Euler paths and circuits on digraphs and genome sequencing

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June 1, 2017



Overview

- Definitions
- 2 Eulerian Graphs
- 3 Applications

Definition (Graph)

A **graph** G consists of a non-empty finite set V(G) of elements called **vertices**, and a finite 'family' E(G) of unordered pairs of (not necessarily distinct) elements of V(G) called **edges**.

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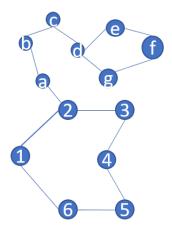
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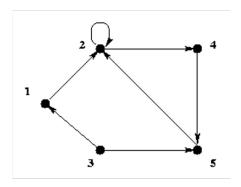
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 NYC grid with all the streets being one-way, which then restricts our movement on the graph.



Graphs and Digraphs





Euler Paths vs. Circuits

Definition (Euler Path)

An **Euler path** on a graph G is a special walk that uses each edge exactly once, and it starts and ends at **different** vertices.

Definition (Euler Circuit)

An **Euler circuit** on a graph G is a walk that uses each edge exactly once, and it starts and ends at the **same** vertex.

Criterion for an Euler path or circuit on a graph

Euler Path

A given graph *G* has an Euler path if and only if the graph is connected and **all but 2 vertices in the graph are of odd degree.**

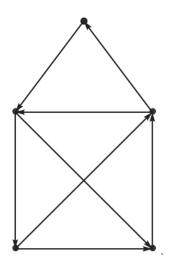
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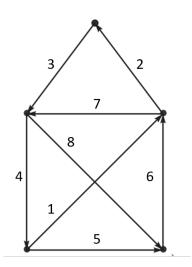
A given graph *G* has an Euler path if and only if the graph is connected and **all but 2 vertices in the graph are of odd degree.**

 What extra condition do you think we need to add for a digraph to have an Euler path?

Can we find an Euler Path?



YES WE CAN!



Criterion for an Euler path on a digraph

Euler Path

A given graph *G* has an Euler path if and only if the graph is connected and **all but 2 vertices in the graph are of odd degree.**

Euler Path on a digraph

A digraph D_g has an Euler path iff

- The graph is connected
- All but 2 vertices in the graph are of odd degree
- the |indegree outdegree| = 1 for those two odd vertices in D_{σ} .



Criterion for an Euler circuit on a digraph

Euler Circuit

A graph G has an Euler circuit if and only if G is connected and all the vertices are of **even degree** .

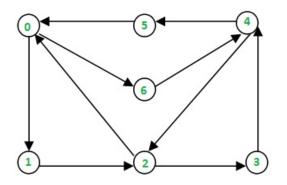
Criterion for an Euler circuit on a digraph

Euler Circuit

A graph G has an Euler circuit if and only if G is connected and all the vertices are of **even degree** .

 What extra condition do you think will be needed on a digraph for it to have an Euler circuit?

Euler Circuit on digraph



Euler Circuit: 0 -> 6 -> 4 -> 5 -> 0 -> 1 -> 2 -> 3 -> 4 -> 2 -> 0

Criterion for an Euler circuit on a digraph

Euler Circuit

A graph G has an Euler circuit if and only if G is connected and all the vertices are of **even degree** .

Euler circuit on a digraph

A graph D_g has an Euler circuit if and only if D_g is connected and all the vertices are of even degree and the **indegree** = **outdegree** for all vertices.

 A formal proof done as part of the final project in Senior Seminar (Spring 2017)



Recall: For an Euler Path all but 2 vertices must be of odd degree and to have an Euler circuit has all vertices must be of even degree.

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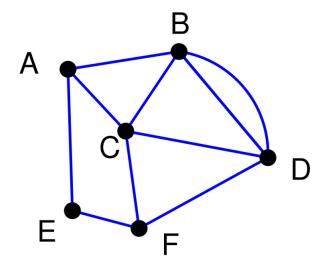
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This is called Fleury's Algorithm

Find an Euler Path?



What's next?

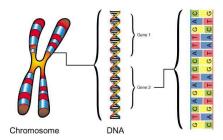
This is cool, but for all the applied mathematicians in the room and computer engineers like me the question becomes:

How does that help me?

Applications

- Mathematical modeling
- ONA fragment reconstruction
- Ostman problem
- Traveling salesman problem
- omany more

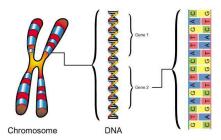
DNA



Genes

 Protein that stores the genetic information of a living organism

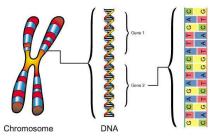
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- Protein that stores the genetic information of a living organism
- Four components to it: A,T,G,C. A connects to T and G connects to C
- Fragments of DNA are used in genetic research and discovery
- Strings of such ATGC pairs have this information stored in them

- Reads are taken of a known DNA strand (Sanger, 1977)
- They vary in size from 30-800 nucleotides
- Reads are taken in an overlapping form
- Reconstructing the specific genome with the overlapping to create a superstring is NP-complete

Shortest Super String Problem

Problem: Given a set of strings, find a shortest string that contains all of them - NP Complete

```
The Shortest Superstring problem
Set of strings: {000, 001, 010, 011, 100, 101, 110, 111}
Concatenation
              000 001 010 011 100 101 110 111
Superstring
                       010
                    110
                011
Shortest
             0001110100
superstring
              001
                   111
                     101
                         100
```

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- The final directed Euler Path is the super string

What is a k-mer composition of a given genome string

Given a string: **TAATGCCATGGGATGTT**, what is a 3-mer composition?

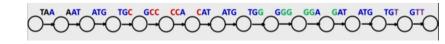
```
= \{TAA, AAT, ATG, TGC, GCC, CCA, CAT, ATG, TGG, GGG, GGA, GAT, ATG, TGT, GTT\}
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We use these 3-mers as labels of directed edges.

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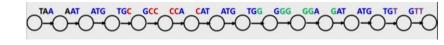
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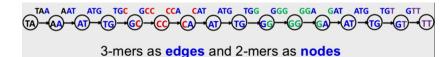


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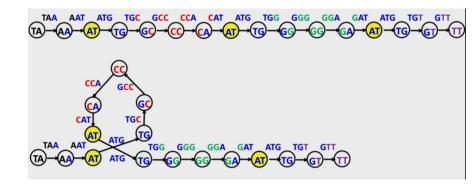
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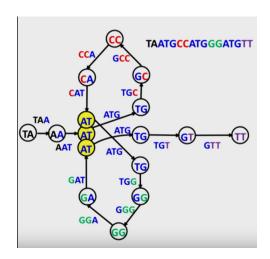




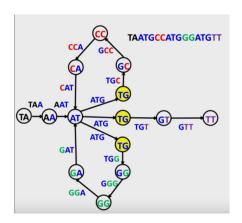
Collapsing like vertices on itself



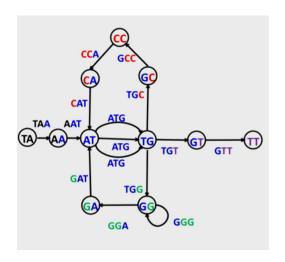
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DeBruijn Graph of TAATGCCATGGGATGTT



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- What if there are multiple Euler paths?
- That is where we use paired Debruijn graphs (A special form of 4-mer and 6-mer pairing)

References

- Euler Circuits, DNA Sequencing by Hybridization, and a New Graph Polynomial that Counts Euler Circuit Decompositions by Richard A. Arratia
- An Eulerian path approach to DNA fragment assemblyPavel
 A. Pevzner*, Haixu Tang, and Michael S. Waterman
- Euler circuits and DNA sequencing by hybridization by Richard Arratiaa, Bela Bollobasb, Don Coppersmithc, Gregory B. Sorkinc
- YouTube channel: Bioinformatics Algorithms: An Active Learning Approach

The End