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 18, 2017

Abstract

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

Deep Learning

[5] J. Bruna, W. Zaremba, A. Szlam, and Y. LeCun. "Spectral Networks and Deep Locally Connected Networks on Graphs". In: *ICLR*. 2014.

[9] 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.

[12] 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.

[14] 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.

[19] 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.

[20] W. L. Hamilton, R. Ying, and J. Leskovec. "Inductive Representation Learning on Large Graphs". In: *Advances in Neural Information Processing Systems*. 2017, pp. 1025–1035.

[21] W. L. Hamilton, R. Ying, and J. Leskovec. "Representation Learning on Graphs: Methods and Applications". In: *IEEE Data Engineering Bulletin* 40.3 (2017), pp. 52–74.

[27] 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.

[33] S. Kearnes, K. McCloskey, M. Berndl, V. Pande, and P. Riley. "Molecular graph convolutions: moving beyond fingerprints". In: *Journal of Computer-Aided Molecular Design* 30.8 (2016), pp. 595–608.

[35] T. N Kipf and M. Welling. "Semi-Supervised Classification with Graph Convolutional Networks". In: *ICLR*. 2016.

[44] 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.

[48] P. Vandergheynst M. Defferrard X. Bresson. "Convolutional Neural Networks on Graphs with Fast Localized Spectral Filtering". In: *Advances in Neural Information Processing Systems*. 2016, pp. 3844–3852.

[52] A. Mayr, G. Klambauer, T. Unterthiner, and S. Hochreiter. "DeepTox: Toxicity Prediction using Deep Learning". In: *Frontiers in Environmental Science* 3.80 (2016).

[53] 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.

[54] A. Micheli. “Neural Network for Graphs: A Contextual Constructive Approach”. In: *IEEE Transactions on Neural Networks* 20.3 (2009), pp. 498–511.

[55] F. Monti, D. Boscaini, J. Masci, E. Rodolà, J. Svoboda, and M. M. Bronstein. “Geometric Deep Learning on Graphs and Manifolds Using Mixture Model CNNs”. In: *IEEE Conference on Computer Vision and Pattern Recognition*. 2017, pp. 5425–5434.

[56] F. Monti, M. M. Bronstein, and X. Bresson. “Geometric Matrix Completion with Recurrent Multi-Graph Neural Networks”. In: *Advances in Neural Information Processing Systems*. 2017, pp. 3700–3710.

[60] M. Niepert, M. Ahmed, and K. Kutzkov. “Learning Convolutional Neural Networks for Graphs”. In: *33rd International Conference on Machine Learning*. 2016, pp. 2014–2023.

[65] T. Pham, T. Tran, D. Q. Phung, and S. Venkatesh. “Column Networks for Collective Classification”. In: *AAAI*. 2017, pp. 2485–2491.

[67] F. Scarselli, M. Gori, A. C. Tsoi, M. Hagenbuchner, and G. Monfardini. “Computational Capabilities of Graph Neural Networks”. In: *IEEE Transactions on Neural Networks* 20.1 (2009), pp. 81–102.

[68] 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.

[69] 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.

[80] L. Yi, H. Su, H. Guo, and L. Guibas. “SyncSpecCNN: Synchronized Spectral CNN for 3D Shape Segmentation”. In: *IEEE Conference on Computer Vision and Pattern Recognition*. 2017, pp. 6584–6592.

Kernel Methods

[1] F. Aiolli, M. Donini, N. Navarin, and A. Sperduti. “Multiple Graph-Kernel Learning”. In: *SSCI*. 2015, pp. 1607–1614.

[2] 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.

[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.

[6] F. Costa and K. De Grave. “Fast Neighborhood Subgraph Pairwise Distance Kernel”. In: *26th International Conference on Machine Learning*. 2010, pp. 255–262.

[7] G. Da San Martino, N. Navarin, and Sperduti A. “A Tree-Based Kernel for Graphs”. In: *SIAM Conference of Data Mining*. 2012, pp. 975–986.

[8] G. Da San Martino, N. Navarin, and A. Sperduti. “A memory efficient graph kernel”. In: *IJCNN*. 2012, pp. 1–7.

[10] 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.

[11] 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.

[13] 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.

[15] 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.

[16] T. Gärtner. "Kernels for Structured Data". PhD thesis. University of Bonn, 2005.

[17] 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] 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.

[22] Z. Harchaoui and F. Bach. "Image Classification with Segmentation Graph Kernels". In: *IEEE Conference on Computer Vision and Pattern Recognition*. 2007, pp. 1–8.

[23] D. Haussler. *Convolution Kernels on Discrete Structures*. Tech. rep. UCS-CRL-99-10. University of California at Santa Cruz, 1999.

[24] L. Hermansson, F. D. Johansson, and O. Watanabe. "Generalized Shortest Path Kernel on Graphs". In: *Discovery Science: 18th International Conference*. 2015, pp. 78–85.

[25] S. Hido and H. Kashima. "A Linear-Time Graph Kernel". In: *9th IEEE International Conference on Data Mining*. 2009, pp. 179–188.

[26] 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.

[28] 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.

[29] 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.

[30] U. Kang, H. Tong, and J. Sun. "Fast Random Walk Graph Kernel". In: *SIAM International Conference on Data Mining*. 2012, pp. 828–838.

[31] H. Kashima, K. Tsuda, and A. Inokuchi. "Marginalized Kernels Between Labeled Graphs". In: *20th International Conference on Machine Learning*. 2003, pp. 321–328.

[32] 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.

[34] K. Kersting, N. M. Kriege, C. Morris, P. Mutzel, and M. Neumann. *Benchmark Data Sets for Graph Kernels*. 2016. URL: `http://graphkernels.cs.tu-dortmund.de`.

[36] R. Kondor and K. M. Borgwardt. "The skew spectrum of graphs". In: *25th International Conference on Machine Learning*. 2008, pp. 496–503.

[37] R. Kondor and H. Pan. "The Multiscale Laplacian Graph Kernel". In: *Advances in Neural Information Processing Systems*. 2016, pp. 2982–2990.

[38] R. Kondor, N. Shervashidze, and K. M. Borgwardt. "The graphlet spectrum". In: *26th International Conference on Machine Learning*. 2009, pp. 529–536.

[39] N. M. Kriege. "Comparing Graphs: Algorithms & Applications". PhD thesis. TU Dortmund University, 2015.

[40] 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, ?

[41] 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.

[42] N. Kriege and P. Mutzel. "Subgraph Matching Kernels for Attributed Graphs". In: *29th International Conference on Machine Learning*. 2012.

[43] 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.

[45] B. Li, X. Zhu, L. Chi, and C. Zhang. “Nested Subtree Hash Kernels for Large-Scale Graph Classification over Streams”. In: *IEEE 12th International Conference on Data Mining*. 2012, pp. 399–408.

[46] L. Li, H. Tong, Y. Xiao, and W. Fan. “*Cheetah*: Fast Graph Kernel Tracking on Dynamic Graphs”. In: *SIAM International Conference on Data Mining*. 2015, pp. 280–288.

[47] W. Li, H. Saidi, H. Sanchez, M. Schäf, and P. Schweitzer. “Detecting Similar Programs via The Weisfeiler-Leman Graph Kernel”. In: *ICSR*. 2016, pp. 315–330.

[49] 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.

[50] 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.

[51] P. Mahé and J.-P. Vert. “Graph kernels based on tree patterns for molecules”. In: *Machine Learning* 75.1 (2009), pp. 3–35.

[57] 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, ?

[58] 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.

[59] 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.

[61] G. Nikolentzos, P. Meladianos, F. Rousseau, Y. Stavrakas, and M. Vazirgiannis. “Shortest-Path Graph Kernels for Document Similarity”. In: *EMNLP*. 2017, pp. 1890–1900.

[62] G. Nikolentzos, P. Meladianos, and M. Vazirgiannis. “Matching Node Embeddings for Graph Similarity”. In: *AAAI*. 2017, pp. 2429–2435.

[63] L. Oneto, N. Navarin, M. Donini, A. Sperduti, F. Aiolli, and D. Anguita. “Measuring the expressivity of graph kernels through Statistical Learning Theory”. In: *Neurocomputing* 268.Supplement C (2017), pp. 4–16.

[64] F. Orsini, P. Frasconi, and L. De Raedt. “Graph Invariant Kernels”. In: *24th International Joint Conference on Artificial Intelligence*. 2015, pp. 3756–3762.

[66] 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.

[70] 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.

[71] 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.

[72] 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.

[73] 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.

[74] M. Sugiyama and K. M. Borgwardt. “Halting in Random Walk Kernels”. In: *Advances in Neural Information Processing Systems*. 2015, pp. 1639–1647.

[75] J.-P. Vert. “The optimal assignment kernel is not positive definite”. In: *CoRR* abs/0801.4061 (2008). URL: `http://arxiv.org/abs/0801.4061`.

[76] 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.

[77] 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.

[78] P. Yanardag and S. V. N. Vishwanathan. “A Structural Smoothing Framework For Robust Graph Comparison”. In: *Advances in Neural Information Processing Systems*. 2015, pp. 2134–2142.

[79] P. Yanardag and S. V. N. Vishwanathan. “Deep Graph Kernels”. In: *21st ACM SIGKDD International Conference on Knowledge Discovery and Data Mining*. 2015, pp. 1365–1374.