A graph theory problem related to the self-assembly of DNA structures

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(based on a joint work with Margherita Maria Ferrari)

The self-assembly of DNA structures can be obtained by several methods that are based on the Watson-Crick complementary properties of DNA strands. We consider the method of branched junction molecules: star-shaped molecules whose arms have cohesive ends that allow the molecules to join together in a prescribed way and form a larger molecule (DNA complex).

In graph theory terminology, a branched junction molecule is called a tile and consists of a vertex with labeled half-edges; labels are the cohesive ends and belong to a finite set of symbols, say $\{a, \hat{a} : a \in \Sigma\}$. A tile is denoted by the multiset consisting of the labels of the half-edges (the tile type). We can create an edge between two vertices u, v if and only if u has a half-edge labeled by a and v has a half-edge labeled by $\hat{a}$; the edge thus obtained is said to be a bond-edge of type $a\hat{a}$. By connecting the vertices according to the labels, we can construct a graph G representing a DNA complex.

The following problem is considered: determine the minimum number of tile types and bond-edge types that are necessary to construct a given graph G.

In this seminar we discuss the above problem and show some techniques providing an upper bound for the number of bond-edge types that are necessary to construct an arbitrary graph.