

Bibliography for Graph Classification

Kernel and Neural Computation Methods

Christopher Morris*

*Department of Computer Science, TU Dortmund University, Dortmund, Germany,
firstname.lastname@tu-dortmund.de

December 13, 2017

Abstract

Bibliography for the area of (supervised) graph classification, both graph kernel and deep learning approaches. We only included published articles.

Deep Learning

- [6] H. Dai, B. Dai, and L. Song. “Discriminative Embeddings of Latent Variable Models for Structured Data”. In: *33rd International Conference on Machine Learning*. 2016, pp. 2702–2711.
- [9] D. K. Duvenaud, D. Maclaurin, J. Iparraguirre, R. Bombarell, T. Hirzel, A. Aspuru-Guzik, and R. P. Adams. “Convolutional Networks on Graphs for Learning Molecular Fingerprints”. In: *Advances in Neural Information Processing Systems*. 2015, pp. 2224–2232.
- [11] A. Fout, J. Byrd, B. Shariat, and A. Ben-Hur. “Protein Interface Prediction using Graph Convolutional Networks”. In: *Advances in Neural Information Processing Systems*. 2017, pp. 6533–6542.
- [16] J. Gilmer, S. S. Schoenholz, P. F. Riley, O. Vinyals, and G. E. Dahl. “Neural Message Passing for Quantum Chemistry”. In: *33rd International Conference on Machine Learning*. 2017.
- [17] W. L. Hamilton, Z. Ying, and J. Leskovec. “Inductive Representation Learning on Large Graphs”. In: *Advances in Neural Information Processing Systems*. 2017, pp. 1025–1035.
- [22] W. Jin, C. W. Coley, R. Barzilay, and T. S. Jaakkola. “Predicting Organic Reaction Outcomes with Weisfeiler-Lehman Network”. In: *Advances in Neural Information Processing Systems*. 2017, pp. 2604–2613.
- [28] T. N Kipf and M. Welling. “Semi-Supervised Classification with Graph Convolutional Networks”. In: *ICLR*. 2016.
- [35] T. Lei, W. Jin, R. Barzilay, and T. S. Jaakkola. “Deriving Neural Architectures from Sequence and Graph Kernels”. In: *34th International Conference on Machine Learning*. 2017, pp. 2024–2033.
- [36] Y. Li, D. Tarlow, M. Brockschmidt, and R. Zemel. “Gated Graph Sequence Neural Networks”. In: *International Conference on Learning Representations*. 2016.
- [40] A. Mayr, G. Klambauer, T. Unterthiner, and S. Hochreiter. “DeepTox: Toxicity Prediction using Deep Learning”. In: *Frontiers in Environmental Science* 3.80 (2016).

- [41] C. Merkwirth and T. Lengauer. “Automatic Generation of Complementary Descriptors with Molecular Graph Networks”. In: *Journal of Chemical Information and Modeling* 45.5 (2005), pp. 1159–1168.
- [45] M. Niepert, M. Ahmed, and K. Kutzkov. “Learning Convolutional Neural Networks for Graphs”. In: *33rd International Conference on Machine Learning*. 2016, pp. 2014–2023.
- [48] T. Pham, T. Tran, D. Q. Phung, and S. Venkatesh. “Column Networks for Collective Classification”. In: *AAAI*. 2017, pp. 2485–2491.
- [50] F. Scarselli, M. Gori, A. C. Tsoi, M. Hagenbuchner, and G. Monfardini. “The Graph Neural Network Model”. In: *Transactions on Neural Networks* 20.1 (2009), pp. 61–80.
- [51] K. Schütt, P.-J. Kindermans, H. E. S. Felix, S. Chmiela, A. Tkatchenko, and K.-R. Müller. “SchNet: A continuous-filter convolutional neural network for modeling quantum interactions”. In: *Advances in Neural Information Processing Systems*. 2017, pp. 992–1002.

Kernel Methods

- [1] L. Bai, L. Rossi, Z. Zhang, and E. R. Hancock. “An Aligned Subtree Kernel for Weighted Graphs”. In: *32nd International Conference on Machine Learning*. 2015, pp. 30–39.
- [2] K. M. Borgwardt and H.-P. Kriegel. “Shortest-path kernels on graphs”. In: *5th IEEE International Conference on Data Mining*. 2005, pp. 74–81.
- [3] K. M. Borgwardt and H.-P. Kriegel. “Shortest-path kernels on graphs”. In: *5th IEEE International Conference on Data Mining*. 2005, pp. 74–81.
- [4] K. M. Borgwardt, C. S. Ong, S. Schönauer, S. V. N. Vishwanathan, A. J. Smola, and H.-P. Kriegel. “Protein function prediction via graph kernels.” In: *Bioinformatics* 21.Supplement 1 (2005), pp. i47–i56.
- [5] F. Costa and K. De Grave. “Fast Neighborhood Subgraph Pairwise Distance Kernel”. In: *26th International Conference on Machine Learning*. 2010, pp. 255–262.
- [7] A. K. Debnath, R. L. Lopez de Compadre, G. Debnath, A. J. Shusterman, and C. Hansch. “Structure-activity relationship of mutagenic aromatic and heteroaromatic nitro compounds. Correlation with molecular orbital energies and hydrophobicity”. In: *Journal of Medicinal Chemistry* 34.2 (1991), pp. 786–797.
- [8] P. D. Dobson and A. J. Doig. “Distinguishing Enzyme Structures from Non-enzymes Without Alignments”. In: *Journal of Molecular Biology* 330.4 (2003), pp. 771–783.
- [10] A. Feragen, N. Kasenburg, J. Petersen, M. D. Bruijne, and Borgwardt K. M. “Scalable kernels for graphs with continuous attributes”. In: *Advances in Neural Information Processing Systems*. Erratum available at http://image.diku.dk/aasa/papers/graphkernels_nips_erratum.pdf. 2013, pp. 216–224.
- [12] H. Fröhlich, J. K. Wegner, F. Sieker, and A. Zell. “Optimal assignment kernels for attributed molecular graphs”. In: *22nd International Conference on Machine learning*. 2005, pp. 225–232.
- [13] T. Gärtner. “Kernels for Structured Data”. PhD thesis. University of Bonn, 2005.
- [14] T. Gärtner, P. Flach, and S. Wrobel. “On Graph Kernels: Hardness Results and Efficient Alternatives”. In: *Learning Theory and Kernel Machines*. 2003, pp. 129–143.

- [15] T. Gärtner, P. Flach, and S. Wrobel. “On Graph Kernels: Hardness Results and Efficient Alternatives”. In: *Learning Theory and Kernel Machines*. 2003, pp. 129–143.
- [18] Z. Harchaoui and F. Bach. “Image Classification with Segmentation Graph Kernels”. In: *IEEE Conference on Computer Vision and Pattern Recognition*. 2007, pp. 1–8.
- [19] D. Haussler. *Convolution Kernels on Discrete Structures*. Tech. rep. UCS-CRL-99-10. University of California at Santa Cruz, 1999.
- [20] S. Hido and H. Kashima. “A Linear-Time Graph Kernel”. In: *9th IEEE International Conference on Data Mining*. 2009, pp. 179–188.
- [21] T. Horváth, T. Gärtner, and S. Wrobel. “Cyclic pattern kernels for predictive graph mining”. In: *10th ACM SIGKDD International Conference on Knowledge Discovery and Data Mining*. 2004, pp. 158–167.
- [23] F. D. Johansson and D. Dubhashi. “Learning with Similarity Functions on Graphs Using Matchings of Geometric Embeddings”. In: *21st ACM SIGKDD International Conference on Knowledge Discovery and Data Mining*. 2015, pp. 467–476.
- [24] F. D. Johansson, V. Jethava, D. P. Dubhashi, and C. Bhattacharyya. “Global graph kernels using geometric embeddings”. In: *31st International Conference on Machine Learning*. 2014, pp. 694–702.
- [25] U. Kang, H. Tong, and J. Sun. “Fast Random Walk Graph Kernel”. In: *SIAM International Conference on Data Mining*. 2012, pp. 828–838.
- [26] H. Kashima, K. Tsuda, and A. Inokuchi. “Marginalized Kernels Between Labeled Graphs”. In: *20th International Conference on Machine Learning*. 2003, pp. 321–328.
- [27] J. Kazius, R. McGuire, and R. Bursi. “Derivation and validation of toxicophores for mutagenicity prediction”. In: *Journal Medicinal Chemistry* 48.13 (2005), pp. 312–320.
- [29] R. Kondor and H. Pan. “The Multiscale Laplacian Graph Kernel”. In: *Advances in Neural Information Processing Systems*. 2016, pp. 2982–2990.
- [30] N. M. Kriege. “Comparing Graphs: Algorithms & Applications”. PhD thesis. TU Dortmund University, 2015.
- [31] N. M. Kriege and C. Morris. “Recent Advances in Kernel-Based Graph Classification”. In: *28th European Conference on Machine Learning & Principles and Practice of Knowledge Discovery in Databases*. 2017, ?
- [32] N. M. Kriege, Giscard. P.-L., and R. C. Wilson. “On Valid Optimal Assignment Kernels and Applications to Graph Classification”. In: *Advances in Neural Information Processing Systems*. 2016, pp. 1615–1623.
- [33] N. Kriege and P. Mutzel. “Subgraph Matching Kernels for Attributed Graphs”. In: *29th International Conference on Machine Learning*. 2012.
- [34] N. Kriege, M. Neumann, K. Kersting, and M. Mutzel. “Explicit versus Implicit Graph Feature Maps: A Computational Phase Transition for Walk Kernels”. In: *14th IEEE International Conference on Data Mining*. 2014, pp. 881–886.
- [37] P. Mahé, L. Ralaivola, V. Stoven, and J.-P. Vert. “The pharmacophore kernel for virtual screening with support vector machines.” In: *Journal of Chemical Information and Modeling* 46.5 (2006), pp. 2003–2014.

- [38] P. Mahé, N. Ueda, T. Akutsu, J.-L. Perret, and J.-P. Vert. “Extensions of marginalized graph kernels”. In: *21st International Conference on Machine Learning*. 2004, pp. 552–559.
- [39] P. Mahé and J.-P. Vert. “Graph kernels based on tree patterns for molecules”. In: *Machine Learning* 75.1 (2009), pp. 3–35.
- [42] C. Morris, K. Kersting, and P. Mutzel. “Glocalized Weisfeiler-Lehman Kernel: Global-Local Feature Maps of Graphs”. In: *17th IEEE International Conference on Data Mining*. 2017, ?
- [43] C. Morris, N. M. Kriege, K. Kersting, and P. Mutzel. “Faster Kernel for Graphs with Continuous Attributes via Hashing”. In: *16th IEEE International Conference on Data Mining*. 2016, pp. 1095–1100.
- [44] M. Neumann, R. Garnett, C. Bauckhage, and K. Kersting. “Propagation kernels: Efficient graph kernels from propagated information”. In: *Machine Learning* 102.2 (2016), pp. 209–245.
- [46] L. Oneto, N. Navarin, M. Donini, A. Sperduti, F. Aioli, and D. Anguita. “Measuring the expressivity of graph kernels through Statistical Learning Theory”. In: *Neurocomputing* 268.Supplement C (2017), pp. 4–16.
- [47] F. Orsini, P. Frasconi, and L. De Raedt. “Graph Invariant Kernels”. In: *24th International Joint Conference on Artificial Intelligence*. 2015, pp. 3756–3762.
- [49] J. Ramon and T. Gärtner. “Expressivity versus Efficiency of Graph Kernels”. In: *1st International Workshop on Mining Graphs, Trees and Sequences*. 2003, pp. 65–74.
- [52] N. Shervashidze, P. Schweitzer, E. J. van Leeuwen, K. Mehlhorn, and K. M. Borgwardt. “Weisfeiler-Lehman Graph Kernels”. In: *Journal of Machine Learning Research* 12 (2011), pp. 2539–2561.
- [53] N. Shervashidze, P. Schweitzer, E. J. van Leeuwen, K. Mehlhorn, and K. M. Borgwardt. “Weisfeiler-Lehman Graph Kernels”. In: *Journal of Machine Learning Research* 12 (2011), pp. 2539–2561.
- [54] N. Shervashidze, S. V. N. Vishwanathan, T. H. Petri, K. Mehlhorn, and K. M. Borgwardt. “Efficient Graphlet Kernels for Large Graph Comparison”. In: *12th International Conference on Artificial Intelligence and Statistics*. 2009, pp. 488–495.
- [55] Y. Su, F. Han, R. E. Harang, and X. Yan. “A fast Kernel for Attributed Graphs”. In: *SIAM International Conference on Data Mining*. 2016, pp. 486–494.
- [56] M. Sugiyama and K. M. Borgwardt. “Halting in Random Walk Kernels”. In: *Advances in Neural Information Processing Systems*. 2015, pp. 1639–1647.
- [57] S. V. N. Vishwanathan, N. N. Schraudolph, R. Kondor, and K. M. Borgwardt. “Graph Kernels”. In: *Journal of Machine Learning Research* 11 (2010), pp. 1201–1242.
- [58] N. Wale, I. A. Watson, and G. Karypis. “Comparison of descriptor spaces for chemical compound retrieval and classification”. In: *Knowledge and Information Systems* 14.3 (2008), pp. 347–375.