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Some Applications of the Geometric Representations of Graphs

1 Individual Project's contribution to the CRP

1.1 Aims and Objectives

Geometric and other representations of graphs or graph-based structures have important applications in mathematics, computer science, social networks, chemistry, bioinformatics, etc. Main goal of the project is development of coherent theory of graph representations, mostly of symmetric or almost symmetric structures and products. The knowledge acquired by the researches will be applied to geometrically interesting combinatorial structures like configurations, maps and polytopes, as to the large partially symmetric networks. The project will consist of the following parts:

1. representation and enumerating of highly symmetric graphs;
2. almost symmetric graph structures;
3. representation of large networks;
4. representations and configurations of symmetric maps and polytopes;
5. graph representations in mathematical chemistry and bioinformatics.

Individual goal of the project is application of graph theory in chemistry, bioinformatics and graph products. Chemical structures can be represented by graphs, where the atoms are represented by vertices and chemical bonds by edges. Many physical and chemical properties can be found knowing the molecular topology. Extremal graph theory helps in finding graphs with extremal values of some molecular descriptors. If some graph-theoretical property is in good correlation with some physical or chemical property, then such results give us the ability to determine molecules with optimal value of the concerned property.

Furthermore, one can model social networks by graphs in such a way that members of the network are represented by vertices, and their relationships by edges. Finding communities inside such networks is important for sociological researches – one can analyze group coherency, subcultures or modularity of investigated group etc. Similar results are important in studying of the spreading of epidemics. Exploring the Internet, one can represent Web pages by vertices and their links by edges. In object oriented programming the objects can be seen as vertices and their dependencies as edges. For the purpose of more efficient development of complex software, it is important to determine module communities. That makes us able to minimize influence of the program code developed by one group of people to the code of other groups.

Another graph theory application that appears in optimizing, organization and analyzing of communication networks, chemistry and algorithm construction are the graphs dominations (k -dominations, total dominations, independent dominations, etc.), see [1, 6, 7, 9, 11], Because networks can be seen as graph products (specially path products), one of the project parts would be studying domination sets on different graph products [12, 14, 9, 8, 10], and also on some graphs with regular structures, for instance m -uniform chains, m -uniform cactus-chains or, in chemistry very important, multiple hexagonal chains (representing benzenoid systems) [2, 16]. We will also study the chains consisting of cycles with n vertices.

1.2 Methodologies

In the research we will use methods of combinatorial theory, graph theory, statistics and data-mining.

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