# Self-Assembly of DNA Graphs and Postman Tours


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## Overview


Self-assembly of DNA graphs has been shown to give polynomial time solutions to hard computational problems such as the 3-SAT and $k$-colorability problems. Jonoska et al. showed that for every graph, there exists a thickened graph with a boundary component, a reporter strand, that traverses every edge at least once and no more than twice. In conjunction with edge weighting algorithms for self-assembly graphs, we consider the relationship between reporter strands and postman tours in solving problems involving minimal weight Eulerian walks, such as the Windy Postman Problem.


## Preliminaries

We consider 3-valent graphs only.

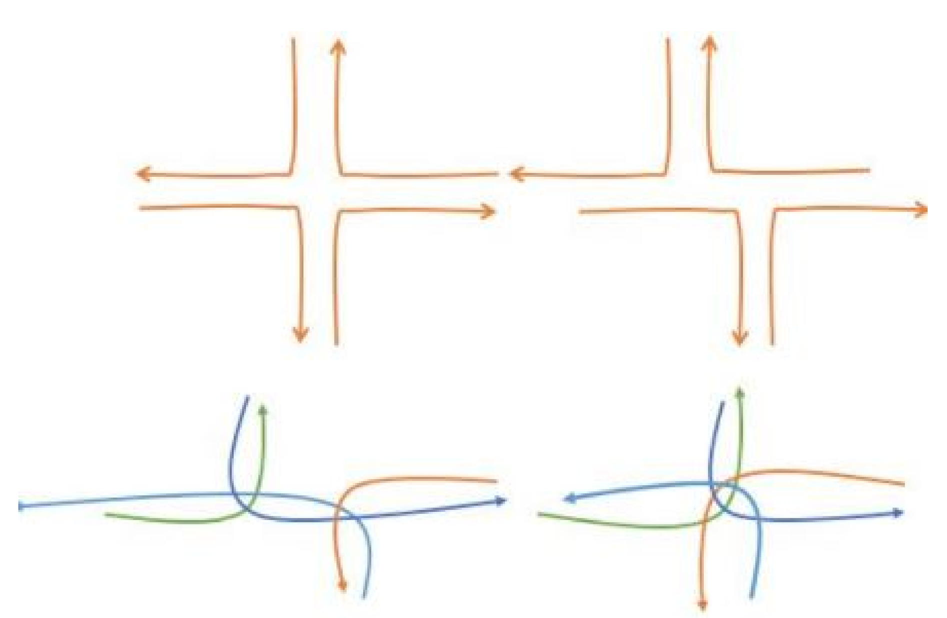

Figure 1: A 3-degree perturbation of a vertex of degree 4

- **Postman Tour:** A cycle that traverses every edge of a weighted, connected graph at least once and no more than twice. (denoted by $\tau$)
- **Windy Postman Problem:** The NP-Hard problem of identifying a postman tour of minimal weight in a directed and weighted graph.
- **Elementary Boundary Operation:** A permutation of the edges incident to a vertex.
- **Reporter Strand:** A boundary component that traverses each edge at least once and no more than twice. (denoted by $\sigma$)

## Thickened Graphs

A thickened graph is a topological manifold which contains the graph $G$ as a deformation retract.

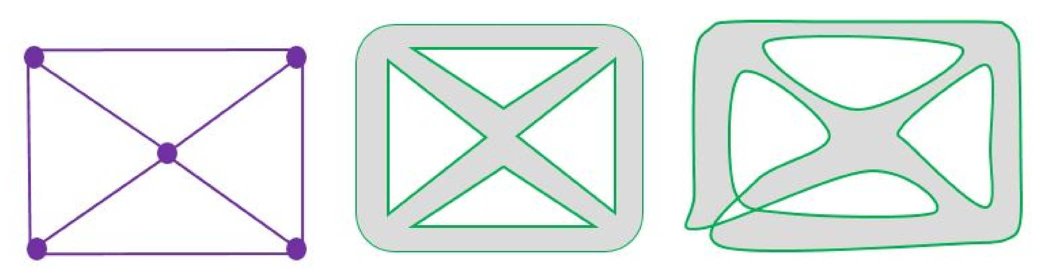

Figure 2: A graph, its thickened graph, and its thickened homomorphism created by one boundary operation.

## Postman Tours of $K_4$

For every graph there exists a maximal length postman tour traversing every edge twice and a minimal length postman tour constructed by connecting pairs of odd vertices. The maximal postman tour is never optimal for 3-valent graphs, and thus, we proceed with identifying non-maximal postman tours. For $K_4$, non-maximal tours traverse exactly 2 or 3 edges twice. As shown in Figure 3, every non-maximal postman tour of $K_4$ can be represented by a reporter strand following 1, 2, or 3 of boundary operations.

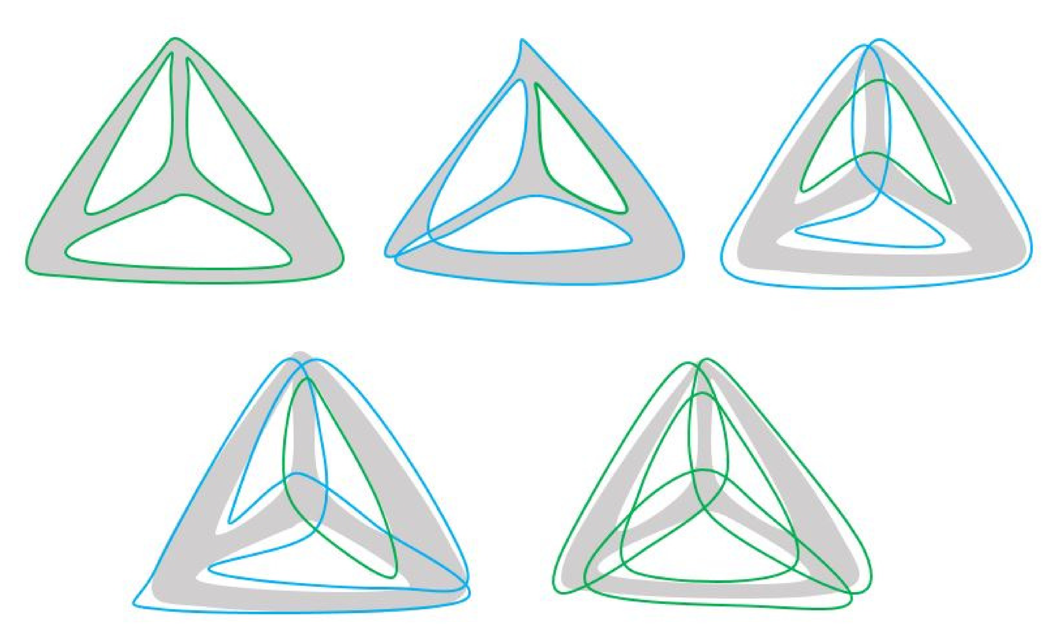

Figure 3: Boundary operations of $K_4$

It is obvious that a reporter strand represents a postman tour, so we consider the converse. Is there a reporter strand for every postman tour? The answer is "yes" for $K_4$, but "no" in general.

## Postman Tours and Reporter Strands

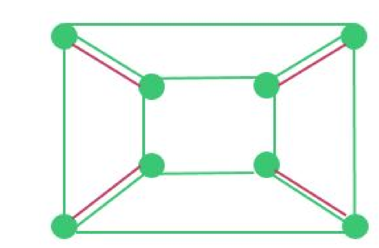

Figure 4: Is there a reporter strand for representing this postman tour?

In the graph shown above, the addition of the four purple lines creates a postman tour of length 16. This postman tour cannot be explicitly represented as a reporter strand while maintaining even parity.

## Theorem

For every non-maximal postman tour $\tau$ of a given graph $G$ there exists a thickened graph $F(G)$ with a reporter strand $\sigma$ that contains $\tau$.

## Outline of the Proof

### Basis Case

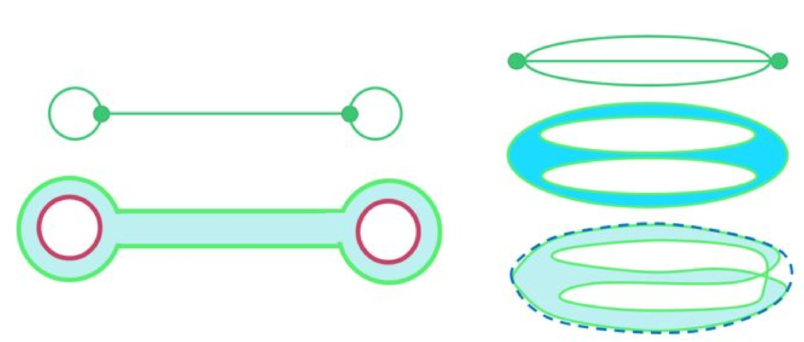

Figure 5: 3-valent multi-graphs of order 2

### Inductive Step

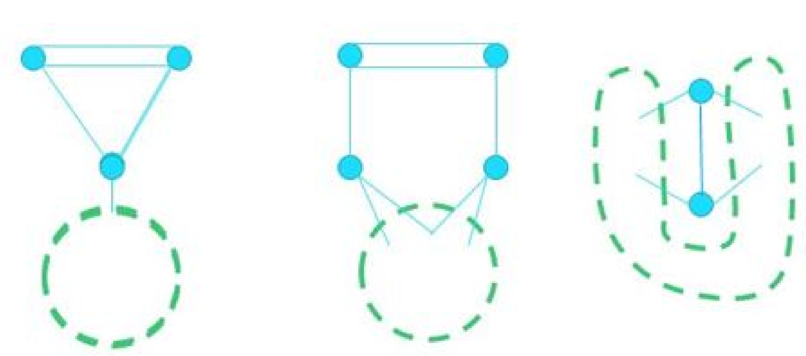

Figure 6: Possible cases for the addition of two vertices

## Outline of the Proof Cont'd

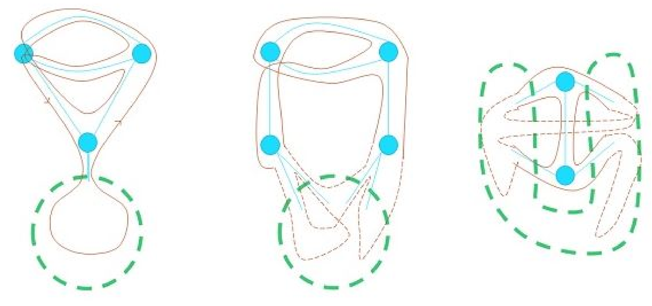

Figure 7: Extension of $\sigma$ to a graph of order $2n+2$

## Conclusions and Future Work

Analysis of the topological structure of thickened graphs proves to be beneficial for studying self-assembly graphs. Algorithms relying on the requisite number of hydrogen bonds necessary within a sequenced strand exist for the inclusion of weight in constructing self-assembly graphs. In conjunction with the analysis of reporter strands, these algorithms could offer solutions to minimal weight Eulerian walk problems. The identification and removal of the superfluous loops included in the resulting reporter strands is necessary to establish a complete algorithm.

## References


[1] N. Jonoska and M. Saito, *Boundary Components of Thickened Graphs*, Lecture Notes in Computer Science **2340** (2002) 70-81.

[2] N. Jonoska, N.C. Seeman, and G. Wu, *On the existence of reporter strands in DNA-based graph structures*, Theoretical Computer Science **410** (2009) 1448-1460.

[3] G. Wu, N. Jonoska, and N.C. Seeman, *Construction of a DNA nano-object directly demonstrates computation*, Biosystems **98** (2009) 80-84.



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