

An exact algorithm to find a maximum weight clique in a weighted undirected graph

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We introduce a new algorithm MaxCliqueWeight for identifying a maximum weight clique in a weighted graph, and its variant MaxCliqueDynWeight with dynamically varying bounds. This algorithm uses an efficient branch-and-bound approach with a new weighted graph coloring algorithm that efficiently determines upper weight bounds for a maximum weighted clique in a graph. We evaluate this algorithm on random weighted graphs with node counts up to 10,000 and on standard DIMACS benchmark graphs used in a variety of research areas. Our findings reveal a remarkable improvement in computational speed when compared to existing algorithms, particularly evident in the case of high-density random graphs and DIMACS graphs, where our newly developed algorithm outperforms existing alternatives by several orders of magnitude. The newly developed algorithm and its variant are freely available to the broader research community at <http://insilab.org/maxcliqueweight>, paving the way for transformative applications in various research areas, including drug discovery.