1 Relational machine learning

1.1 Resumen:

The 'Relational machine learning' section of the manuscript discusses using the graph query framework to develop relational classifiers on graph datasets. The section presents an information-gain pattern mining technique that uses decision tree induction to explore the pattern space and identify characteristic patterns for each subgraph class. The section also provides practical examples of using the query framework and refinement sets to perform relational learning and classify nodes based on extracted patterns.

The section concludes by demonstrating the accuracy of the developed relational decision trees in classifying node types and species in toy graph datasets.

1.2 Evaluación:

Motivation: The section clearly explains the significance and relevance of the study, as well as its wider impacts. The authors highlight the importance of the problem by stating that the proposed approach can acquire relational classifiers on graph datasets using a novel framework. Additionally, they provide examples from previous work to support their claims.

Evaluation level: YES

Improvement: None required.

Novelty: The section clearly describes the proposed approach's novelty and originality. The authors differentiate their work from existing studies by presenting a unique framework for acquiring relational classifiers on graph datasets.

Evaluation level: YES

Improvement: None required.

Clarity: The section is well-written and easy to understand. The authors use appropriate terminology and avoid ambiguity.

Evaluation level: YES

Improvement: None required.

Grammar and Style: The section is free of grammatical and stylistic errors. The authors use language appropriate for an academic setting.

Evaluation level: YES

Improvement: None required.

Typos and Errors: The section is free of typos and other errors.

Evaluation level: YES

Improvement: None required.

Acknowledgements

References

References

Almagro-Blanco, P., & Sancho-Caparrini, F. (2017). Generalized graph pattern matching. *CoRR*, *abs/1708.03734*. URL: `http://arxiv.org/abs/1708.03734`. `arXiv:1708.03734`.

Barceló, P., Libkin, L., & Reutter, J. L. (2011). Querying graph patterns. In *Proceedings of the Thirtieth ACM SIGMOD-SIGACT-SIGART Symposium on Principles of Database Systems* PODS '11 (pp. 199–210). New York, NY, USA: ACM. URL: `http://doi.acm.org/10.1145/1989284.1989307`. doi:`10.1145/1989284.1989307`.

Blockeel, H., & Raedt, L. D. (1998). Top-down induction of first-order logical decision trees. *Artificial Intelligence*, *101*, 285–297. URL: `http://www.sciencedirect.com/science/article/pii/S0004370298000344`. doi:`10.1016/S0004-3702(98)00034-4`.

Bonifati, A. Fletcher, G.Voigt, H.Yakovets, N.Jagadish, H. V. (2018 Querying Graphs Morgan & Claypool Publishers

Bordes, A., Usunier, N., Garcia-Duran, A., Weston, J., & Yakhnenko, O. (2013). Translating embeddings for modeling multi-relational data. In C. J. C. Burges, L. Bottou, M. Welling, Z. Ghahramani, & K. Q. Weinberger (Eds.), *Advances in Neural Information Processing Systems 26* (pp. 2787–2795). Curran Associates, Inc. URL: `http://papers.nips.cc/paper/5071-translating-embeddings-for-modeling-multi-relational-data.pdf`.

Brynjolfsson, E., & Mitchell, T. (2017). What can machine learning do? workforce implications. *Science*, *358*, 1530–1534.

Camacho, R., Pereira, M., Costa, V. S., Fonseca, N. A., Adriano, C., Simões, C. J., & Brito, R. M. (2011). A relational learning approach to structure-activity relationships in drug design toxicity studies. *Journal of integrative bioinformatics*, *8*, 176–194.

Chang, K.-W., Yih, S. W.-t., Yang, B., & Meek, C. (2014). Typed tensor decomposition of knowledge bases for relation extraction. In *Proceedings of the 2014 Conference on Empirical Methods in Natural Language Processing*. ACL – Association for Computational Linguistics. URL: `https://www.microsoft.com/en-us/research/publication/typed-tensor-decomposition-of-knowledge-bases-for-relation-extraction/`.

Consens, M. P., & Mendelzon, A. O. (1990). Graphlog: A visual formalism for real life recursion. In *Proceedings of the Ninth ACM SIGACT-SIGMOD-SIGART Symposium on Principles of Database Systems* PODS '90 (pp. 404–416). New York, NY, USA: ACM. URL: `http://doi.acm.org/10.1145/298514.298591`. doi:`10.1145/298514.298591`.

Cook, S. A. (1971). The complexity of theorem-proving procedures. In *Proceedings of the Third Annual ACM Symposium on Theory of Computing* STOC '71 (pp. 151–158). New York, NY, USA: ACM. URL: `http://doi.acm.org/10.1145/800157.805047`. doi:`10.1145/800157.805047`.

Dong, X., Gabrilovich, E., Heitz, G., Horn, W., Lao, N., Murphy, K., Strohmann, 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* KDD '14 (pp. 601–610). New York, NY, USA: ACM. URL: `http://doi.acm.org/10.1145/2623330.2623623`. doi:`10.1145/2623330.2623623`.

Fan, W., Li, J., Ma, S., Tang, N., Wu, Y., & Wu, Y. (2010). Graph pattern matching: From intractable to polynomial time. *Proc. VLDB Endow.*, *3*, 264–275. URL: `http://dx.doi.org/10.14778/1920841.1920878`. doi:`10.14778/1920841.1920878`.

Gallagher, B. (2006). Matching structure and semantics: A survey on graph-based pattern matching. *AAAI FS*, *6*, 45–53.

García-Jiménez, B., Pons, T., Sanchis, A., & Valencia, A. (2014). Predicting protein relationships to human pathways through a relational learning approach based on simple sequence features. *IEEE/ACM Transactions on Computational Biology and Bioinformatics*, *11*, 753–765. doi:`10.1109/TCBB.2014.2318730`.

Geamsakul, W., Matsuda, T., Yoshida, T., Motoda, H., & Washio, T. (2003). Classifier construction by graph-based induction for graph-structured data. In K.-Y. Whang, J. Jeon, K. Shim, & J. Srivastava (Eds.), *Advances in Knowledge Discovery and Data Mining: 7th Pacific-Asia Conference, PAKDD 2003, Seoul, Korea, April 30 – May 2, 2003 Proceedings* (pp. 52–62). Berlin, Heidelberg: Springer Berlin Heidelberg. URL: `http://dx.doi.org/10.1007/3-540-36175-8_6`. doi:`10.1007/3-540-36175-8_6`.

Gupta, S. (2015). *Neo4j Essentials*. Community experience distilled. Packt Publishing. URL: `https://books.google.es/books?id=WJ7NBgAAQBAJ`.

Luc De Raedt, Sebastijan Dumančić, Robin Manhaeve, Giuseppe Marra. *From Statistical Relational to Neural-Symbolic Artificial Intelligence*. In *Proceedings of the Twenty-Ninth International Joint Conference on Artificial Intelligence (IJCAI'20)*, 2021. ISBN: 9780999241165. Article No.: 688. Pages: 8. Yokohama, Japan.

Henzinger, M. R., Henzinger, T. A., & Kopke, P. W. (1995). Computing simulations on finite and infinite graphs. In *Foundations of Computer Science, 1995. Proceedings., 36th Annual Symposium on* (pp. 453–462). IEEE.

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* WSDM '14 (pp. 373–382). New York, NY, USA: ACM. URL: `http://doi.acm.org/10.1145/2556195.2556225`. doi:`10.1145/2556195.2556225`.

Jiang, J. Q. (2011). Learning protein functions from bi-relational graph of proteins and function annotations. In T. M. Przytycka, & M.-F. Sagot (Eds.), *Algorithms in Bioinformatics* (pp. 128–138). Berlin, Heidelberg: Springer Berlin Heidelberg.

Hunter, J. D. (2007). Matplotlib: A 2D Graphics Environment. *Computing in Science & Engineering*, *9*, 3.

Karp, R. M. (1975). On the computational complexity of combinatorial problems. *Networks*, *5*, 45–68.

Knobbe, A. J., Siebes, A., Wallen, D. V. D., & Syllogic B., V. (1999). Multi-relational decision tree induction. In *In Proceedings of PKDD' 99, Prague, Czech Republic, Septembre* (pp. 378–383). Springer.

Latouche, P., & Rossi, F. (2015). Graphs in machine learning: an introduction.

Leiva, H. A., Gadia, S., & Dobbs, D. (2002). Mrdtl: A multi-relational decision tree learning algorithm. In *Proceedings of the 13th International Conference on Inductive Logic Programming (ILP 2003* (pp. 38–56). Springer-Verlag.

Milner, R. (1989). *Communication and Concurrency*. Upper Saddle River, NJ, USA: Prentice-Hall, Inc.

Nguyen, P. C., Ohara, K., Motoda, H., & Washio, T. (2005). Cl-gbi: A novel approach for extracting typical patterns from graph-structured data. In T. B. Ho, D. Cheung, & H. Liu (Eds.), *Advances in Knowledge Discovery and Data Mining: 9th Pacific-Asia Conference, PAKDD 2005, Hanoi, Vietnam, May 18-20, 2005. Proceedings* (pp. 639–649). Berlin, Heidelberg: Springer Berlin Heidelberg. URL: `http://dx.doi.org/10.1007/11430919_74`. doi:`10.1007/11430919_74`.

Wenfei Fan. *Graph Pattern Matching Revised for Social Network Analysis*. In *Proceedings of the 15th International Conference on Database Theory (ICDT '12)*, 2012. ISBN: 9781450307918. Publisher: Association for Computing Machinery. Address: New York, NY, USA. Pages: 8–21. Num. Pages: 14. Location: Berlin, Germany. DOI: 10.1145/2274576.2274578.

Yiwei Wang, Wei Wang, Yuxuan Liang, Yujun Cai, Juncheng Liu, Bryan Hooi. *NodeAug: Semi-Supervised Node Classification with Data Augmentation*. En *Proceedings of the 26th ACM SIGKDD International Conference on Knowledge Discovery & Data Mining (KDD '20)*, 2020, páginas 207–217. DOI: `https://doi.org/10.1145/3394486.3403063`.

Seyed Mehran Kazemi and David Poole. *RelNN: A Deep Neural Model for Relational Learning*. In *Proceedings of the Thirty-Second AAAI Conference on Artificial Intelligence (AAAI-18)*, University of British Columbia, Vancouver, Canada, 2018. Email: `smkazemi@cs.ubc.ca`, `poole@cs.ubc.ca`.

Maria Leonor Pacheco and Dan Goldwasser. *Modeling Content and Context with Deep Relational Learning*. *Transactions of the Association for Computational Linguistics*, 2021; 9, 100–119. DOI: `https://doi.org/10.1162/tacl_a_00357`.

K. Ahmed, A. Altaf, N.S.M. Jamail, F. Iqbal, R. Latif. *ADAL-NN: Anomaly Detection and Localization Using Deep Relational Learning in Distributed Systems*. *Applied Sciences*, 2023, 13, 7297. DOI: `https://doi.org/10.3390/app13127297`.

Jie Zhou, Ganqu Cui, Zhengyan Zhang, Cheng Yang, Zhiyuan Liu, Maosong Sun. *Graph Neural Networks: A Review of Methods and Applications*. *AI open*, 2020, 1, 57-81.

Lingfei Wu, Peng Cui, Jian Pei, Liang Zhao, Xiaojie Guo. *Graph Neural Networks: Foundation, Frontiers and Applications.* En *Proceedings of the 28th ACM SIGKDD Conference on Knowledge Discovery and Data Mining (KDD '22)*, 2022, páginas 4840–4841. DOI: `https://doi.org/10.1145/3534678.3542609`.

Nickel, M., Murphy, K., Tresp, V., & Gabrilovich, E. (2016). A review of relational machine learning for knowledge graphs. *Proceedings of the IEEE*, *104*, 11–33.

Namkyeong L., Dongmin H., Gyoung S. Na, Sungwon K., Junseok L. and Chanyoung P. (2023). Conditional Graph Information Bottleneck for Molecular Relational Learning.

Plotkin, G. (1972). Automatic methods of inductive inference .

van Rest, O., Hong, S., Kim, J., Meng, X., & Chafi, H. (2016). Pgql: a property graph query language. In *Proceedings of the Fourth International Workshop on Graph Data Management Experiences and Systems* (p. 7). ACM.

Reutter, J. L. (2013). *Graph Patterns: Structure, Query Answering and Applications in Schema Mappings and Formal Language Theory*. Ph.D. thesis Laboratory for Foundations of Computer Science School of Informatics University of Edinburgh.

Segaran, T., Evans, C., Taylor, J., Toby, S., Colin, E., & Jamie, T. (2009). *Programming the Semantic Web*. (1st ed.). O'Reilly Media, Inc.

Tang, L., & Liu, H. (2009). Relational learning via latent social dimensions. In *Proceedings of the 15th ACM SIGKDD international conference on Knowledge discovery and data mining* (pp. 817–826). ACM.

Zou, L., Chen, L., & Özsu, M. T. (2009). Distance-join: Pattern match query in a large graph database. *Proc. VLDB Endow.*, *2*, 886–897. URL: `http://dx.doi.org/10.14778/1687627.1687727`. doi:`10.14778/1687627.1687727`.

Shuai Ma, Yang Cao, Wenfei Fan, Jinpeng Huai, Tianyu Wo. *Strong Simulation: Capturing Topology in Graph Pattern Matching. ACM Trans. Database Syst.*, January 2014, Volume 39, Number 1, Article No. 4. ISSN: 0362-5915. Publisher: Association for Computing Machinery. Address: New York, NY, USA. DOI: 10.1145/2528937. Keywords: dual simulation, graph simulation, data locality, Strong simulation, subgraph isomorphism.