Algorithmic Generation of DNA Self-Assembly Graphs

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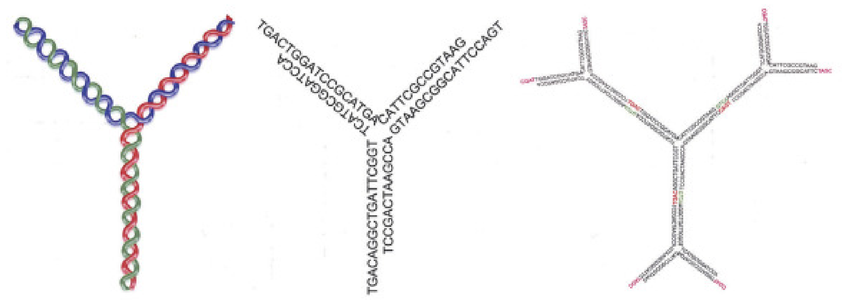
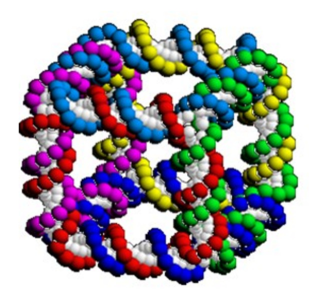
Introduction

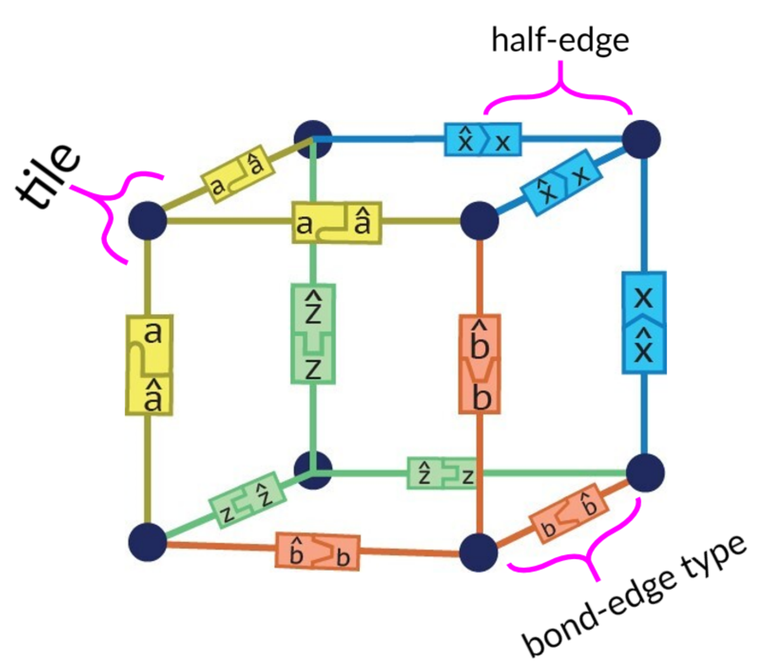
Self-assembling nanostructures are constructed through the process of branched-junction DNA molecules bonding with each other without external guidance. We use graph theory and a *flexible* tile-based model to predict what structures can be produced in a laboratory setting. [1]



3-armed junction-branched DNA molecules [3]



DNA cube



Graph realized by pot $P = \{\{a^3\}, \{\hat{a}, \hat{x}, \hat{z}\}, \{x^3\}, \{\hat{a}, \hat{b}, \hat{x}\}, \{\hat{a}, \hat{b}, z\}, \{z, \hat{z}^2\}, \{\hat{b}, \hat{x}, z\}, \{b^3\}\}$ using tile distribution $(1, 1, 1, 1, 1, 1, 1, 1)$

Goal

Given a pot of tiles, P, can we algorithmically construct at least one graph and possibly all non-isomorphic graphs realized by P?

- Input: A pot containing any number of bond-edge types
- Output: All non-isomorphic graphs realized by P

Construction Matrix Algorithm

Input: $P = \{\{\hat{a}, b\}, \{\hat{a}, \hat{b}\}, \{a^2, b\}, \{a^2, \hat{b}\}\}$

$$\begin{array}{c} \begin{matrix} t_1 & t_2 & t_3 & t_4 \end{matrix} \\ \left[\begin{array}{cccc|c} -1 & -1 & 2 & 2 & 0 \\ 1 & -1 & 1 & -1 & 0 \\ 1 & 1 & 1 & 1 & 1 \end{array}\right] \begin{matrix} a \\ b \\ \\ \end{matrix} \end{array} \xrightarrow{RREF} \begin{array}{c} \begin{matrix} t_1 & t_2 & t_3 & t_4 \end{matrix} \\ \left[\begin{array}{cccc|c} 1 & 0 & 0 & -1 & 1/6 \\ 0 & 1 & 0 & 1 & 1/2 \\ 0 & 0 & 1 & 1 & 1/3 \end{array}\right] \begin{matrix} a \\ b \\ \\ \end{matrix} \end{array}$$

Output: Minimum possible order = 6

Tile proportions = $\langle \frac{1}{6}, \frac{3}{6}, \frac{2}{6}, \frac{0}{6} \rangle, \langle \mathbf{\frac{2}{6}}, \mathbf{\frac{2}{6}}, \mathbf{\frac{1}{6}}, \mathbf{\frac{1}{6}} \rangle, \langle \frac{3}{6}, \frac{1}{6}, \frac{0}{6}, \frac{2}{6} \rangle$

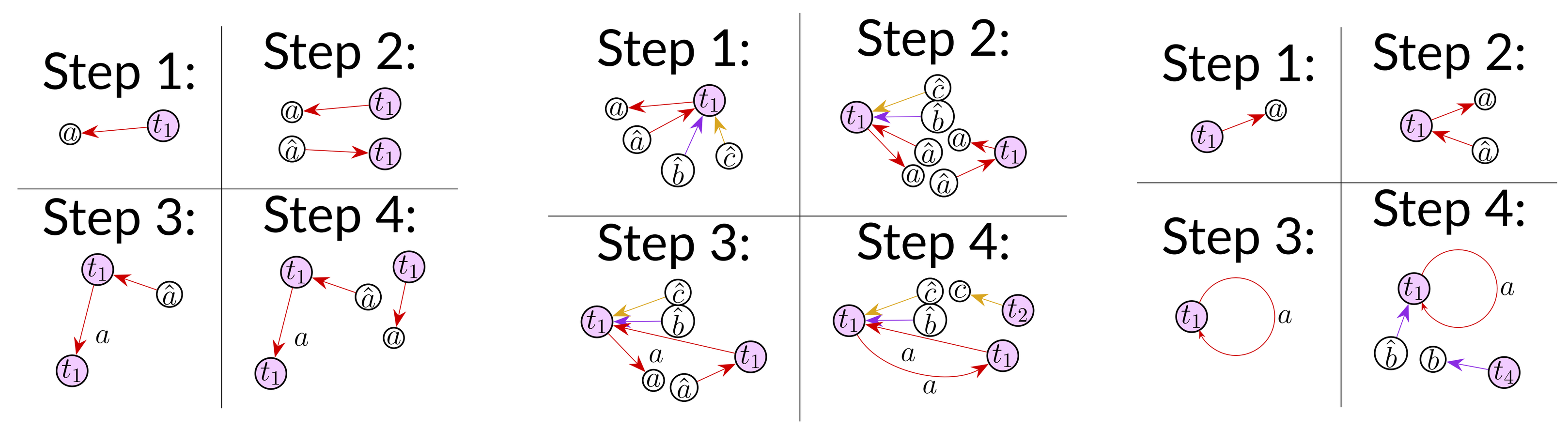
Prioritization Algorithms

Organizing

We can order the list of tiles by:

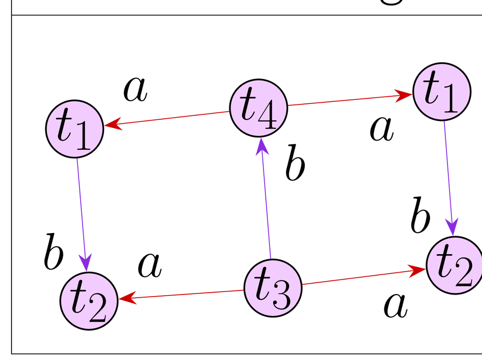
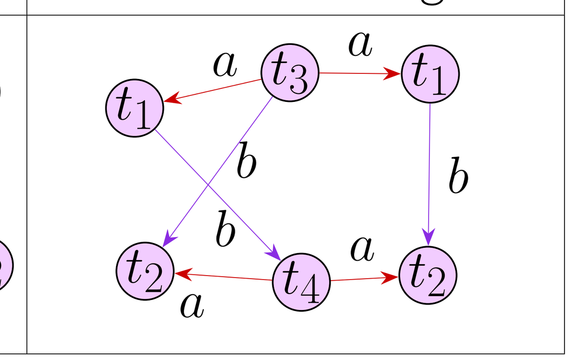
degree	$\{a^2, b\}, \{a^2, \hat{b}\}, \{\hat{a}, b\}, \{\hat{a}, \hat{b}\}$
diversity	$\{\hat{a}, b\}, \{\hat{a}, \hat{b}\}, \{a^2, b\}, \{a^2, \hat{b}\}$
lexicographic	$\{a^2, b\}, \{a^2, \hat{b}\}, \{\hat{a}, b\}, \{\hat{a}, \hat{b}\}$

Connecting Process



Avoid both Allow multi-edges Allow loops

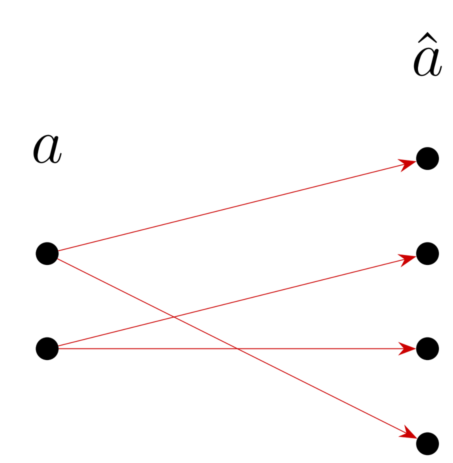
Connected Examples

ordering: degree avoid multi-edges	ordering: lexicographic avoid multi-edges
	

Combinatorics

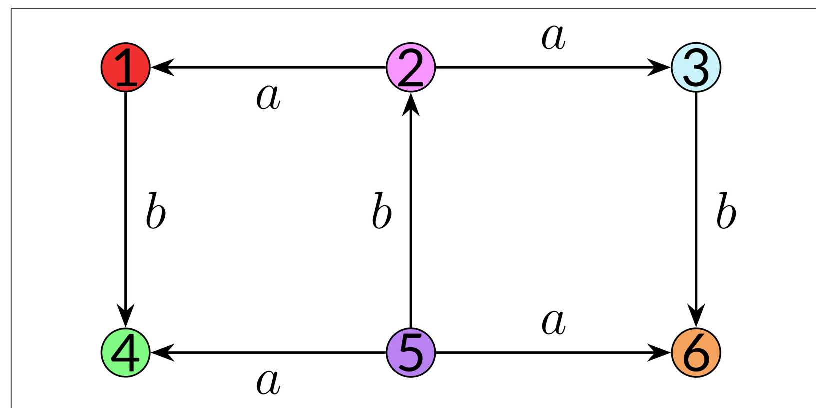
We count the number of permutations of edge-swaps.

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



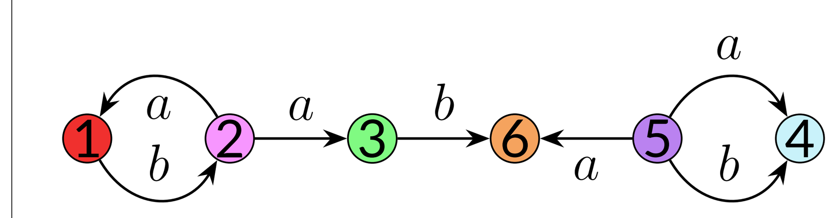
$$\prod_{\alpha \in A} \binom{e_\alpha(G)}{\deg_\alpha(v_1)} \binom{e_\alpha(G) - \deg_\alpha(v_1)}{\deg_\alpha(v_2)} \cdots \binom{e_\alpha(G) - \deg_\alpha(v_1) - \cdots - \deg_\alpha(v_{k-1})}{\deg_\alpha(v_k)} = 36$$

Isomorphism Algorithm



dict$(G) = \{a\colon [2,1], [2,3], [5,4], [5,6],$ $b\colon [1,4], [5,2], [3,6]\}$

canonical label: $[1|6|2|4|5|3]$



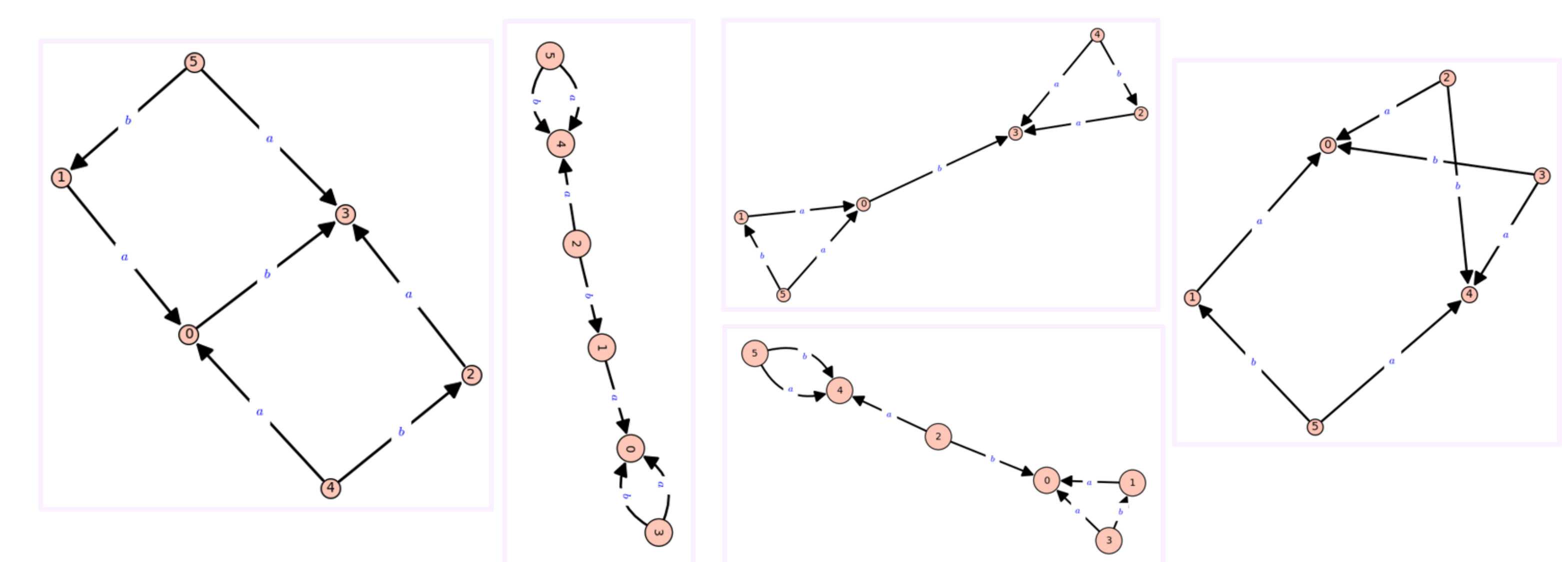
dict$(G') = \{a\colon [2,1], [2,3], [5,4], [5,6],$ $b\colon [1,2], [5,4], [3,6]\}$

canonical label: $[1|6|4|2|5|3]$

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

Theorem (Canonical Labeling) [2]: $G_1 \cong G_2$ iff $c(G_1) = c(G_2)$

Algorithm Output



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

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