Eulerian and Hamiltonian Cycles

Alexander S. Kulikov

Steklov Mathematical Institute at St. Petersburg, Russian Academy of Sciences
and
University of California, San Diego

Toy Genome Assembly Problem

Find a string whose all substrings of length 3 are

AGC, ATC, CAG, CAT, CCA, GCA, TCA, TCC.

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How is it related to cycles in graphs?..

Outline

Eulerian Cycles

Hamiltonian Cycles

Genome Assembly

Eulerian Cycle

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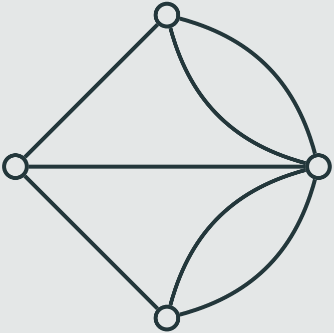
- The definition works for both directed and undirected graphs
- A cycle must have the same starting and ending nodes
- While in a path the starting and ending node should not necessarily be equal

Example

Non-Eulerian graph



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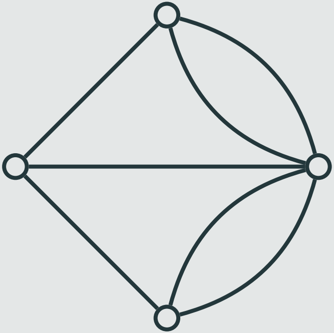
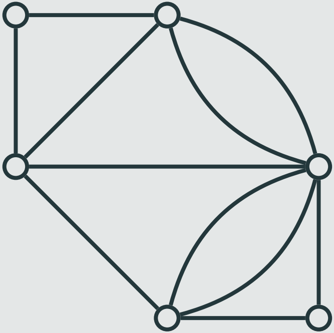


Eulerian graph



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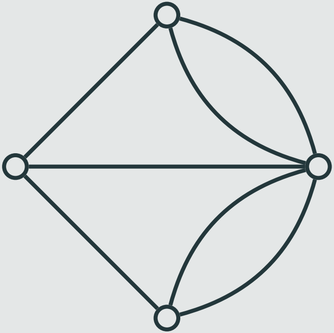
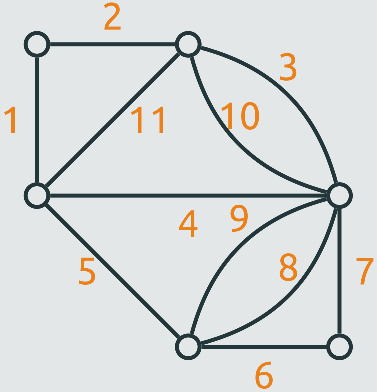


Eulerian graph



Criteria

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A connected *undirected* graph contains an Eulerian cycle, if and only if the degree of every node is even.

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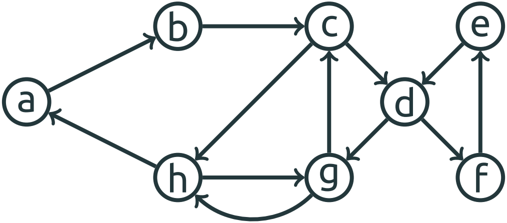
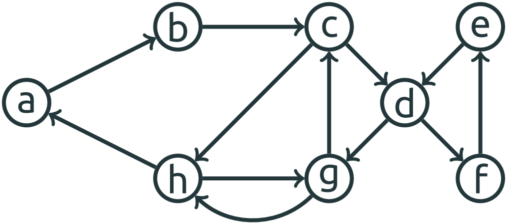
A strongly connected *directed* graph contains an Eulerian cycle, if and only if, for every node, its in-degree is equal to its out-degree.

Proof (Directed Case)



if some node is imbalanced,
there is clearly no Eulerian cycle

Proof (Directed Case)



thus, assume that the graph is balanced

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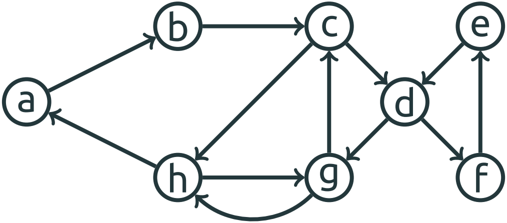
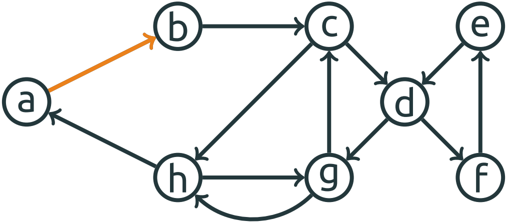


start walking from some node

Proof (Directed Case)



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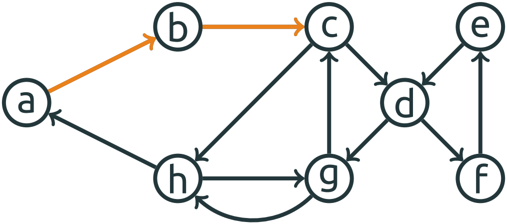

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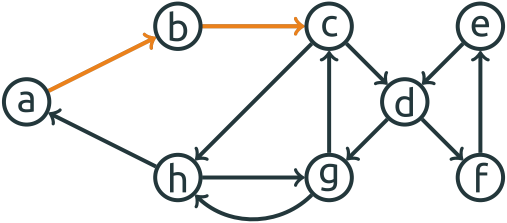
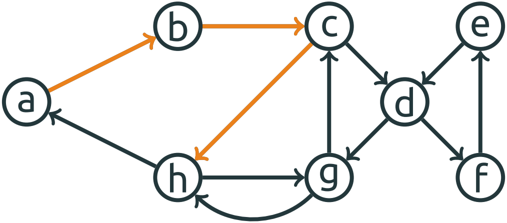


since the graph is balanced, at some point we'll return back to the starting node

Proof (Directed Case)



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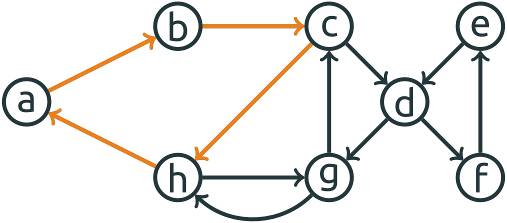

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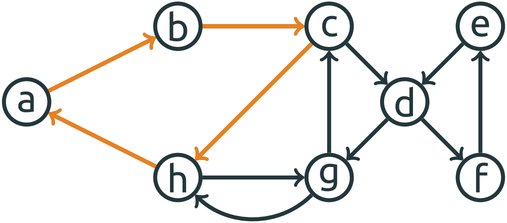

OK, what’s next? we haven’t traversed all the edges and now we are stuck

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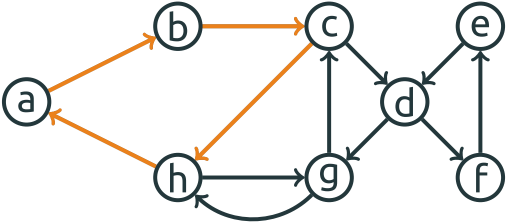

since the graph is strongly connected, there must be untraversed edges going out of a node from the current cycle

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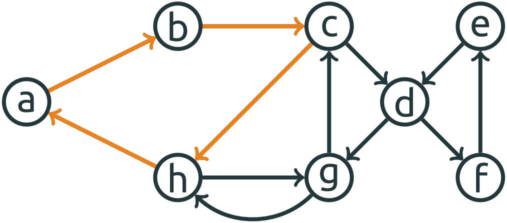

the current cycle has neither beginning nor end

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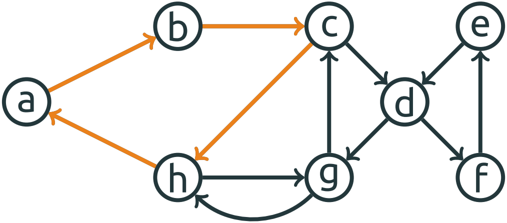

so, we may assume that its starting and ending point is the node c

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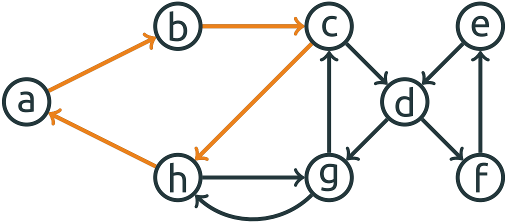

we then continue exploring the graph from the node c

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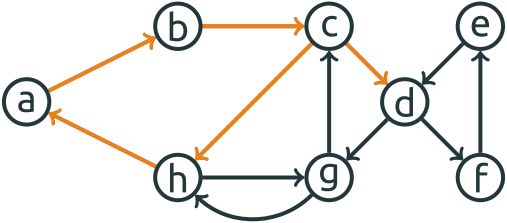

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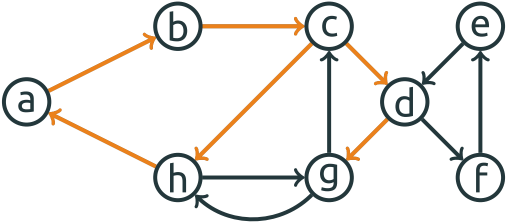

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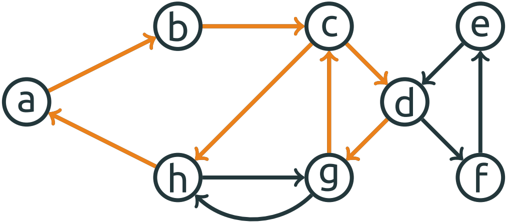

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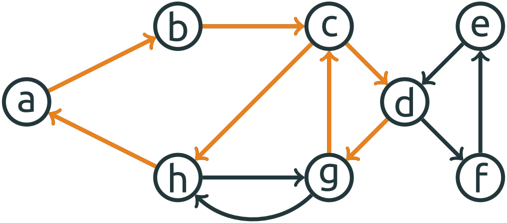
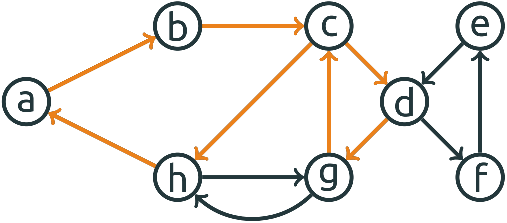


we got larger cycle

Proof (Directed Case)



continue from g

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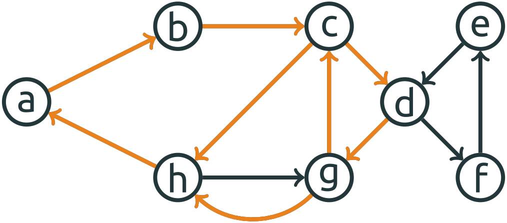

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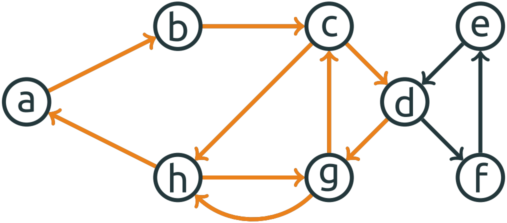

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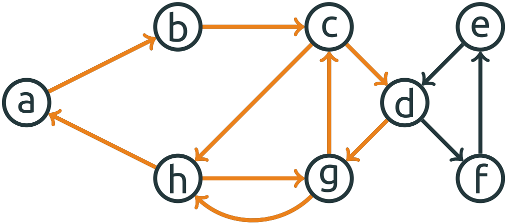

continue from d

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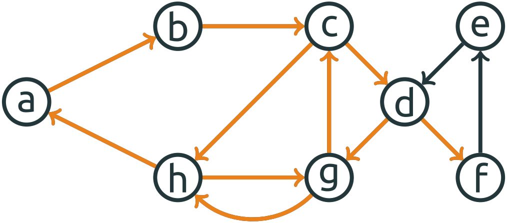

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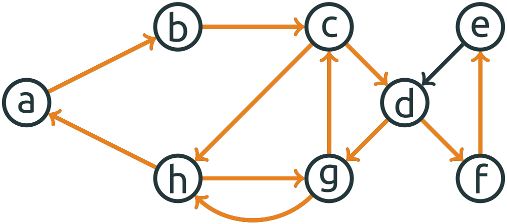

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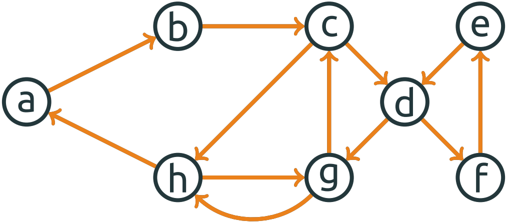
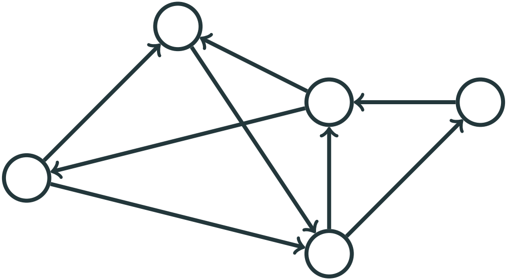


Path Instead of Cycle

- The criteria for a path is similar
- A graph is allowed to contain two imbalanced nodes: one for the starting point and one for the ending point of a path
- By adding an edge between these two nodes, one gets a graph with an Eulerian cycle

Path to Cycle



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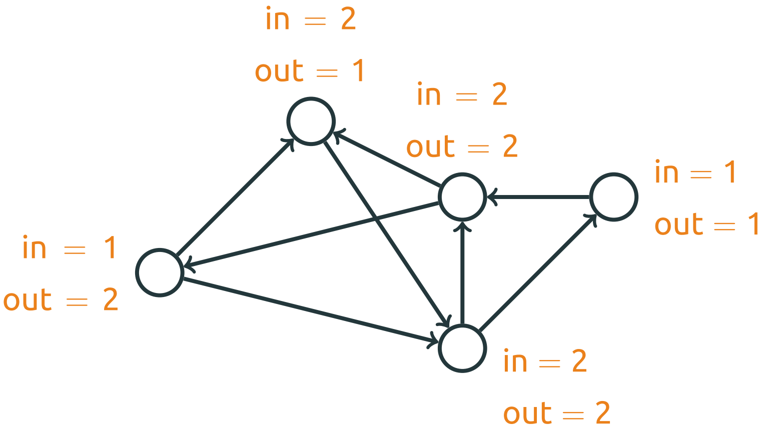

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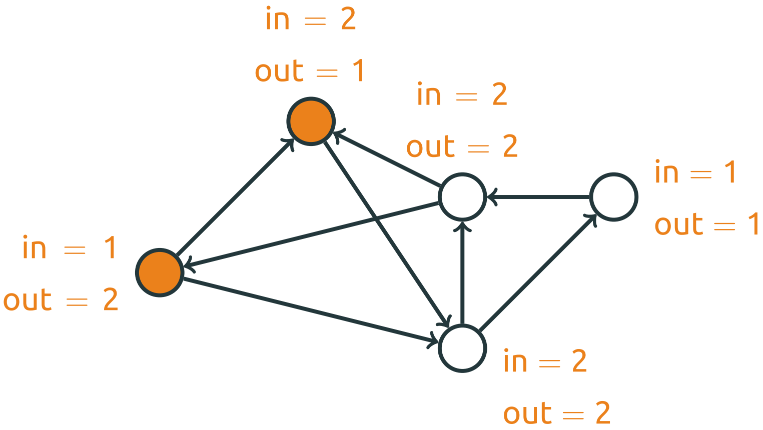

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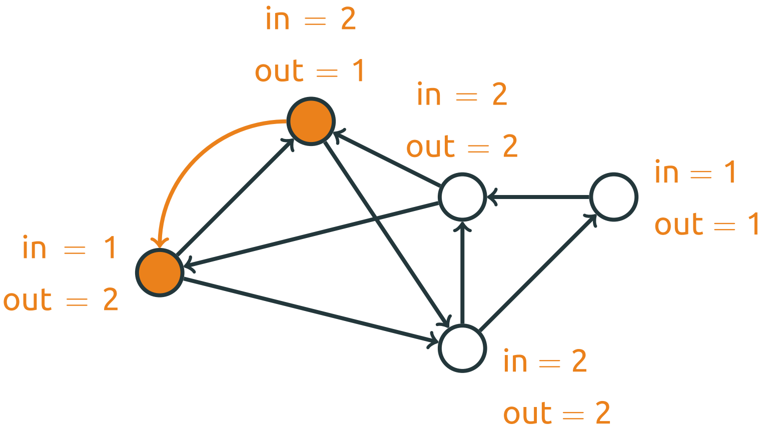

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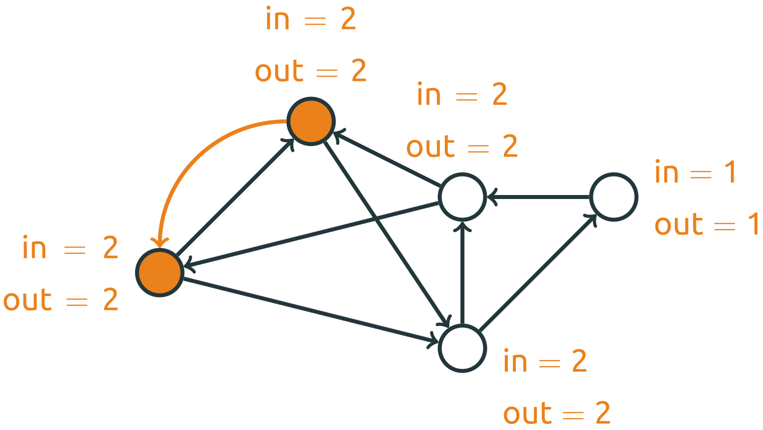


Efficient Algorithms

The proof of existence of an Eulerian cycle can be transformed into an efficient algorithm for constructing an Eulerian cycle

Outline

Eulerian Cycles

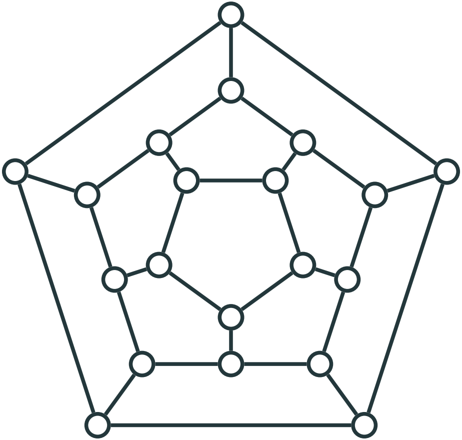
Hamiltonian Cycles

Genome Assembly

Hamiltonian Cycle

A Hamiltonian cycle visits every node of a graph exactly once.

Example



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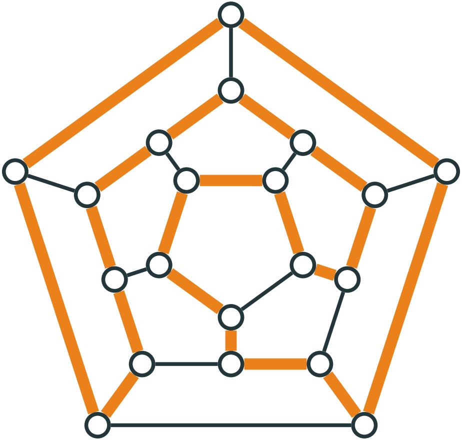

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- No polynomial time algorithm known
- The question whether there is a polynomial time algorithm for the Hamiltonian cycle problem is the P versus NP problem, the most important open problem in Computer Science, with a prize of $1M from the Clay Mathematics Institute (`http://www.claymath.org/millennium-problems`)

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All Substrings of Length 3

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DISCRETE
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 ISC
  SCR
   CRE
    RET
     ETE
```

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Every two neighbor 3-substrings have
a common part, called an overlap, of length 2

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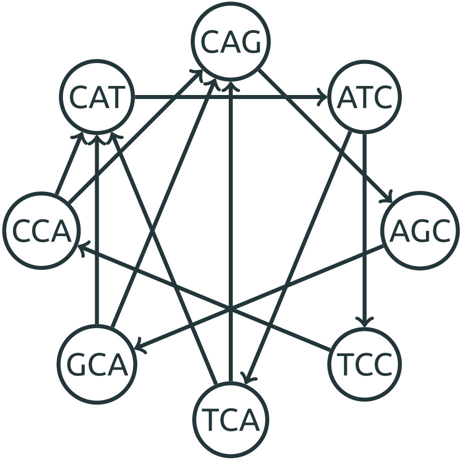
Finding a Permutation

- Goal: Find a string whose all substrings of length 3 are AGC, ATC, CAG, CAT, CCA, GCA, TCA, TCC
- Hence, we need to find an order of these 3-strings such that the overlap between any two consecutive strings is equal to 2

Overlap Graph



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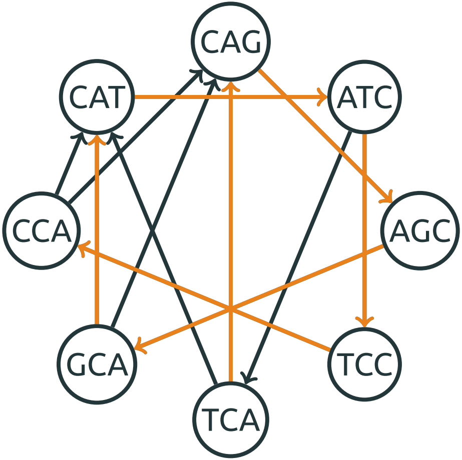

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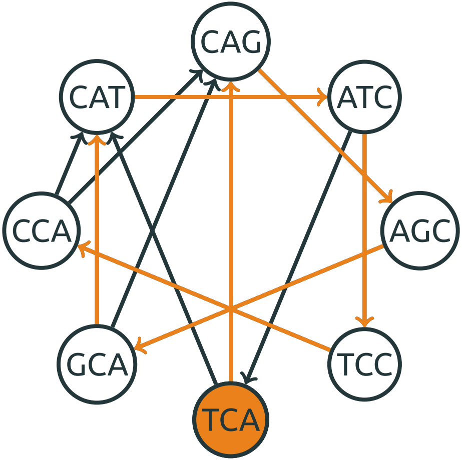
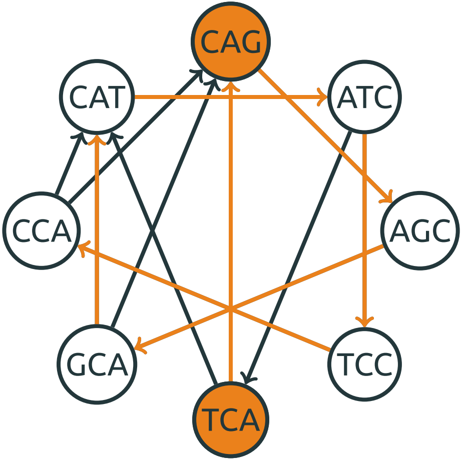


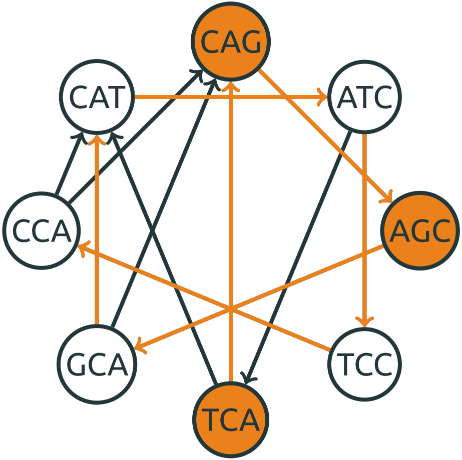
TCA

Overlap Graph



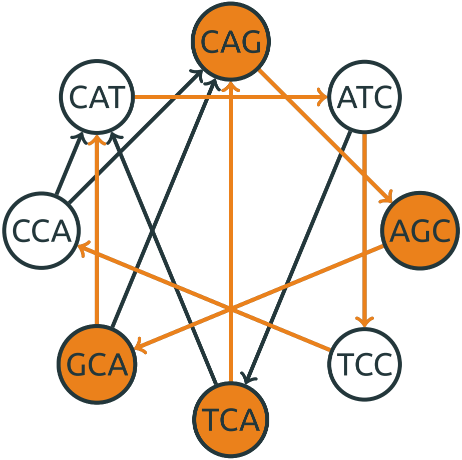
TCAG

Overlap Graph



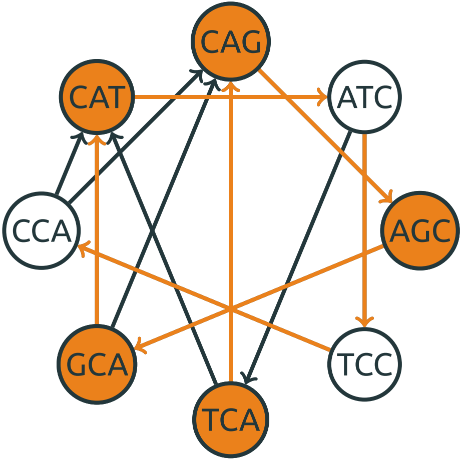
TCAGC

Overlap Graph



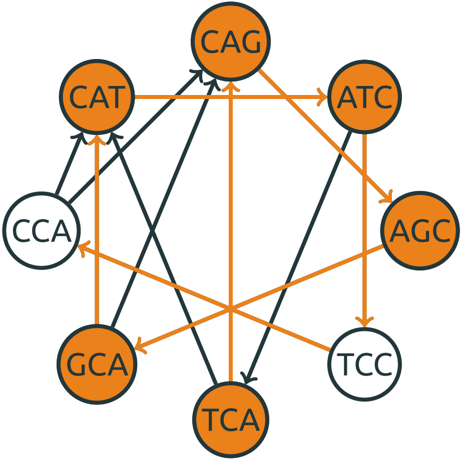
TCAGCA

Overlap Graph



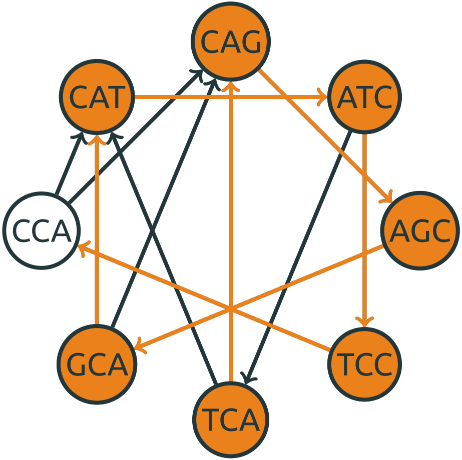
TCAGCAT

Overlap Graph



TCAGCATC

Overlap Graph



TCAGCATCC

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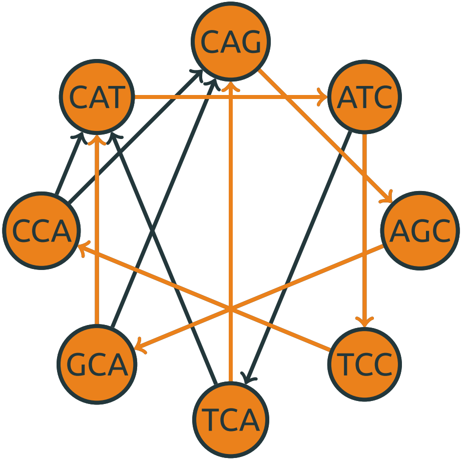

TCAGCATCCA

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- OK, we’ve reduced the problem of genome assembly to the Hamiltonian cycle problem
- But we don’t have efficient algorithms for the Hamiltonian cycle problem!
- The approach is useless for the case when there are thousands or millions of input strings

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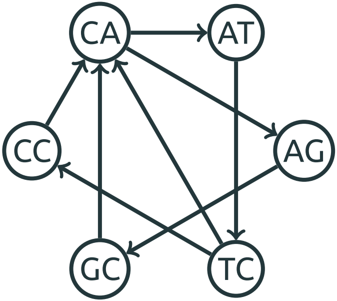
Speculating

- In the overlap graph, each input string is represented by a node
- Let’s instead try to represent each string by an edge (De Bruijn; Pevzner, Tang, Waterman)
- E.g., represent the string CAT as an edge CA $\rightarrow$ AT
- Used in state-of-the-art genome assemblers

De Bruijn Graph

AGC, ATC, CAG, CAT, CCA, GCA, TCA, TCC



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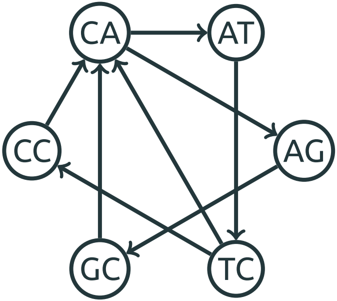
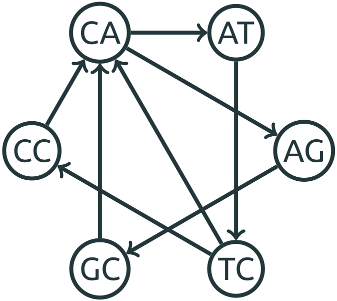


now, we need to find an order of edges

De Bruijn Graph

AGC, ATC, CAG, CAT, CCA, GCA, TCA, TCC



that is, an Eulerian cycle

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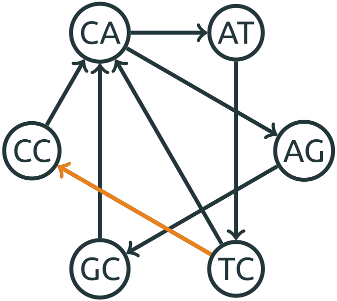

TCC

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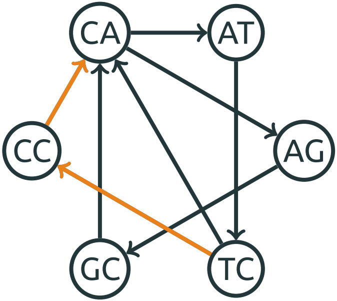

TCCA

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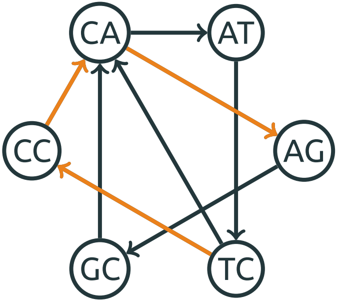
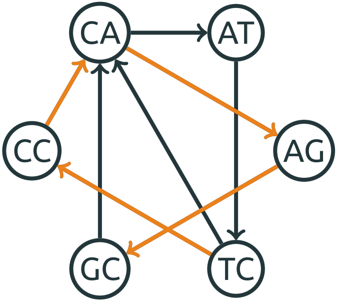


TCCAG

De Bruijn Graph

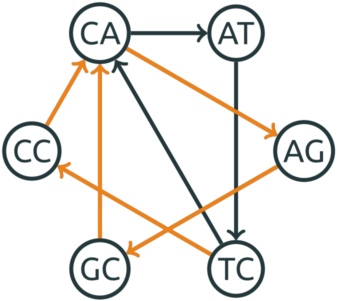
AGC, ATC, CAG, CAT, CCA, GCA, TCA, TCC



TCCAGC

De Bruijn Graph

AGC, ATC, CAG, CAT, CCA, GCA, TCA, TCC



TCCAGCA

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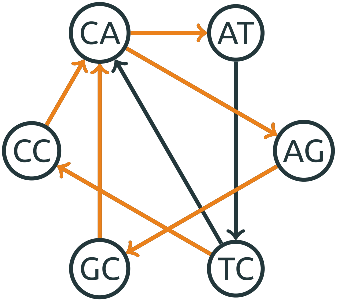

TCCAGCAT

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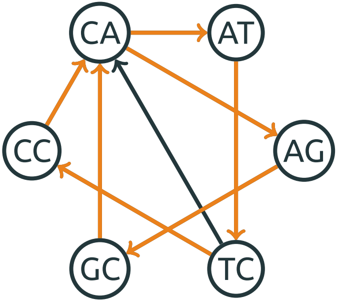
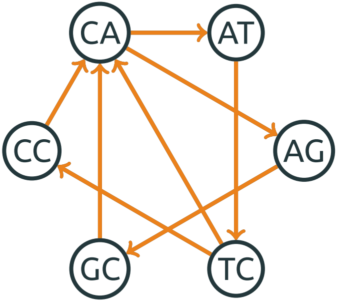


TCCAGCATC

De Bruijn Graph

AGC, ATC, CAG, CAT, CCA, GCA, TCA, TCC



TCCAGCATCA

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- Genome assembly: the right problem formulation makes all the difference!