Algorithmic Generation of DNA Self-Assembly Graphs

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Introduction

Self-assembling nanostructures are constructed through the process of branched-junction DNA molecules bonding with each other without external guidance. We use graph theory and a flexible tile-based model to predict what structures can be produced in a laboratory setting. [1]

Prioritization Algorithms

Organizing

We can order the list of tiles by:

- degree: $\{a^2, b, \{a, b\}, \{a, b\}, \{a, b\}\}$
- lexicographic: $\{a^2, b\}$

Connecting Process

Step 1: Avoid both
Step 2: Allow multi-edges
Step 3: Avoid both
Step 4: Allow loops

Connected Examples

Ordering: degree
Avoid multi-edges

Ordering: lexicographic
Avoid multi-edges

Combinatorics

We count the number of permutations of edge-swaps.

$P = \{(a, b), \{a, b\}, \{a, b\}, \{a, b\}\}$, Tile Distribution = (2, 2, 1, 1)

$$a \prod_{\alpha \in A} \left( e_{\alpha}(G) - \deg_{\alpha}(v_1) \right) \cdots \left( e_{\alpha}(G) - \deg_{\alpha}(v_k) \right) = 36$$

Acknowledgement

This material is based upon work supported by the National Science Foundation under Grant No. DMS-1929284 while the authors were in residence at the Institute for Computational and Experimental Research in Mathematics in Providence, RI, during the Summer@ICERM program.

References


Isomorphism Algorithm

Permuting graph $G$ using (2, 1, 3) gives graph $G'$. $G$ and $G'$ are non-isomorphic.

Algorithm Output

The given pot with tile distribution (2, 2, 1, 1) has 5 non-isomorphic graphs.