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Weisfeiler-Lehman graph kernels. (English) Zbl 1280.68194

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Summary: We propose a family of efficient kernels for large graphs with discrete node labels. Key to our method is a rapid feature extraction scheme based on the Weisfeiler-Lehman test of isomorphism on graphs. It maps the original graph to a sequence of graphs, whose node attributes capture topological and label information. A family of kernels can be defined based on this Weisfeiler-Lehman sequence of graphs, including a highly efficient kernel comparing subtree-like patterns. Its runtime scales only linearly in the number of edges of the graphs and the length of the Weisfeiler-Lehman graph sequence. In our experimental evaluation, our kernels outperform state-of-the-art graph kernels on several graph classification benchmark data sets in terms of accuracy and runtime. Our kernels open the door to large-scale applications of graph kernels in various disciplines such as computational biology and social network analysis.

MSC:

68T05 Learning and adaptive systems in artificial intelligence
62H30 Classification and discrimination; cluster analysis (statistical aspects)
05C90 Applications of graph theory

Cited in **26** Documents

Keywords:

[graph kernels](#)

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