A, Bradbury J, Chanan G, Killeen T, Lin Z, Gimelshein N, Antiga L, Desmaison A, Kopf A, Yang E, DeVito Z, Raison M, Tejani A, Chilamkurthy S, Steiner B, Fang L, Bai J, Chintala S (2019) Pytorch: An imperative style, high-performance deep learning library. In: Advances in Neural Information Processing Systems, vol 32
- Pathak D, Krahenbuhl P, Donahue J, Darrell T, Efros AA (2016) Context encoders: Feature learning by inpainting. In: Proceedings of the IEEE conference on computer vision and pattern recognition, pp 2536–2544
- Peña-Castillo L, Tasan M, Myers CL, et al (2008) A critical assessment of mus musculus gene function prediction using integrated genomic evidence. *Genome Biology* 9(Suppl 1):S2, DOI 10.1186/gb-2008-9-s1-s2
- Peng H, Li J, He Y, Liu Y, Bao M, Wang L, Song Y, Yang Q (2018) Large-scale hierarchical text classification with recursively regularized deep graph-cnn. In: Proceedings of the 2018 world wide web conference, pp 1063–1072
- Peng H, Pappas N, Yogatama D, Schwartz R, Smith N, Kong L (2021) Random feature attention. In: International Conference on Learning Representations
- Peng Z, Dong Y, Luo M, Wu XM, Zheng Q (2020) Self-supervised graph representation learning via global context prediction. arXiv preprint arXiv:200301604
- Pennington J, Socher R, Manning CD (2014) Glove: Global vectors for word representation. In: Proceedings of the 2014 conference on empirical methods in natural language processing (EMNLP), pp 1532–1543

- Percha B, Altman RB (2018) A global network of biomedical relationships derived from text. *Bioinformatics* 34(15):2614–2624
- Perez E, Strub F, De Vries H, Dumoulin V, Courville A (2018) Film: Visual reasoning with a general conditioning layer. In: *Proceedings of the AAAI Conference on Artificial Intelligence*, vol 32
- Perozzi B, Al-Rfou R, Skiena S (2014) Deepwalk: Online learning of social representations. In: *Proceedings of the 20th ACM SIGKDD international conference on Knowledge discovery and data mining*, pp 701–710
- Petar V, Guillem C, Arantxa C, Adriana R, Pietro L, Yoshua B (2018) Graph attention networks. In: *International Conference on Learning Representations*
- Pham H, Guan M, Zoph B, Le Q, Dean J (2018) Efficient neural architecture search via parameter sharing. In: *International Conference on Machine Learning*, pp 4092–4101
- Pham T, Tran T, Phung D, Venkatesh S (2017) Column networks for collective classification. In: *Proceedings of the Thirty-First AAAI Conference on Artificial Intelligence*, AAAI Press, AAAI'17, p 2485–2491
- Piñero J, Ramírez-Anguita JM, Saüch-Pitarch J, Ronzano F, Centeno E, Sanz F, Furlong LI (2020) The disgenet knowledge platform for disease genomics: 2019 update. *Nucleic acids research* 48(D1):D845–D855
- Pires DE, Blundell TL, Ascher DB (2015) pkcsm: predicting small-molecule pharmacokinetic and toxicity properties using graph-based signatures. *Journal of medicinal chemistry* 58(9):4066–4072
- Pletscher-Frankild S, Pallegà A, Tsafou K, Binder JX, Jensen LJ (2015) Diseases: Text mining and data integration of disease–gene associations. *Methods* 74:83–89
- Pogancic MV, Paulus A, Musil V, Martius G, Rolinek M (2020) Differentiation of blackbox combinatorial solvers. In: *International Conference on Learning Representations*, OpenReview.net
- Pope PE, Kolouri S, Rostami M, Martin CE, Hoffmann H (2019) Explainability methods for graph convolutional neural networks. In: *Proceedings of the IEEE/CVF Conference on Computer Vision and Pattern Recognition*, pp 10,772–10,781
- Pradel M, Sen K (2018) Deepbugs: A learning approach to name-based bug detection. *Proceedings of the ACM on Programming Languages* 2(OOPSLA):1–25
- Pradel M, Gousios G, Liu J, Chandra S (2020) TypeWriter: Neural type prediction with search-based validation. In: *Proceedings of the 28th ACM Joint Meeting on European Software Engineering Conference and Symposium on the Foundations of Software Engineering*, pp 209–220
- Pushpakom S, Iorio F, Eyers PA, Escott KJ, Hopper S, Wells A, Doig A, Williams T, Latimer J, McNamee C, et al (2019) Drug repurposing: progress, challenges and recommendations. *Nature reviews Drug discovery* 18(1):41–58
- Putra JWG, Tokunaga T (2017) Evaluating text coherence based on semantic similarity graph. In: *Proceedings of TextGraphs-11: the Workshop on Graph-based Methods for Natural Language Processing*, pp 76–85

- Qi Y, Bar-Joseph Z, Klein-Seetharaman J (2006) Evaluation of different biological data and computational classification methods for use in protein interaction prediction. *Proteins: Structure, Function, and Bioinformatics* 63(3):490–500
- Qiu J, Dong Y, Ma H, Li J, Wang K, Tang J (2018) Network embedding as matrix factorization: Unifying deepwalk, line, pte, and node2vec. In: *Proceedings of the eleventh ACM international conference on web search and data mining*, pp 459–467
- Qiu J, Chen Q, Dong Y, Zhang J, Yang H, Ding M, Wang K, Tang J (2020a) Gcc: Graph contrastive coding for graph neural network pre-training. In: *Proceedings of the 26th ACM SIGKDD International Conference on Knowledge Discovery & Data Mining*, pp 1150–1160
- Qiu J, Cen Y, Chen Q, Zhou C, Zhou J, Yang H, Tang J (2021) Local clustering graph neural networks. *OpenReview*
- Qiu X, Sun T, Xu Y, Shao Y, Dai N, Huang X (2020b) Pre-trained models for natural language processing: A survey. *Science China Technological Sciences* pp 1–26
- Qu Y, Cai H, Ren K, Zhang W, Yu Y, Wen Y, Wang J (2016) Product-based neural networks for user response prediction. In: *2016 IEEE 16th International Conference on Data Mining (ICDM)*, IEEE, pp 1149–1154
- Radford A, Narasimhan K, Salimans T, Sutskever I (2018) Improving language understanding with unsupervised learning. Tech. rep., OpenAI
- Radivojac P, Clark WT, Oron TR, et al (2013) A large-scale evaluation of computational protein function prediction. *Nature Methods* 10(3):221–227
- Raghothaman M, Kulkarni S, Heo K, Naik M (2018) User-guided program reasoning using Bayesian inference. In: *Proceedings of the 39th ACM SIGPLAN Conference on Programming Language Design and Implementation*, pp 722–735
- Rahman TA, Surma B, Backes M, Zhang Y (2019) Fairwalk: Towards fair graph embedding. In: *IJCAI*, pp 3289–3295
- Ramakrishnan R, Dral PO, Rupp M, Von Lilienfeld OA (2014) Quantum chemistry structures and properties of 134 kilo molecules. *Scientific data* 1(1):1–7
- Ramos PIP, Arge LWP, Lima NCB, Fukutani KF, de Queiroz ATL (2019) Leveraging user-friendly network approaches to extract knowledge from high-throughput omics datasets. *Frontiers in genetics* 10:1120
- Rastkar S, Murphy GC (2013) Why did this code change? In: *Proceedings of the 2013 International Conference on Software Engineering*, IEEE Press, pp 1193–1196
- Rastkar S, Murphy GC, Bradley AW (2011) Generating natural language summaries for crosscutting source code concerns. In: *2011 27th IEEE International Conference on Software Maintenance (ICSM)*, IEEE, pp 103–112
- Rastkar S, Murphy GC, Murray G (2014) Automatic summarization of bug reports. *IEEE Transactions on Software Engineering* 40(4):366–380
- Ratti C, Sobolevsky S, Calabrese F, Andris C, Reades J, Martino M, Claxton R, Strogatz SH (2010) Redrawing the map of great britain from a network of human interactions. *PloS one* 5(12)

- Raychev V, Vechev M, Yahav E (2014) Code completion with statistical language models. In: Proceedings of the 35th ACM SIGPLAN Conference on Programming Language Design and Implementation, pp 419–428
- Raychev V, Vechev M, Krause A (2015) Predicting program properties from Big Code. In: Principles of Programming Languages (POPL)
- Real E, Moore S, Selle A, Saxena S, Suematsu YL, Tan J, Le Q, Kurakin A (2017) Large-scale evolution of image classifiers. arXiv preprint arXiv:170301041
- Real E, Aggarwal A, Huang Y, Le QV (2019) Regularized evolution for image classifier architecture search. In: Proceedings of the AAAI Conference on Artificial Intelligence, vol 33, pp 4780–4789
- Ren H, Hu W, Leskovec J (2020) Query2box: Reasoning over knowledge graphs in vector space using box embeddings. In: International Conference on Learning Representations
- Ren S, He K, Girshick R, Sun J (2015) Faster r-cnn: towards real-time object detection with region proposal networks. In: Proceedings of the 28th International Conference on Neural Information Processing Systems-Volume 1, pp 91–99
- Ren Z, Wang X, Zhang N, Lv X, Li LJ (2017) Deep reinforcement learning-based image captioning with embedding reward. In: Proceedings of the IEEE conference on computer vision and pattern recognition, pp 290–298
- Rendle S (2010) Factorization machines. In: 10th IEEE International Conference on Data Mining (ICDM), IEEE, pp 995–1000
- Rezende DJ, Mohamed S, Wierstra D (2014) Stochastic backpropagation and approximate inference in deep generative models. In: International conference on machine learning, PMLR, pp 1278–1286
- Rhodes G (2010) Crystallography made crystal clear: a guide for users of macromolecular models. Elsevier
- Ribeiro LF, Saverese PH, Figueiredo DR (2017) struc2vec: Learning node representations from structural identity. In: the ACM SIGKDD International Conference on Knowledge Discovery and Data Mining, pp 385–394
- Ribeiro MT, Ziviani N, Moura ESD, Hata I, Lacerda A, Veloso A (2014) Multiobjective pareto-efficient approaches for recommender systems. *ACM Transactions on Intelligent Systems and Technology (TIST)* 5(4):1–20
- Ribeiro MT, Singh S, Guestrin C (2016) ” why should i trust you?” explaining the predictions of any classifier. In: Proceedings of the 22nd ACM SIGKDD international conference on knowledge discovery and data mining, pp 1135–1144
- Richiardi J, Achard S, Bunke H, Van De Ville D (2013) Machine learning with brain graphs: predictive modeling approaches for functional imaging in systems neuroscience. *IEEE Signal Processing Magazine* 30(3):58–70
- Riesen K (2015) Structural Pattern Recognition with Graph Edit Distance Approximation Algorithms and Applications. Springer
- Riesen K, Fankhauser S, Bunke H (2007) Speeding up graph edit distance computation with a bipartite heuristic. In: *MLG, Citeseer*, pp 21–24
- Riloff E (1996) Automatically generating extraction patterns from untagged text. In: Proceedings of the national conference on artificial intelligence, pp 1044–1049

- Rink B, Bejan CA, Harabagiu SM (2010) Learning textual graph patterns to detect causal event relations. In: FLAIRS Conference
- Rizvi RF, Vasilakes JA, Adam TJ, Melton GB, Bishop JR, Bian J, Tao C, Zhang R (2019) Integrated dietary supplement knowledge base (idisk)
- Robinson PN, Köhler S, Bauer S, et al (2008) The human phenotype ontology: A tool for annotating and analyzing human hereditary disease. *The American Journal of Human Genetics* 83(5):610–615
- Rocco I, Cimpoi M, Arandjelović R, Torii A, Pajdla T, Sivic J (2018) Neighbourhood consensus networks. In: *Advances in Neural Information Processing Systems*, vol 31
- Rodeghero P, McMillan C, McBurney PW, Bosch N, D’Mello S (2014) Improving automated source code summarization via an eye-tracking study of programmers. In: *Proceedings of the 36th international conference on Software engineering*, ACM, pp 390–401
- Rodeghero P, Jiang S, Armaly A, McMillan C (2017) Detecting user story information in developer-client conversations to generate extractive summaries. In: *2017 IEEE/ACM 39th International Conference on Software Engineering (ICSE)*, IEEE, pp 49–59
- Roehm T, Tiarks R, Koschke R, Maalej W (2012) How do professional developers comprehend software? In: *2012 34th International Conference on Software Engineering (ICSE)*, IEEE, pp 255–265
- Rogers D, Hahn M (2010) Extended-connectivity fingerprints. *Journal of Chemical Information and Modeling* 50(5):742–754
- Rolínek M, Swoboda P, Zietlow D, Paulus A, Musil V, Martius G (2020) Deep graph matching via blackbox differentiation of combinatorial solvers. In: *European Conference on Computer Vision*, Springer, pp 407–424
- Rong Y, Bian Y, Xu T, Xie W, Wei Y, Huang W, Huang J (2020a) Self-supervised graph transformer on large-scale molecular data. *Advances in Neural Information Processing Systems* 33
- Rong Y, Huang W, Xu T, Huang J (2020b) Dropedge: Towards deep graph convolutional networks on node classification. In: *International Conference on Learning Representations*
- Rong Y, Xu T, Huang J, Huang W, Cheng H, Ma Y, Wang Y, Derr T, Wu L, Ma T (2020c) Deep graph learning: Foundations, advances and applications. In: *Proceedings of the 26th ACM SIGKDD International Conference on Knowledge Discovery & Data Mining*, ACM, Virtual Event, pp 3555–3556
- Rossi A, Barbosa D, Firmani D, Matinata A, Merialdo P (2021) Knowledge graph embedding for link prediction: A comparative analysis. *ACM Transactions on Knowledge Discovery from Data (TKDD)* 15(2):1–49
- Rossi E, Chamberlain B, Frasca F, Eynard D, Monti F, Bronstein M (2020) Temporal graph networks for deep learning on dynamic graphs. *arXiv preprint arXiv:2006.10637*
- Rotmensch M, Halpern Y, Tlimat A, Horng S, Sontag D (2017) Learning a health knowledge graph from electronic medical records. *Scientific reports* 7(1):5994

- Rousseau F, Vazirgiannis M (2013) Graph-of-word and tw-idf: new approach to ad hoc ir. In: Proceedings of the 22nd ACM international conference on Information & Knowledge Management, pp 59–68
- Rousseau F, Kiagias E, Vazirgiannis M (2015) Text categorization as a graph classification problem. In: Proceedings of the 53rd Annual Meeting of the Association for Computational Linguistics and the 7th International Joint Conference on Natural Language Processing (Volume 1: Long Papers), pp 1702–1712
- Roweis ST, Saul LK (2000) Nonlinear dimensionality reduction by locally linear embedding. *science* 290(5500):2323–2326
- Rubner Y, Tomasi C, Guibas LJ (1998) A metric for distributions with applications to image databases. In: Sixth International Conference on Computer Vision (IEEE Cat. No. 98CH36271), IEEE, pp 59–66
- Rue H, Held L (2005) Gaussian Markov random fields: theory and applications. CRC press
- Rui SCLDJZJL T (2005) A character recognition based on feature extraction. *Journal of Chinese Computer Systems*, 26(2), 289–292 26(2):289–292
- Sabour S, Frosst N, Hinton GE (2017) Dynamic routing between capsules. In: Proceedings of the 31st International Conference on Neural Information Processing Systems, pp 3859–3869
- Sachdev S, Li H, Luan S, Kim S, Sen K, Chandra S (2018) Retrieval on source code: a neural code search. In: Proceedings of the 2nd ACM SIGPLAN International Workshop on Machine Learning and Programming Languages, pp 31–41
- Sahu S, Gupta R, Sivaraman G, AbdAlmageed W, Espy-Wilson C (2017) Adversarial auto-encoders for speech based emotion recognition. *Proc Interspeech 2017* pp 1243–1247
- Sahu SK, Anand A (2018) Drug-drug interaction extraction from biomedical texts using long short-term memory network. *Journal of biomedical informatics* 86:15–24
- Saire D, Ramírez Rivera A (2019) Graph learning network: A structure learning algorithm. In: Workshop on Learning and Reasoning with Graph-Structured Data (ICMLW 2019)
- Samanta B, Abir D, Jana G, Chattaraj PK, Ganguly N, Rodriguez MG (2019) Nevae: A deep generative model for molecular graphs. In: Proceedings of the AAAI Conference on Artificial Intelligence, vol 33, pp 1110–1117
- Sanchez-Lengeling B, Wei J, Lee B, Reif E, Wang P, Qian W, McCloskey K, Colwell L, Wiltschko A (2020) Evaluating attribution for graph neural networks. In: Larochelle H, Ranzato M, Hadsell R, Balcan MF, Lin H (eds) *Advances in Neural Information Processing Systems*, Curran Associates, Inc., vol 33, pp 5898–5910
- Sandryhaila A, Moura JF (2013) Discrete signal processing on graphs. *IEEE Trans Signal Process* 61(7):1644–1656
- Sangeetha J, Jayasankar T (2019) Emotion speech recognition based on adaptive fractional deep belief network and reinforcement learning. In: *Cognitive Informatics and Soft Computing*, Springer, pp 165–174

- Santini S, Ostermaier B, Vitaletti A (2008) First experiences using wireless sensor networks for noise pollution monitoring. In: *Proceedings of the workshop on Real-world wireless sensor networks*, pp 61–65
- Santos A, Colaço AR, Nielsen AB, Niu L, Geyer PE, Coscia F, Albrechtsen NJW, Mundt F, Jensen LJ, Mann M (2020) Clinical knowledge graph integrates proteomics data into clinical decision-making. *bioRxiv*
- Sato R (2020) A survey on the expressive power of graph neural networks. *arXiv preprint arXiv:200304078*
- Sato R, Yamada M, Kashima H (2021) Random features strengthen graph neural networks. In: *Proceedings of the 2021 SIAM International Conference on Data Mining (SDM)*, SIAM, pp 333–341
- Satorras VG, Estrach JB (2018) Few-shot learning with graph neural networks. In: *International Conference on Learning Representations*
- Scarselli F, Gori M, Tsoi AC, Hagenbuchner M, Monfardini G (2008) The graph neural network model. *IEEE transactions on neural networks* 20(1):61–80
- Schenker A, Last M, Bunke H, Kandel A (2003) Clustering of web documents using a graph model. In: *Web Document Analysis: Challenges and Opportunities*, World Scientific, pp 3–18
- Schlichtkrull M, Kipf TN, Bloem P, Van Den Berg R, Titov I, Welling M (2018) Modeling relational data with graph convolutional networks. In: *European semantic web conference*, Springer, pp 593–607
- Schlichtkrull MS, De Cao N, Titov I (2021) Interpreting graph neural networks for nlp with differentiable edge masking. In: *International Conference on Learning Representations*
- Schnake T, Eberle O, Lederer J, Nakajima S, Schütt KT, Müller KR, Montavon G (2020) Xai for graphs: Explaining graph neural network predictions by identifying relevant walks. *arXiv preprint arXiv:200603589*
- Schneider N, Flanigan J, O’Gorman T (2015) The logic of amr: Practical, unified, graph-based sentence semantics for nlp. In: *Proceedings of the 2015 Conference of the North American Chapter of the Association for Computational Linguistics: Tutorial Abstracts*, pp 4–5
- Schriml LM, Mitraka E, Munro J, Tauber B, Schor M, Nickle L, Felix V, Jeng L, Bearer C, Lichenstein R, et al (2019) Human disease ontology 2018 update: classification, content and workflow expansion. *Nucleic acids research* 47(D1):D955–D962
- Schuchardt J, Bojchevski A, Klicpera J, Günnemann S (2021) Collective robustness certificates. In: *International Conference on Learning Representations, ICLR*
- Schug J (2002) Predicting gene ontology functions from ProDom and CDD protein domains. *Genome Research* 12(4):648–655
- Schulman J, Wolski F, Dhariwal P, Radford A, Klimov O (2017) Proximal policy optimization algorithms. *arXiv preprint arXiv:170706347*
- Schuster M, Paliwal KK (1997) Bidirectional recurrent neural networks. *IEEE Transactions on Signal Processing* 45(11):2673–2681

- Schwarzenberg R, Hübner M, Harbecke D, Alt C, Hennig L (2019) Layerwise relevance visualization in convolutional text graph classifiers. In: Proceedings of the EMNLP 2019 Workshop on Graph-Based Natural Language Processing
- Schweidtmann AM, Rittig JG, König A, Grohe M, Mitsos A, Dahmen M (2020) Graph neural networks for prediction of fuel ignition quality. *Energy & Fuels* 34(9):11,395–11,407
- Schwikowski B, Uetz P, Fields S (2000) A network of protein–protein interactions in yeast. *Nature Biotechnology* 18(12):1257–1261
- Seide F, Li G, Yu D (2011) Conversational speech transcription using context-dependent deep neural networks. In: Twelfth annual conference of the international speech communication association
- Seidman SB (1983) Network structure and minimum degree. *Social Networks* 5(3):269–287
- Selsam D, Bjørner N (2019) Guiding high-performance SAT solvers with unsat-core predictions. In: International Conference on Theory and Applications of Satisfiability Testing, Springer, pp 336–353
- Semasaba AOA, Zheng W, Wu X, Agyemang SA (2020) Literature survey of deep learning-based vulnerability analysis on source code. *IET Software*
- Seo Y, Defferrard M, Vandergheynst P, Bresson X (2018) Structured sequence modeling with graph convolutional recurrent networks. In: *Neural Information Processing*, Springer, pp 362–373
- Shah M, Chen X, Rohrbach M, Parikh D (2019) Cycle-consistency for robust visual question answering. In: Proceedings of the IEEE/CVF Conference on Computer Vision and Pattern Recognition, pp 6649–6658
- Shang C, Tang Y, Huang J, Bi J, He X, Zhou B (2019) End-to-end structure-aware convolutional networks for knowledge base completion. In: Proceedings of the AAAI Conference on Artificial Intelligence, vol 33, pp 3060–3067
- Shang J, Zheng Y, Tong W, Chang E, Yu Y (2014) Inferring gas consumption and pollution emission of vehicles throughout a city. In: Proceedings of the 20th ACM SIGKDD international conference on Knowledge discovery and data mining, pp 1027–1036
- Shanthamallu US, Thiagarajan JJ, Spanias A (2021) Uncertainty-Matching Graph Neural Networks to Defend Against Poisoning Attacks. In: AAAI Conference on Artificial Intelligence
- Sharp ME (2017) Toward a comprehensive drug ontology: extraction of drug-indication relations from diverse information sources. *Journal of biomedical semantics* 8(1):1–10
- Shehu A, Barbará D, Molloy K (2016) A survey of computational methods for protein function prediction. In: Wong KC (ed) *Big Data Analytics in Genomics*, Springer Verlag, pp 225–298
- Shen J, Zhang J, Luo X, et al (2007) Predicting protein-protein interactions based only on sequences information. *Proceedings of the National Academy of Sciences* 104(11):4337–4341
- Shen K, Wu L, Xu F, Tang S, Xiao J, Zhuang Y (2020) Hierarchical attention based spatial-temporal graph-to-sequence learning for grounded video description. In:

- Bessiere C (ed) Proceedings of the Twenty-Ninth International Joint Conference on Artificial Intelligence, IJCAI-20, International Joint Conferences on Artificial Intelligence Organization, pp 941–947, main track
- Shen YL, Huang CY, Wang SS, Tsao Y, Wang HM, Chi TS (2019) Reinforcement learning based speech enhancement for robust speech recognition. In: ICASSP 2019-2019 IEEE International Conference on Acoustics, Speech and Signal Processing (ICASSP), IEEE, pp 6750–6754
- Shen Z, Zhang M, Zhao H, Yi S, Li H (2021) Efficient attention: Attention with linear complexities. In: Proceedings of the IEEE/CVF Winter Conference on Applications of Computer Vision, pp 3531–3539
- Shervashidze N, Schweitzer P, van Leeuwen EJ, Mehlhorn K, Borgwardt KM (2011a) Weisfeiler-Lehman graph kernels. *Journal of Machine Learning Research* 12:2539–2561
- Shervashidze N, Schweitzer P, Leeuwen EJv, Mehlhorn K, Borgwardt KM (2011b) Weisfeiler-lehman graph kernels. *Journal of Machine Learning Research* 12(Sep):2539–2561
- Shi C, Li Y, Zhang J, Sun Y, Philip SY (2016) A survey of heterogeneous information network analysis. *IEEE Transactions on Knowledge and Data Engineering* 29(1):17–37
- Shi C, Hu B, Zhao WX, Philip SY (2018a) Heterogeneous information network embedding for recommendation. *IEEE Transactions on Knowledge and Data Engineering* 31(2):357–370
- Shi C, Xu M, Zhu Z, Zhang W, Zhang M, Tang J (2019a) Graphaf: a flow-based autoregressive model for molecular graph generation. In: International Conference on Learning Representations
- Shi J, Malik J (2000) Normalized cuts and image segmentation. *IEEE Transactions on Pattern Analysis and Machine Intelligence* 22(8):888–905, DOI 10.1109/34.868688
- Shi L, Zhang Y, Cheng J, Lu H (2019b) Skeleton-based action recognition with directed graph neural networks. In: IEEE/CVF Conference on Computer Vision and Pattern Recognition, pp 7912–7921
- Shi M, Wilson DA, Zhu X, Huang Y, Zhuang Y, Liu J, Tang Y (2020) Evolutionary architecture search for graph neural networks. *arXiv preprint arXiv:2009.10199*
- Shi W, Rajkumar R (2020) Point-gnn: Graph neural network for 3d object detection in a point cloud. In: Proceedings of the IEEE/CVF conference on computer vision and pattern recognition, pp 1711–1719
- Shi Y, Gui H, Zhu Q, Kaplan L, Han J (2018b) Aspem: Embedding learning by aspects in heterogeneous information networks. In: Proceedings of the 2018 SIAM International Conference on Data Mining, SIAM, pp 144–152
- Shi Y, Zhu Q, Guo F, Zhang C, Han J (2018c) Easing embedding learning by comprehensive transcription of heterogeneous information networks. In: Proceedings of the 24th ACM SIGKDD International Conference on Knowledge Discovery & Data Mining, pp 2190–2199
- Shibata N, Kajikawa Y, Sakata I (2012) Link prediction in citation networks. *Journal of the American society for information science and technology* 63(1):78–85

- Shorten C, Khoshgoftaar TM (2019) A survey on image data augmentation for deep learning. *Journal of Big Data* 6(1):1–48
- Shou Z, Wang D, Chang SF (2016) Temporal action localization in untrimmed videos via multi-stage cnns. In: *Proceedings of the IEEE conference on computer vision and pattern recognition*, pp 1049–1058
- Shou Z, Chan J, Zareian A, Miyazawa K, Chang SF (2017) Cdc: Convolutional-de-convolutional networks for precise temporal action localization in untrimmed videos. In: *Proceedings of the IEEE conference on computer vision and pattern recognition*, pp 5734–5743
- Shrivastava S (2017) Bring rich knowledge of people places things and local businesses to your apps. Bing Blogs
- Shu DW, Park SW, Kwon J (2019) 3d point cloud generative adversarial network based on tree structured graph convolutions. In: *Proceedings of the IEEE/CVF International Conference on Computer Vision*, pp 3859–3868
- Shu K, Mahudeswaran D, Wang S, Liu H (2020) Hierarchical propagation networks for fake news detection: Investigation and exploitation. In: *International AAAI Conference on Web and Social Media*
- Shuman DI, Narang SK, Frossard P, Ortega A, Vandergheynst P (2013) The emerging field of signal processing on graphs: Extending high-dimensional data analysis to networks and other irregular domains. *IEEE Signal Process Mag* 30(3):83–98
- Si X, Dai H, Raghothaman M, Naik M, Song L (2018) Learning loop invariants for program verification. *Advances in Neural Information Processing Systems* 31:7751–7762
- Si Y, Du J, Li Z, Jiang X, Miller T, Wang F, Zheng J, Roberts K (2020) Deep representation learning of patient data from electronic health records (ehr): A systematic review. *Journal of Biomedical Informatics* pp 103,671–103,671
- Siddharth N, Paige B, van de Meent JW, Desmaison A, Goodman ND, Kohli P, Wood F, Torr PH (2017) Learning disentangled representations with semi-supervised deep generative models. In: *Proceedings of the 31st International Conference on Neural Information Processing Systems*, pp 5927–5937
- Siegelmann HT, Sontag ED (1995) On the computational power of neural nets. *Journal of computer and system sciences* 50(1):132–150
- Silander T, Myllymäki P (2006) A simple approach for finding the globally optimal bayesian network structure. In: *Proceedings of the Twenty-Second Conference on Uncertainty in Artificial Intelligence*, pp 445–452
- Sillito J, Murphy GC, De Volder K (2008) Asking and answering questions during a programming change task. *IEEE Transactions on Software Engineering* 34(4):434–451
- Silva J (2012) A vocabulary of program slicing-based techniques. *ACM computing surveys (CSUR)* 44(3):1–41
- Silver D, Lever G, Heess N, Degris T, Wierstra D, Riedmiller M (2014) Deterministic policy gradient algorithms. In: *International conference on machine learning*, PMLR, pp 387–395

- Simonovsky M, Komodakis N (2017) Dynamic edge-conditioned filters in convolutional neural networks on graphs. In: IEEE Conference on Computer Vision and Pattern Recognition, pp 29–38
- Simonovsky M, Komodakis N (2018) Graphvae: Towards generation of small graphs using variational autoencoders. arXiv preprint arXiv:180203480
- Simonyan K, Zisserman A (2014a) Two-stream convolutional networks for action recognition in videos. In: Proceedings of the 27th International Conference on Neural Information Processing Systems, pp 568–576
- Simonyan K, Zisserman A (2014b) Very deep convolutional networks for large-scale image recognition. arXiv preprint arXiv:14091556
- Simonyan K, Vedaldi A, Zisserman A (2013) Deep inside convolutional networks: Visualising image classification models and saliency maps. arXiv preprint arXiv:13126034
- Singhal A (2012) Introducing the knowledge graph: things, not strings. Official google blog 5:16
- Skarding J, Gabrys B, Musial K (2020) Foundations and modelling of dynamic networks using dynamic graph neural networks: A survey. arXiv preprint arXiv:200507496
- Smilkov D, Thorat N, Kim B, Viégas F, Wattenberg M (2017) Smoothgrad: removing noise by adding noise. Workshop on Visualization for Deep Learning, ICML
- Socher R, Huang EH, Pennington J, Ng AY, Manning CD (2011) Dynamic pooling and unfolding recursive autoencoders for paraphrase detection. In: NIPS, vol 24, pp 801–809
- Socher R, Chen D, Manning CD, Ng A (2013) Reasoning with neural tensor networks for knowledge base completion. In: Advances in neural information processing systems, Citeseer, pp 926–934
- Sohn K, Lee H, Yan X (2015) Learning structured output representation using deep conditional generative models. Advances in neural information processing systems 28:3483–3491
- Song C, Lin Y, Guo S, Wan H (2020a) Spatial-temporal synchronous graph convolutional networks: A new framework for spatial-temporal network data forecasting. In: Proceedings of the AAAI Conference on Artificial Intelligence, vol 34, pp 914–921
- Song L, Zhang Y, Wang Z, Gildea D (2018) A graph-to-sequence model for amr-to-text generation. In: Proceedings of the 56th Annual Meeting of the Association for Computational Linguistics (Volume 1: Long Papers), pp 1616–1626
- Song L, Wang A, Su J, Zhang Y, Xu K, Ge Y, Yu D (2020b) Structural information preserving for graph-to-text generation. In: Proceedings of the 58th Annual Meeting of the Association for Computational Linguistics, pp 7987–7998
- Song W, Xiao Z, Wang Y, Charlin L, Zhang M, Tang J (2019a) Session-based social recommendation via dynamic graph attention networks. In: ACM International Conference on Web Search and Data Mining, pp 555–563
- Song X, Sun H, Wang X, Yan J (2019b) A survey of automatic generation of source code comments: Algorithms and techniques. IEEE Access 7:111,411–111,428

- Sridhara G, Pollock L, Vijay-Shanker K (2011) Automatically detecting and describing high level actions within methods. In: Proceedings of the 33rd International Conference on Software Engineering, ACM, pp 101–110
- Srinivasan B, Ribeiro B (2020a) On the equivalence between node embeddings and structural graph representations. In: International Conference on Learning Representations
- Srinivasan B, Ribeiro B (2020b) On the equivalence between positional node embeddings and structural graph representations. In: 8th International Conference on Learning Representations, ICLR 2020, Addis Ababa, Ethiopia, April 26–30, 2020, OpenReview.net
- Srivastava N, Hinton G, Krizhevsky A, Sutskever I, Salakhutdinov R (2014) Dropout: a simple way to prevent neural networks from overfitting. *The journal of machine learning research* 15(1):1929–1958
- Stanfield Z, Coşkun M, Koyutürk M (2017) Drug response prediction as a link prediction problem. *Scientific reports* 7(1):1–13
- Stanic A, van Steenkiste S, Schmidhuber J (2021) Hierarchical relational inference. In: Proceedings of the AAAI Conference on Artificial Intelligence
- Stark C (2006) BioGRID: a general repository for interaction datasets. *Nucleic Acids Research* 34(90001):D535–D539
- van Steenkiste S, Chang M, Greff K, Schmidhuber J (2018) Relational neural expectation maximization: Unsupervised discovery of objects and their interactions. In: International Conference on Learning Representations
- Sterling T, Irwin JJ (2015) ZINC 15 – ligand discovery for everyone. *Journal of Chemical Information and Modeling* 55(11):2324–2337
- Stokes J, Yang K, Swanson K, Jin W, Cubillos-Ruiz A, Donghia N, MacNair C, French S, Carfrae L, Bloom-Ackerman Z, Tran V, Chiappino-Pepe A, Badran A, Andrews I, Chory E, Church G, Brown E, Jaakkola T, Barzilay R, Collins J (2020) A deep learning approach to antibiotic discovery. *Cell* 180:688–702.e13
- Su C, Aseltine R, Doshi R, Chen K, Rogers SC, Wang F (2020a) Machine learning for suicide risk prediction in children and adolescents with electronic health records. *Translational psychiatry* 10(1):1–10
- Su C, Tong J, Wang F (2020b) Mining genetic and transcriptomic data using machine learning approaches in parkinson's disease. *npj Parkinson's Disease* 6(1):1–10
- Su C, Tong J, Zhu Y, Cui P, Wang F (2020c) Network embedding in biomedical data science. *Briefings in bioinformatics* 21(1):182–197
- Su C, Xu Z, Hoffman K, Goyal P, Safford MM, Lee J, Alvarez-Mulett S, Gomez-Escobar L, Price DR, Harrington JS, et al (2020d) Identifying organ dysfunction trajectory-based subphenotypes in critically ill patients with covid-19. medRxiv
- Su C, Xu Z, Pathak J, Wang F (2020e) Deep learning in mental health outcome research: a scoping review. *Translational Psychiatry* 10(1):1–26
- Su C, Zhang Y, Flory JH, Weiner MG, Kaushal R, Schenck EJ, Wang F (2021) Novel clinical subphenotypes in covid-19: derivation, validation, prediction, temporal patterns, and interaction with social determinants of health. medRxiv

- Subramanian I, Verma S, Kumar S, Jere A, Anamika K (2020) Multi-omics data integration, interpretation, and its application. *Bioinformatics and biology insights* 14:1177932219899,051
- Sugiyama M, Borgwardt KM (2015) Halting in random walk kernels. In: *Advances in Neural Information Processing Systems*, pp 1639–1647
- Sukhbaatar S, Fergus R, et al (2016) Learning multiagent communication with back-propagation. *Advances in neural information processing systems* 29:2244–2252
- Sun C, Gong Y, Wu Y, Gong M, Jiang D, Lan M, Sun S, Duan N (2019) Joint type inference on entities and relations via graph convolutional networks. In: *Proceedings of the 57th Annual Meeting of the Association for Computational Linguistics*, pp 1361–1370
- Sun H, Xiao J, Zhu W, He Y, Zhang S, Xu X, Hou L, Li J, Ni Y, Xie G (2020a) Medical knowledge graph to enhance fraud, waste, and abuse detection on claim data: Model development and performance evaluation. *JMIR Medical Informatics* 8(7):e17,653
- Sun J, Jiang Q, Lu C (2020b) Recursive social behavior graph for trajectory prediction. In: *Proceedings of the IEEE/CVF Conference on Computer Vision and Pattern Recognition*, pp 660–669
- Sun K, Lin Z, Zhu Z (2020c) Multi-stage self-supervised learning for graph convolutional networks on graphs with few labeled nodes. In: *Proceedings of the AAAI Conference on Artificial Intelligence*, vol 34, pp 5892–5899
- Sun M, Li P (2019) Graph to graph: a topology aware approach for graph structures learning and generation. In: *The 22nd International Conference on Artificial Intelligence and Statistics*, PMLR, pp 2946–2955
- Sun S, Zhang B, Xie L, Zhang Y (2017) An unsupervised deep domain adaptation approach for robust speech recognition. *Neurocomputing* 257:79–87
- Sun Y, Han J (2013) Mining heterogeneous information networks: a structural analysis approach. *Acm Sigkdd Explorations Newsletter* 14(2):20–28
- Sun Y, Han J, Yan X, Yu PS, Wu T (2011) Pathsime: Meta path-based top-k similarity search in heterogeneous information networks. *Proceedings of the VLDB Endowment* 4(11):992–1003
- Sun Y, Wang S, Tang X, Hsieh TY, Honavar V (2020d) Adversarial attacks on graph neural networks via node injections: A hierarchical reinforcement learning approach. In: *Proceedings of The Web Conference 2020*, Association for Computing Machinery, WWW '20, p 673–683, DOI 10.1145/3366423.3380149
- Sun Y, Yuan F, Yang M, Wei G, Zhao Z, Liu D (2020e) A generic network compression framework for sequential recommender systems. In: *Proceedings of the 43rd International ACM SIGIR Conference on Research and Development in Information Retrieval*, pp 1299–1308
- Sundararajan M, Taly A, Yan Q (2017) Axiomatic attribution for deep networks. In: *International Conference on Machine Learning*, PMLR, pp 3319–3328
- Sutskever I, Vinyals O, Le QV (2014) Sequence to sequence learning with neural networks. *Advances in Neural Information Processing Systems* 27:3104–3112
- Sutton RS, Barto AG (2018) *Reinforcement learning: An introduction*. MIT press

- Sutton RS, McAllester DA, Singh SP, Mansour Y (2000) Policy gradient methods for reinforcement learning with function approximation. In: *Advances in Neural Information Processing Systems*, pp 1057–1063
- Swietojanski P, Li J, Renals S (2016) Learning hidden unit contributions for unsupervised acoustic model adaptation. *IEEE/ACM Transactions on Audio, Speech, and Language Processing* 24(8):1450–1463
- Szegedy C, Liu W, Jia Y, Sermanet P, Reed S, Anguelov D, Erhan D, Vanhoucke V, Rabinovich A (2015) Going deeper with convolutions. In: *Proceedings of the IEEE conference on computer vision and pattern recognition*, pp 1–9
- Szklarczyk D, Gable AL, Lyon D, Junge A, Wyder S, Huerta-Cepas J, Simonovic M, Doncheva NT, Morris JH, Bork P, et al (2019) String v11: protein–protein association networks with increased coverage, supporting functional discovery in genome-wide experimental datasets. *Nucleic acids research* 47(D1):D607–D613
- Takahashi T (2019) Indirect adversarial attacks via poisoning neighbors for graph convolutional networks. In: *2019 IEEE International Conference on Big Data (Big Data)*, IEEE, pp 1395–1400
- Tang J, Wang K (2018) Personalized top-n sequential recommendation via convolutional sequence embedding. In: *Proceedings of the Eleventh ACM International Conference on Web Search and Data Mining*, pp 565–573
- Tang J, Qu M, Mei Q (2015a) Pte: Predictive text embedding through large-scale heterogeneous text networks. In: *Proceedings of the 21th ACM SIGKDD international conference on knowledge discovery and data mining*, pp 1165–1174
- Tang J, Qu M, Wang M, Zhang M, Yan J, Mei Q (2015b) Line: Large-scale information network embedding. In: *Proceedings of the 24th international conference on world wide web*, pp 1067–1077
- Tang R, Du M, Liu N, Yang F, Hu X (2020a) An embarrassingly simple approach for trojan attack in deep neural networks. In: *Proceedings of the 26th ACM SIGKDD International Conference on Knowledge Discovery & Data Mining*, pp 218–228
- Tang X, Li Y, Sun Y, Yao H, Mitra P, Wang S (2020b) Transferring robustness for graph neural network against poisoning attacks. In: *Proceedings of the 13th International Conference on Web Search and Data Mining*, pp 600–608
- Tao J, Lin J, Zhang S, Zhao S, Wu R, Fan C, Cui P (2019) Mvan: Multi-view attention networks for real money trading detection in online games. In: *Proceedings of the 25th ACM SIGKDD International Conference on Knowledge Discovery & Data Mining*, pp 2536–2546
- Tarlow D, Moitra S, Rice A, Chen Z, Manzagol PA, Sutton C, Aftandilian E (2020) Learning to fix build errors with Graph2Diff neural networks. In: *Proceedings of the IEEE/ACM 42nd International Conference on Software Engineering Workshops*, pp 19–20
- Tate JG, Bamford S, Jubb HC, Sondka Z, Beare DM, Bindal N, Boutselakis H, Cole CG, Creatore C, Dawson E, et al (2019) Cosmic: the catalogue of somatic mutations in cancer. *Nucleic acids research* 47(D1):D941–D947
- Te G, Hu W, Zheng A, Guo Z (2018) Rgcnn: Regularized graph cnn for point cloud segmentation. In: *Proceedings of the 26th ACM international conference on Multimedia*, pp 746–754

- Tenenbaum JB, De Silva V, Langford JC (2000) A global geometric framework for nonlinear dimensionality reduction. *science* 290(5500):2319–2323
- Teru K, Denis E, Hamilton W (2020) Inductive relation prediction by subgraph reasoning. In: International Conference on Machine Learning, PMLR, pp 9448–9457
- Thomas S, Seltzer ML, Church K, Hermansky H (2013) Deep neural network features and semi-supervised training for low resource speech recognition. In: 2013 IEEE international conference on acoustics, speech and signal processing, IEEE, pp 6704–6708
- Tian Z, Guo M, Wang C, Liu X, Wang S (2017) Refine gene functional similarity network based on interaction networks. *BMC bioinformatics* (16)
- Tornig W, Altman RB (2018) High precision protein functional site detection using 3d convolutional neural networks. *Bioinformatics* 35(9):1503–1512
- Train K (1986) Qualitative choice analysis: Theory, econometrics, and an application to automobile demand, vol 10. MIT press
- Tramer F, Carlini N, Brendel W, Madry A (2020) On adaptive attacks to adversarial example defenses. In: Larochelle H, Ranzato M, Hadsell R, Balcan MF, Lin H (eds) *Advances in Neural Information Processing Systems*, Curran Associates, Inc., vol 33, pp 1633–1645
- Tran D, Bourdev L, Fergus R, Torresani L, Paluri M (2015) Learning spatiotemporal features with 3d convolutional networks. In: *Proceedings of the IEEE international conference on computer vision*, pp 4489–4497
- Trivedi R, Dai H, Wang Y, Song L (2017) Know-evolve: Deep temporal reasoning for dynamic knowledge graphs. In: International Conference on Machine Learning, PMLR, pp 3462–3471
- Trivedi R, Farajtabar M, Biswal P, Zha H (2019) Dyrep: Learning representations over dynamic graphs. In: *International Conference on Learning Representations*
- Trouillon T, Welbl J, Riedel S, Gaussier É, Bouchard G (2016) Complex embeddings for simple link prediction. In: International Conference on Machine Learning, pp 2071–2080
- Tsai YHH, Bai S, Yamada M, Morency LP, Salakhutdinov R (2019) Transformer dissection: An unified understanding for transformer’s attention via the lens of kernel. In: *Proceedings of the 2019 Conference on Empirical Methods in Natural Language Processing and the 9th International Joint Conference on Natural Language Processing (EMNLP-IJCNLP)*, pp 4335–4344
- Tsuyuzaki K, Nikaido I (2017) Biological systems as heterogeneous information networks: a mini-review and perspectives. *WSDM HeteroNAM 18 - International Workshop on Heterogeneous Networks Analysis and Mining*
- Tu C, Zhang W, Liu Z, Sun M, et al (2016) Max-margin deepwalk: Discriminative learning of network representation. In: *IJCAI*, vol 2016, pp 3889–3895
- Tu K, Cui P, Wang X, Wang F, Zhu W (2018) Structural deep embedding for hypernetworks. In: *Proceedings of the AAAI Conference on Artificial Intelligence*, vol 32
- Tu M, Wang G, Huang J, Tang Y, He X, Zhou B (2019) Multi-hop reading comprehension across multiple documents by reasoning over heterogeneous graphs. In:

- Proceedings of the 57th Annual Meeting of the Association for Computational Linguistics, pp 2704–2713
- Tufano M, Drain D, Svyatkovskiy A, Sundaresan N (2020) Generating accurate assert statements for unit test cases using pretrained transformers. arXiv preprint arXiv:200905634
- Tzirakis P, Zhang J, Schuller BW (2018) End-to-end speech emotion recognition using deep neural networks. In: 2018 IEEE international conference on acoustics, speech and signal processing (ICASSP), IEEE, pp 5089–5093
- Ulutun O, Iftekhhar A, Manjunath BS (2020) Vsgnet: Spatial attention network for detecting human object interactions using graph convolutions. In: Proceedings of the IEEE/CVF Conference on Computer Vision and Pattern Recognition, pp 13,617–13,626
- Vahedian A, Zhou X, Tong L, Li Y, Luo J (2017) Forecasting gathering events through continuous destination prediction on big trajectory data. In: Proceedings of the 25th ACM SIGSPATIAL International Conference on Advances in Geographic Information Systems, pp 1–10
- Vahedian A, Zhou X, Tong L, Street WN, Li Y (2019) Predicting urban dispersal events: A two-stage framework through deep survival analysis on mobility data. In: Proceedings of the AAAI Conference on Artificial Intelligence, vol 33, pp 5199–5206
- Van Hasselt H, Guez A, Silver D (2016) Deep reinforcement learning with double q-learning. In: Proceedings of the AAAI Conference on Artificial Intelligence, vol 30
- Van Oord A, Kalchbrenner N, Kavukcuoglu K (2016) Pixel recurrent neural networks. In: International Conference on Machine Learning, pp 1747–1756
- Vashishth S, Yadati N, Talukdar P (2019) Graph-based deep learning in natural language processing. In: Proceedings of the 2019 Conference on Empirical Methods in Natural Language Processing and the 9th International Joint Conference on Natural Language Processing (EMNLP-IJCNLP): Tutorial Abstracts
- Vashishth S, Sanyal S, Nitin V, Talukdar P (2020) Composition-based multi-relational graph convolutional networks. In: International Conference on Learning Representations
- Vasic M, Kanade A, Maniatis P, Bieber D, Singh R (2018) Neural program repair by jointly learning to localize and repair. In: International Conference on Learning Representations
- Vaswani A, Shazeer N, Parmar N, Uszkoreit J, Jones L, Gomez AN, Kaiser u, Polosukhin I (2017) Attention is all you need. In: Proceedings of the 31st International Conference on Neural Information Processing Systems, Curran Associates Inc., Red Hook, NY, USA, NIPS'17, p 6000–6010
- Veličković P, Cucurull G, Casanova A, Romero A, Lio P, Bengio Y (2018) Graph attention networks. In: International Conference on Learning Representations
- Velickovic P, Fedus W, Hamilton WL, Liò P, Bengio Y, Hjelm RD (2019) Deep graph infomax. In: ICLR (Poster)
- Veličković P, Ying R, Padovano M, Hadsell R, Blundell C (2019) Neural execution of graph algorithms. In: International Conference on Learning Representations

- Velickovic P, Buesing L, Overlan M, Pascanu R, Vinyals O, Blundell C (2020) Pointer graph networks. In: Larochelle H, Ranzato M, Hadsell R, Balcan MF, Lin H (eds) *Advances in Neural Information Processing Systems*, Curran Associates, Inc., vol 33, pp 2232–2244
- Veličković P, Fedus W, Hamilton WL, Liò P, Bengio Y, Hjelm RD (2019) Deep graph infomax. In: *International Conference on Learning Representations*
- Vento M, Foggia P (2013) Graph matching techniques for computer vision. In: *Image Processing: Concepts, Methodologies, Tools, and Applications*, IGI Global, chap 21, pp 381–421
- Vignac C, Loukas A, Frossard P (2020a) Building powerful and equivariant graph neural networks with structural message-passing. *arXiv e-prints* pp arXiv–2006
- Vignac C, Loukas A, Frossard P (2020b) Building powerful and equivariant graph neural networks with structural message-passing. In: Larochelle H, Ranzato M, Hadsell R, Balcan MF, Lin H (eds) *Advances in Neural Information Processing Systems*, Curran Associates, Inc., vol 33, pp 14,143–14,155
- Vincent P, Larochelle H, Bengio Y, Manzagol P (2008) Extracting and composing robust features with denoising autoencoders. In: Cohen WW, McCallum A, Roweis ST (eds) *Machine Learning, Proceedings of the Twenty-Fifth International Conference (ICML 2008)*, Helsinki, Finland, June 5-9, 2008, ACM, ACM International Conference Proceeding Series, vol 307, pp 1096–1103, DOI 10.1145/1390156.1390294
- Vinyals O, Fortunato M, Jaitly N (2015) Pointer networks. In: *Neural Information Processing Systems (NeurIPS)*, pp 2692–2700
- Vinyals O, Bengio S, Kudlur M (2016) Order matters: Sequence to sequence for sets. In: *International Conference on Learning Representations*
- Vishwanathan SVN, Schraudolph NN, Kondor R, Borgwardt KM (2010) Graph kernels. *Journal of Machine Learning Research* 11(Apr):1201–1242
- VONLUXBURG U (2007) A tutorial on spectral clustering. *Statistics and Computing* 17:395–416
- Vrandečić D, Krötzsch M (2014) Wikidata: a free collaborative knowledgebase. *Communications of the ACM* 57(10):78–85
- Vu MN, Thai MT (2020) Pgm-explainer: Probabilistic graphical model explanations for graph neural networks. *arXiv preprint arXiv:201005788*
- Wald J, Dhama H, Navab N, Tombari F (2020) Learning 3d semantic scene graphs from 3d indoor reconstructions. In: *Proceedings of the IEEE/CVF Conference on Computer Vision and Pattern Recognition*, pp 3961–3970
- Wan S, Lan Y, Guo J, Xu J, Pang L, Cheng X (2016) A deep architecture for semantic matching with multiple positional sentence representations. In: *Proceedings of the AAAI Conference on Artificial Intelligence*, vol 30
- Wan Y, Zhao Z, Yang M, Xu G, Ying H, Wu J, Yu PS (2018) Improving automatic source code summarization via deep reinforcement learning. In: *Proceedings of the 33rd ACM/IEEE International Conference on Automated Software Engineering*, ACM, pp 397–407

- Wang B, Gong NZ (2019) Attacking graph-based classification via manipulating the graph structure. In: Proceedings of the 2019 ACM SIGSAC Conference on Computer and Communications Security, pp 2023–2040
- Wang C, Pan S, Long G, Zhu X, Jiang J (2017a) Mgae: Marginalized graph autoencoder for graph clustering. In: Proceedings of the 2017 ACM on Conference on Information and Knowledge Management, pp 889–898
- Wang D, Cui P, Zhu W (2016) Structural deep network embedding. In: Proceedings of the 22nd ACM SIGKDD international conference on Knowledge discovery and data mining, pp 1225–1234
- Wang D, Jamnik M, Lio P (2019a) Abstract diagrammatic reasoning with multiplex graph networks. In: International Conference on Learning Representations
- Wang D, Lin J, Cui P, Jia Q, Wang Z, Fang Y, Yu Q, Zhou J, Yang S, Qi Y (2019b) A semi-supervised graph attentive network for financial fraud detection. In: 2019 IEEE International Conference on Data Mining (ICDM), IEEE, pp 598–607
- Wang D, Jiang M, Syed M, Conway O, Juneja V, Subramanian S, Chawla NV (2020a) Calendar graph neural networks for modeling time structures in spatiotemporal user behaviors. In: Proceedings of the 26th ACM SIGKDD International Conference on Knowledge Discovery & Data Mining, pp 2581–2589
- Wang F, Preininger A (2019) Ai in health: State of the art, challenges, and future directions. Yearbook of medical informatics 28(1):16–26
- Wang F, Zhang C (2007) Label propagation through linear neighborhoods. IEEE Transactions on Knowledge and Data Engineering 20(1):55–67
- Wang G, Dunbrack RL (2003) PISCES: a protein sequence culling server. Bioinformatics 19(12):1589–1591, DOI 10.1093/bioinformatics/btg224
- Wang H, Huan J (2019) Agan: Towards automated design of generative adversarial networks. arXiv preprint arXiv:1906.11080
- Wang H, Schmid C (2013) Action recognition with improved trajectories. In: Proceedings of the IEEE international conference on computer vision, pp 3551–3558
- Wang H, Wang J, Wang J, Zhao M, Zhang W, Zhang F, Xie X, Guo M (2018a) Graphgan: Graph representation learning with generative adversarial nets. In: Proceedings of the AAAI conference on artificial intelligence, vol 32
- Wang H, Zhang F, Zhang M, Leskovec J, Zhao M, Li W, Wang Z (2019c) Knowledge-aware graph neural networks with label smoothness regularization for recommender systems. In: KDD'19, pp 968–977
- Wang H, Zhao M, Xie X, Li W, Guo M (2019d) Knowledge graph convolutional networks for recommender systems. In: The world wide web conference, pp 3307–3313
- Wang H, Zhao M, Xie X, Li W, Guo M (2019e) Knowledge graph convolutional networks for recommender systems. In: WWW'19, pp 3307–3313
- Wang H, Wang K, Yang J, Shen L, Sun N, Lee HS, Han S (2020b) Gcn-rl circuit designer: Transferable transistor sizing with graph neural networks and reinforcement learning. In: Design Automation Conference, IEEE, pp 1–6
- Wang J, Zheng VW, Liu Z, Chang KCC (2017b) Topological recurrent neural network for diffusion prediction. In: 2017 IEEE International Conference on Data Mining (ICDM), IEEE, pp 475–484

- Wang J, Huang P, Zhao H, Zhang Z, Zhao B, Lee DL (2018b) Billion-scale commodity embedding for e-commerce recommendation in alibaba. In: Proceedings of the 24th ACM SIGKDD International Conference on Knowledge Discovery & Data Mining, pp 839–848
- Wang J, Oh J, Wang H, Wiens J (2018c) Learning credible models. In: Proceedings of the 24th ACM SIGKDD International Conference on Knowledge Discovery & Data Mining, pp 2417–2426
- Wang J, Luo M, Suya F, Li J, Yang Z, Zheng Q (2020c) Scalable attack on graph data by injecting vicious nodes. *Data Mining and Knowledge Discovery* 34(5):1363–1389
- Wang K, Singh R, Su Z (2018d) Dynamic neural program embeddings for program repair. In: International Conference on Learning Representations
- Wang M, Liu M, Liu J, Wang S, Long G, Qian B (2017c) Safe medicine recommendation via medical knowledge graph embedding. arXiv preprint arXiv:171005980
- Wang M, Yu L, Zheng D, Gan Q, Gai Y, Ye Z, Li M, Zhou J, Huang Q, Ma C, Huang Z, Guo Q, Zhang H, Lin H, Zhao J, Li J, Smola AJ, Zhang Z (2019f) Deep graph library: Towards efficient and scalable deep learning on graphs. In: International Conference on Learning Representations Workshop on Representation Learning on Graphs and Manifolds
- Wang M, Lin Y, Lin G, Yang K, Wu Xm (2020d) M2grl: A multi-task multi-view graph representation learning framework for web-scale recommender systems. In: Proceedings of the 26th ACM SIGKDD International Conference on Knowledge Discovery & Data Mining, pp 2349–2358
- Wang Q, Mao Z, Wang B, Guo L (2017d) Knowledge graph embedding: A survey of approaches and applications. *IEEE Transactions on Knowledge and Data Engineering* 29(12):2724–2743
- Wang Q, Li M, Wang X, Parulian N, Han G, Ma J, Tu J, Lin Y, Zhang H, Liu W, et al (2020e) Covid-19 literature knowledge graph construction and drug repurposing report generation. arXiv preprint arXiv:200700576
- Wang R, Yan J, Yang X (2019g) Learning combinatorial embedding networks for deep graph matching. In: Proceedings of the IEEE/CVF International Conference on Computer Vision, pp 3056–3065
- Wang R, Zhang T, Yu T, Yan J, Yang X (2020f) Combinatorial learning of graph edit distance via dynamic embedding. arXiv preprint arXiv:201115039
- Wang S, He L, Cao B, Lu CT, Yu PS, Ragin AB (2017e) Structural deep brain network mining. In: Proceedings of the 23rd ACM SIGKDD International Conference on Knowledge Discovery and Data Mining, pp 475–484
- Wang S, Tang J, Aggarwal C, Chang Y, Liu H (2017f) Signed network embedding in social media. In: Proceedings of the 2017 SIAM international conference on data mining, SIAM, pp 327–335
- Wang S, Chen Z, Li D, Li Z, Tang LA, Ni J, Rhee J, Chen H, Yu PS (2019h) Attentional heterogeneous graph neural network: Application to program reidentification. In: Proceedings of the 2019 SIAM International Conference on Data Mining, SIAM, pp 693–701

- Wang S, Chen Z, Yu X, Li D, Ni J, Tang L, Gui J, Li Z, Chen H, Yu PS (2019i) Heterogeneous graph matching networks for unknown malware detection. In: Proceedings of the Twenty-Eighth International Joint Conference on Artificial Intelligence, IJCAI, pp 3762–3770
- Wang S, Li BZ, Khabsa M, Fang H, Ma H (2020g) Linformer: Self-attention with linear complexity. CoRR abs/2006.04768
- Wang S, Li Y, Zhang J, Meng Q, Meng L, Gao F (2020h) Pm2. 5-gnn: A domain knowledge enhanced graph neural network for pm2. 5 forecasting. In: Proceedings of the 28th International Conference on Advances in Geographic Information Systems, pp 163–166
- Wang S, Wang R, Yao Z, Shan S, Chen X (2020i) Cross-modal scene graph matching for relationship-aware image-text retrieval. In: Proceedings of the IEEE/CVF Winter Conference on Applications of Computer Vision, pp 1508–1517
- Wang T, Ling H (2017) Gracker: A graph-based planar object tracker. IEEE transactions on pattern analysis and machine intelligence 40(6):1494–1501
- Wang T, Liu H, Li Y, Jin Y, Hou X, Ling H (2020j) Learning combinatorial solver for graph matching. In: Proceedings of the IEEE/CVF conference on computer vision and pattern recognition, pp 7568–7577
- Wang T, Wan X, Jin H (2020k) Amr-to-text generation with graph transformer. Transactions of the Association for Computational Linguistics 8:19–33
- Wang X, Gupta A (2018) Videos as space-time region graphs. In: Proceedings of the European conference on computer vision (ECCV), pp 399–417
- Wang X, Cui P, Wang J, Pei J, Zhu W, Yang S (2017g) Community preserving network embedding. In: Proceedings of the AAAI Conference on Artificial Intelligence, vol 31
- Wang X, Girshick R, Gupta A, He K (2018e) Non-local neural networks. In: Proceedings of the IEEE conference on computer vision and pattern recognition, pp 7794–7803
- Wang X, Ye Y, Gupta A (2018f) Zero-shot recognition via semantic embeddings and knowledge graphs. In: Proceedings of the IEEE conference on computer vision and pattern recognition, pp 6857–6866
- Wang X, He X, Cao Y, Liu M, Chua TS (2019j) Kgat: Knowledge graph attention network for recommendation. In: KDD'19, pp 950–958
- Wang X, He X, Wang M, Feng F, Chua TS (2019k) Neural graph collaborative filtering. In: Proceedings of the 42nd international ACM SIGIR conference on Research and development in Information Retrieval, pp 165–174
- Wang X, Ji H, Shi C, Wang B, Ye Y, Cui P, Yu PS (2019l) Heterogeneous graph attention network. In: The World Wide Web Conference, pp 2022–2032
- Wang X, Ji H, Shi C, Wang B, Ye Y, Cui P, Yu PS (2019m) Heterogeneous graph attention network. In: The World Wide Web Conference, pp 2022–2032
- Wang X, Zhang Y, Shi C (2019n) Hyperbolic heterogeneous information network embedding. In: Proceedings of the AAAI conference on artificial intelligence, vol 33, pp 5337–5344

- Wang X, Bo D, Shi C, Fan S, Ye Y, Yu PS (2020l) A survey on heterogeneous graph embedding: Methods, techniques, applications and sources. arXiv preprint arXiv:201114867
- Wang X, Lu Y, Shi C, Wang R, Cui P, Mou S (2020m) Dynamic heterogeneous information network embedding with meta-path based proximity. *IEEE Transactions on Knowledge and Data Engineering* pp 1–1, DOI 10.1109/TKDE.2020.2993870
- Wang X, Wang R, Shi C, Song G, Li Q (2020n) Multi-component graph convolutional collaborative filtering. In: *Proceedings of the AAAI Conference on Artificial Intelligence*, vol 34, pp 6267–6274
- Wang X, Wu Y, Zhang A, He X, seng Chua T (2021) Causal screening to interpret graph neural networks
- Wang Y, Ni X, Sun JT, Tong Y, Chen Z (2011) Representing document as dependency graph for document clustering. In: *Proceedings of the 20th ACM international conference on Information and knowledge management*, pp 2177–2180
- Wang Y, Shen H, Liu S, Gao J, Cheng X (2017h) Cascade dynamics modeling with attention-based recurrent neural network. In: *Proceedings of the 26th International Joint Conference on Artificial Intelligence*, pp 2985–2991
- Wang Y, Che W, Guo J, Liu T (2018g) A neural transition-based approach for semantic dependency graph parsing. In: *Proceedings of the AAAI Conference on Artificial Intelligence*, vol 32
- Wang Y, Yin H, Chen H, Wo T, Xu J, Zheng K (2019o) Origin-destination matrix prediction via graph convolution: a new perspective of passenger demand modeling. In: *Proceedings of the 25th ACM SIGKDD International Conference on Knowledge Discovery & Data Mining*, pp 1227–1235
- Wang Y, Liu S, Yoon M, Lamba H, Wang W, Faloutsos C, Hooi B (2020o) Provably robust node classification via low-pass message passing. In: *2020 IEEE International Conference on Data Mining (ICDM)*, pp 621–630, DOI 10.1109/ICDM50108.2020.00071
- Wang Z, Zhang J, Feng J, Chen Z (2014) Knowledge graph embedding by translating on hyperplanes. In: *Proceedings of the AAAI Conference on Artificial Intelligence*, vol 28
- Wang Z, Zheng L, Li Y, Wang S (2019p) Linkage based face clustering via graph convolution network. In: *Proceedings of the IEEE/CVF Conference on Computer Vision and Pattern Recognition*, pp 1117–1125
- Wass MN, Barton G, Sternberg MJE (2012) CombFunc: predicting protein function using heterogeneous data sources. *Nucleic Acids Research* 40(W1):W466–W470
- Watkins KE, Ferris B, Borning A, Rutherford GS, Layton D (2011) Where is my bus? impact of mobile real-time information on the perceived and actual wait time of transit riders. *Transportation Research Part A: Policy and Practice* 45(8):839–848
- Watts DJ, Strogatz SH (1998) Collective dynamics of ‘small-world’ networks. *nature* 393(6684):440–442
- Wei J, Goyal M, Durrett G, Dillig I (2019) LambdaNet: Probabilistic type inference using graph neural networks. In: *International Conference on Learning Representations*

- Wei X, Yu R, Sun J (2020) View-gcn: View-based graph convolutional network for 3d shape analysis. In: Proceedings of the IEEE/CVF Conference on Computer Vision and Pattern Recognition, pp 1850–1859
- Weihua Hu MZYDHRBLMCJL Matthias Fey (2020) Open graph benchmark: Datasets for machine learning on graphs. arXiv preprint arXiv:200500687
- Weininger D (1988) Smiles, a chemical language and information system. 1. introduction to methodology and encoding rules. *Journal of chemical information and computer sciences* 28(1):31–36
- Weisfeiler B (1976) On Construction and Identification of Graphs. *Lecture Notes in Mathematics*, Vol. 558, Springer
- Weisfeiler B, Leman A (1968) The reduction of a graph to canonical form and the algebra which appears therein. *Nauchno-Tekhnicheskaya Informatsia* 2(9):12–16
- Weisfeiler B, Leman A (1968) The reduction of a graph to canonical form and the algebra which appears therein. *NTI, Series* 2(9):12–16
- Weng C, Shah NH, Hripcsak G (2020) Deep phenotyping: embracing complexity and temporality—towards scalability, portability, and interoperability. *Journal of biomedical informatics* 105:103,433
- Weston J, Bengio S, Usunier N (2010) Large scale image annotation: learning to rank with joint word-image embeddings. *Machine learning* 81(1):21–35
- Whirl-Carrillo M, McDonagh EM, Hebert J, Gong L, Sangkuhl K, Thorn C, Altman RB, Klein TE (2012) Pharmacogenomics knowledge for personalized medicine. *Clinical Pharmacology & Therapeutics* 92(4):414–417
- White M, Tufano M, Vendome C, Poshyvanyk D (2016) Deep learning code fragments for code clone detection. In: 2016 31st IEEE/ACM International Conference on Automated Software Engineering (ASE), IEEE, pp 87–98
- Williams RJ (1992) Simple statistical gradient-following algorithms for connectionist reinforcement learning. *Machine learning* 8(3-4):229–256
- Wishart DS, Feunang YD, Guo AC, Lo EJ, Marcu A, Grant JR, Sajed T, Johnson D, Li C, Sayeeda Z, et al (2018) Drugbank 5.0: a major update to the drugbank database for 2018. *Nucleic acids research* 46(D1):D1074–D1082
- Wold S, Esbensen K, Geladi P (1987) Principal component analysis. *Chemometrics and intelligent laboratory systems* 2(1-3):37–52
- Woźnica A, Kalousis A, Hilario M (2010) Adaptive matching based kernels for labelled graphs. In: *Advances in Knowledge Discovery and Data Mining*, Springer, *Lecture Notes in Computer Science*, vol 6119, pp 374–385
- Wu B, Xu C, Dai X, Wan A, Zhang P, Tomizuka M, Keutzer K, Vajda P (2020a) Visual transformers: Token-based image representation and processing for computer vision. arXiv preprint arXiv:200603677
- Wu F, Souza A, Zhang T, Fifty C, Yu T, Weinberger K (2019a) Simplifying graph convolutional networks. In: *International conference on machine learning*, PMLR, pp 6861–6871
- Wu H, Wang C, Tyshetskiy Y, Docherty A, Lu K, Zhu L (2019b) Adversarial examples for graph data: Deep insights into attack and defense. In: *Proceedings of the Twenty-Eighth International Joint Conference on Artificial Intelligence*,

- IJCAI-19, International Joint Conferences on Artificial Intelligence Organization, pp 4816–4823
- Wu H, Ma Y, Xiang Z, Yang C, He K (2021a) A spatial-temporal graph neural network framework for automated software bug triaging. *arXiv preprint arXiv:210111846*
- Wu J, Cao M, Cheung JCK, Hamilton WL (2020b) Temp: Temporal message passing for temporal knowledge graph completion. In: *Proceedings of the 2020 Conference on Empirical Methods in Natural Language Processing (EMNLP)*, pp 5730–5746
- Wu L, Chen Y, Ji H, Li Y (2021b) Deep learning on graphs for natural language processing. In: *Proceedings of the 2021 Conference of the North American Chapter of the Association for Computational Linguistics: Human Language Technologies: Tutorials*, pp 11–14
- Wu L, Chen Y, Shen K, Guo X, Gao H, Li S, Pei J, Long B (2021c) Graph neural networks for natural language processing: A survey. *arXiv preprint arXiv:210606090*
- Wu N, Zhao XW, Wang J, Pan D (2020c) Learning effective road network representation with hierarchical graph neural networks. In: *Proceedings of the 26th ACM SIGKDD International Conference on Knowledge Discovery & Data Mining*, pp 6–14
- Wu S, Tang Y, Zhu Y, Wang L, Xie X, Tan T (2019c) Session-based recommendation with graph neural networks. In: *Proceedings of the AAAI Conference on Artificial Intelligence*, vol 33, pp 346–353
- Wu T, Ren H, Li P, Leskovec J (2020d) Graph information bottleneck. In: Larochelle H, Ranzato M, Hadsell R, Balcan MF, Lin H (eds) *Advances in Neural Information Processing Systems*, Curran Associates, Inc., vol 33, pp 20,437–20,448
- Wu Y, Warner JL, Wang L, Jiang M, Xu J, Chen Q, Nian H, Dai Q, Du X, Yang P, et al (2019d) Discovery of noncancer drug effects on survival in electronic health records of patients with cancer: a new paradigm for drug repurposing. *JCO clinical cancer informatics* 3:1–9
- Wu Z, Ramsundar B, Feinberg EN, Gomes J, Geniesse C, Pappu AS, Leswing K, Pande V (2018) MoleculeNet: A benchmark for molecular machine learning. *Chemical Science* 9:513–530
- Wu Z, Pan S, Chen F, Long G, Zhang C, Yu PS (2019e) A comprehensive survey on graph neural networks. *CoRR abs/1901.00596*
- Wu Z, Pan S, Chen F, Long G, Zhang C, Philip SY (2021d) A comprehensive survey on graph neural networks. *IEEE Transactions on Neural Networks and Learning Systems* 32(1):4–24
- Xhonneux LP, Qu M, Tang J (2020) Continuous graph neural networks. In: *Proceedings of the International Conference on Machine Learning*
- Xia R, Liu Y (2015) A multi-task learning framework for emotion recognition using 2d continuous space. *IEEE Transactions on Affective Computing* 8(1):3–14
- Xiao C, Choi E, Sun J (2018) Opportunities and challenges in developing deep learning models using electronic health records data: a systematic review. *Journal of the American Medical Informatics Association* 25(10):1419–1428

- Xie L, Yuille A (2017) Genetic cnn. In: Proceedings of the IEEE International Conference on Computer Vision, pp 1379–1388
- Xie M, Yin H, Wang H, Xu F, Chen W, Wang S (2016) Learning graph-based poi embedding for location-based recommendation. In: Proceedings of the 25th ACM International on Conference on Information and Knowledge Management, Association for Computing Machinery, CIKM '16, p 15–24, DOI 10.1145/2983323.2983711
- Xie S, Kirillov A, Girshick R, He K (2019a) Exploring randomly wired neural networks for image recognition. In: Proceedings of the IEEE/CVF International Conference on Computer Vision, pp 1284–1293
- Xie T, Grossman JC (2018) Crystal graph convolutional neural networks for an accurate and interpretable prediction of material properties. *Physical Review Letters* 120:145,301
- Xie Y, Xu Z, Wang Z, Ji S (2021) Self-supervised learning of graph neural networks: A unified review. *arXiv preprint arXiv:2102.10757*
- Xie Z, Lv W, Huang S, Lu Z, Du B, Huang R (2019b) Sequential graph neural network for urban road traffic speed prediction. *IEEE Access* 8:63,349–63,358
- Xiu H, Yan X, Wang X, Cheng J, Cao L (2020) Hierarchical graph matching network for graph similarity computation. *arXiv preprint arXiv:2006.16551*
- Xu D, Zhu Y, Choy CB, Fei-Fei L (2017a) Scene graph generation by iterative message passing. In: Proceedings of the IEEE conference on computer vision and pattern recognition, pp 5410–5419
- Xu D, Cheng W, Luo D, Liu X, Zhang X (2019a) Spatio-temporal attentive rnn for node classification in temporal attributed graphs. In: International Joint Conference on Artificial Intelligence, pp 3947–3953
- Xu D, Ruan C, Korceoglu E, Kumar S, Achan K (2020a) Inductive representation learning on temporal graphs. In: International Conference on Learning Representations
- Xu H, Jiang C, Liang X, Li Z (2019b) Spatial-aware graph relation network for large-scale object detection. In: Proceedings of the IEEE/CVF Conference on Computer Vision and Pattern Recognition, pp 9298–9307
- Xu J, Gan Z, Cheng Y, Liu J (2020b) Discourse-aware neural extractive text summarization. In: Proceedings of the 58th Annual Meeting of the Association for Computational Linguistics, pp 5021–5031
- Xu K, Ba J, Kiros R, Cho K, Courville A, Salakhudinov R, Zemel R, Bengio Y (2015) Show, attend and tell: Neural image caption generation with visual attention. In: International conference on machine learning, PMLR, pp 2048–2057
- Xu K, Li C, Tian Y, Sonobe T, Kawarabayashi K, Jegelka S (2018a) Representation learning on graphs with jumping knowledge networks. In: International Conference on Machine Learning, pp 5453–5462
- Xu K, Wu L, Wang Z, Feng Y, Sheinin V (2018b) Sql-to-text generation with graph-to-sequence model. *arXiv preprint arXiv:1809.05255*
- Xu K, Wu L, Wang Z, Feng Y, Witbrock M, Sheinin V (2018c) Graph2seq: Graph to sequence learning with attention-based neural networks. *arXiv preprint arXiv:1804.00823*

- Xu K, Wu L, Wang Z, Yu M, Chen L, Sheinin V (2018d) Exploiting rich syntactic information for semantic parsing with graph-to-sequence model. In: Proceedings of the 2018 Conference on Empirical Methods in Natural Language Processing, Association for Computational Linguistics, Brussels, Belgium, pp 918–924
- Xu K, Chen H, Liu S, Chen PY, Weng TW, Hong M, Lin X (2019c) Topology attack and defense for graph neural networks: An optimization perspective. In: Proceedings of the Twenty-Eighth International Joint Conference on Artificial Intelligence, IJCAI-19, International Joint Conferences on Artificial Intelligence Organization, pp 3961–3967, DOI 10.24963/ijcai.2019/550
- Xu K, Hu W, Leskovec J, Jegelka S (2019d) How powerful are graph neural networks? In: International Conference on Learning Representations
- Xu K, Hu W, Leskovec J, Jegelka S (2019e) How powerful are graph neural networks? In: International Conference on Learning Representations
- Xu K, Wang L, Yu M, Feng Y, Song Y, Wang Z, Yu D (2019f) Cross-lingual knowledge graph alignment via graph matching neural network. In: Proceedings of the 57th Annual Meeting of the Association for Computational Linguistics, pp 3156–3161
- Xu K, Li J, Zhang M, Du SS, Kawarabayashi Ki, Jegelka S (2020c) What can neural networks reason about? In: International Conference on Learning Representations
- Xu L, Wei X, Cao J, Yu PS (2017b) Embedding of embedding (eoe) joint embedding for coupled heterogeneous networks. In: Proceedings of the Tenth ACM International Conference on Web Search and Data Mining, pp 741–749
- Xu M, Li L, Wai D, Liu Q, Chao LS, et al (2020d) Document graph for neural machine translation. arXiv preprint arXiv:201203477
- Xu Q, Sun X, Wu CY, Wang P, Neumann U (2020e) Grid-gcn for fast and scalable point cloud learning. In: Proceedings of the IEEE/CVF Conference on Computer Vision and Pattern Recognition, pp 5661–5670
- Xu R, Li L, Wang Q (2013) Towards building a disease-phenotype knowledge base: extracting disease-manifestation relationship from literature. *Bioinformatics* 29(17):2186–2194
- Yamaguchi F, Golde N, Arp D, Rieck K (2014) Modeling and discovering vulnerabilities with code property graphs. In: 2014 IEEE Symposium on Security and Privacy, IEEE, pp 590–604
- Yan J, Yin XC, Lin W, Deng C, Zha H, Yang X (2016) A short survey of recent advances in graph matching. In: Proceedings of the 2016 ACM on International Conference on Multimedia Retrieval, pp 167–174
- Yan J, Yang S, Hancock E (2020a) Learning for graph matching and related combinatorial optimization problems. In: Bessiere C (ed) Proceedings of the Twenty-Ninth International Joint Conference on Artificial Intelligence, IJCAI-20, International Joint Conferences on Artificial Intelligence Organization, pp 4988–4996
- Yan S, Xiong Y, Lin D (2018a) Spatial temporal graph convolutional networks for skeleton-based action recognition. In: AAAI Conference on Artificial Intelligence, vol 32
- Yan X, Han J (2002) gspan: Graph-based substructure pattern mining. In: Proceedings of IEEE International Conference on Data Mining, IEEE, pp 721–724

- Yan Y, Mao Y, Li B (2018b) Second: Sparsely embedded convolutional detection. *Sensors* 18(10):3337
- Yan Y, Zhang Q, Ni B, Zhang W, Xu M, Yang X (2019) Learning context graph for person search. In: *Proceedings of the IEEE/CVF Conference on Computer Vision and Pattern Recognition*, pp 2158–2167
- Yan Y, Qin J, Chen J, Liu L, Zhu F, Tai Y, Shao L (2020b) Learning multi-granular hypergraphs for video-based person re-identification. In: *Proceedings of the IEEE/CVF Conference on Computer Vision and Pattern Recognition*, pp 2899–2908
- Yanardag P, Vishwanathan S (2015) Deep graph kernels. In: *Proceedings of the 21th ACM SIGKDD International Conference on Knowledge Discovery and Data Mining*, ACM, pp 1365–1374
- Yang B, Yih W, He X, Gao J, Deng L (2015a) Embedding entities and relations for learning and inference in knowledge bases. In: Bengio Y, LeCun Y (eds) 3rd International Conference on Learning Representations, ICLR 2015, San Diego, CA, USA, May 7-9, 2015, Conference Track Proceedings
- Yang B, Luo W, Urtasun R (2018a) Pixor: Real-time 3d object detection from point clouds. In: *Proceedings of the IEEE conference on Computer Vision and Pattern Recognition*, pp 7652–7660
- Yang C, Liu Z, Zhao D, Sun M, Chang EY (2015b) Network representation learning with rich text information. In: *IJCAI*, vol 2015, pp 2111–2117
- Yang C, Zhuang P, Shi W, Luu A, Li P (2019a) Conditional structure generation through graph variational generative adversarial nets. In: *NeurIPS*, pp 1338–1349
- Yang F, Fan K, Song D, et al (2020a) Graph-based prediction of protein-protein interactions with attributed signed graph embedding. *BMC Bioinformatics* 21(1):323
- Yang H, Qin C, Li YH, Tao L, Zhou J, Yu CY, Xu F, Chen Z, Zhu F, Chen YZ (2016a) Therapeutic target database update 2016: enriched resource for bench to clinical drug target and targeted pathway information. *Nucleic acids research* 44(D1):D1069–D1074
- Yang J, Zheng WS, Yang Q, Chen YC, Tian Q (2020b) Spatial-temporal graph convolutional network for video-based person re-identification. In: *Proceedings of the IEEE/CVF Conference on Computer Vision and Pattern Recognition*, pp 3289–3299
- Yang K, Swanson K, Jin W, Coley C, Eiden P, Gao H, Guzman-Perez A, Hopper T, Kelley B, Mathea M, et al (2019b) Analyzing learned molecular representations for property prediction. *Journal of chemical information and modeling* 59(8):3370–3388
- Yang L, Kang Z, Cao X, Jin D, Yang B, Guo Y (2019c) Topology optimization based graph convolutional network. In: *Proceedings of the Twenty-Eighth International Joint Conference on Artificial Intelligence*, pp 4054–4061
- Yang L, Zhan X, Chen D, Yan J, Loy CC, Lin D (2019d) Learning to cluster faces on an affinity graph. In: *Proceedings of the IEEE/CVF Conference on Computer Vision and Pattern Recognition*, pp 2298–2306

- Yang Q, Liu Y, Chen T, Tong Y (2019e) Federated machine learning: Concept and applications. *ACM Transactions on Intelligent Systems and Technology (TIST)* 10(2):1–19
- Yang S, Li G, Yu Y (2019f) Dynamic graph attention for referring expression comprehension. In: *Proceedings of the IEEE/CVF International Conference on Computer Vision*, pp 4644–4653
- Yang S, Liu J, Wu K, Li M (2020c) Learn to generate time series conditioned graphs with generative adversarial nets. *arXiv preprint arXiv:200301436*
- Yang X, Tang K, Zhang H, Cai J (2019g) Auto-encoding scene graphs for image captioning. In: *Proceedings of the IEEE/CVF Conference on Computer Vision and Pattern Recognition*, pp 10,685–10,694
- Yang Y, Abrego GH, Yuan S, Guo M, Shen Q, Cer D, Sung YH, Strophe B, Kurzweil R (2019h) Improving multilingual sentence embedding using bi-directional dual encoder with additive margin softmax. In: *Proceedings of the 28th International Joint Conference on Artificial Intelligence, AAAI Press*, pp 5370–5378
- Yang Z, Cohen W, Salakhudinov R (2016b) Revisiting semi-supervised learning with graph embeddings. In: *International conference on machine learning*, PMLR, pp 40–48
- Yang Z, Qi P, Zhang S, Bengio Y, Cohen W, Salakhutdinov R, Manning CD (2018b) Hotpotqa: A dataset for diverse, explainable multi-hop question answering. In: *Proceedings of the 2018 Conference on Empirical Methods in Natural Language Processing*, pp 2369–2380
- Yang Z, Zhao J, Dhingra B, He K, Cohen WW, Salakhutdinov RR, LeCun Y (2018c) Glomo: Unsupervised learning of transferable relational graphs. In: *Advances in Neural Information Processing Systems*, pp 8950–8961
- Yang Z, Ding M, Zhou C, Yang H, Zhou J, Tang J (2020d) Understanding negative sampling in graph representation learning. In: *Proceedings of the 26th ACM SIGKDD International Conference on Knowledge Discovery & Data Mining*, pp 1666–1676
- Yao L, Wang L, Pan L, Yao K (2016) Link prediction based on common-neighbors for dynamic social network. *Procedia Computer Science* 83:82–89
- Yao L, Mao C, Luo Y (2019) Graph convolutional networks for text classification. In: *Proceedings of the AAAI Conference on Artificial Intelligence*, vol 33, pp 7370–7377
- Yao S, Wang T, Wan X (2020) Heterogeneous graph transformer for graph-to-sequence learning. In: *Proceedings of the 58th Annual Meeting of the Association for Computational Linguistics*, pp 7145–7154
- Yao T, Pan Y, Li Y, Mei T (2018) Exploring visual relationship for image captioning. In: *Proceedings of the European conference on computer vision (ECCV)*, pp 684–699
- Yarotsky D (2017) Error bounds for approximations with deep relu networks. *Neural Networks* 94:103–114
- Yasunaga M, Liang P (2020) Graph-based, self-supervised program repair from diagnostic feedback. In: *International Conference on Machine Learning*, PMLR, pp 10,799–10,808

- Ye Y, Hou S, Chen L, Lei J, Wan W, Wang J, Xiong Q, Shao F (2019a) Out-of-sample node representation learning for heterogeneous graph in real-time android malware detection. In: Proceedings of the Twenty-Eighth International Joint Conference on Artificial Intelligence, IJCAI-19, International Joint Conferences on Artificial Intelligence Organization, pp 4150–4156
- Ye Y, Wang X, Yao J, Jia K, Zhou J, Xiao Y, Yang H (2019b) Bayes embedding (bem): Refining representation by integrating knowledge graphs and behavior-specific networks. In: Proceedings of the 28th ACM International Conference on Information and Knowledge Management, Association for Computing Machinery, CIKM '19, p 679–688, DOI 10.1145/3357384.3358014
- Yefet N, Alon U, Yahav E (2020) Adversarial examples for models of code. Proceedings of the ACM on Programming Languages 4(OOPSLA):1–30
- Yeung DY, Chang H (2007) A kernel approach for semisupervised metric learning. IEEE Transactions on Neural Networks 18(1):141–149
- Yi J, Park J (2020) Hypergraph convolutional recurrent neural network. In: Proceedings of the 26th ACM SIGKDD International Conference on Knowledge Discovery & Data Mining, pp 3366–3376
- YILMAZ B, Genc H, Agriman M, Demirdover BK, Erdemir M, Simsek G, Karagoz P (2020) Recent trends in the use of graph neural network models for natural language processing. In: Deep Learning Techniques and Optimization Strategies in Big Data Analytics, IGI Global, pp 274–289
- Ying J, de Miranda Cardoso JV, Palomar D (2020a) Nonconvex sparse graph learning under laplacian constrained graphical model. Advances in Neural Information Processing Systems 33
- Ying R, He R, Chen K, Eksombatchai P, Hamilton WL, Leskovec J (2018a) Graph convolutional neural networks for web-scale recommender systems. In: Proceedings of the 24th ACM SIGKDD International Conference on Knowledge Discovery & Data Mining, pp 974–983
- Ying R, He R, Chen K, Eksombatchai P, Hamilton WL, Leskovec J (2018b) Graph convolutional neural networks for web-scale recommender systems. In: Proceedings of the 24th ACM SIGKDD International Conference on Knowledge Discovery & Data Mining, pp 974–983
- Ying R, Bourgeois D, You J, Zitnik M, Leskovec J (2019) Gnnexplainer: Generating explanations for graph neural networks. Advances in neural information processing systems 32:9240
- Ying R, Lou Z, You J, Wen C, Canedo A, Leskovec J, et al (2020b) Neural subgraph matching. arXiv preprint arXiv:200703092
- Ying Z, You J, Morris C, Ren X, Hamilton W, Leskovec J (2018c) Hierarchical graph representation learning with differentiable pooling. In: Advances in Neural Information Processing Systems, pp 4800–4810
- YLow, JGonzalez, AKyrola, DBickson, CGuestrin, JHellerstein (2012) Distributed graphlab: A framework for machine learning in the cloud. PVLDB 5(8):716–727
- You J, Liu B, Ying Z, Pande V, Leskovec J (2018a) Graph convolutional policy network for goal-directed molecular graph generation. In: Advances in Neural Information Processing Systems, pp 6412–6422

- You J, Ying R, Ren X, Hamilton W, Leskovec J (2018b) Graphrnn: Generating realistic graphs with deep auto-regressive models. In: International Conference on Machine Learning, PMLR, pp 5708–5717
- You J, Ying R, Leskovec J (2019) Position-aware graph neural networks. In: International Conference on Machine Learning, PMLR, pp 7134–7143
- You J, Ying Z, Leskovec J (2020a) Design space for graph neural networks. *Advances in Neural Information Processing Systems* 33
- You J, Gomes-Selman J, Ying R, Leskovec J (2021) Identity-aware graph neural networks. *CoRR* abs/2101.10320, [2101.10320](#)
- You Y, Chen T, Sui Y, Chen T, Wang Z, Shen Y (2020b) Graph contrastive learning with augmentations. In: Larochelle H, Ranzato M, Hadsell R, Balcan MF, Lin H (eds) *Advances in Neural Information Processing Systems*, Curran Associates, Inc., vol 33, pp 5812–5823
- You Y, Chen T, Wang Z, Shen Y (2020c) When does self-supervision help graph convolutional networks? In: International Conference on Machine Learning, PMLR, pp 10,871–10,880
- You ZH, Chan KCC, Hu P (2015a) Predicting protein-protein interactions from primary protein sequences using a novel multi-scale local feature representation scheme and the random forest. *PLOS ONE* 10:1–19
- You ZH, Li J, Gao X, et al (2015b) Detecting protein-protein interactions with a novel matrix-based protein sequence representation and support vector machines. *BioMed Research International* 2015:1–9
- Yu B, Yin H, Zhu Z (2018a) Spatio-temporal graph convolutional networks: a deep learning framework for traffic forecasting. In: *Proceedings of the 27th International Joint Conference on Artificial Intelligence*, pp 3634–3640
- Yu D, Fu J, Mei T, Rui Y (2017a) Multi-level attention networks for visual question answering. In: *Proceedings of the IEEE Conference on Computer Vision and Pattern Recognition*, pp 4709–4717
- Yu D, Zhang R, Jiang Z, Wu Y, Yang Y (2021a) Graph-revised convolutional network. In: Hutter F, Kersting K, Lijffijt J, Valera I (eds) *Machine Learning and Knowledge Discovery in Databases*, Springer International Publishing, Cham, pp 378–393
- Yu H, Wu Z, Wang S, Wang Y, Ma X (2017b) Spatiotemporal recurrent convolutional networks for traffic prediction in transportation networks. *Sensors* 17(7):1501
- Yu J, Lu Y, Qin Z, Zhang W, Liu Y, Tan J, Guo L (2018b) Modeling text with graph convolutional network for cross-modal information retrieval. In: *Pacific Rim Conference on Multimedia*, Springer, pp 223–234
- Yu L, Du B, Hu X, Sun L, Han L, Lv W (2021b) Deep spatio-temporal graph convolutional network for traffic accident prediction. *Neurocomputing* 423:135–147
- Yu T, Wang R, Yan J, Li B (2020) Learning deep graph matching with channel-independent embedding and hungarian attention. In: *International conference on learning representations*

- Yu Y, Chen J, Gao T, Yu M (2019a) Dag-gnn: Dag structure learning with graph neural networks. In: International Conference on Machine Learning, pp 7154–7163
- Yu Y, Wang Y, Xia Z, Zhang X, Jin K, Yang J, Ren L, Zhou Z, Yu D, Qing T, et al (2019b) Premedkb: an integrated precision medicine knowledgebase for interpreting relationships between diseases, genes, variants and drugs. *Nucleic acids research* 47(D1):D1090–D1101
- Yuan F, He X, Karatzoglou A, Zhang L (2020a) Parameter-efficient transfer from sequential behaviors for user modeling and recommendation. In: Proceedings of the 43rd International ACM SIGIR Conference on Research and Development in Information Retrieval, pp 1469–1478
- Yuan H, Tang J, Hu X, Ji S (2020b) Xggn: Towards model-level explanations of graph neural networks. In: Proceedings of the 26th ACM SIGKDD International Conference on Knowledge Discovery & Data Mining, pp 430–438
- Yuan J, Zheng Y, Zhang C, Xie W, Xie X, Sun G, Huang Y (2010) T-drive: driving directions based on taxi trajectories. In: Proceedings of the 18th SIGSPATIAL International conference on advances in geographic information systems, pp 99–108
- Yuan J, Zheng Y, Xie X (2012) Discovering regions of different functions in a city using human mobility and pois. In: Proceedings of the 18th ACM SIGKDD international conference on Knowledge discovery and data mining, pp 186–194
- Yuan Y, Liang X, Wang X, Yeung DY, Gupta A (2017) Temporal dynamic graph lstm for action-driven video object detection. In: Proceedings of the IEEE international conference on computer vision, pp 1801–1810
- Yuan Z, Zhou X, Yang T (2018) Hetero-convlstm: A deep learning approach to traffic accident prediction on heterogeneous spatio-temporal data. In: Proceedings of the 24th ACM SIGKDD International Conference on Knowledge Discovery & Data Mining, pp 984–992
- Yue-Hei Ng J, Hausknecht M, Vijayanarasimhan S, Vinyals O, Monga R, Toderici G (2015) Beyond short snippets: Deep networks for video classification. In: Proceedings of the IEEE conference on computer vision and pattern recognition, pp 4694–4702
- Yun S, Jeong M, Kim R, Kang J, Kim HJ (2019) Graph transformer networks. *Advances in Neural Information Processing Systems* 32:11,983–11,993
- Zaheer M, Kottur S, Ravanbakhsh S, Poczos B, Salakhutdinov RR, Smola AJ (2017) Deep sets. In: Advances in Neural Information Processing Systems, pp 3391–3401
- Zanfir A, Sminchisescu C (2018) Deep learning of graph matching. In: Proceedings of the IEEE conference on computer vision and pattern recognition, pp 2684–2693
- Zelnik-Manor L, Perona P (2004) Self-tuning spectral clustering. *Advances in neural information processing systems* 17:1601–1608
- Zeng H, Zhou H, Srivastava A, Kannan R, Prasanna V (2020a) Graphsaint: Graph sampling based inductive learning method. In: International Conference on Learning Representations

- Zeng R, Huang W, Tan M, Rong Y, Zhao P, Huang J, Gan C (2019) Graph convolutional networks for temporal action localization. In: Proceedings of the IEEE/CVF International Conference on Computer Vision, pp 7094–7103
- Zeng X, Song X, Ma T, Pan X, Zhou Y, Hou Y, Zhang Z, Li K, Karypis G, Cheng F (2020b) Repurpose open data to discover therapeutics for covid-19 using deep learning. *Journal of proteome research* 19(11):4624–4636
- Zeng Z, Tung AK, Wang J, Feng J, Zhou L (2009) Comparing stars: On approximating graph edit distance. *Proceedings of the VLDB Endowment* 2(1):25–36
- Zhang B, Hill E, Clause J (2016a) Towards automatically generating descriptive names for unit tests. In: Proceedings of the 31st IEEE/ACM International Conference on Automated Software Engineering, ACM, pp 625–636
- Zhang C, Huang C, Yu L, Zhang X, Chawla NV (2018a) Camel: Content-aware and meta-path augmented metric learning for author identification. In: Proceedings of the 2018 World Wide Web Conference, pp 709–718
- Zhang C, Chao WL, Xuan D (2019a) An empirical study on leveraging scene graphs for visual question answering. *arXiv preprint arXiv:1907.12133*
- Zhang C, Song D, Huang C, Swami A, Chawla NV (2019b) Heterogeneous graph neural network. In: Proceedings of the 25th ACM SIGKDD International Conference on Knowledge Discovery & Data Mining, pp 793–803
- Zhang C, Swami A, Chawla NV (2019c) Shne: Representation learning for semantic-associated heterogeneous networks. In: Proceedings of the Twelfth ACM International Conference on Web Search and Data Mining, pp 690–698
- Zhang D, Yin J, Zhu X, Zhang C (2016b) Collective classification via discriminative matrix factorization on sparsely labeled networks. In: Proceedings of the 25th ACM International on Conference on Information and Knowledge Management, pp 1563–1572
- Zhang D, Yin J, Zhu X, Zhang C (2018b) Metagraph2vec: Complex semantic path augmented heterogeneous network embedding. In: Pacific-Asia conference on knowledge discovery and data mining, Springer, pp 196–208
- Zhang D, Yin J, Zhu X, Zhang C (2018c) Network representation learning: A survey. *IEEE transactions on Big Data* 6(1):3–28
- Zhang G, He H, Katabi D (2019d) Circuit-GNN: Graph neural networks for distributed circuit design. In: International Conference on Machine Learning, pp 7364–7373
- Zhang H, Zheng T, Gao J, Miao C, Su L, Li Y, Ren K (2019e) Data poisoning attack against knowledge graph embedding. In: Proceedings of the Twenty-Eighth International Joint Conference on Artificial Intelligence, IJCAI-19, International Joint Conferences on Artificial Intelligence Organization, pp 4853–4859
- Zhang J (2020) Graph neural distance metric learning with graph-bert. *arXiv preprint arXiv:2002.03427*
- Zhang J, Bargal SA, Lin Z, Brandt J, Shen X, Sclaroff S (2018d) Top-down neural attention by excitation backprop. *International Journal of Computer Vision* 126(10):1084–1102

- Zhang J, Shi X, Xie J, Ma H, King I, Yeung DY (2018e) Gaan: Gated attention networks for learning on large and spatiotemporal graphs. arXiv preprint arXiv:180307294
- Zhang J, Wang X, Zhang H, Sun H, Wang K, Liu X (2019f) A novel neural source code representation based on abstract syntax tree. In: 2019 IEEE/ACM 41st International Conference on Software Engineering (ICSE), IEEE, pp 783–794
- Zhang J, Zhang H, Xia C, Sun L (2020a) Graph-bert: Only attention is needed for learning graph representations. arXiv preprint arXiv:200105140
- Zhang L, Lu H (2020) A Feature-Importance-Aware and Robust Aggregator for GCN. In: ACM International Conference on Information & Knowledge Management, DOI 10.1145/3340531.3411983
- Zhang M, Chen Y (2018a) Link prediction based on graph neural networks. In: Advances in Neural Information Processing Systems, pp 5165–5175
- Zhang M, Chen Y (2018b) Link prediction based on graph neural networks. In: Proceedings of the 32nd International Conference on Neural Information Processing Systems, pp 5171–5181
- Zhang M, Chen Y (2019) Inductive matrix completion based on graph neural networks. In: International Conference on Learning Representations
- Zhang M, Chen Y (2020) Inductive matrix completion based on graph neural networks. In: International Conference on Learning Representations
- Zhang M, Schmitt-Ulms G, Sato C, Xi Z, Zhang Y, Zhou Y, St George-Hyslop P, Rogaeva E (2016c) Drug repositioning for alzheimer’s disease based on systematic ‘omics’ data mining. *PloS one* 11(12):e0168,812
- Zhang M, Cui Z, Neumann M, Chen Y (2018f) An end-to-end deep learning architecture for graph classification. In: Association for the Advancement of Artificial Intelligence
- Zhang M, Cui Z, Neumann M, Chen Y (2018g) An end-to-end deep learning architecture for graph classification. In: the AAAI Conference on Artificial Intelligence, pp 4438–4445
- Zhang M, Hu L, Shi C, Wang X (2020b) Adversarial label-flipping attack and defense for graph neural networks. In: 2020 IEEE International Conference on Data Mining (ICDM), IEEE, pp 791–800
- Zhang M, Li P, Xia Y, Wang K, Jin L (2020c) Revisiting graph neural networks for link prediction. arXiv preprint arXiv:201016103
- Zhang N, Deng S, Li J, Chen X, Zhang W, Chen H (2020d) Summarizing chinese medical answer with graph convolution networks and question-focused dual attention. In: Proceedings of the 2020 Conference on Empirical Methods in Natural Language Processing: Findings, pp 15–24
- Zhang Q, Chang J, Meng G, Xiang S, Pan C (2020e) Spatio-temporal graph structure learning for traffic forecasting. In: Proceedings of the AAAI Conference on Artificial Intelligence, vol 34, pp 1177–1185
- Zhang R, Isola P, Efros AA (2016d) Colorful image colorization. In: European conference on computer vision, Springer, pp 649–666
- Zhang S, Hu Z, Subramonian A, Sun Y (2020f) Motif-driven contrastive learning of graph representations. arXiv preprint arXiv:201212533

- Zhang W, Tang S, Cao Y, Pu S, Wu F, Zhuang Y (2019g) Frame augmented alternating attention network for video question answering. *IEEE Transactions on Multimedia* 22(4):1032–1041
- Zhang W, Fang Y, Liu Z, Wu M, Zhang X (2020g) mg2vec: Learning relationship-preserving heterogeneous graph representations via metagraph embedding. *IEEE Transactions on Knowledge and Data Engineering* 14(8):1
- Zhang W, Liu H, Liu Y, Zhou J, Xiong H (2020h) Semi-supervised hierarchical recurrent graph neural network for city-wide parking availability prediction. In: *Proceedings of the AAAI Conference on Artificial Intelligence*, vol 34, pp 1186–1193
- Zhang W, Wang XE, Tang S, Shi H, Shi H, Xiao J, Zhuang Y, Wang WY (2020i) Relational graph learning for grounded video description generation. In: *Proceedings of the 28th ACM International Conference on Multimedia*, pp 3807–3828
- Zhang X, Zitnik M (2020) GnnGuard: Defending graph neural networks against adversarial attacks. *Advances in Neural Information Processing Systems* 33
- Zhang X, Li Y, Zhou X, Luo J (2019) Unveiling taxi drivers' strategies via cgail: Conditional generative adversarial imitation learning. In: *2019 IEEE International Conference on Data Mining (ICDM)*, pp 1480–1485, DOI 10.1109/ICDM.2019.00194
- Zhang X, Li Y, Zhou X, Luo J (2020a) cgail: Conditional generative adversarial imitation learning—an application in taxi drivers' strategy learning. *IEEE Transactions on Big Data* pp 1–1, DOI 10.1109/TBDATA.2020.3039810
- Zhang X, Li Y, Zhou X, Zhang Z, Luo J (2020b) Trajgail: Trajectory generative adversarial imitation learning for long-term decision analysis. In: *2020 IEEE International Conference on Data Mining (ICDM)*, pp 801–810, DOI 10.1109/ICDM50108.2020.00089
- Zhang Y, Zheng W, Lin H, Wang J, Yang Z, Dumontier M (2018h) Drug–drug interaction extraction via hierarchical rnns on sequence and shortest dependency paths. *Bioinformatics* 34(5):828–835
- Zhang Y, Fan Y, Ye Y, Zhao L, Shi C (2019a) Key player identification in underground forums over attributed heterogeneous information network embedding framework. In: *Proceedings of the 28th ACM International Conference on Information and Knowledge Management*, pp 549–558
- Zhang Y, Khan S, Coates M (2019b) Comparing and detecting adversarial attacks for graph deep learning. In: *Representation Learning on Graphs and Manifolds Workshop at ICLR*
- Zhang Y, Li Y, Zhou X, Kong X, Luo J (2019c) Trafficgan: Off-deployment traffic estimation with traffic generative adversarial networks. *2019 IEEE International Conference on Data Mining (ICDM)* pp 1474–1479
- Zhang Y, Pal S, Coates M, Ustebay D (2019d) Bayesian graph convolutional neural networks for semi-supervised classification. In: *Proceedings of the AAAI Conference on Artificial Intelligence*, vol 33, pp 5829–5836
- Zhang Y, Defazio D, Ramesh A (2020a) Relx: A model-agnostic relational model explainer. *arXiv preprint arXiv:200600305*

- Zhang Y, Deng W, Wang M, Hu J, Li X, Zhao D, Wen D (2020b) Global-local gcn: Large-scale label noise cleansing for face recognition. In: Proceedings of the IEEE/CVF Conference on Computer Vision and Pattern Recognition, pp 7731–7740
- Zhang Y, Guo Z, Teng Z, Lu W, Cohen SB, Liu Z, Bing L (2020c) Lightweight, dynamic graph convolutional networks for amr-to-text generation. In: Proceedings of the 2020 Conference on Empirical Methods in Natural Language Processing (EMNLP), pp 2162–2172
- Zhang Y, Yu X, Cui Z, Wu S, Wen Z, Wang L (2020d) Every document owns its structure: Inductive text classification via graph neural networks. In: Proceedings of the 58th Annual Meeting of the Association for Computational Linguistics, pp 334–339
- Zhang Z, Wang M, Xiang Y, Huang Y, Nehorai A (2018i) Retgk: Graph kernels based on return probabilities of random walks. In: Advances in Neural Information Processing Systems, pp 3964–3974
- Zhang Z, Cui P, Zhu W (2020e) Deep learning on graphs: A survey. *IEEE Transactions on Knowledge and Data Engineering* pp 1–1, DOI 10.1109/TKDE.2020.2981333
- Zhang Z, Zhang Z, Zhou Y, Shen Y, Jin R, Dou D (2020f) Adversarial attacks on deep graph matching. *Advances in Neural Information Processing Systems* 33
- Zhang Z, Zhao Z, Lin Z, Huai B, Yuan NJ (2020g) Object-aware multi-branch relation networks for spatio-temporal video grounding. *arXiv preprint arXiv:200806941*
- Zhang Z, Zhao Z, Zhao Y, Wang Q, Liu H, Gao L (2020h) Where does it exist: Spatio-temporal video grounding for multi-form sentences. In: Proceedings of the IEEE/CVF Conference on Computer Vision and Pattern Recognition, pp 10,668–10,677
- Zhang Z, Zhuang F, Zhu H, Shi Z, Xiong H, He Q (2020i) Relational graph neural network with hierarchical attention for knowledge graph completion. In: Proceedings of the AAAI Conference on Artificial Intelligence, vol 34, pp 9612–9619
- Zhao H, Du L, Buntine W (2017) Leveraging node attributes for incomplete relational data. In: International Conference on Machine Learning, pp 4072–4081
- Zhao H, Zhou Y, Song Y, Lee DL (2019a) Motif enhanced recommendation over heterogeneous information network. In: Proceedings of the 28th ACM international conference on information and knowledge management, pp 2189–2192
- Zhao H, Wei L, Yao Q (2020a) Simplifying architecture search for graph neural network. In: Conrad S, Tiddi I (eds) Proceedings of the CIKM 2020 Workshops co-located with 29th ACM International Conference on Information and Knowledge Management (CIKM 2020), Galway, Ireland, October 19-23, 2020, CEUR-WS.org, CEUR Workshop Proceedings, vol 2699
- Zhao J, Zhou Z, Guan Z, Zhao W, Ning W, Qiu G, He X (2019b) Intentgc: a scalable graph convolution framework fusing heterogeneous information for recommendation. In: Proceedings of the 25th ACM SIGKDD International Conference on Knowledge Discovery & Data Mining, pp 2347–2357

- Zhao J, Wang X, Shi C, Liu Z, Ye Y (2020b) Network schema preserving heterogeneous information network embedding. In: Bessiere C (ed) Proceedings of the Twenty-Ninth International Joint Conference on Artificial Intelligence, IJCAI-20, International Joint Conferences on Artificial Intelligence Organization, pp 1366–1372
- Zhao J, Wang X, Shi C, Hu B, Song G, Ye Y (2021) Heterogeneous graph structure learning for graph neural networks. In: Proceedings of the AAAI Conference on Artificial Intelligence
- Zhao K, Bai T, Wu B, Wang B, Zhang Y, Yang Y, Nie JY (2020c) Deep adversarial completion for sparse heterogeneous information network embedding. In: Proceedings of The Web Conference 2020, pp 508–518
- Zhao L, Akoglu L (2019) Pairnorm: Tackling oversmoothing in gnns. In: International Conference on Learning Representations
- Zhao L, Song Y, Zhang C, Liu Y, Wang P, Lin T, Deng M, Li H (2019c) T-GCN: A temporal graph convolutional network for traffic prediction. *IEEE Transactions on Intelligent Transportation Systems* 21(9):3848–3858
- Zhao M, Wang D, Zhang Z, Zhang X (2015) Music removal by convolutional denoising autoencoder in speech recognition. In: 2015 Asia-Pacific Signal and Information Processing Association Annual Summit and Conference (APSIPA), IEEE, pp 338–341
- Zhao S, Su C, Sboner A, Wang F (2019d) Graphene: A precise biomedical literature retrieval engine with graph augmented deep learning and external knowledge empowerment. In: Proceedings of the 28th ACM International Conference on Information and Knowledge Management, pp 149–158
- Zhao S, Qin B, Liu T, Wang F (2020d) Biomedical knowledge graph refinement with embedding and logic rules. *arXiv preprint arXiv:201201031*
- Zhao S, Su C, Lu Z, Wang F (2020e) Recent advances in biomedical literature mining. *Briefings in Bioinformatics*
- Zhao T, Deng C, Yu K, Jiang T, Wang D, Jiang M (2020f) Error-bounded graph anomaly loss for gnns. In: Proceedings of the 29th ACM International Conference on Information & Knowledge Management, pp 1873–1882
- Zhao Y, Wang D, Gao X, Mullins R, Lio P, Jamnik M (2020g) Probabilistic dual network architecture search on graphs. *arXiv preprint arXiv:200309676*
- Zheng C, Fan X, Wang C, Qi J (2020a) Gman: A graph multi-attention network for traffic prediction. In: Proceedings of the AAAI Conference on Artificial Intelligence, vol 34, pp 1234–1241
- Zheng C, Zong B, Cheng W, Song D, Ni J, Yu W, Chen H, Wang W (2020b) Robust graph representation learning via neural sparsification. In: International Conference on Machine Learning, pp 11,458–11,468
- Zheng D, Song X, Ma C, Tan Z, Ye Z, Dong J, Xiong H, Zhang Z, Karypis G (2020c) Dgl-ke: Training knowledge graph embeddings at scale. In: Proceedings of the 43rd International ACM SIGIR Conference on Research and Development in Information Retrieval, pp 739–748

- Zheng L, Lu CT, Jiang F, Zhang J, Yu PS (2018a) Spectral collaborative filtering. In: Proceedings of the 12th ACM Conference on Recommender Systems, ACM, pp 311–319
- Zheng L, Li Z, Li J, Li Z, Gao J (2019) Addgraph: Anomaly detection in dynamic graph using attention-based temporal gcn. In: Proceedings of the Twenty-Eighth International Joint Conference on Artificial Intelligence, IJCAI-19, pp 4419–4425
- Zheng X, Aragam B, Ravikumar PK, Xing EP (2018b) Dags with no tears: Continuous optimization for structure learning. *Advances in Neural Information Processing Systems* 31:9472–9483
- Zheng Y, Liu F, Hsieh HP (2013) U-air: When urban air quality inference meets big data. In: Proceedings of the 19th ACM SIGKDD international conference on Knowledge discovery and data mining, pp 1436–1444
- Zheng Y, Capra L, Wolfson O, Yang H (2014) Urban computing: Concepts, methodologies, and applications 5(3), DOI 10.1145/2629592
- Zhou C, Liu Y, Liu X, Liu Z, Gao J (2017) Scalable graph embedding for asymmetric proximity. In: Proceedings of the AAAI Conference on Artificial Intelligence, vol 31
- Zhou C, Bai J, Song J, Liu X, Zhao Z, Chen X, Gao J (2018a) Atrank: An attention-based user behavior modeling framework for recommendation. In: Proceedings of the AAAI Conference on Artificial Intelligence, vol 32
- Zhou C, Ma J, Zhang J, Zhou J, Yang H (2020a) Contrastive learning for debiased candidate generation in large-scale recommender systems. *arXiv preprint csIR/200512964*
- Zhou D, Bousquet O, Lal TN, Weston J, Schölkopf B (2004) Learning with local and global consistency. *Advances in neural information processing systems* 16(16):321–328
- Zhou F, De la Torre F (2012) Factorized graph matching. In: 2012 IEEE Conference on Computer Vision and Pattern Recognition, IEEE, pp 127–134
- Zhou G, Zhu X, Song C, Fan Y, Zhu H, Ma X, Yan Y, Jin J, Li H, Gai K (2018b) Deep interest network for click-through rate prediction. In: Proceedings of the 24th ACM SIGKDD, pp 1059–1068
- Zhou G, Wang J, Zhang X, Guo M, Yu G (2020b) Predicting functions of maize proteins using graph convolutional network. *BMC Bioinformatics* 21(16):420
- Zhou J, Cui G, Zhang Z, Yang C, Liu Z, Sun M (2018c) Graph neural networks: A review of methods and applications. *arXiv preprint arXiv:181208434*
- Zhou K, Song Q, Huang X, Hu X (2019a) Auto-gnn: Neural architecture search of graph neural networks. *arXiv preprint arXiv:190903184*
- Zhou K, Dong Y, Wang K, Lee WS, Hooi B, Xu H, Feng J (2020c) Understanding and resolving performance degradation in graph convolutional networks. *arXiv preprint arXiv:200607107*
- Zhou K, Huang X, Li Y, Zha D, Chen R, Hu X (2020d) Towards deeper graph neural networks with differentiable group normalization. In: *Advances in Neural Information Processing Systems*, vol 33

- Zhou K, Song Q, Huang X, Zha D, Zou N, Hu X (2020e) Multi-channel graph neural networks. In: International Joint Conference on Artificial Intelligence, pp 1352–1358
- Zhou N, Jiang Y, Bergquist TR, et al (2019b) The CAFA challenge reports improved protein function prediction and new functional annotations for hundreds of genes through experimental screens. *Genome Biology* 20(1), DOI 10.1186/s13059-019-1835-8
- Zhou T, Lü L, Zhang YC (2009) Predicting missing links via local information. *The European Physical Journal B* 71(4):623–630
- Zhou Y, Tuzel O (2018) Voxelnet: End-to-end learning for point cloud based 3d object detection. In: Proceedings of the IEEE Conference on Computer Vision and Pattern Recognition, pp 4490–4499
- Zhou Y, Hou Y, Shen J, Huang Y, Martin W, Cheng F (2020f) Network-based drug repurposing for novel coronavirus 2019-ncov/sars-cov-2. *Cell discovery* 6(1):1–18
- Zhou Z, Kearnes S, Li L, Zare RN, Riley P (2019c) Optimization of molecules via deep reinforcement learning. *Scientific reports* 9(1):1–10
- Zhou Z, Wang Y, Xie X, Chen L, Liu H (2020g) Riskoracle: A minute-level citywide traffic accident forecasting framework. In: Proceedings of the AAAI Conference on Artificial Intelligence, vol 34, pp 1258–1265
- Zhou Z, Wang Y, Xie X, Chen L, Zhu C (2020h) Foresee urban sparse traffic accidents: A spatiotemporal multi-granularity perspective. *IEEE Transactions on Knowledge and Data Engineering* pp 1–1, DOI 10.1109/TKDE.2020.3034312
- Zhu D, Cui P, Wang D, Zhu W (2018) Deep variational network embedding in wasserstein space. In: Proceedings of the 24th ACM SIGKDD International Conference on Knowledge Discovery & Data Mining, pp 2827–2836
- Zhu D, Zhang Z, Cui P, Zhu W (2019a) Robust graph convolutional networks against adversarial attacks. In: Proceedings of the 25th ACM SIGKDD International Conference on Knowledge Discovery and Data Mining, Association for Computing Machinery, KDD '19, p 1399–1407, DOI 10.1145/3292500.3330851
- Zhu J, Li J, Zhu M, Qian L, Zhang M, Zhou G (2019b) Modeling graph structure in transformer for better AMR-to-text generation. In: Proceedings of the 2019 Conference on Empirical Methods in Natural Language Processing and the 9th International Joint Conference on Natural Language Processing (EMNLP-IJCNLP), Association for Computational Linguistics, Hong Kong, China, pp 5459–5468
- Zhu JY, Park T, Isola P, Efros AA (2017) Unpaired image-to-image translation using cycle-consistent adversarial networks. In: Proceedings of the IEEE international conference on computer vision, pp 2223–2232
- Zhu Q, Du B, Yan P (2020a) Self-supervised training of graph convolutional networks. *arXiv preprint arXiv:200602380*
- Zhu R, Zhao K, Yang H, Lin W, Zhou C, Ai B, Li Y, Zhou J (2019c) Aligraph: a comprehensive graph neural network platform. *Proceedings of the VLDB Endowment* 12(12):2094–2105
- Zhu S, Yu K, Chi Y, Gong Y (2007) Combining content and link for classification using matrix factorization. In: Proceedings of the 30th annual international ACM

- SIGIR conference on Research and development in information retrieval, pp 487–494
- Zhu S, Zhou C, Pan S, Zhu X, Wang B (2019d) Relation structure-aware heterogeneous graph neural network. In: 2019 IEEE International Conference on Data Mining (ICDM), IEEE, pp 1534–1539
- ZHU X (2002) Learning from labeled and unlabeled data with label propagation. Tech Report
- Zhu Y, Elemento O, Pathak J, Wang F (2019e) Drug knowledge bases and their applications in biomedical informatics research. *Briefings in bioinformatics* 20(4):1308–1321
- Zhu Y, Che C, Jin B, Zhang N, Su C, Wang F (2020b) Knowledge-driven drug repurposing using a comprehensive drug knowledge graph. *Health Informatics Journal* 26(4):2737–2750
- Zhu Y, Xu Y, Yu F, Liu Q, Wu S, Wang L (2020c) Deep graph contrastive representation learning. arXiv preprint arXiv:200604131
- Zhu Y, Xu Y, Yu F, Liu Q, Wu S, Wang L (2021) Graph Contrastive Learning with Adaptive Augmentation. In: *Proceedings of The Web Conference 2021*, ACM, WWW '21
- Zhuang Y, Jain R, Gao W, Ren L, Aizawa K (2017) Panel: cross-media intelligence. In: *Proceedings of the 25th ACM international conference on Multimedia*, pp 1173–1173
- Zimmermann T, Zeller A, Weissgerber P, Diehl S (2005) Mining version histories to guide software changes. *IEEE Transactions on Software Engineering* 31(6):429–445
- Zitnik M, Leskovec J (2017) Predicting multicellular function through multi-layer tissue networks. *Bioinformatics* 33(14):i190–i198
- Zitnik M, Agrawal M, Leskovec J (2018) Modeling polypharmacy side effects with graph convolutional networks. *Bioinformatics* 34(13):i457–i466
- Zoete V, Cuendet MA, Grosdidier A, Michielin O (2011) SwissParam: A fast force field generation tool for small organic molecules. *Journal of Computational Chemistry* 32(11):2359–2368
- Zoph B, Le QV (2016) Neural architecture search with reinforcement learning. arXiv preprint arXiv:161101578
- Zoph B, Yuret D, May J, Knight K (2016) Transfer learning for low-resource neural machine translation. In: *Proceedings of the 2016 Conference on Empirical Methods in Natural Language Processing*, pp 1568–1575
- Zoph B, Vasudevan V, Shlens J, Le QV (2018) Learning transferable architectures for scalable image recognition. In: *Proceedings of the IEEE Conference on Computer Vision and Pattern Recognition*, pp 8697–8710
- Zügner D, Günnemann S (2019) Adversarial attacks on graph neural networks via meta learning. In: *International Conference on Learning Representations, ICLR*
- Zügner D, Günnemann S (2019) Certifiable robustness and robust training for graph convolutional networks. In: *Proceedings of the 25th ACM SIGKDD International Conference on Knowledge Discovery & Data Mining*, pp 246–256

- Zügner D, Günnemann S (2020) Certifiable robustness of graph convolutional networks under structure perturbations. In: Proceedings of the 26th ACM SIGKDD International Conference on Knowledge Discovery and Data Mining, Association for Computing Machinery, KDD '20, p 1656–1665, DOI 10.1145/3394486.3403217
- Zügner D, Akbarnejad A, Günnemann S (2018) Adversarial attacks on neural networks for graph data. In: Proceedings of the 24th ACM SIGKDD International Conference on Knowledge Discovery & Data Mining, pp 2847–2856
- Zügner D, Borchert O, Akbarnejad A, Günnemann S (2020) Adversarial attacks on graph neural networks: Perturbations and their patterns. *ACM Trans Knowl Discov Data* 14(5):57:1–57:31
- Zügner D, Kirschstein T, Catasta M, Leskovec J, Günnemann S (2021) Language-agnostic representation learning of source code from structure and context. In: International Conference on Learning Representations

