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Isometric Embeddings into Product-Like Graphs

## 1 Individual Project's contribution to the CRP

### 1.1 Aims and Objectives

Networks and graphs that appear in practical applications can be quite large. This fact imposes a serious limitation on methods that provide geometric representations and/or drawings of such structures (that are in turn aimed to better understand the structures). Therefore, one wishes to decompose large structures into pieces that are small enough for the above mentioned methods to be effectively used. After this is done on the pieces of a large structure, the partial information is used to get an insight for the complete structure.

A standard approach for decomposing graphs into smaller parts is via graph products [7]. Ideally, a large graph (or a network) decomposes as a product of smaller graphs, where the product involved is one of the standard graph products. For these products, that is, for the Cartesian product, the direct product, the strong product, and the lexicographic product, the factorization theory is well developed from theoretical as well as from algorithmic point of view. However, in reality it is very unlikely to expect that a (random) graph will be a product. For instance, it is known that asymptotically almost every graph is indecomposable with respect to the Cartesian product. Hence one needs additional ideas to find decompositions of large graphs into smaller pieces.

A recent idea is the one of the approximate graph products [5]. It gives a larger variety of graphs than the standard graph products and already showed to be fruitful. But even this larger class of graphs might be too small. If this happens we are forced to make a step forward by considering the possibility that a given graph only embeds into a graph product, an approximate graph product, or some other product-like structure. Of course, numerous trivial embeddings are possible, however, we wish to have an embedding that reflects the properties of a graph from the structure of the product into which it is embedded. Hence the overall process of analyzing a large graph can be partitioned into the following steps:

- 1) For a given graph  $G$ , find an embedding of  $G$  into an (approximate) graph product or some other product-like structure  $X$ ;
- 2) Decompose  $X$  into factors and determine properties of the factors, for instance find their geometric representations and/or drawings;
- 3) Determine the corresponding factors of the embedded graph  $G$ ;
- 4) From the properties of the factors of the embedded graph, using the properties of  $X$ , deduce properties of  $G$ .

The above describes the framework via which this IP fits into the overall project. The aim of this IP is to focus on points 1) and 4) of the above process as described in the following.

One of the most important and applicable properties of a given graph is its metric structure. Every connected graph gives rise to a metric space on its vertex set, where the metric is given by the path distance in the graph. This connection enriched in many ways both the theory of metric spaces and the graph theory. The metric point of view leads to distinguishing classes of graphs with particularly nice properties of the associated metrics. Examples of these are the classes of  $L1$ -graphs, out of which most prominent so far was the class of  $L1$ -graphs [2]. In the bipartite case, this class is represented by the partial cubes, which received a lot of attention in recent years. Moreover, partial cubes are strongly related to geometry [3]. The combination of the graph theory setup with the metric point of view found applications in other parts of mathematics and even outside of mathematics. In organic chemistry, where the structure of a

molecule can be represented by a connected graph, this point of view led to the development of a number of numerical invariants (or indices) which correlate with various physical and chemical properties of the molecule. One of the better known such invariants is the Wiener index of the graph, defined as the half of the sum of all mutual distances between the vertices, but there is also a number of other important indices defined in terms of distances and paths.

The isometric dimension of a graph is by now well understood. Recently, the Fibonacci dimension of a graph  $G$  was introduced as the smallest integer  $f$  such that  $G$  admits an isometric embedding into the  $f$ -dimensional Fibonacci cube [1]. This dimension has several appealing properties and is also very interesting from the algorithmic point of view. The corresponding isometric embeddability is based on binary strings with forbidden substring 11. This leads to the general problem when embeddability is defined via binary strings with some forbidden substring(s).

An even more recent idea than the approximate graph products is the idea of the so-called tensor 2-sums [8]. The idea came from mathematical physics, more precisely from quantum mechanics, and appears to be a completely new area of research. In order to define a minimal mathematical framework for isolating some of the characteristic properties of quantum entanglement tensor 2-sums were introduced that can be described as a modulo 2 superpositions of standard direct product graphs. Of course, this picture is a much impoverished version of quantum states, however, it is still possible, for instance, prove a combinatorial analogue of the Peres-Horodecki criterion for testing separability.

## 1.2 Methodologies

For our purposes the main method to realize step 1) in the above process of analyzing a large graph is to embed a graph into a product-like graph  $X$  such that the distances of  $G$  are preserved in  $X$  [4]. This enables us that, provided the given embedding is selected appropriately, step 4) can also be realized based on the facts that the embedding is distance preserving and that allows to deduce properties of the embedded graph from the corresponding factors. In this respect, (approximate) graph products are one of the best environments for embeddings. For example, the Cartesian product of graphs can be viewed as the realization of the sum of the graph metrics of the factors. In the same spirit, the strong product of graphs realizes the maximum of the graph metrics of the factors, which is a second natural way to define a metric on the Cartesian product of two metric spaces. Embeddings into product-like graphs uses as one of the main methods partitions of the edge set of a graph into classes imposed by a carefully selected relation. The breakthrough in the area was done in [4]. Another relevant idea is the 3 trees embedding of a Chepoi that provided a breakthrough to linear algorithms for computing invariants on hexagonal graphs. The embedding is defined by unifying certain Theta-classes of a given hexagonal graph based on its geometric representation and then embedding it into the Cartesian product of the standard quotient graphs. These graphs turns out to be trees, hence the name of the embedding. Hence one of the methods method to study embeddings into product-like graphs is a search for appropriate equivalence relations.

Among the applications of embeddings into product graphs metric graph theory, there are numerous theorems using isometric embeddings and the canonical metric representation to give expressions for computing various indices that are used to predict of physical and chemical properties of molecular graphs. Among them, let us mention the Wiener index, the Szeged index, the hyper-Wiener index, the PI index, and the degree distance index. It seems that there should be a way to unify all these approaches into some general framework that would not only enable to deduce existing theorems as corollaries but also to give tools to deduce new results whenever a need for them would appear. A newly introduced method to define a minimal mathematical framework for isolating some of the characteristic property is to decompose a given graph as the superposition of (direct) product graphs. It seems that a connection between 2-sums and approximate graph products is possible. This would provide a promising method to

apply results from one approach to the other. From the natural algorithmic question–design a recognition algorithm for (tensor) 2-sum graphs—one could apply (at least in polynomial cases) the fact that the unique prime factorization with respect to the direct product of nonbipartite connected graphs can be found in polynomial time [6].

## References

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