A colored approach for the self-assembly of DNA structures

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We study a graph theory problem related to the self-assembly of DNA structures. The self-assembly can be obtained by several methods that are based on the Watson-Crick complementary properties of DNA strands. We consider the method based on branched junction molecules, that is, 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 the language of graphs, a branched junction molecule is called a tile and consists of a vertex with labeled half-edges; labels represent the cohesive ends and belong to a set $\{a, \hat{a} : a \in \Sigma\}$, where Σ is a finite set of symbols; a tile is denoted by the multiset consisting of the labels of the half-edges; and two tiles are of the same tile type if they are denoted by the same multiset.

We can create an edge between the 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: given a graph G, determine the minimum number of tile types and bond-edge types that are necessary to construct G. We describe the problem by edge-colored graphs and show some upper bounds for the number of bond-edge types that are necessary to construct an arbitrary graph.