Optimal Constructions for DNA Self-Assembly of k-Regular Graphs

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Introduction

Central Idea

Instead of constructing nanostructures directly, create smaller pieces that will self-assemble into target compounds. In our model, we assume the use of branched junction DNA molecules, referred as *tile*. Each tile contains one vertex and flexible unpaired cohesive ends. When those ends pair up, they form a *bond-edge*. The set of tiles used to form a graph is called a *pot*. [1]

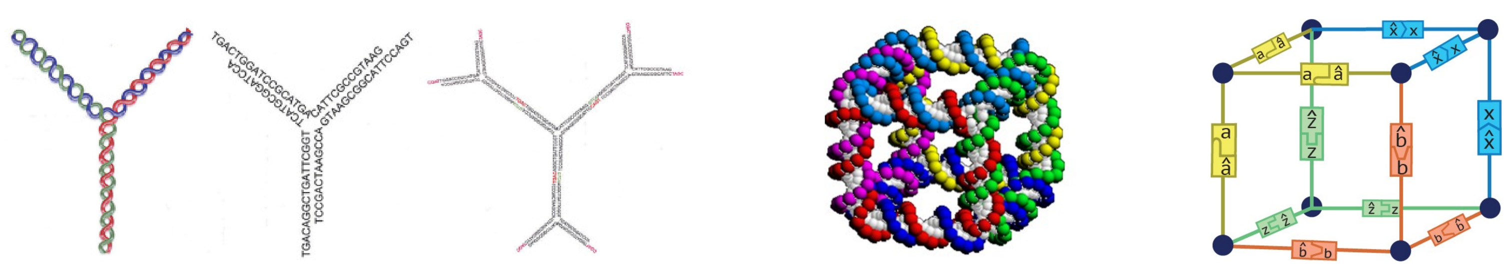

Figure 1. Cube as a molecule and as a graph.

Goal

Given a k-regular graph G, we aim to find the minimum number of bond-edge types or tile types required for a valid pot to form G, denoted $B_3(G)$ and $T_3(G)$, respectively. A pot is valid if for every G' realized by the pot, either $|V(G')| > |V(G)|$ or $G \simeq G'$.

Upper Bound for $B_3(G)$

Upper Bound Theorem. Suppose that G is a k-regular graph and $K \subseteq V(G)$ such that: K is a vertex cover for G, K is neighborhood independent, and the induced subgraph on K is 2-edge-connected. Then $B_3(G) \leq |K|$.

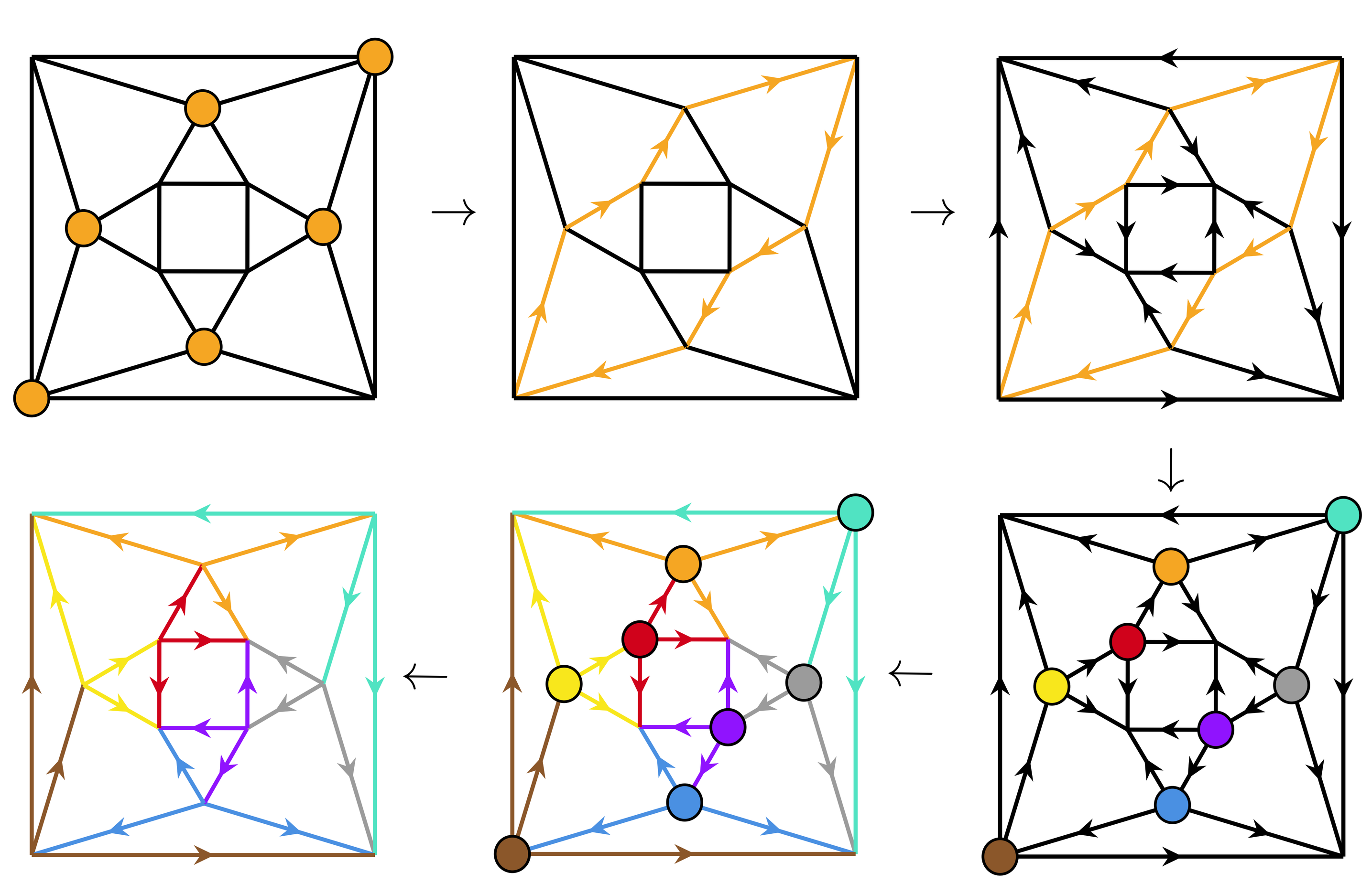

Figure 2. Pot construction for above theorem, with vertex cover K (orange).

Lower Bound for $B_3(G)$

We say that a graph G is **unswappable** if, for all pairs of disjoint edges, swapping the endpoints of the edges gives a nonisomorphic graph.

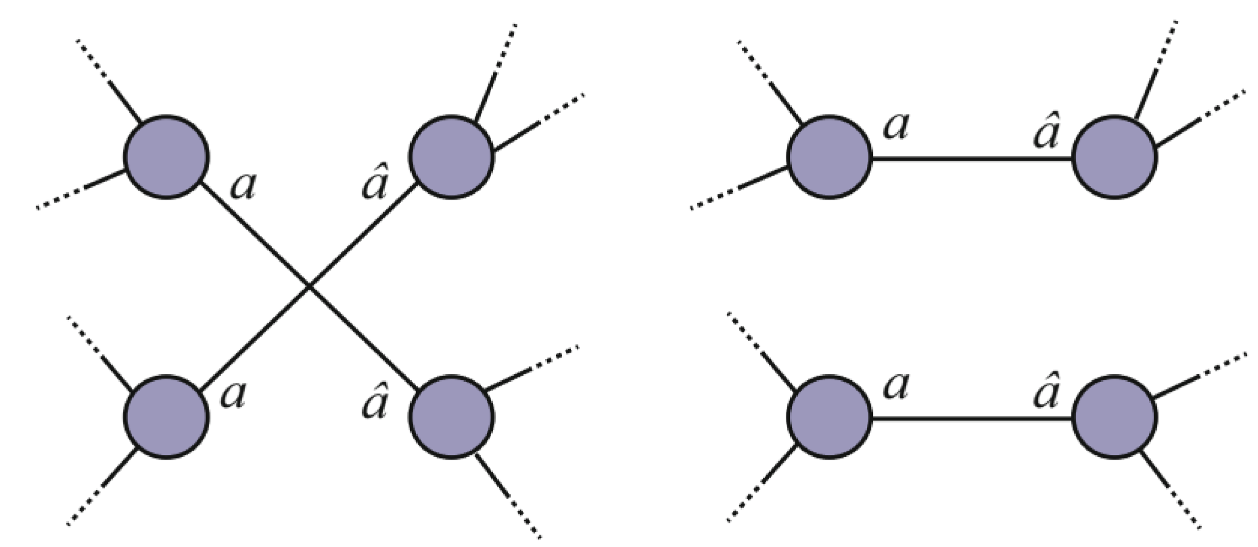

Figure 3. Half-edges may be swapped during self-assembly. [1]

For unswappable graphs, all edges of a particular bond-edge type must be incident to one shared vertex, which we refer to as a **source** of that bond-edge type.

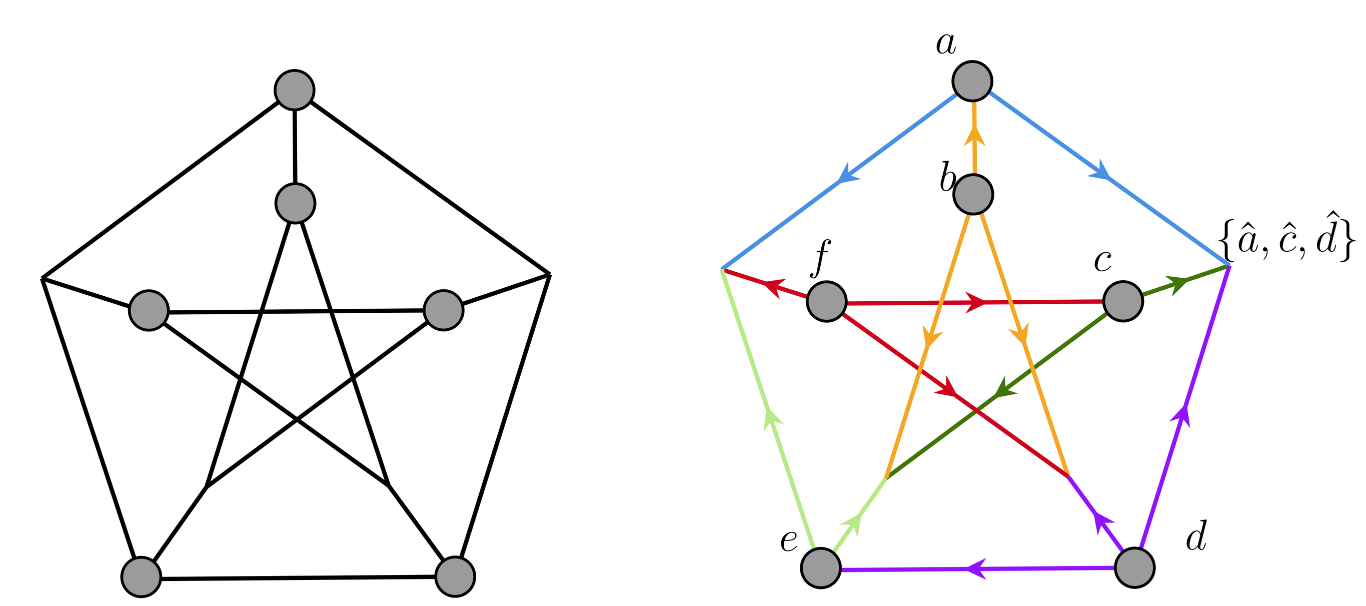

Figure 4. Bond-edge labelling of the Petersen graph, using a vertex cover as source vertices for distinct bond-edge types.

A **vertex cover** is a set of vertices K such that every edge is incident to at least one vertex in K. The set of all bond-edge sources must be a vertex cover; thus,

Lower Bound Theorem. Let G is an unswappable graph, and let K be a minimal vertex cover of G, then $B_3(G) \geq |K|$.

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Prism Graph

The **prism graph**, denoted Y_n, has an inner and an outer cycle each of order n, and vertices directly oppose each other are connected.

Theorem. Let $n \geq 5$ be an integer and Y_n the prism graph. Then

$$n + \left\lfloor \frac{n}{6} \right\rfloor \leq B_3(Y_n) \leq n + \left\lceil \frac{n}{2} \right\rceil \leq T_3(Y_n).$$

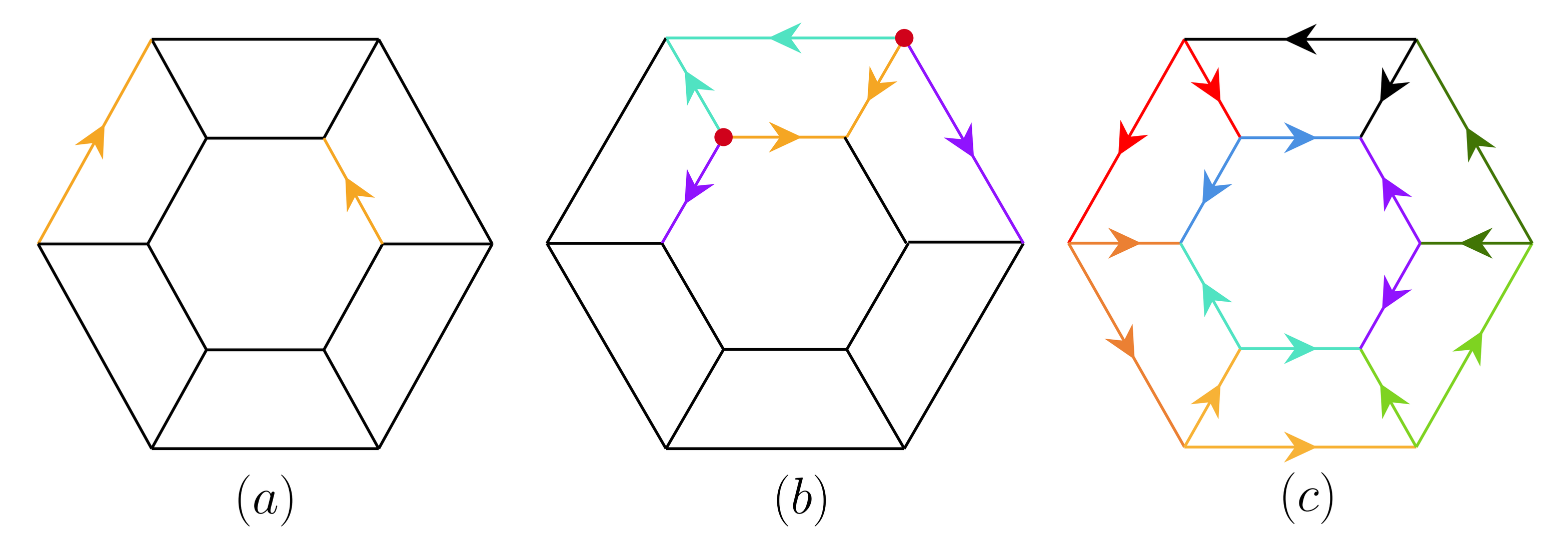

Figure 5. (a) Where bond-edges can repeat. (b) Where tiles can repeat. (c) A sample pot for Y_6.

Crown Graph

A crown graph, denoted Cr_n, is a bipartite graph - $\{v_1, ..., v_n\}$ and $\{u_1, ..., u_n\}$. An edge exists between any v_i, u_j where $i \neq j$.

Theorem. Let $n \geq 4$ be an integer and Cr_n the crown graph. Then

$$B_3(Cr_n) = n + 1 \quad \text{and} \quad T_3(Cr_n) \geq 2n - \left\lfloor \frac{n}{2} \right\rfloor.$$

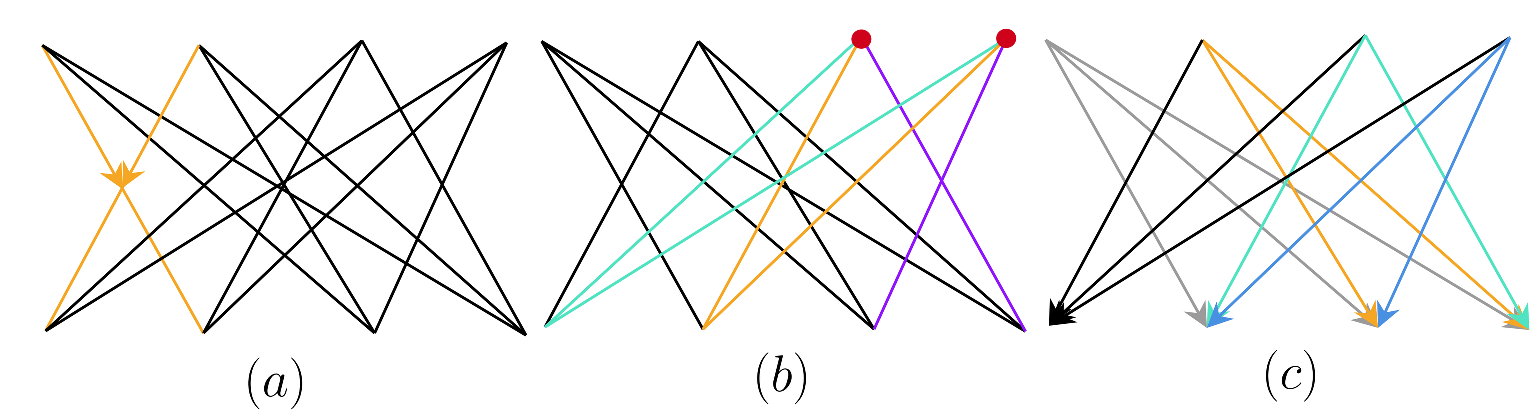

Figure 6. (a) where bond-edges can repeat. (b) where tiles can repeat. (c) a sample pot for Cr_4.

References

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