Modelling and Optimisation with Graphs

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Abstract. Optimisation problems involving graphs are common. For example, network epidemiology investigates the dynamics of a disease spreading over a graph, where the vertices represent agents that can be infected, and edges the potentially infectious contacts between agents. We are interested in modifying the graph to limit the scope of an epidemic, by deleting vertices or edges to limit its maximum component size.
In kidney exchange programs such as the UK Living Kidney Sharing Schemes, patients requiring a kidney transplant who have a willing but incompatible donor may exchange donors with other similar patients. The scheme seeks to maximise the number of transplants that take place, subject to additional criteria; this problem can be modelled as a form of cycle packing in a weighted directed graph.
A major goal in metabolomics is improving metabolite identification from mass spectrometry experiments. One route is through the comparison of measured fragmentation spectra with a database. Constraining results by shared graph substructure could lead to more specific result sets.
And in computational algebra, many problems involving semigroups and monoids can be reinterpreted as graph homomorpism questions.
This talk discusses the work we plan to carry out over the next three years, aimed at simplifying and improving the modelling and solving process for such problems. We will develop high level modelling support for graphs for the Essence' constraint modelling language. Being able to express graph operations directly will reduce the modelling cost, and compiling from high-level models will simplify automatic reformulation and the use of alternative encodings.
To solve these problems, we envision a hybrid approach, combining constraint programming or mixed integer solvers with dedicated subgraph algorithms. Although state-of-the-art subgraph algorithms often have a constraint-based feel to them, they use tailored data structures and propagation routines, which are critical for scalability. Propagating certain kinds of constraints (such as connectivity) can be done directly inside subgraph algorithms, but we believe a "subgraphs modulo theories" approach involving multiple communicating solvers is necessary for more complex problems. A final advantage of high level modelling, then, is in automating the configuration of such approaches.

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