

GTDM – 2019/20

## - Introduction to Graph Theory

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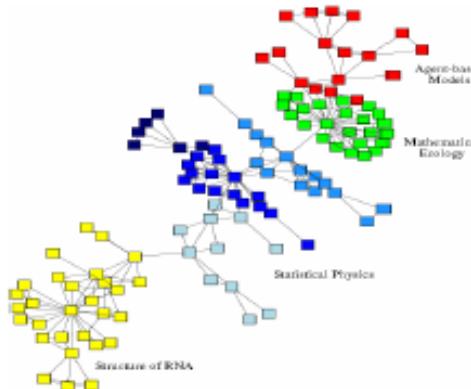
Partially based on Lecture Notes of Keijo Ruohonen

**Why graphs?** Graphs are a general language for describing and modeling complex systems

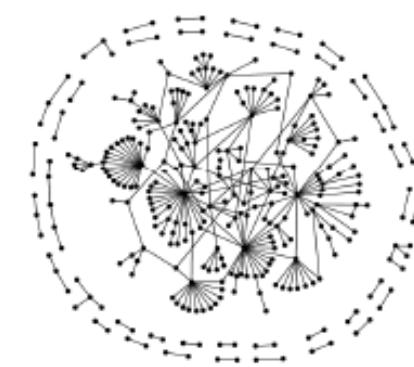
## Many Data are Graphs



Social networks



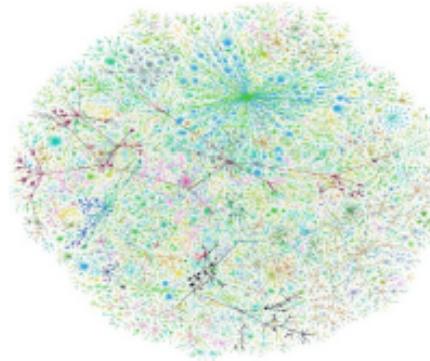
Economic networks



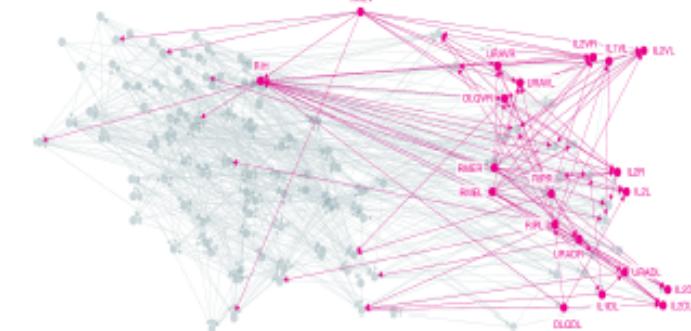
Biomedical networks



Information networks:  
Web & citations



Internet



Networks of neurons

# Graph: A representation of data

## Why Graphs? Why Now?

Universal language for describing complex data

Networks/graphs from science, nature, and technology are more similar than one would expect

Shared vocabulary between fields

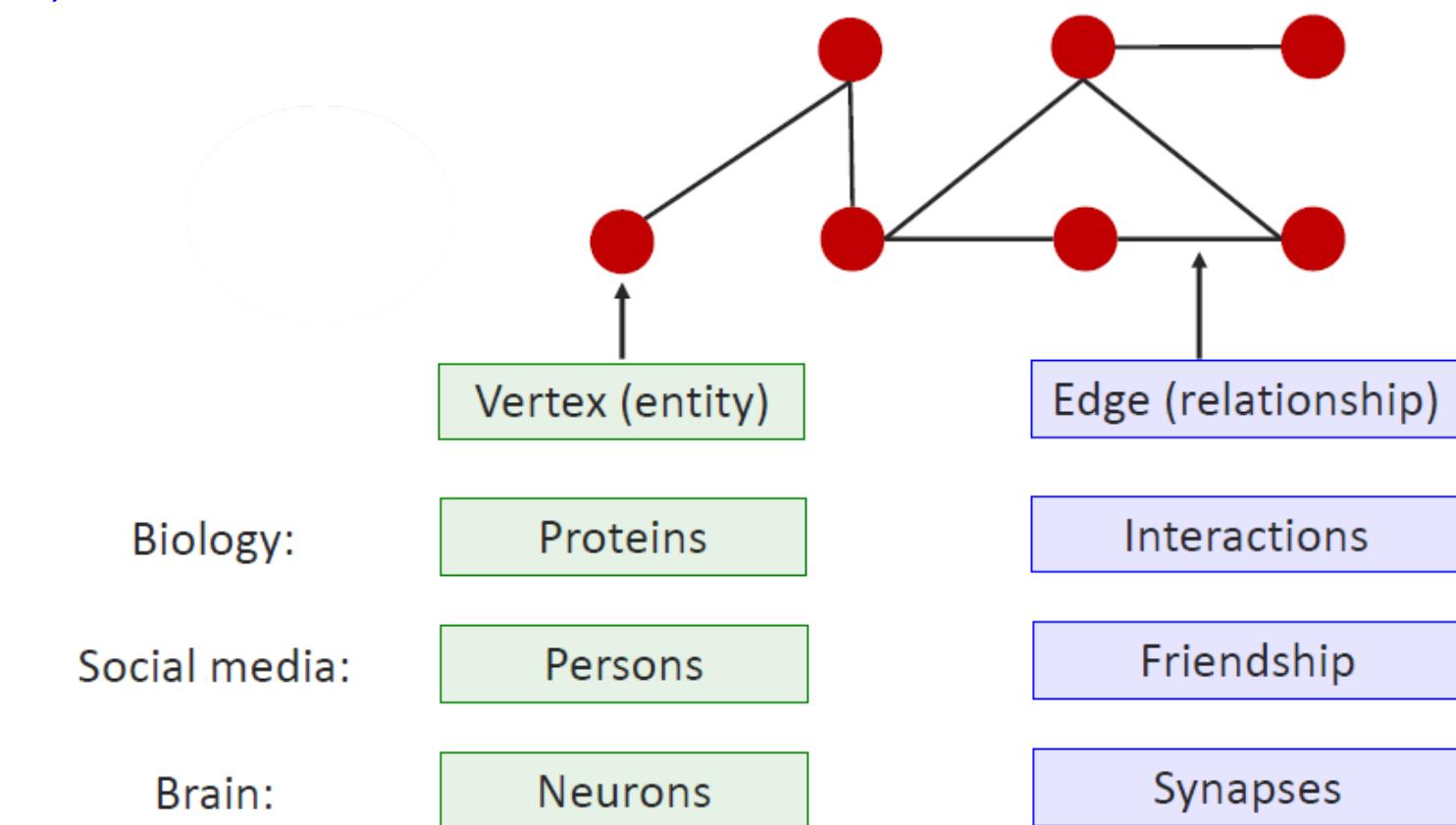
Computer Science, Social science, Physics, Economics, Statistics, Biology

Data availability (+computational challenges)

Web/mobile, bio, health, and medical

Impact!

Social networking, Social media, Drug design



# Social networks

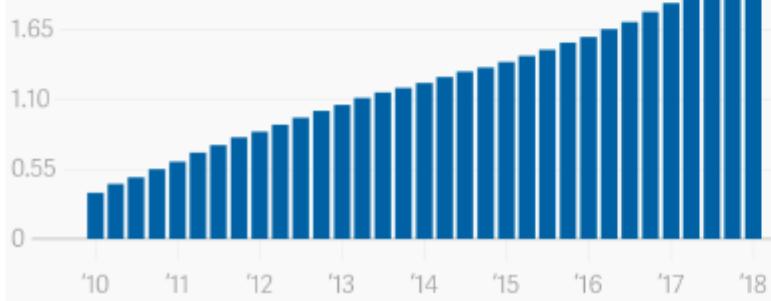
## Problems

- Information spread
- Recommend friend
- Advertisement



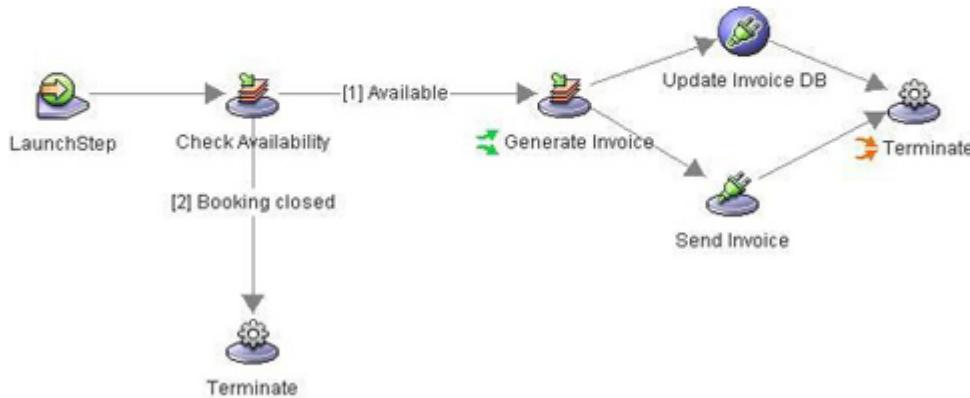
Facebook's monthly active users

2.20 billion active users



Facebook: > 2.2 billion active users

Workflow: It's sequence of processes through which a piece of work passes from initiation to completion. Can be also represented as directed graph.



## Google Maps:



## Hyperlink network

### Problems

- Page ranking
- Advertisement
- Reachability



Google: > 100 trillion indexed pages

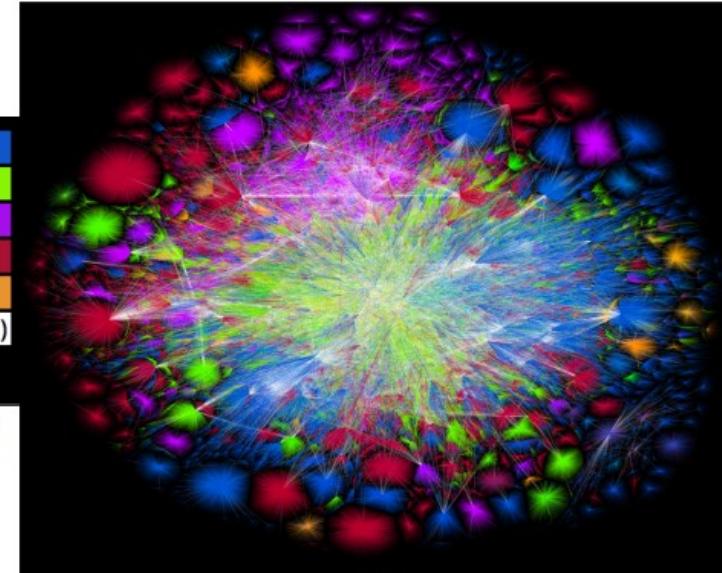
# The Internet

# Biological network

North America (ARIN)  
Europe (RIPE)  
Latin America (LACNIC)  
Asia Pacific (APNIC)  
Africa (AFRINIC)  
"Backbone" (highly connected networks)

Date: July 11 2015

<http://www.opte.org/the-internet/>

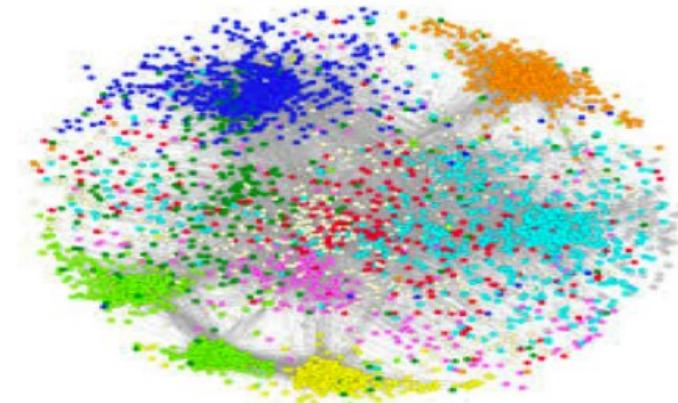


The Web: >50B webpages

## Problems

- Information propagation
- Fake news
- Anomalies

- New protein family
- Gene/protein functions



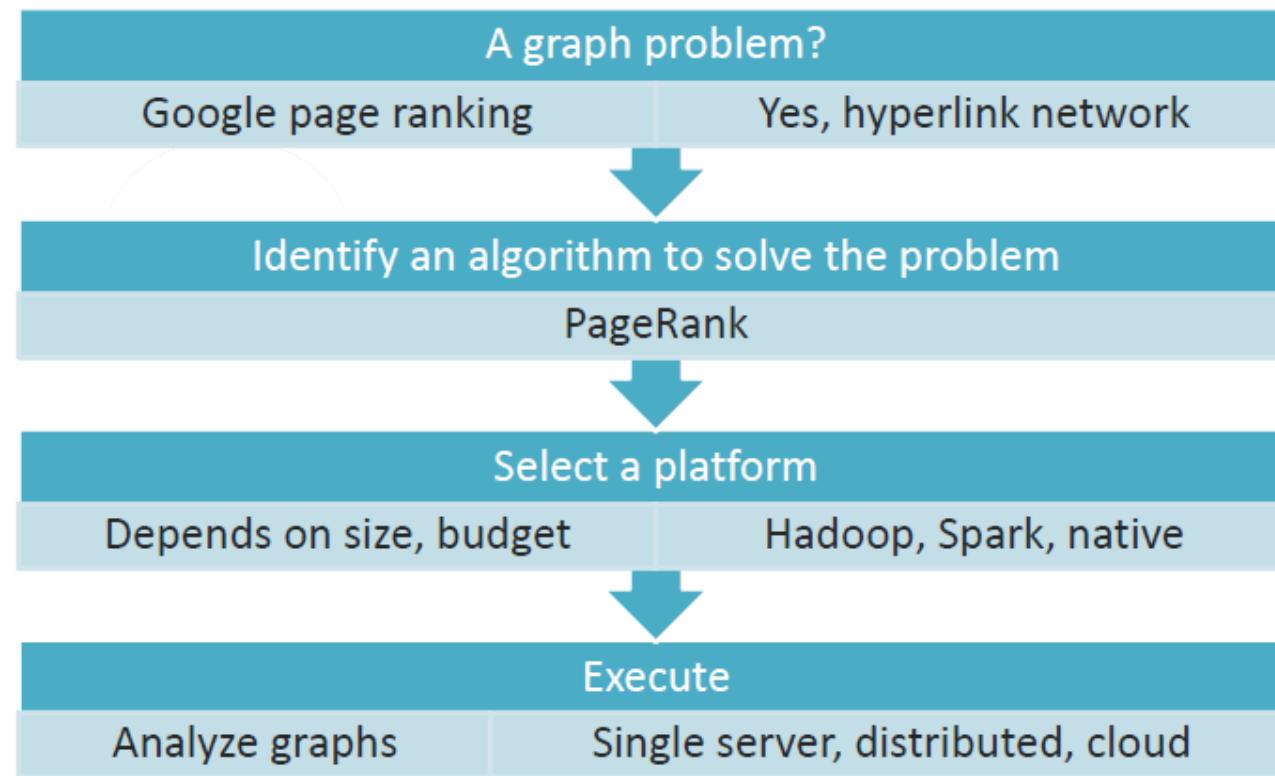
Metagenomic data: > 50 trillion edges among 50B proteins (IMG database)

# Graph analytics

## □ Graph analytics has three components

- **Data model:** Leverage graph structures to model and understand entities and their relationships in data
  - Not every dataset can be mapped to graphs
- **Graph algorithms:** Use graph theory and algorithms to solve problems in graphs
  - Finding suitable algorithms is important
- **Analytics platforms:** Use a suitable platform to analyze graphs with appropriate graph algorithms.
  - Depends on the scale of the problem and available resources
  - Underlying hardware needs to be considered

## Graph analytics: how to solve a problem?



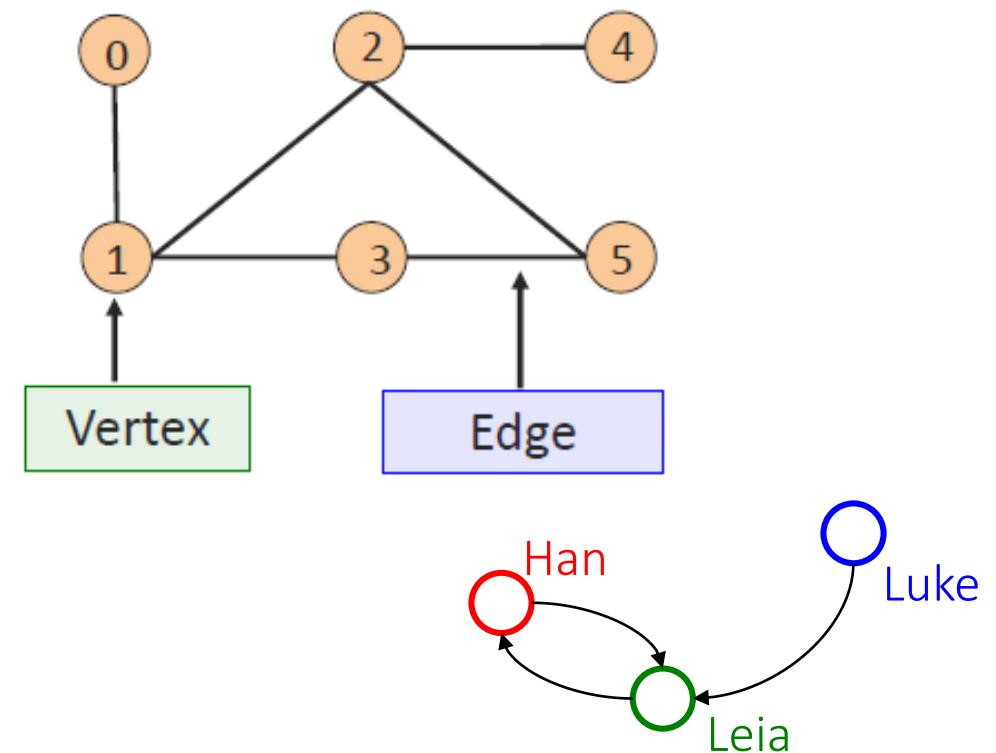
# Graphs

A graph is a formalism for representing relationships among items

- Very general definition
- Very general concept

A **graph** is a pair:  $G = (V, E)$

- A set of **vertices**, also known as **nodes**:  $V = \{v_1, v_2, \dots, v_n\}$
- A set of **edges**  $E = \{e_1, e_2, \dots, e_m\}$ 
  - Each edge  $e_i$  is a pair of vertices  $(v_j, v_k)$
  - An edge "connects" the vertices



Graphs can be **directed** or **undirected**

$$\begin{aligned} V &= \{\text{Han}, \text{Leia}, \text{Luke}\} \\ E &= \{(\text{Luke}, \text{Leia}), \\ &\quad (\text{Han}, \text{Leia}), \\ &\quad (\text{Leia}, \text{Han})\} \end{aligned}$$

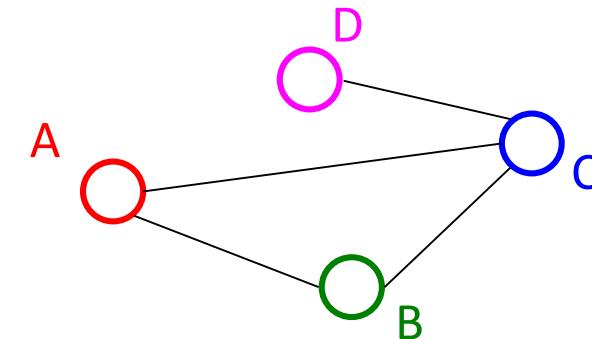
# Undirected Graphs

In **undirected graphs**, edges have no specific direction

- Edges are always "two-way"

Thus,  $(u, v) \in E$  implies  $(v, u) \in E$ .

- Only one of these edges needs to be in the set
- The other is implicit, so normalize how you check for it

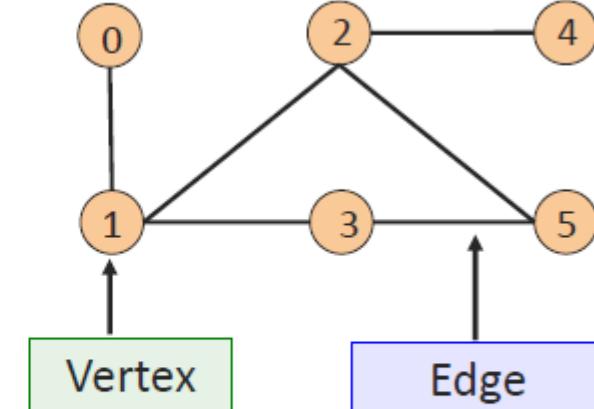


**Degree of a vertex:** number of edges containing that vertex

- Put another way: the number of adjacent vertices

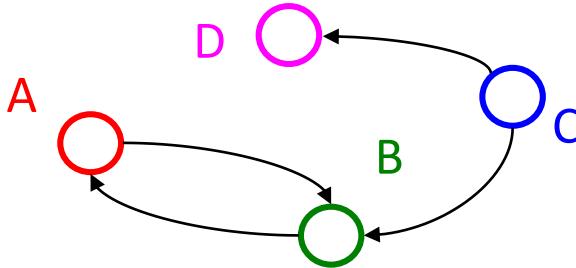
**Degree of a vertex:**  
number of vertices  
adjacent to  $v$   
 $- d(1) = 3$

In directed networks we  
define an **in-degree** and  
**out-degree**.

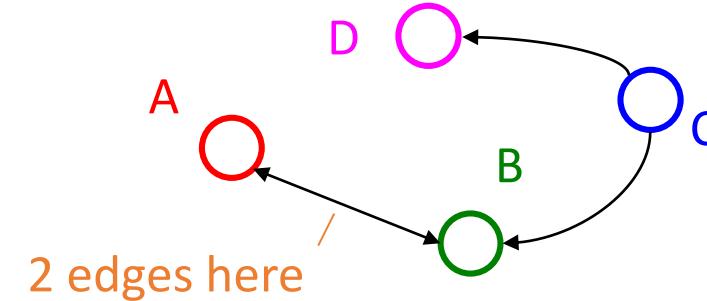


# Directed Graphs

In **directed graphs** (or **digraphs**), edges have direction



or



Thus,  $(u, v) \in E$  does not imply  $(v, u) \in E$ .

Let  $(u, v) \in E$  mean  $u \rightarrow v$

- Call  $u$  the **source** and  $v$  the **destination**
- **In-Degree** of a vertex: number of in-bound edges (edges where the vertex is the destination)
- **Out-Degree** of a vertex: number of out-bound edges (edges where the vertex is the source)

## Self-Edges

A **self-edge** a.k.a. a **loop** edge is of the form  $(u, u)$

- The use/algorithm usually dictates if a graph has:
  - No self edges
  - Some self edges
  - All self edges

A node can have a(n) degree / in-degree / out-degree of **zero**

**Theorem 1.1.** *The graph  $G = (V, E)$ , where  $V = \{v_1, \dots, v_n\}$  and  $E = \{e_1, \dots, e_m\}$ , satisfies*

$$\sum_{i=1}^n d(v_i) = 2m.$$

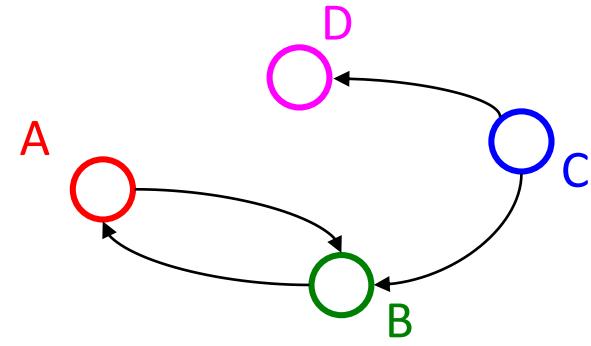
**Corollary.** *Every graph has an even number of vertices of odd degree.*

*Proof.* If the vertices  $v_1, \dots, v_k$  have odd degrees and the vertices  $v_{k+1}, \dots, v_n$  have even degrees, then (Theorem 1.1)

$$d(v_1) + \dots + d(v_k) = 2m - d(v_{k+1}) - \dots - d(v_n)$$

is even. Therefore,  $k$  is even. □

## More Notation



For a graph  $G = (V, E)$ :

- $|V|$  is the number of vertices
- $|E|$  is the number of edges
  - Minimum?
  - Maximum for undirected?
  - Maximum for directed?

0

$|V|(|V|-1)/2$

$|V|(|V|-1)$

$$V = \{A, B, C, D\}$$

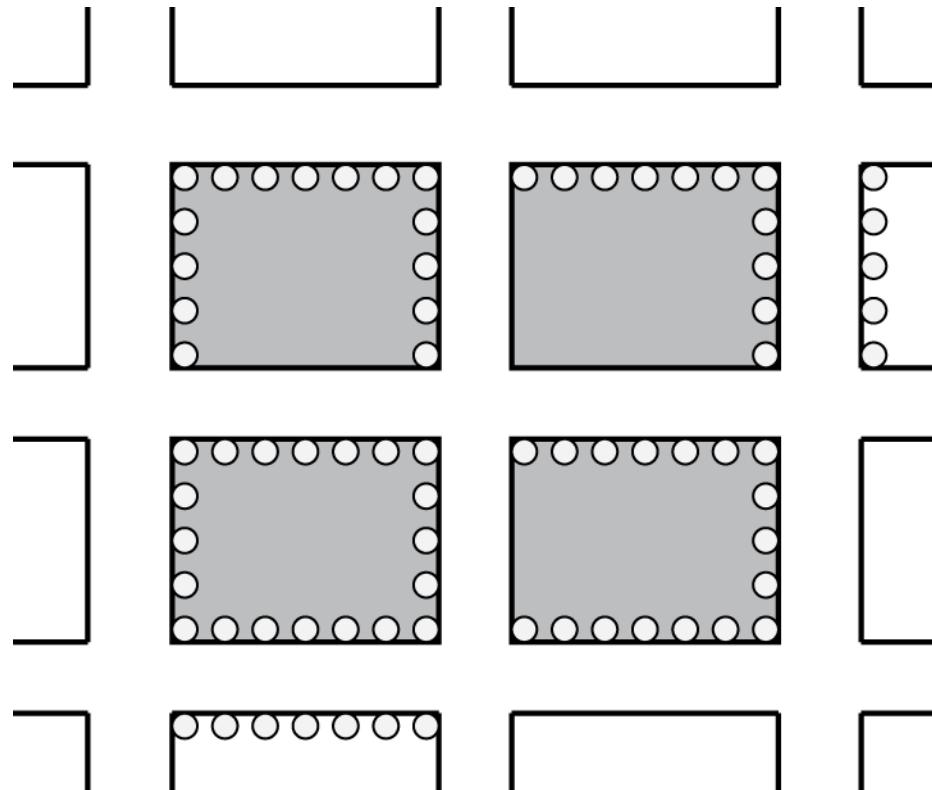
$$E = \{(C, B), (A, B), (B, A), (C, D)\}$$

If  $(u, v) \in E$ , then  $v$  is a **neighbor** of  $u$  (i.e.,  $v$  is **adjacent** to  $u$ )

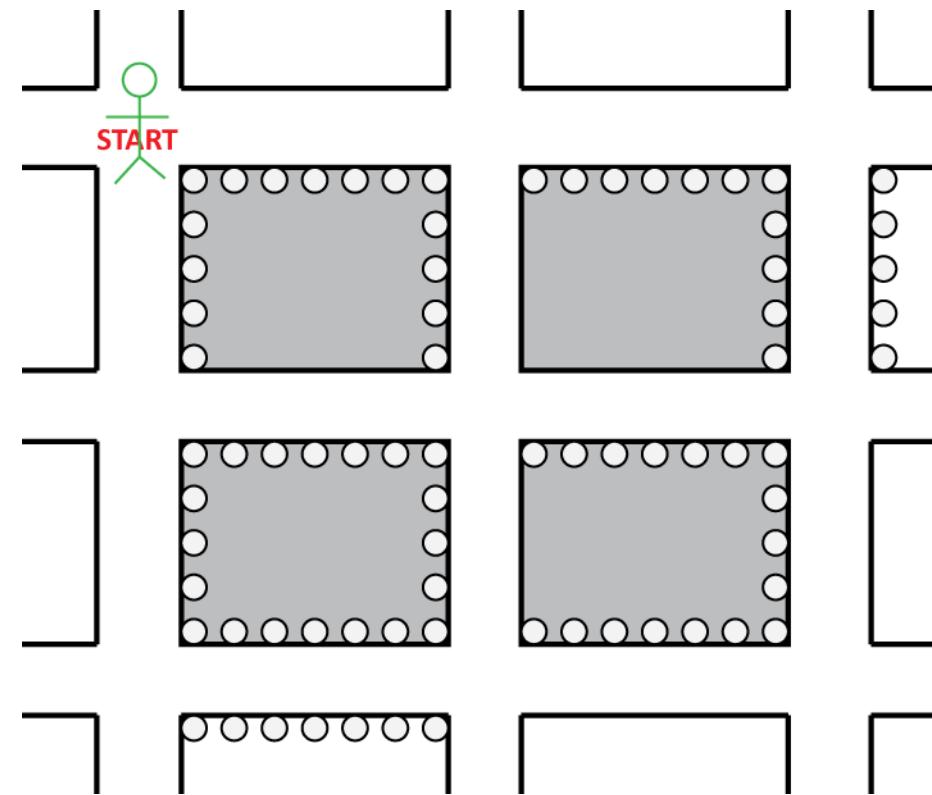
- Order matters for directed edges:  
 $u$  is not adjacent to  $v$  unless  $(v, u) \in E$

# Parking Meters

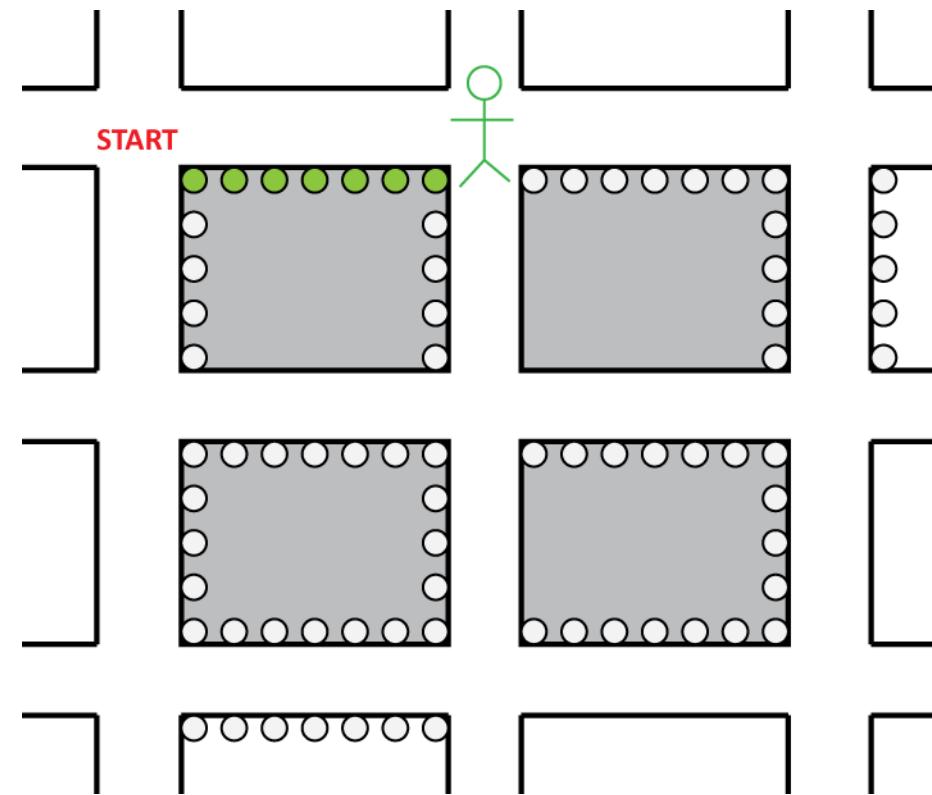
- Here is a map of the parking meters in a small neighborhood
- Our goal is to start at an intersection, check the meters, and return to our starting point...
- ...without retracing our steps!



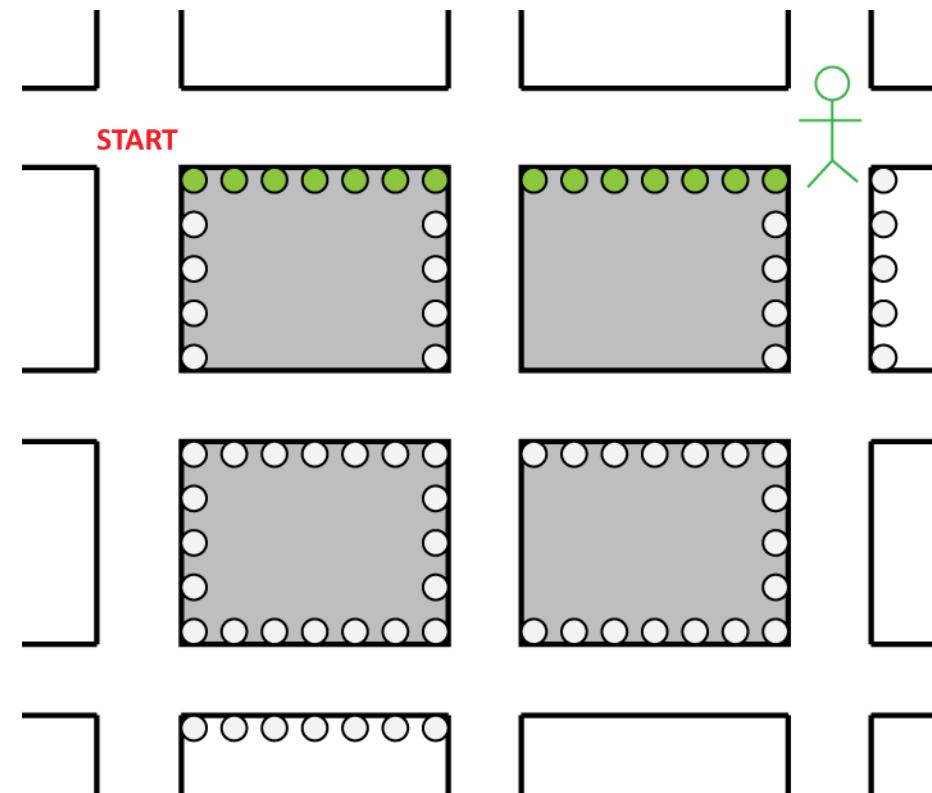
# Solution Attempt #1



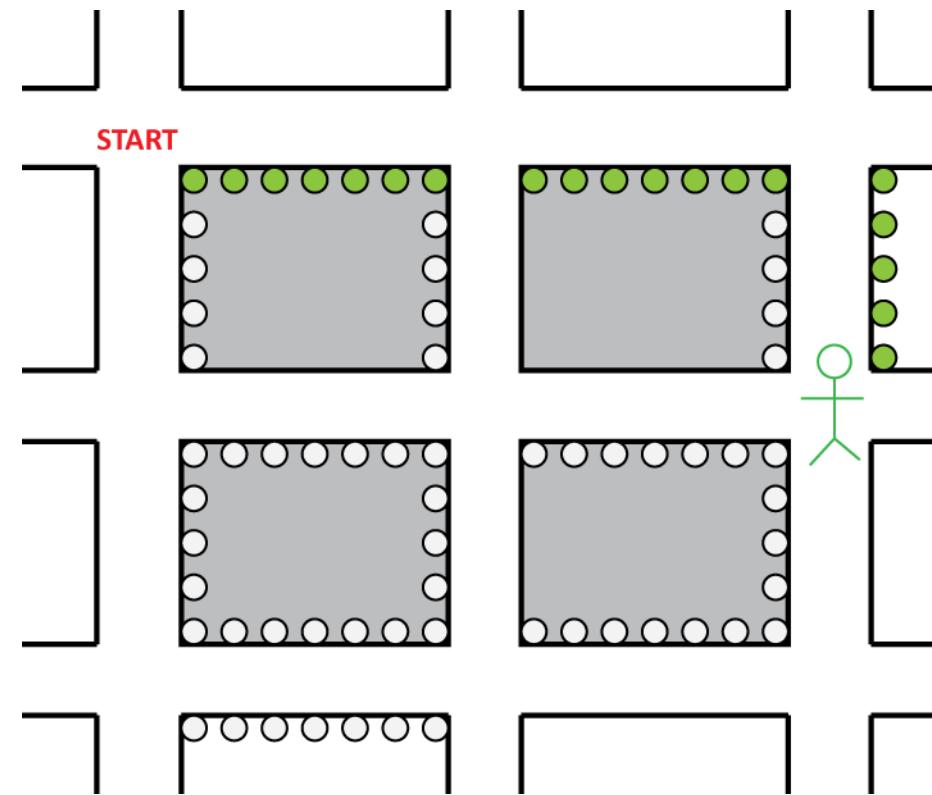
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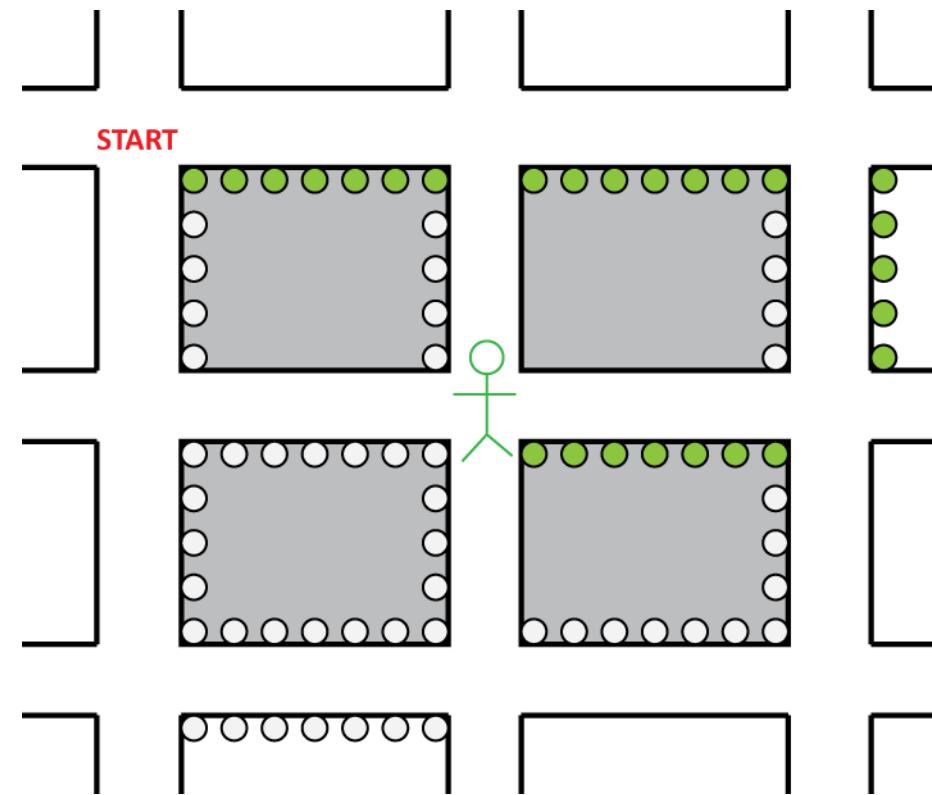
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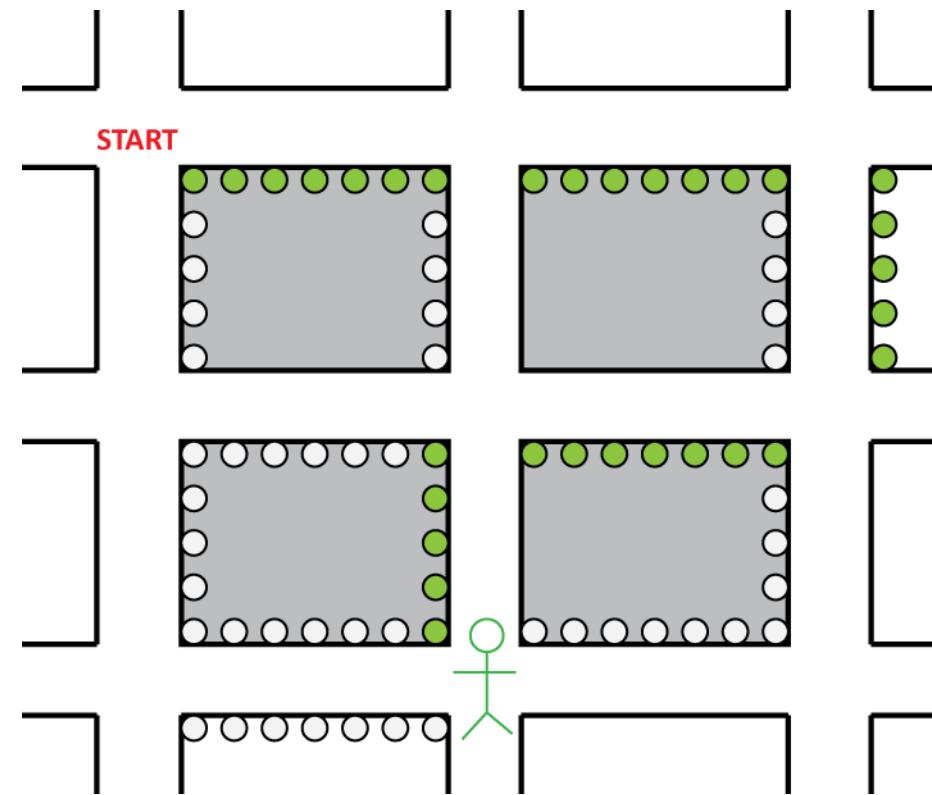
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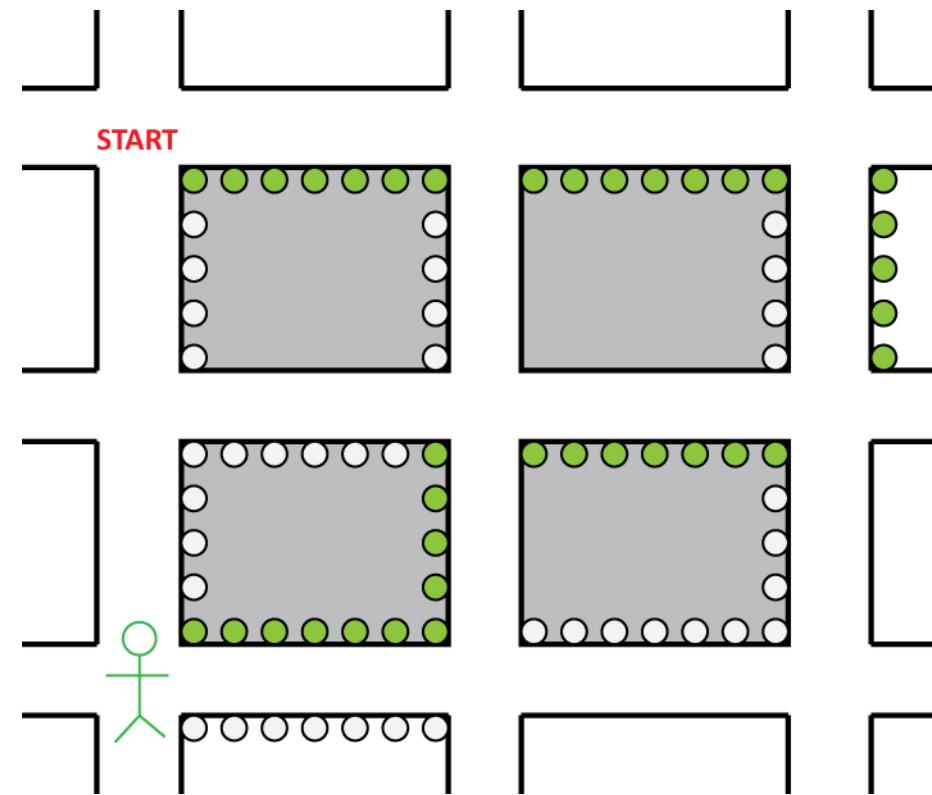
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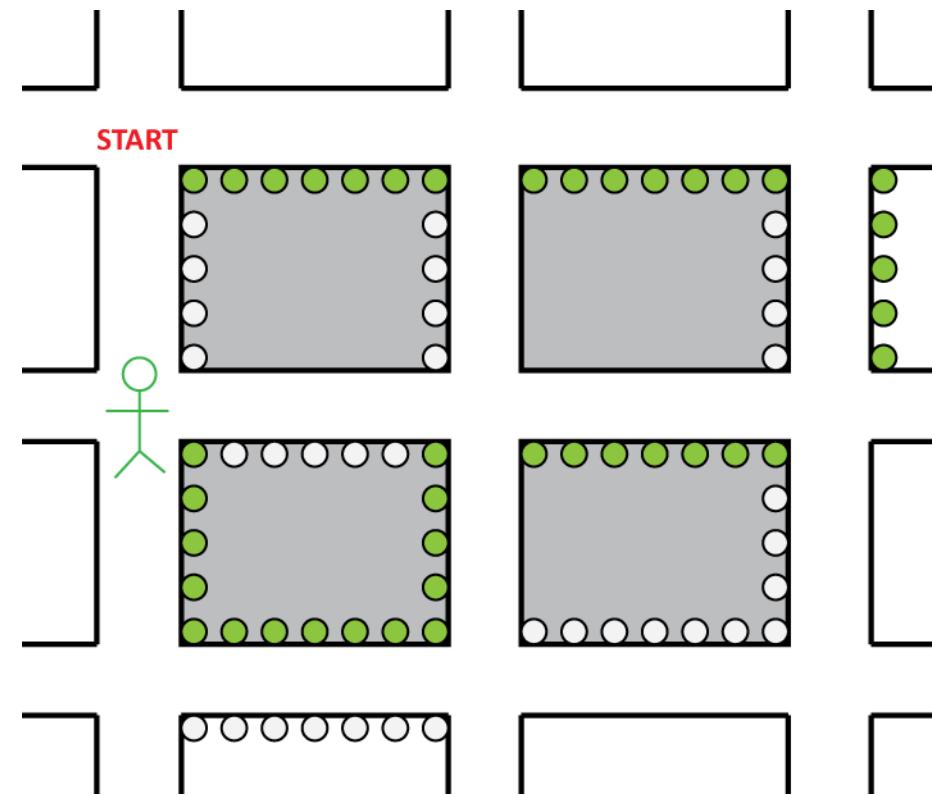
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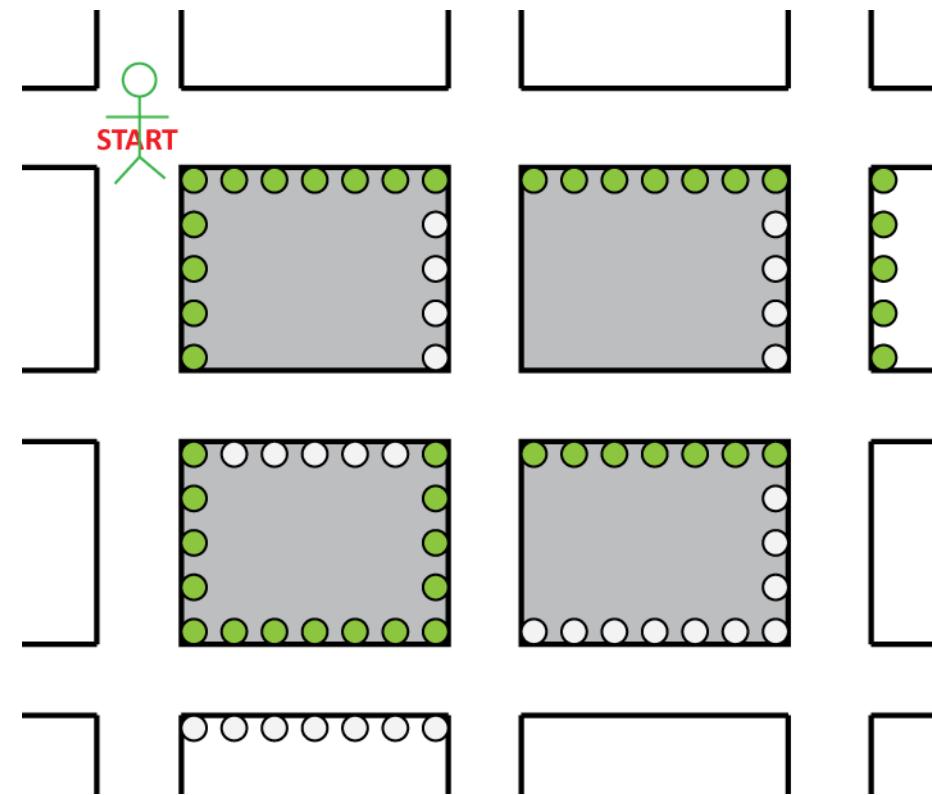
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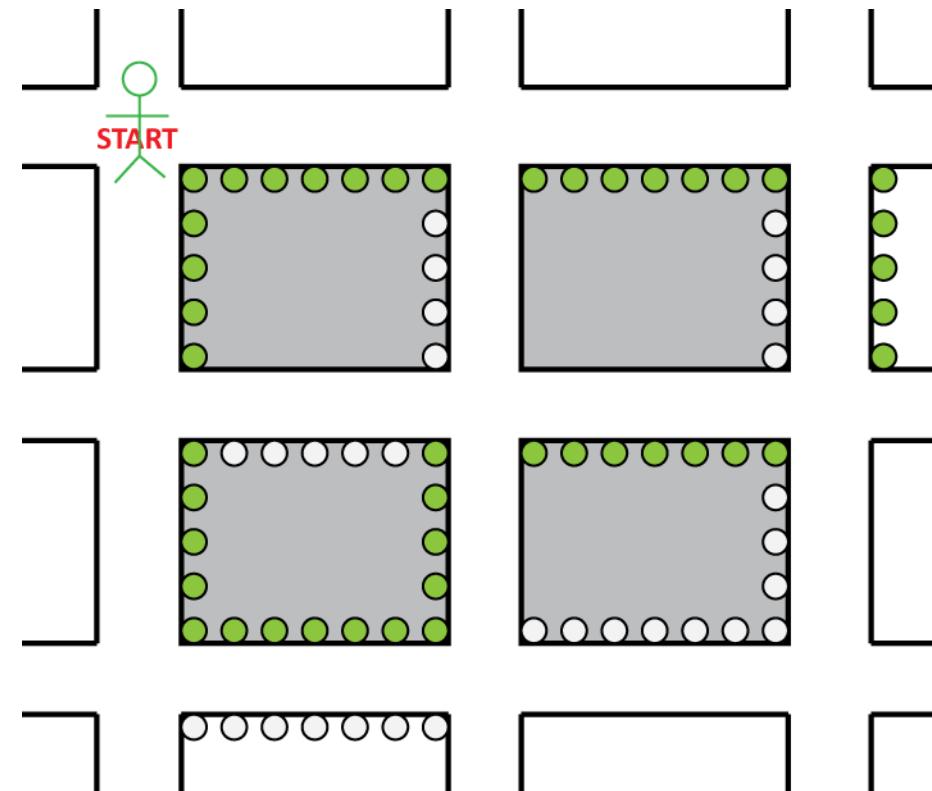


# Solution Attempt #1



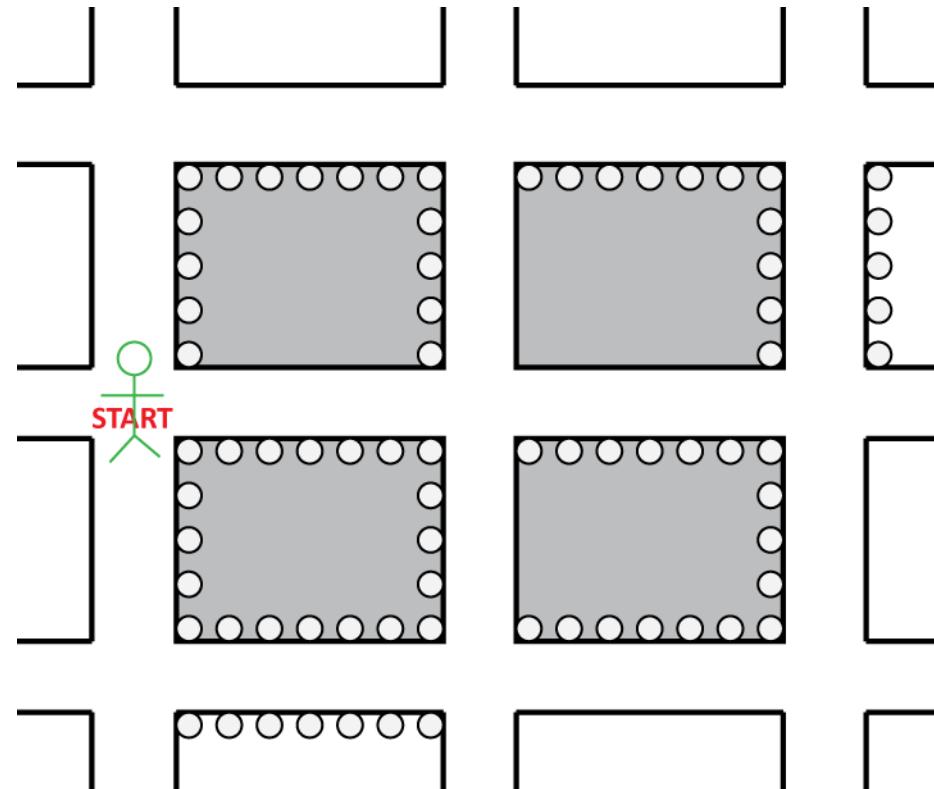
# Solution Attempt #1

Now we're stuck, so we know this can't be a solution to the problem!

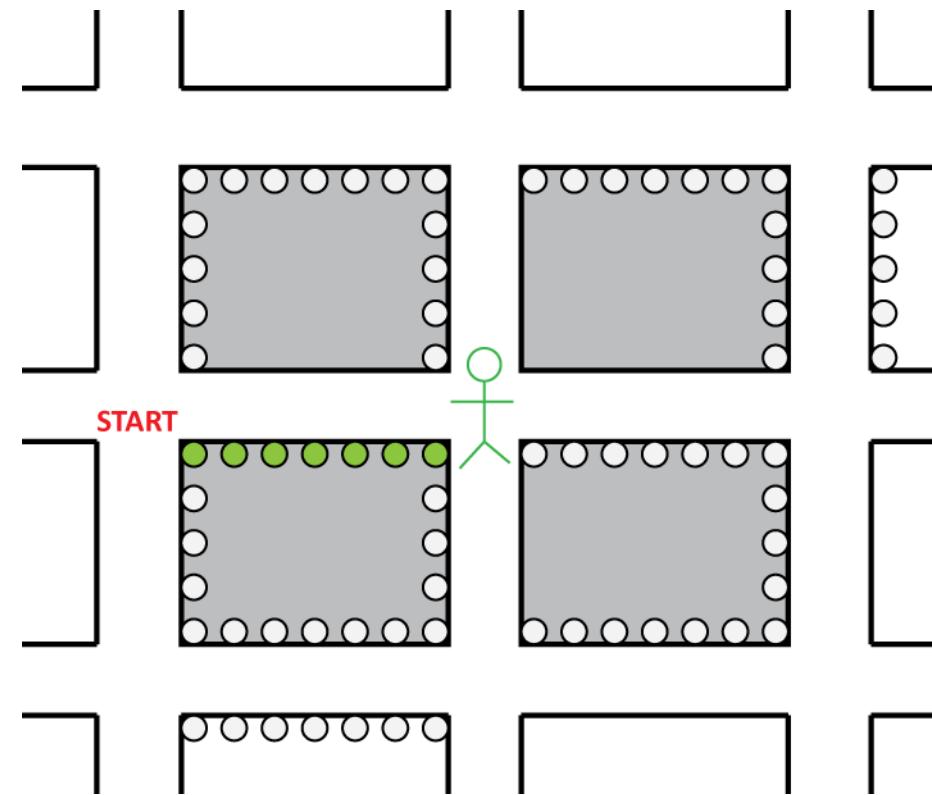


# Solution Attempt #2

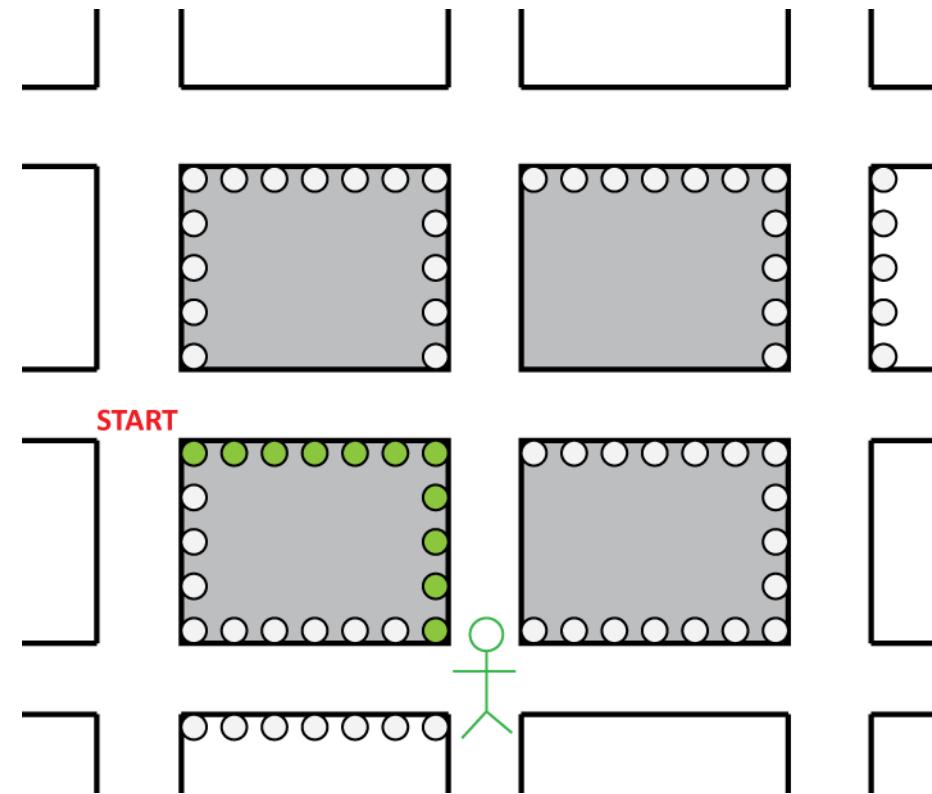
Let's try again, this time with a different starting point...



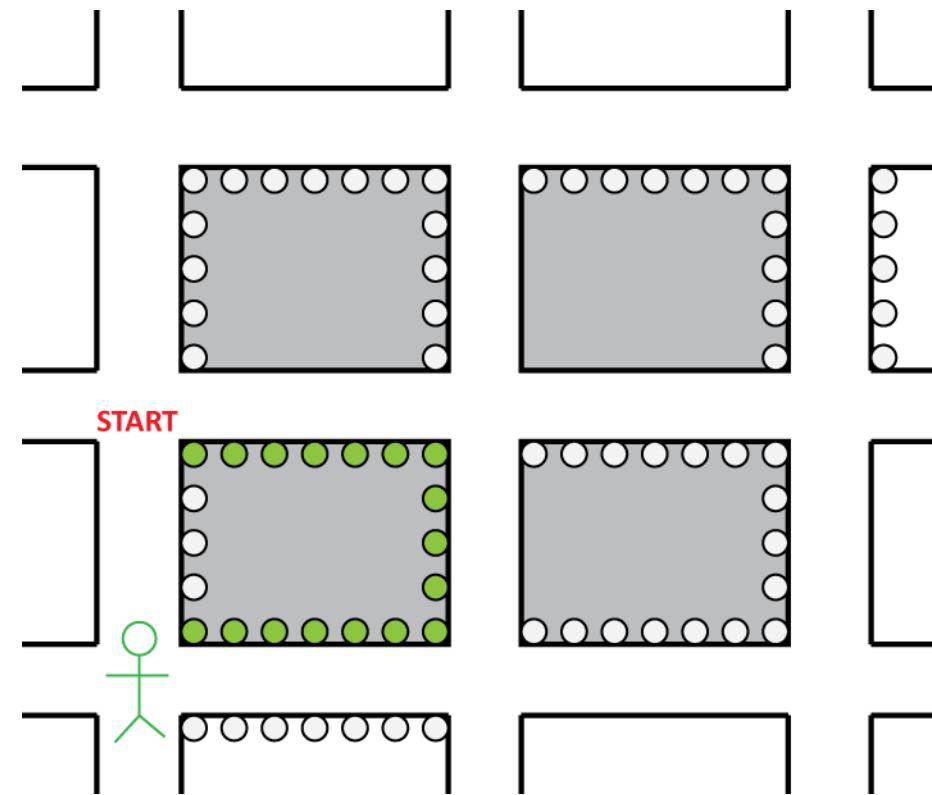
# Solution Attempt #2



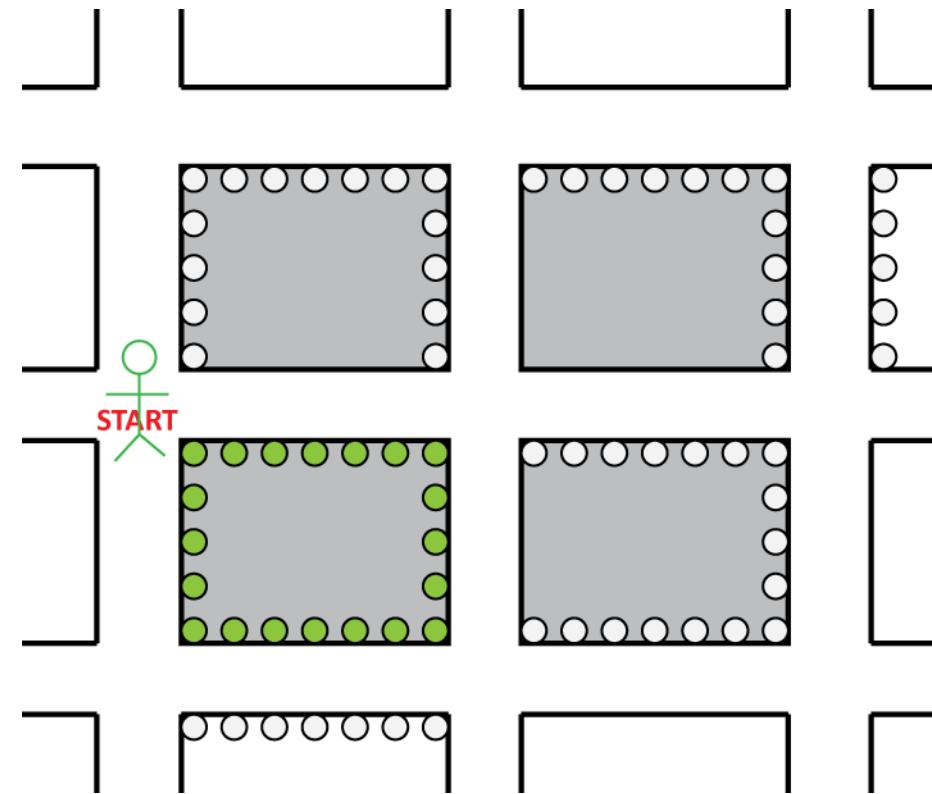
# Solution Attempt #2



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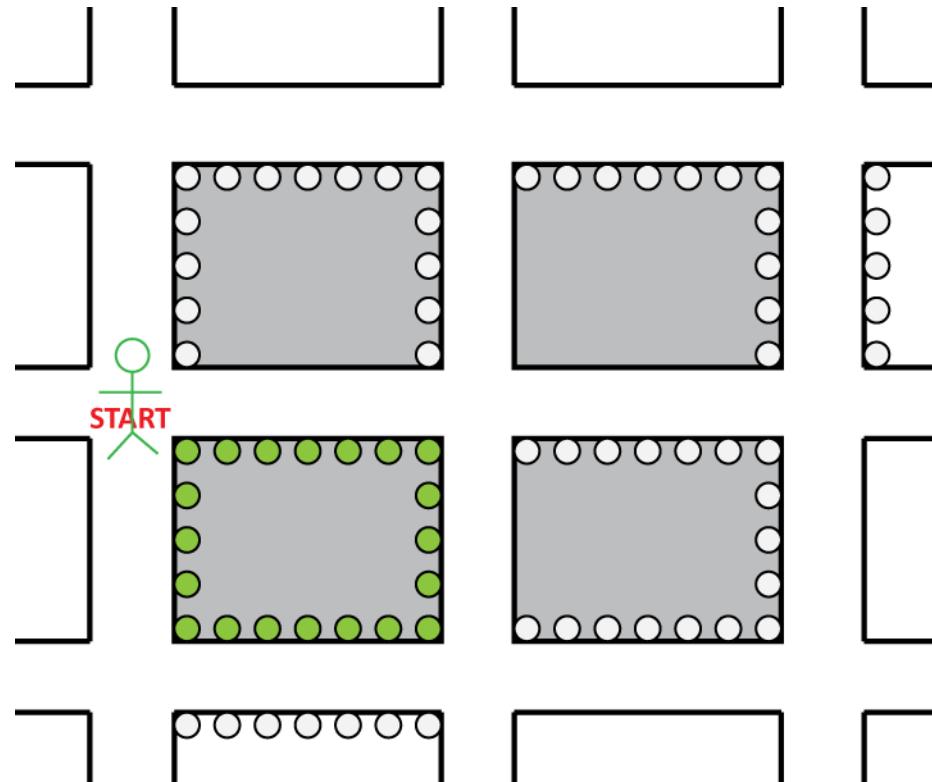


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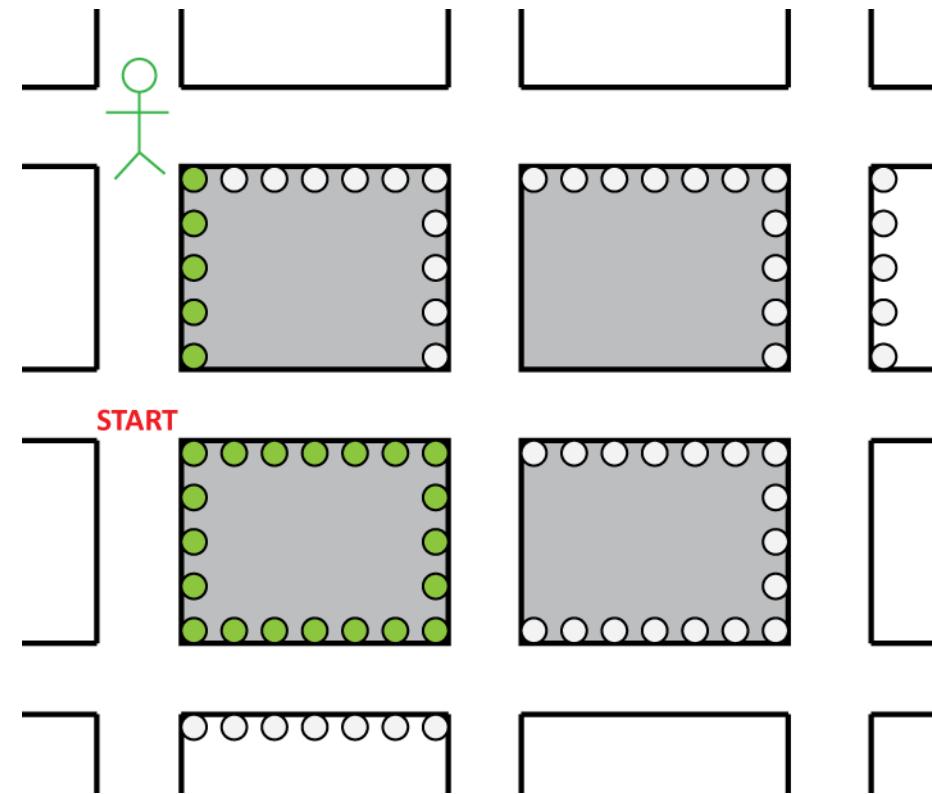


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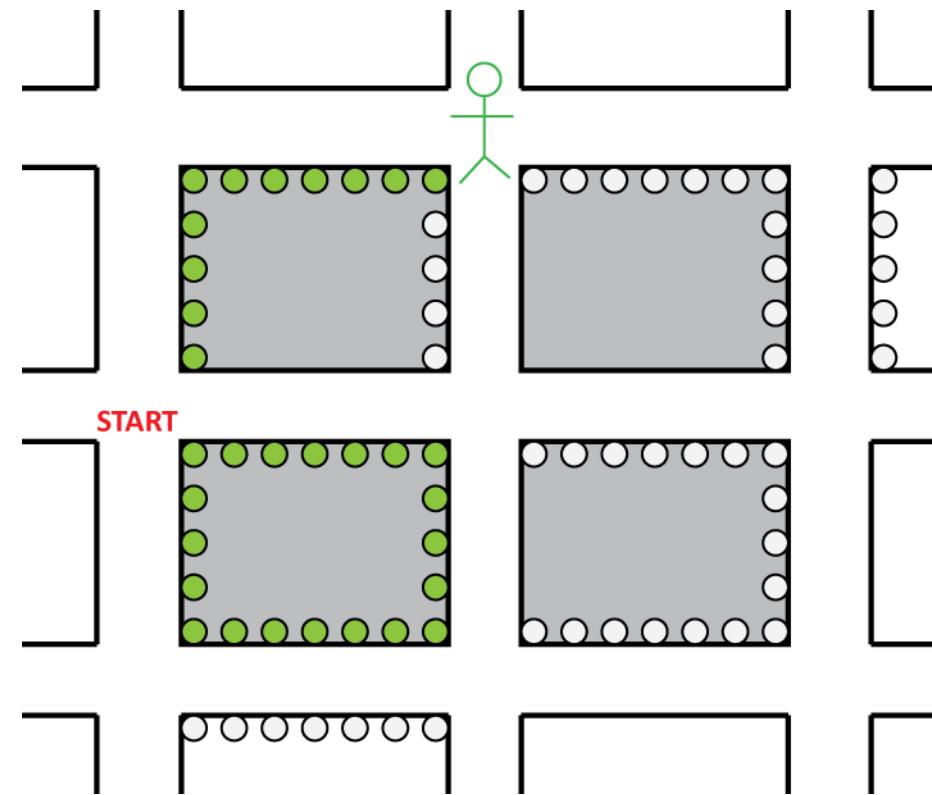
Notice that it's OK for us to return to the start since there is still a way to leave this spot without retracing our steps.



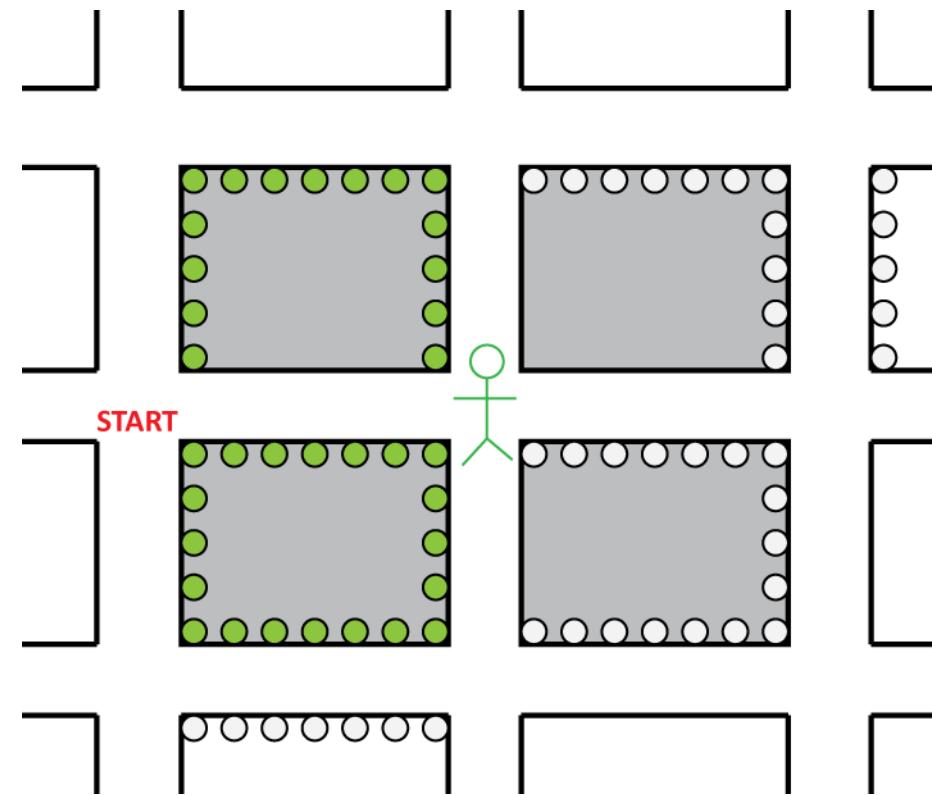
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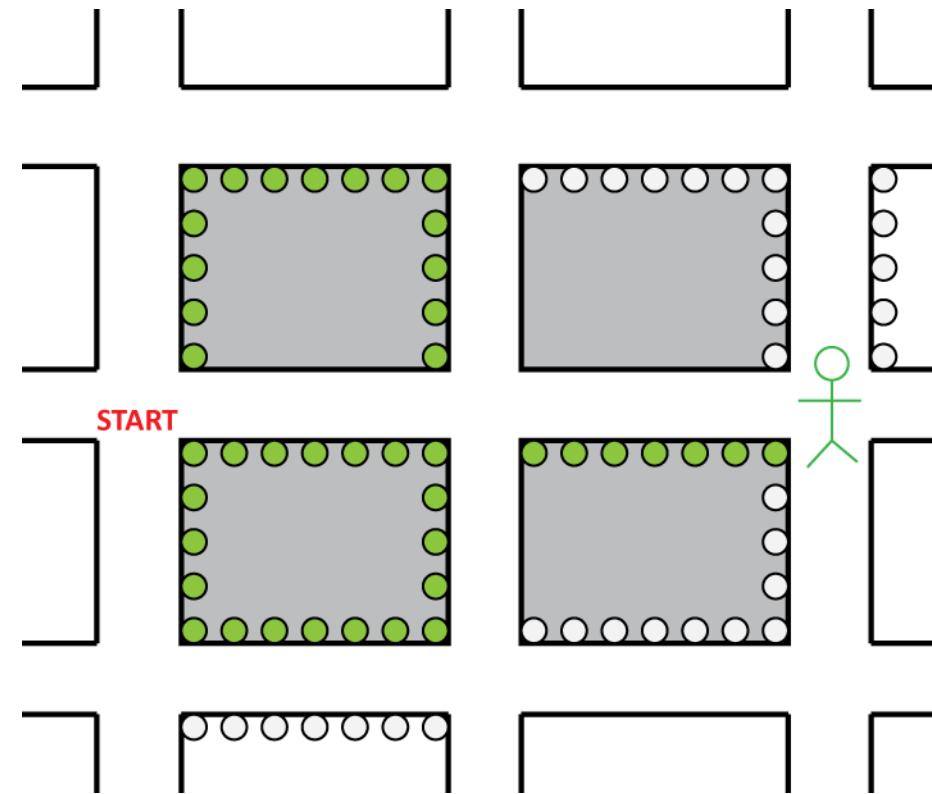
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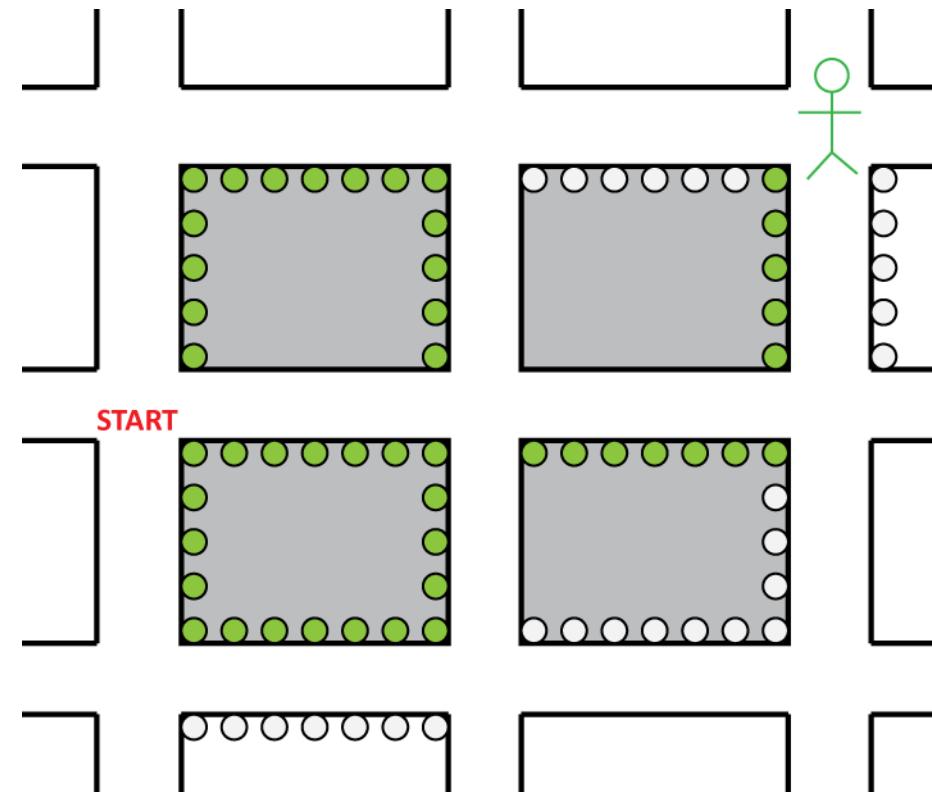
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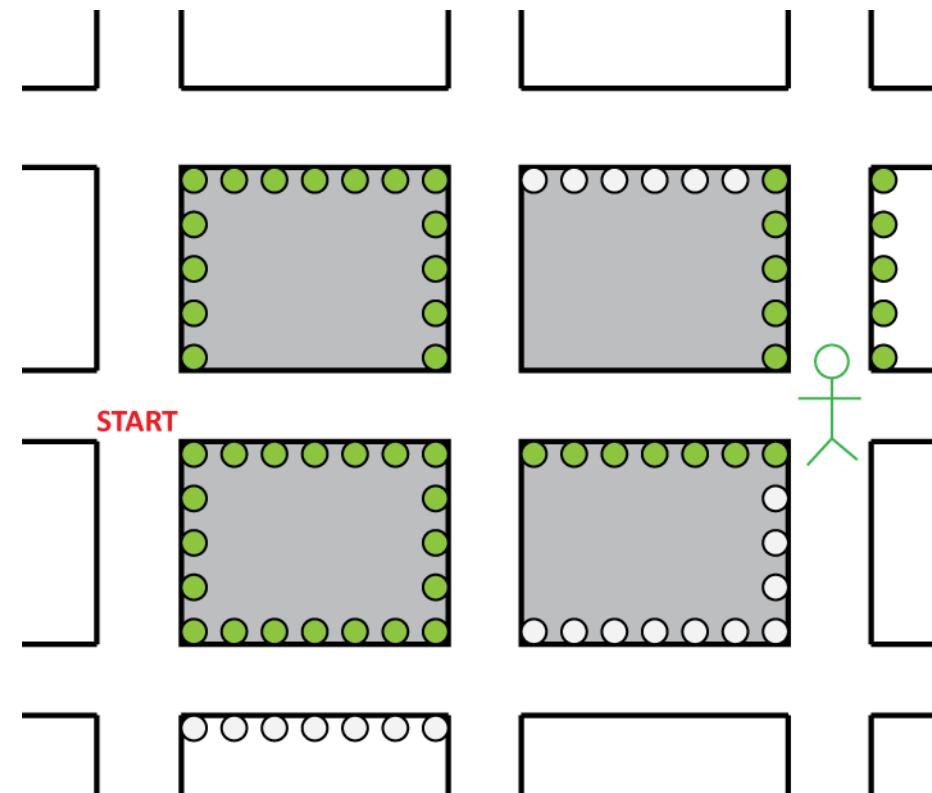
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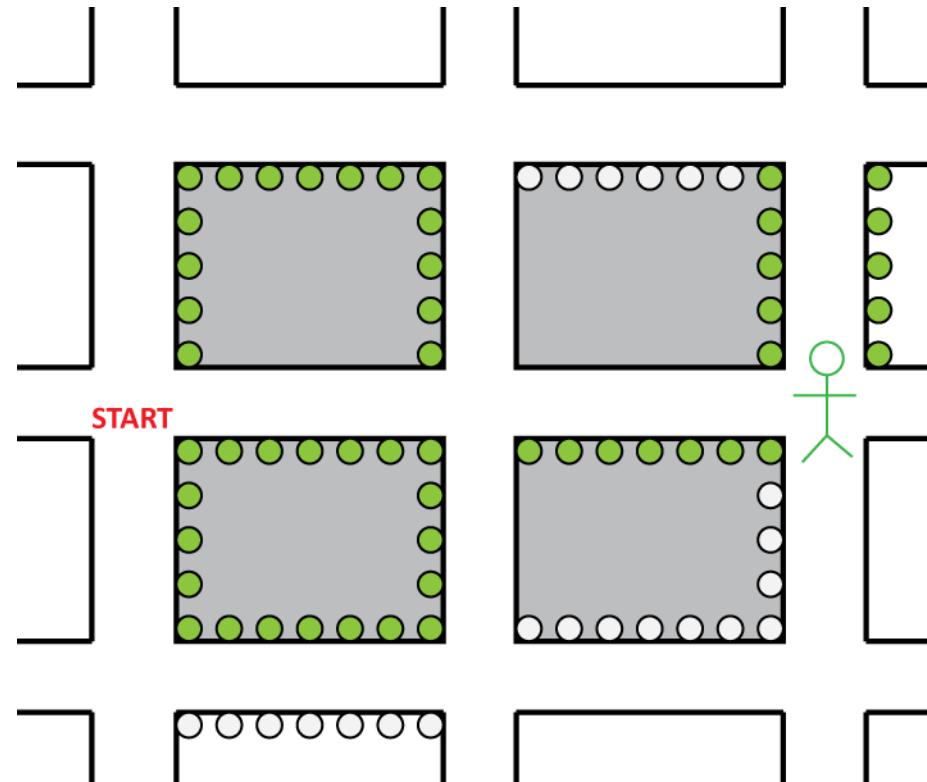
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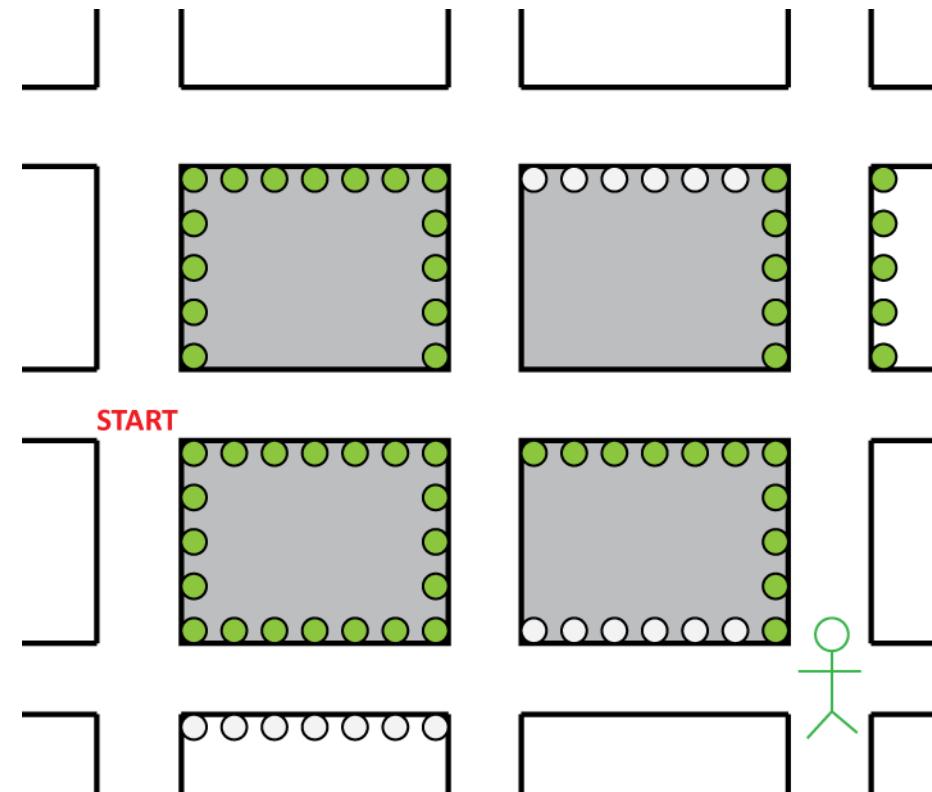
# Solution Attempt #2

Notice how  
we just went  
back the way  
we came.

This is not a  
“retrace”  
because  
there are  
meters on  
both sides of  
the street.



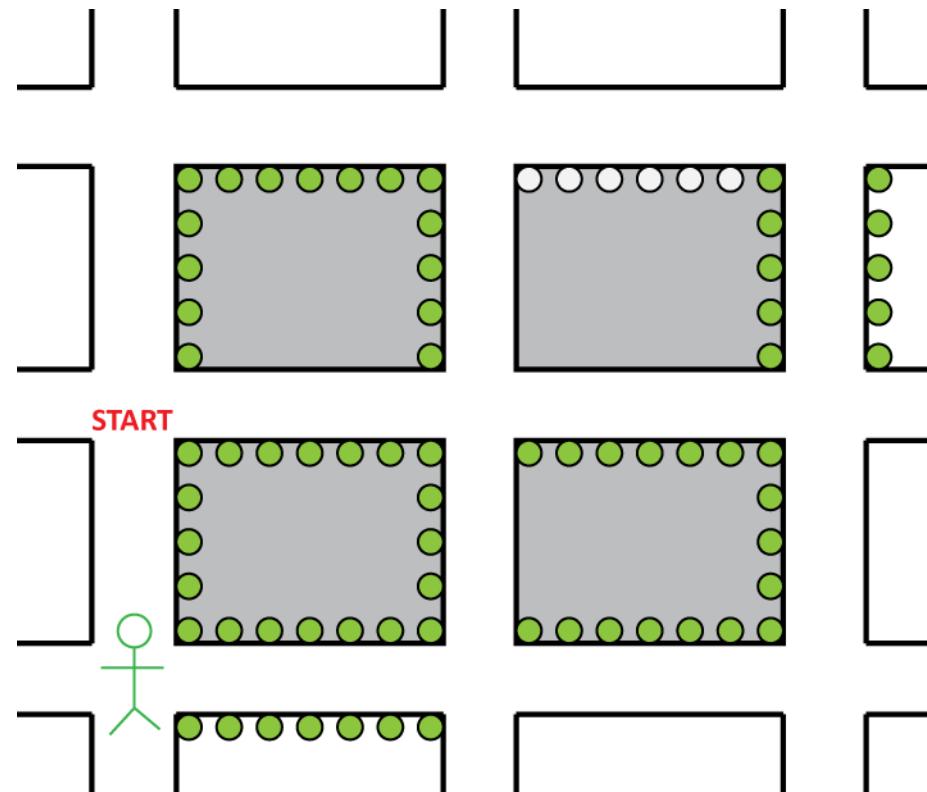
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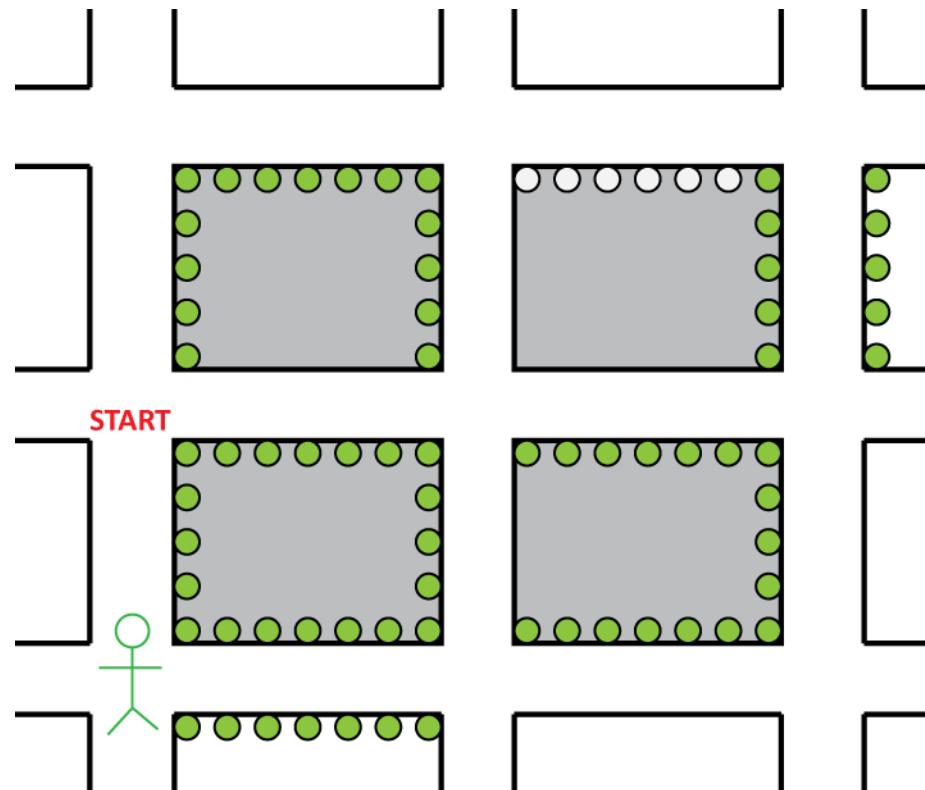


# Solution Attempt #2



# Solution Attempt #2

And we're stuck again, so we know this can't be a solution to the problem either!

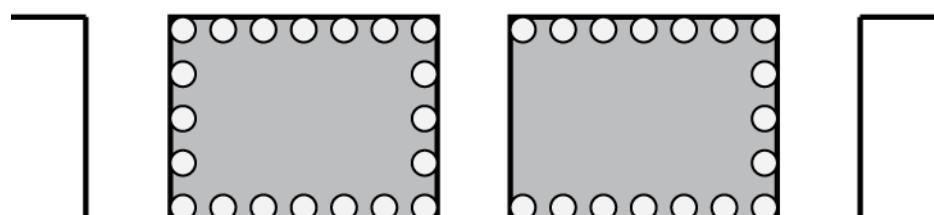
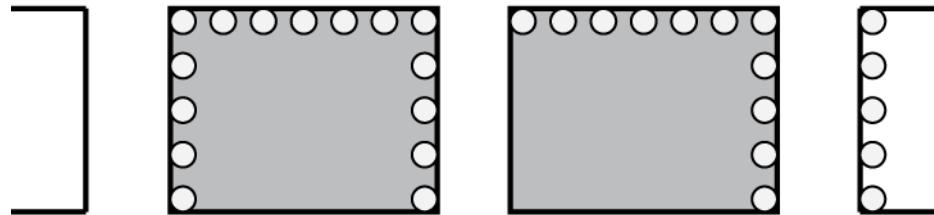


# You Try It

- We haven't had any luck so far... now it's your turn to give it a try



- Can you choose a starting point, visit all the parking meters, and return to the start without retracing?



# Now What?

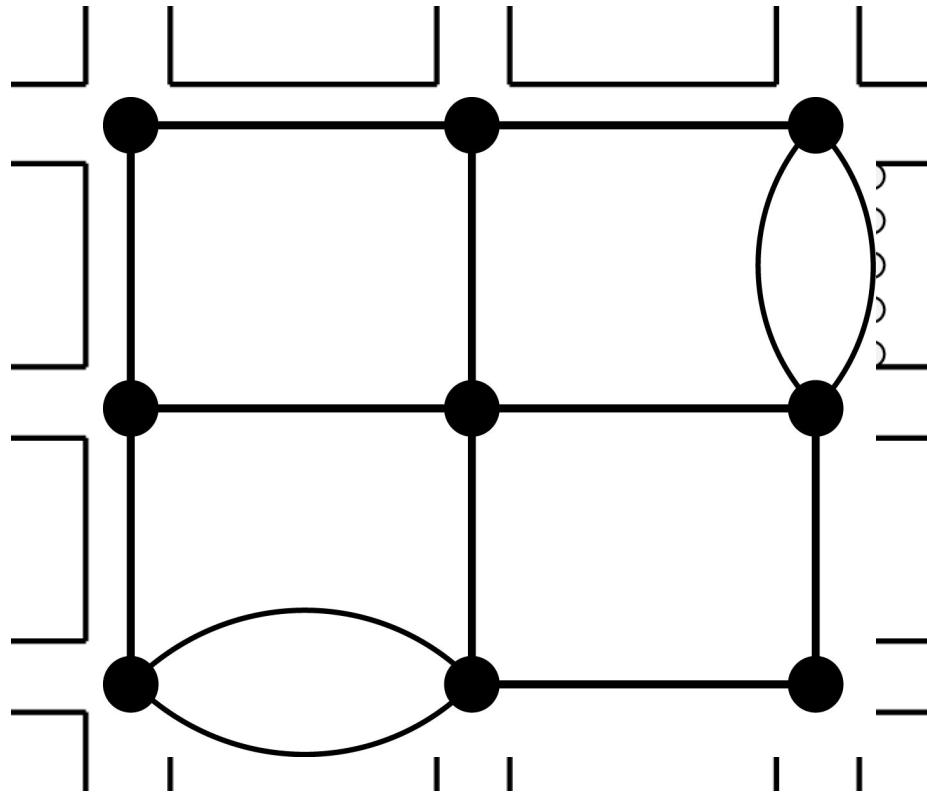
- We could continue to use trial and error to see if we can find a solution
- We might eventually become convinced that there is no solution
- We're going to use a *model* to represent this problem to make it easier to study

# Models and Math

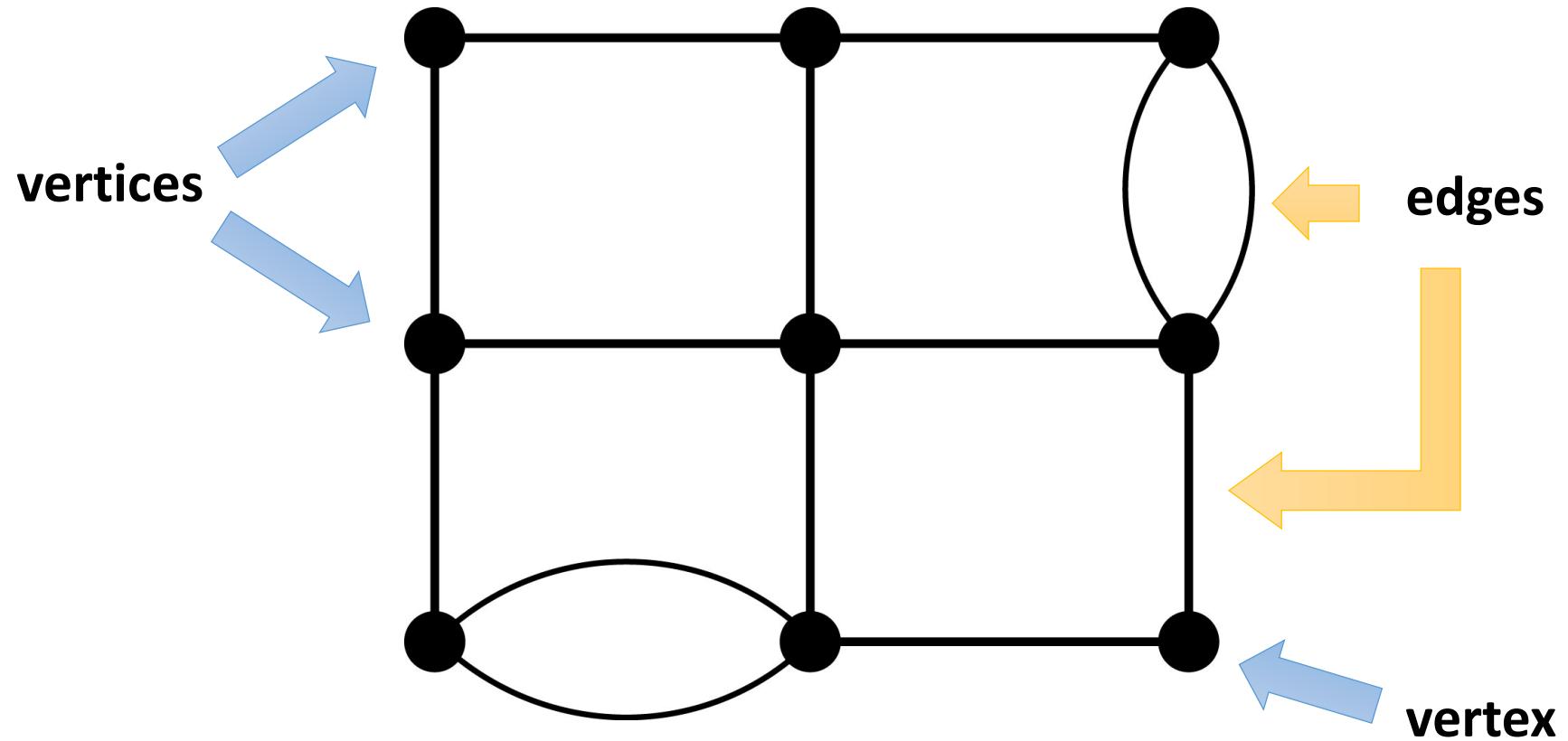
- A *model* is a mathematical tool that simplifies a problem, but keeps all of the important information
- For example, if you ever had to read a word problem and create an equation that you used to solve it, then you have created a mathematical model

# Our Model: A “Graph”

- In our model, we will represent each intersection by a big black dot called a “**vertex**”
- Each row of parking meters is connected by a line called an “**edge**”



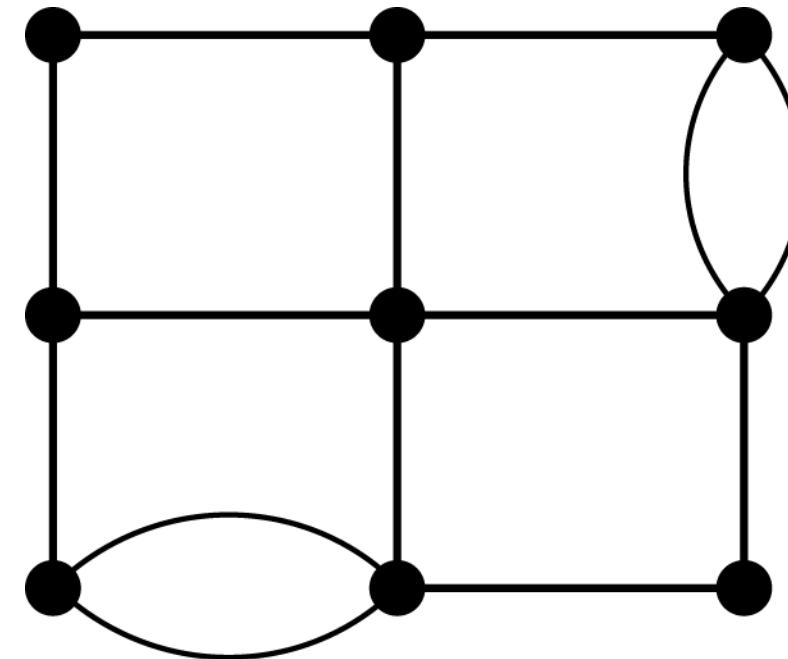
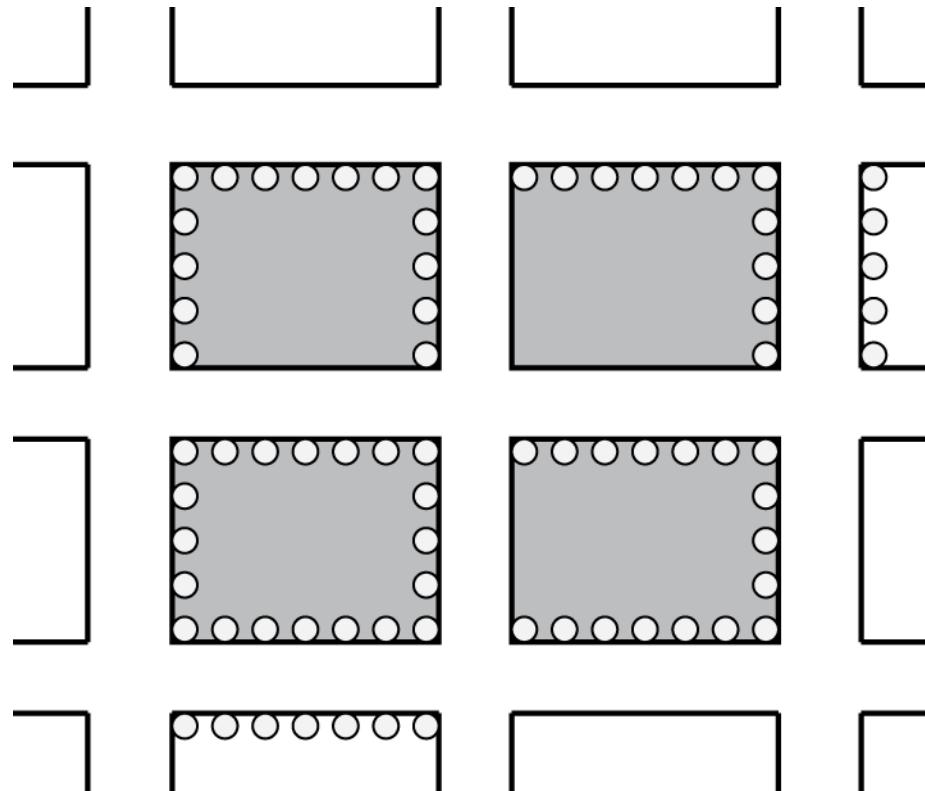
# Graph



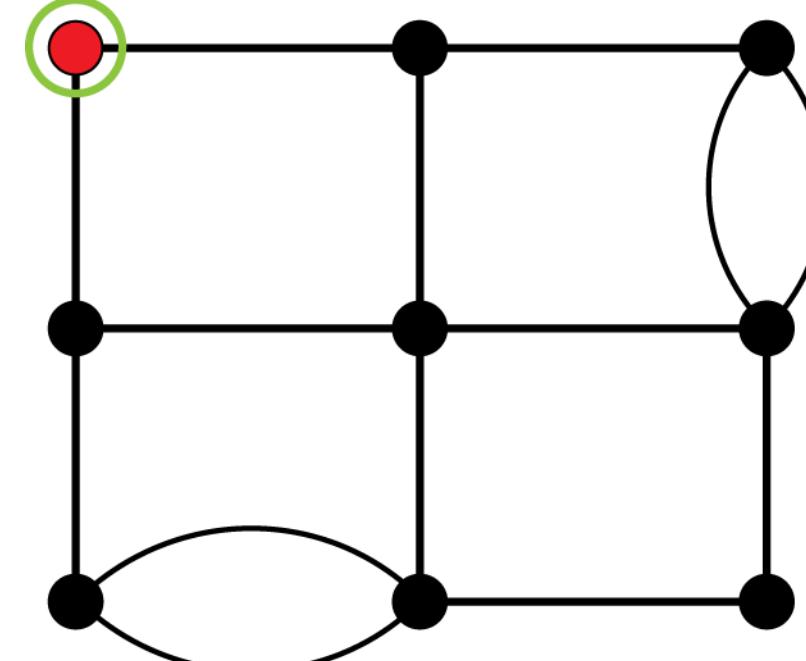
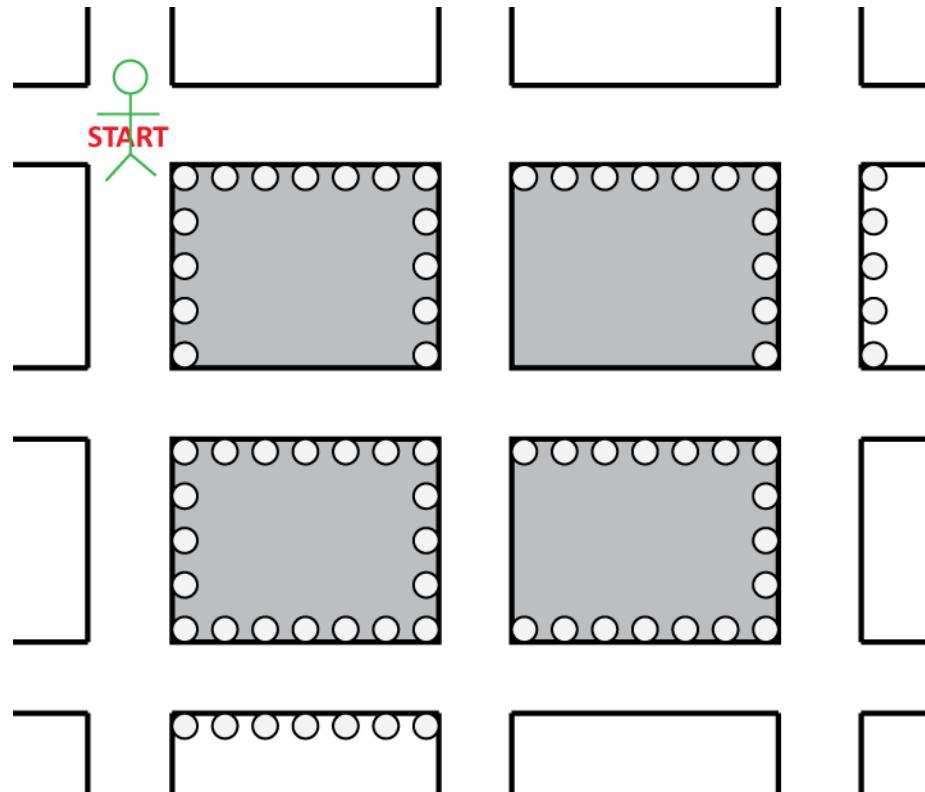
# Using the Graph

- The graph contains all of the information we need to solve our parking meter problem
- We don't need to know the names of the streets or how long they are
- All we need to know is which streets have parking meters, and how they intersect each other

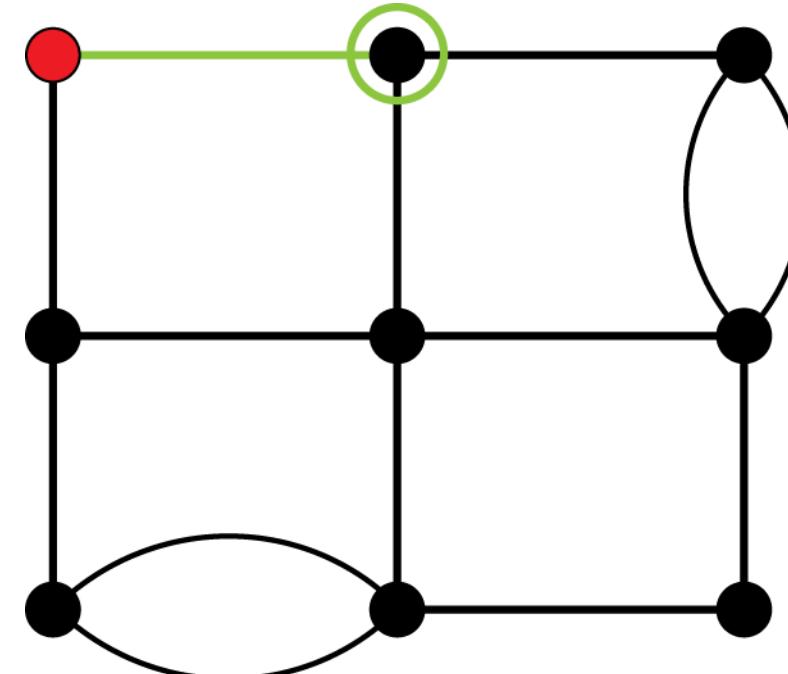
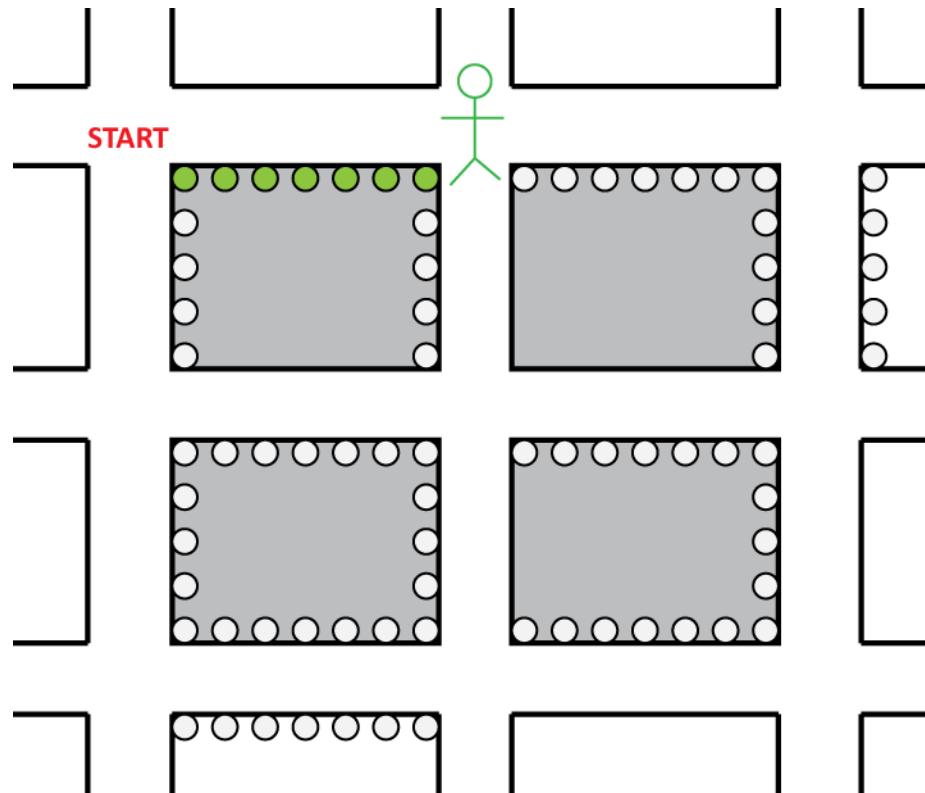
# Two Paths: Map vs. Graph



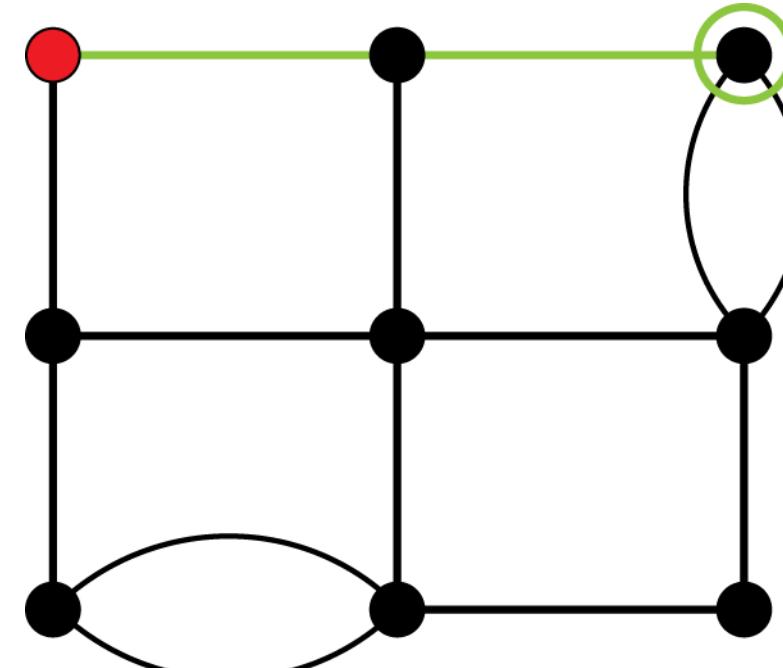
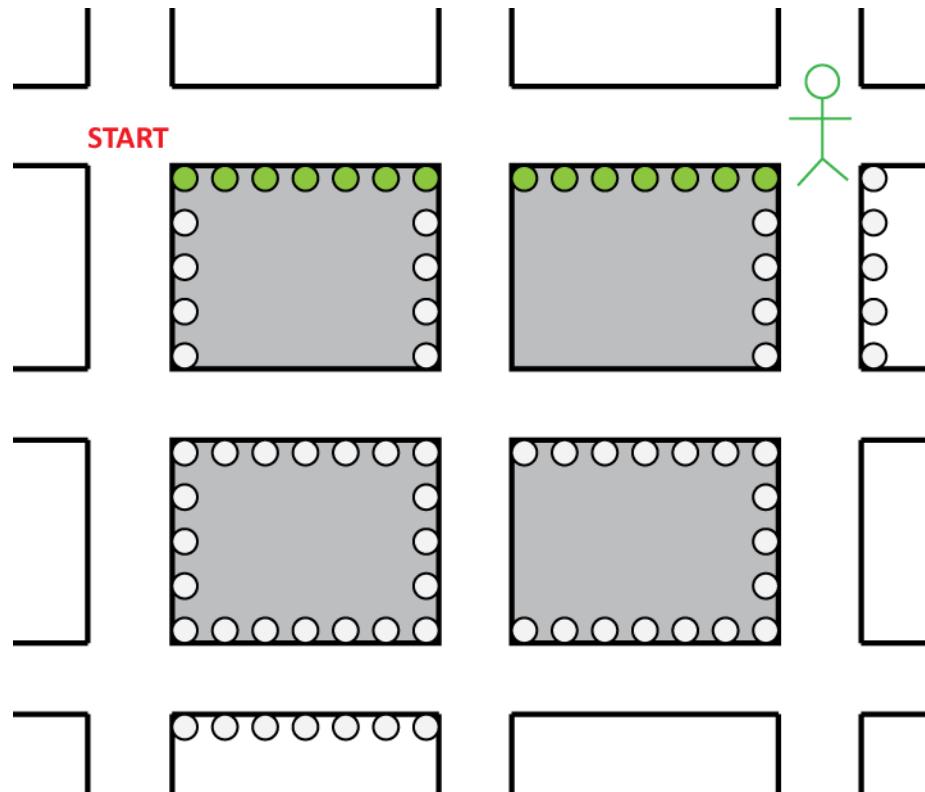
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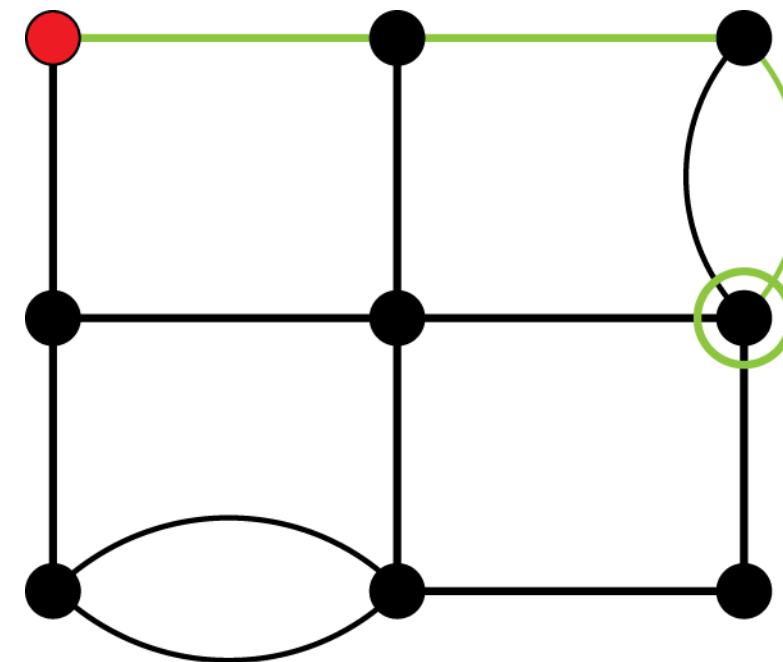
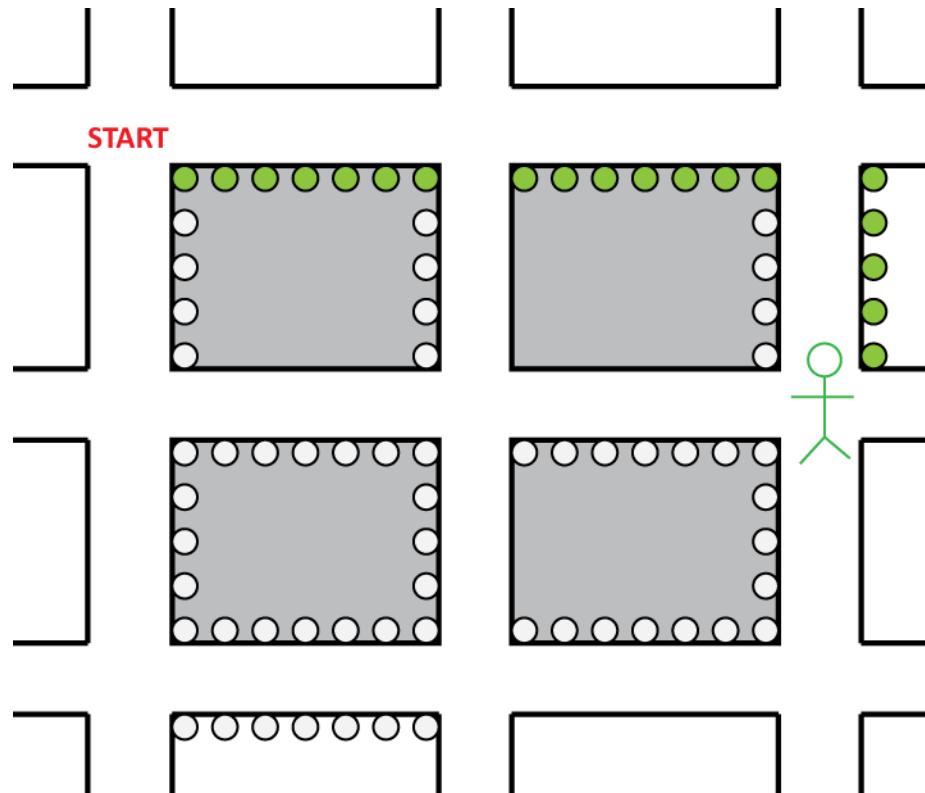
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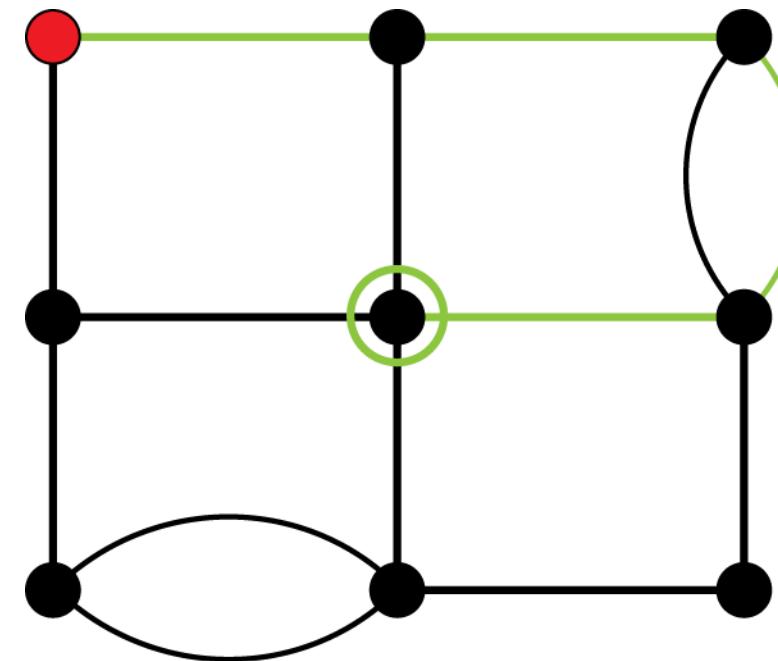
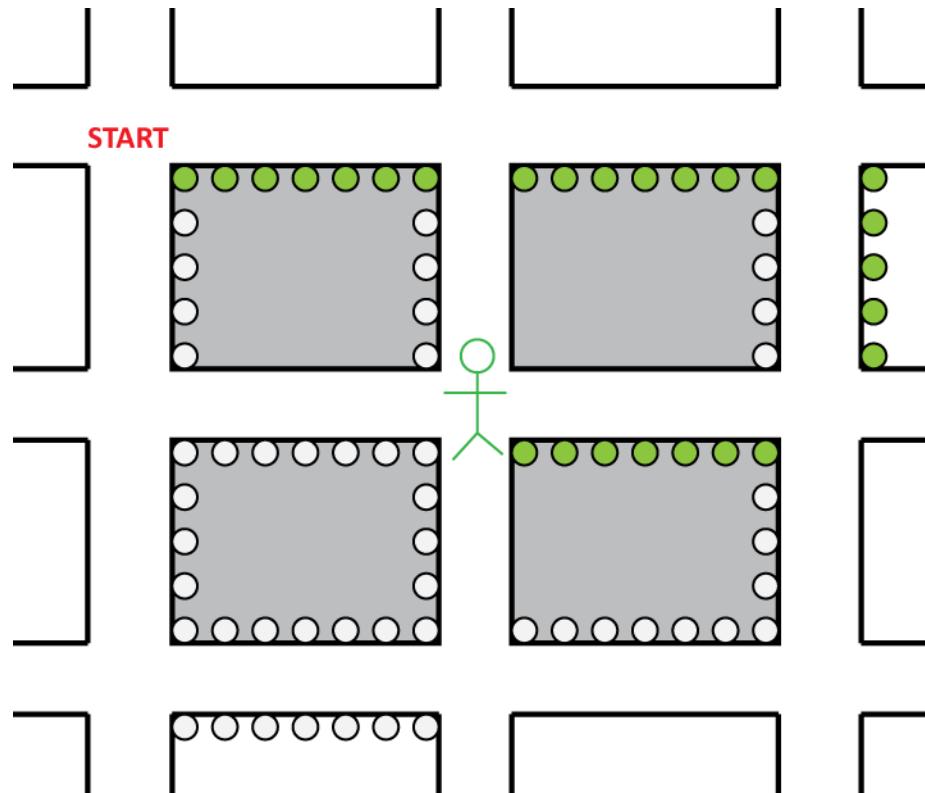
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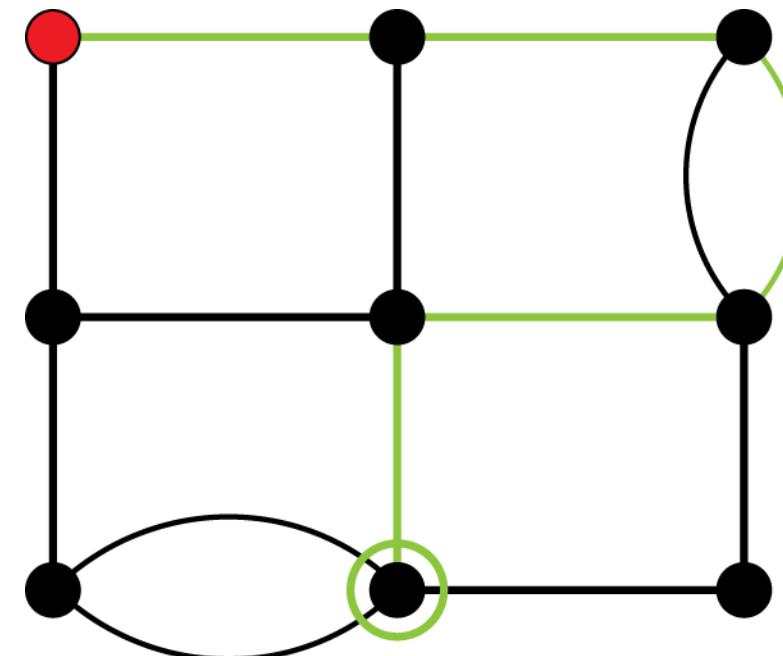
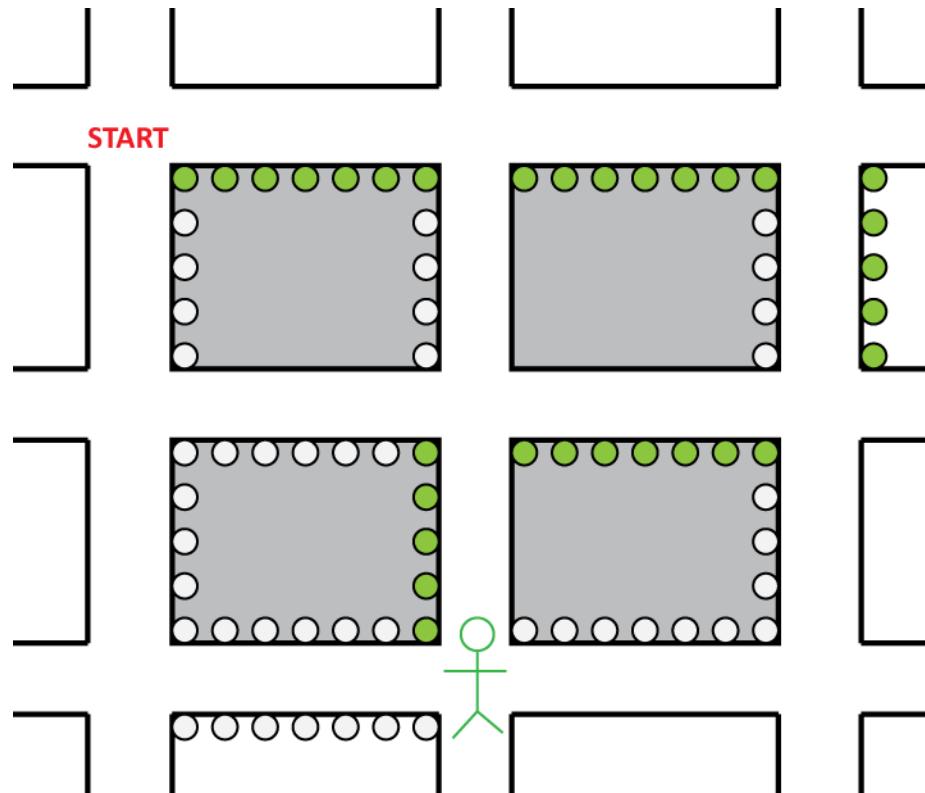
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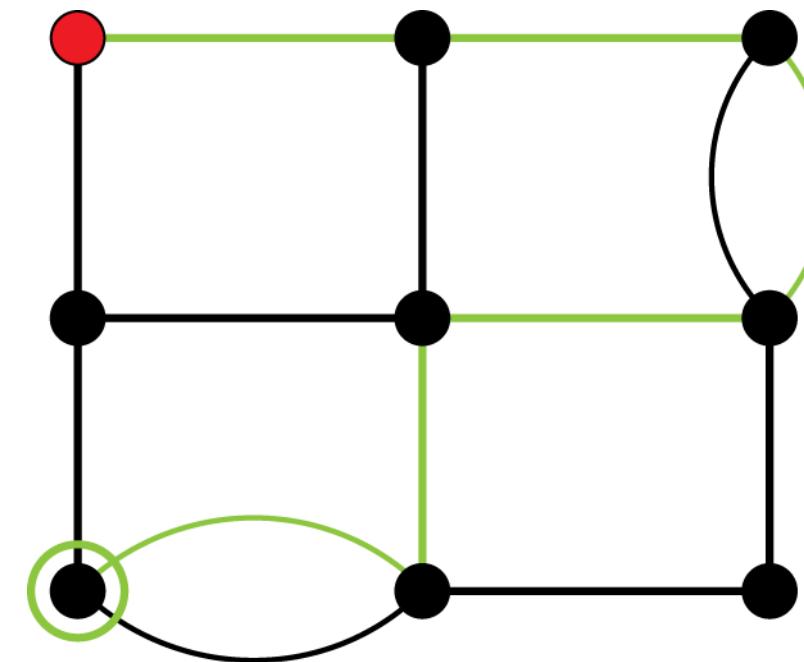
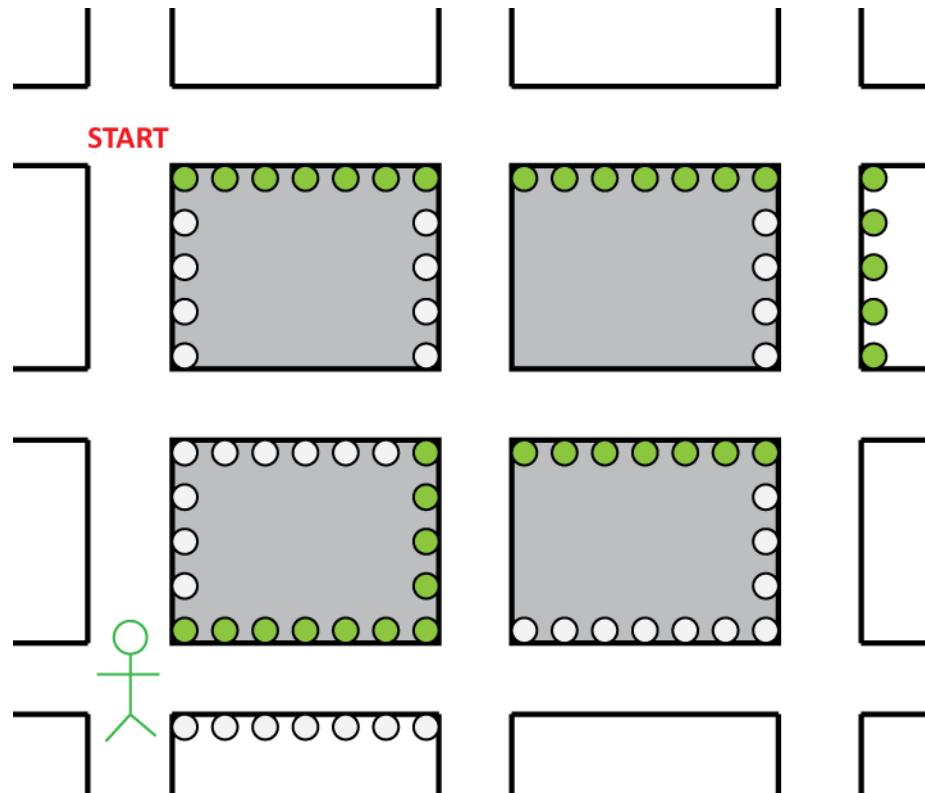
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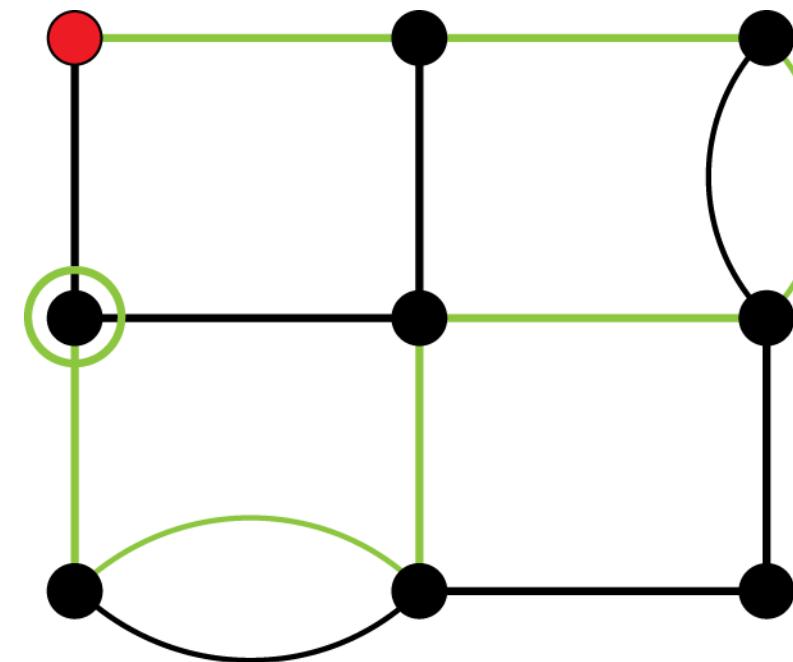
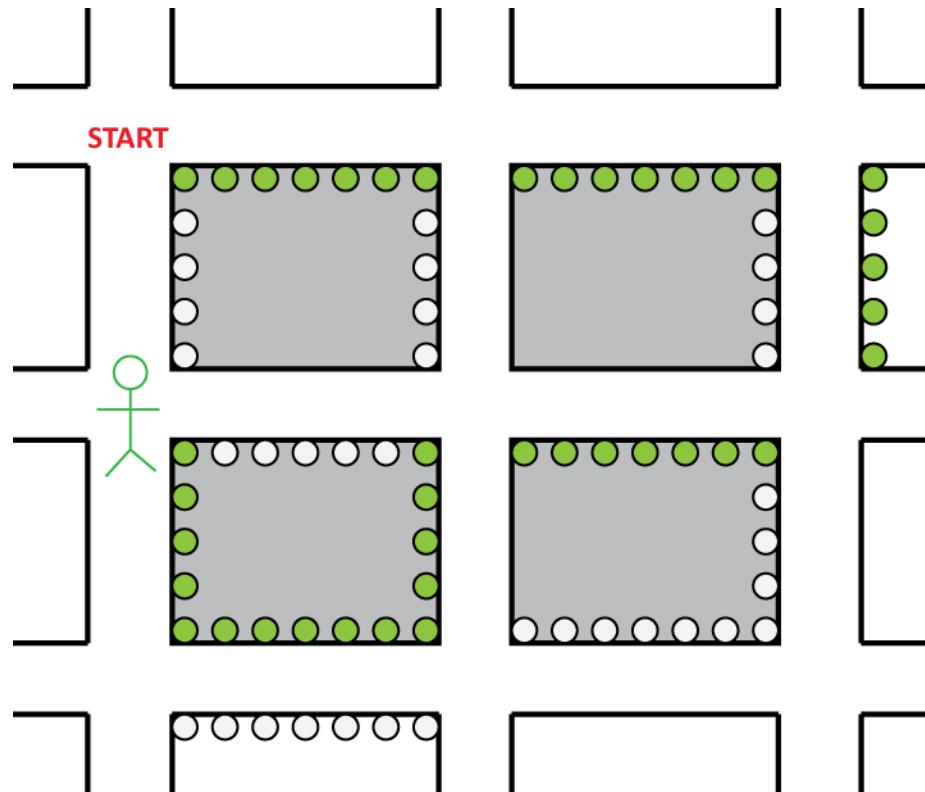
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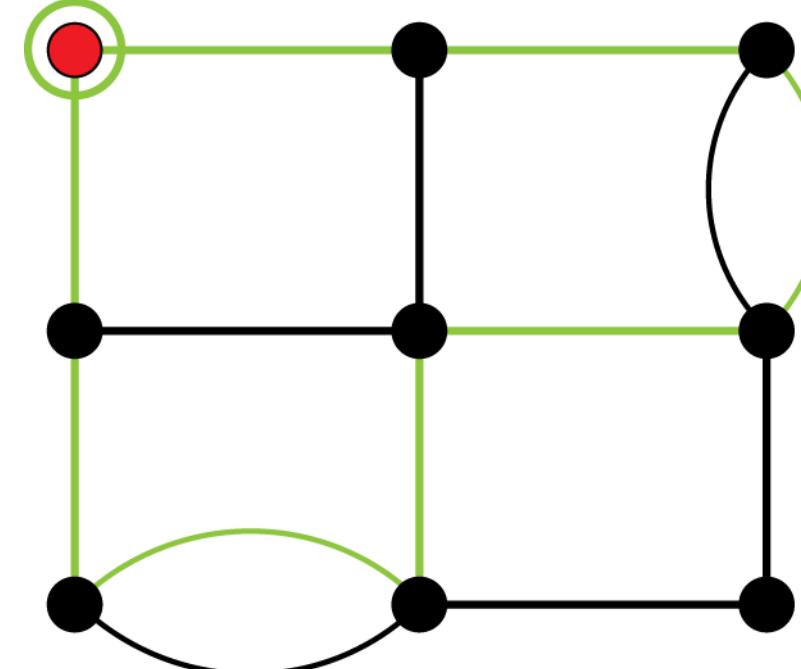
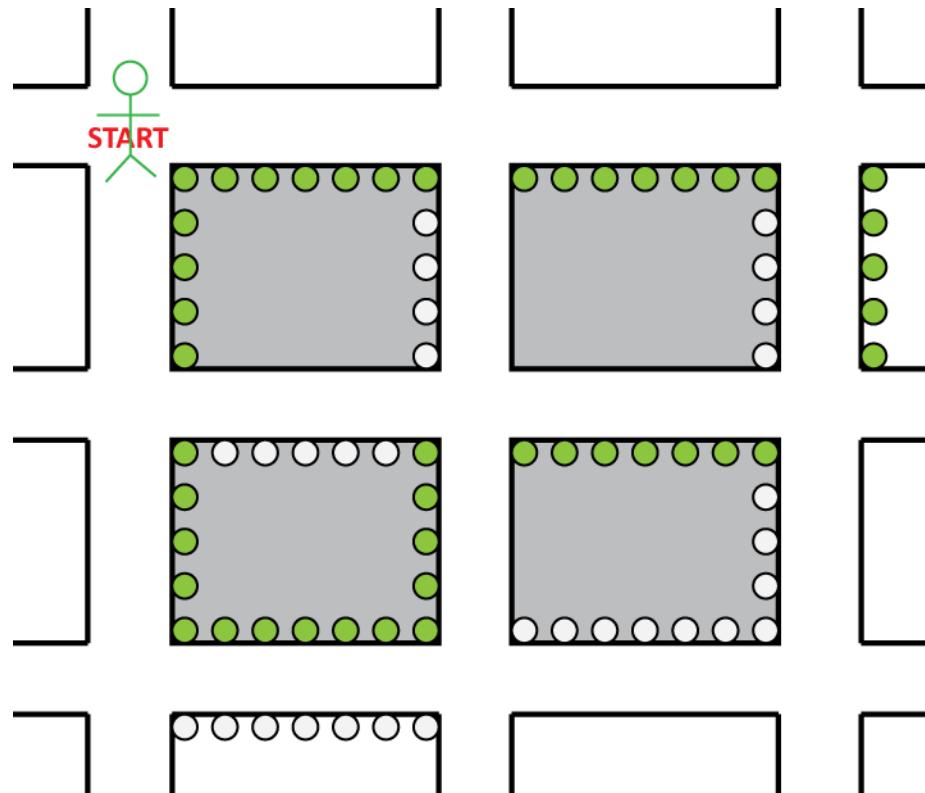
# Two Paths: Map vs. Graph



# Two Paths: Map vs. Graph



# Two Paths: Map vs. Graph



# From Now On: Graphs Only

- From now on, we will only use graphs to study these kinds of problems
- We will eventually learn how to tell which graphs have solutions to the parking meter problem and which do not
- For now, we'll establish some vocabulary and practice creating graphs

# Definitions

- A **path** is a sequence of vertices that are connected by edges. A path can repeat the same edge or vertex multiple times, and doesn't have to end at the same place it begins.
- A **circuit** is a path that ends at the same place it begins.

# Definitions

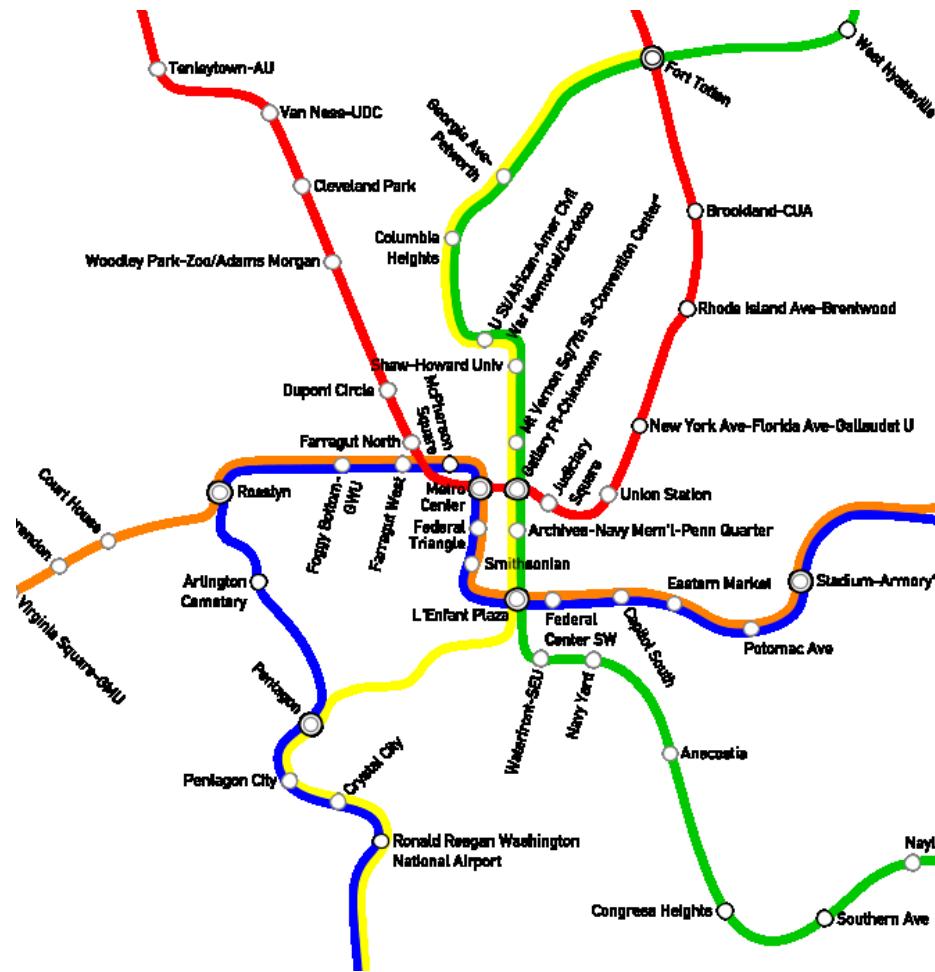
- An **Euler circuit** is a circuit that includes every edge of the graph exactly once.
- This Euler circuit (pronounced “oiler”) is exactly what we are looking for in our parking meter problem
- It turns out there are many other kinds of problems for which we want Euler circuits

# Applications of Euler circuits

- checking parking meters
- street cleaning
- snow plowing
- mail delivery
- garbage collection
- bridge inspection
- etc.

# Applications of Euler Circuits

- Here is a map of a portion of the DC Metro system
  - This map already looks like a graph



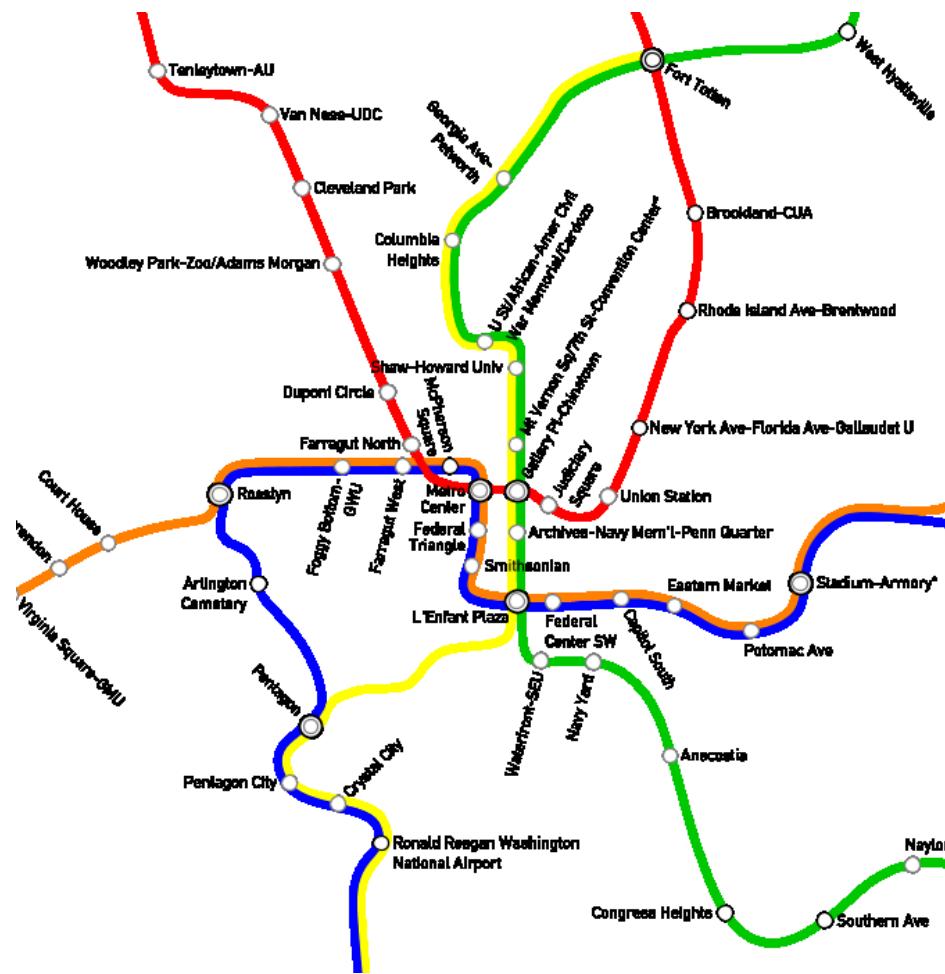
# Applications of Euler Circuits

- Each station is a vertex
- The connections between stations are edges



# Applications of Euler Circuits

- A maintenance worker might need to inspect every tunnel in the system and return to his/her starting point and minimize retracing



# Applications of Euler Circuits

- Here is a map of some of the bridges in New York City

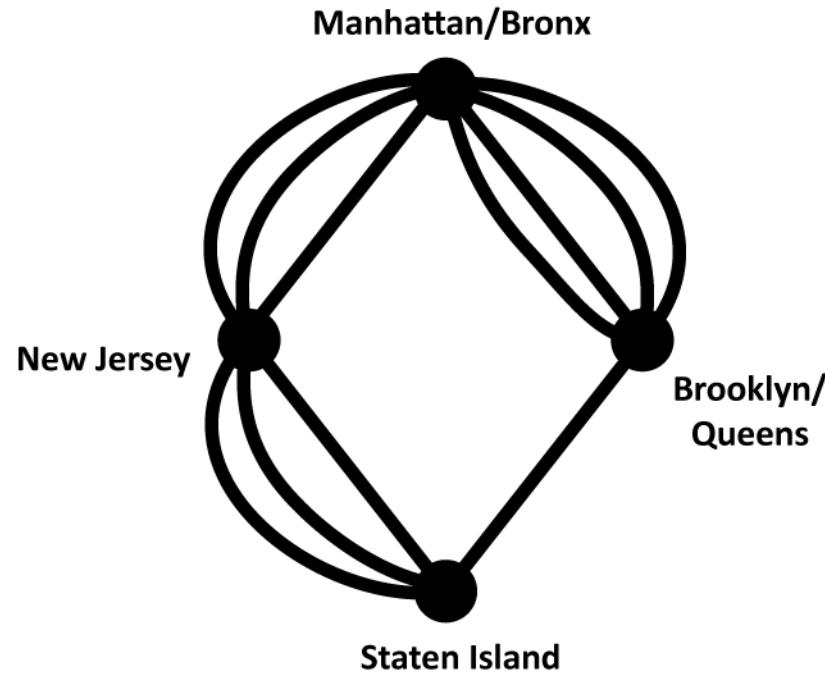


# Applications of Euler Circuits

- We can represent this system with a graph
- Each bridge is represented by an edge
- Each location is represented by a vertex



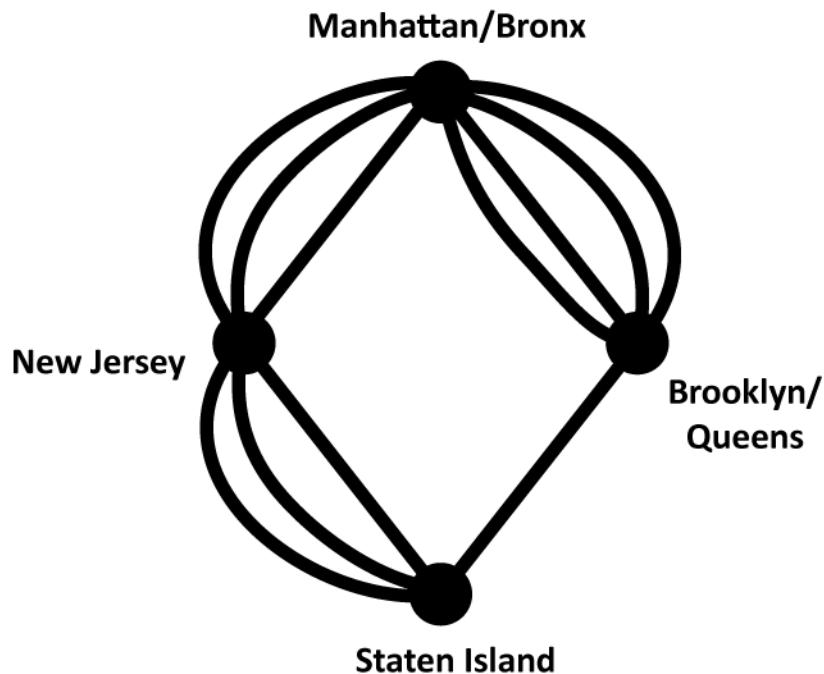
# Applications of Euler Circuits



The graph on the left represents the map on the right.

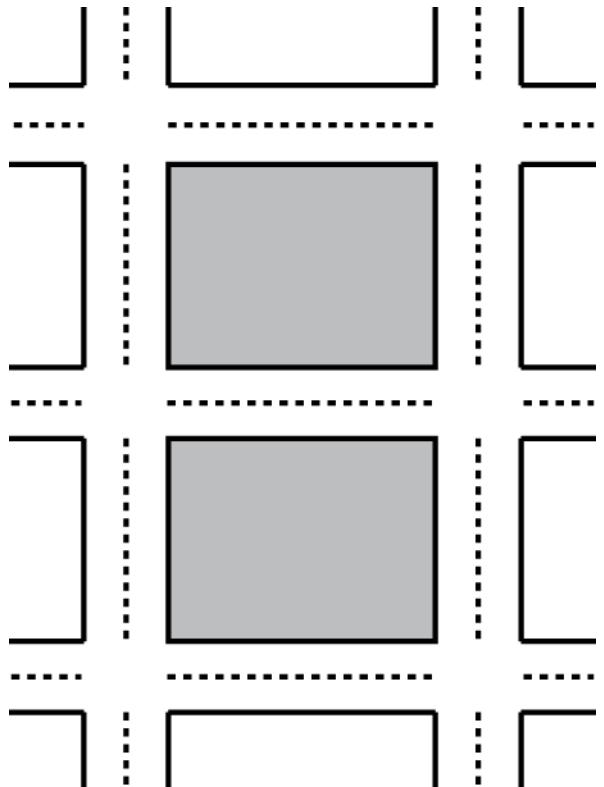


# Applications of Euler Circuits



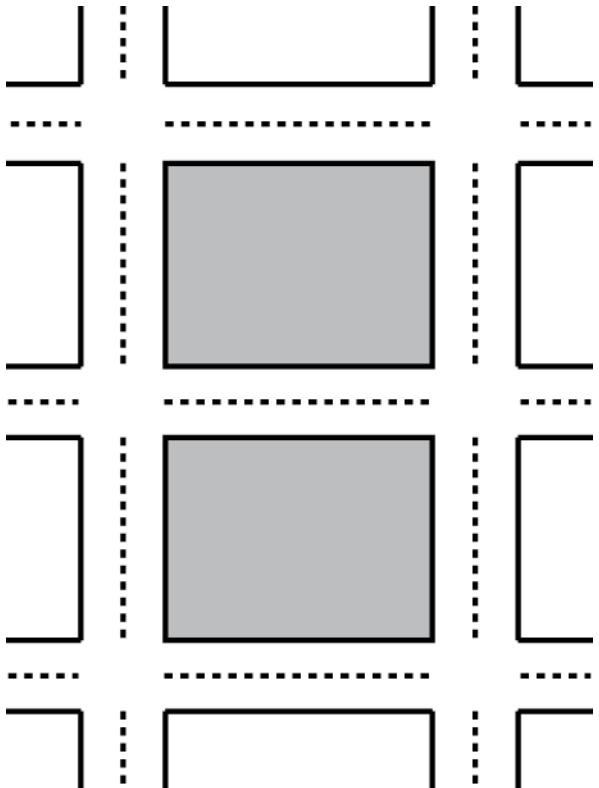
- Using this graph, we can more easily solve problems that involve traveling over these bridges
- For example, a bridge inspector might want to find an Euler circuit for this graph

# Applications of Euler Circuits



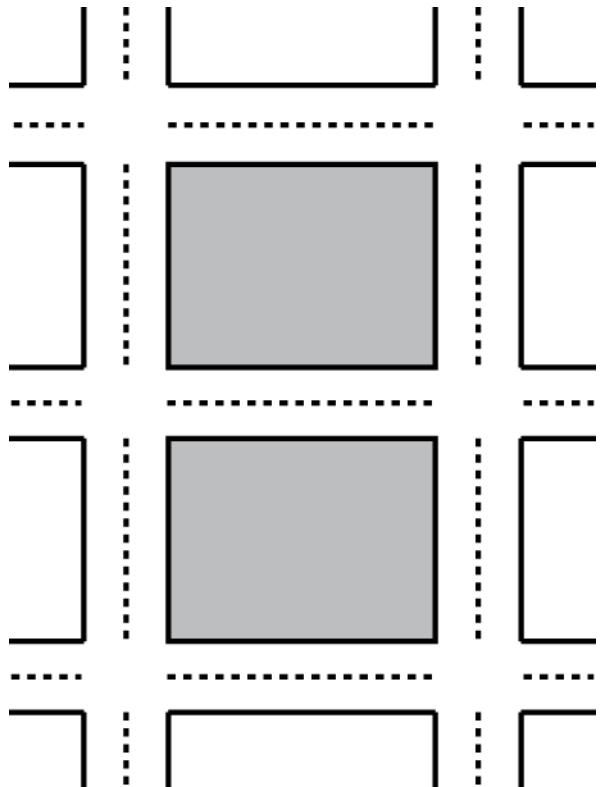
- Now consider this map of a small neighborhood
- Suppose it is your job to drive a snow plow and clean the streets of this neighborhood after a snowstorm

# Applications of Euler Circuits



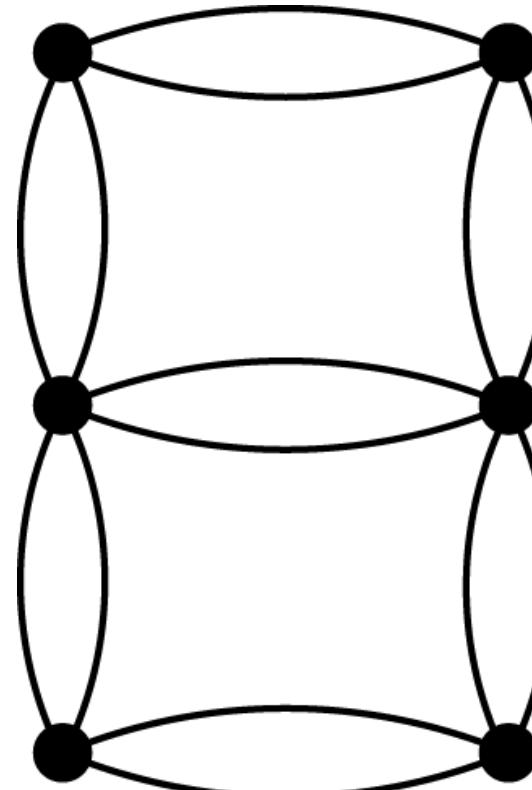
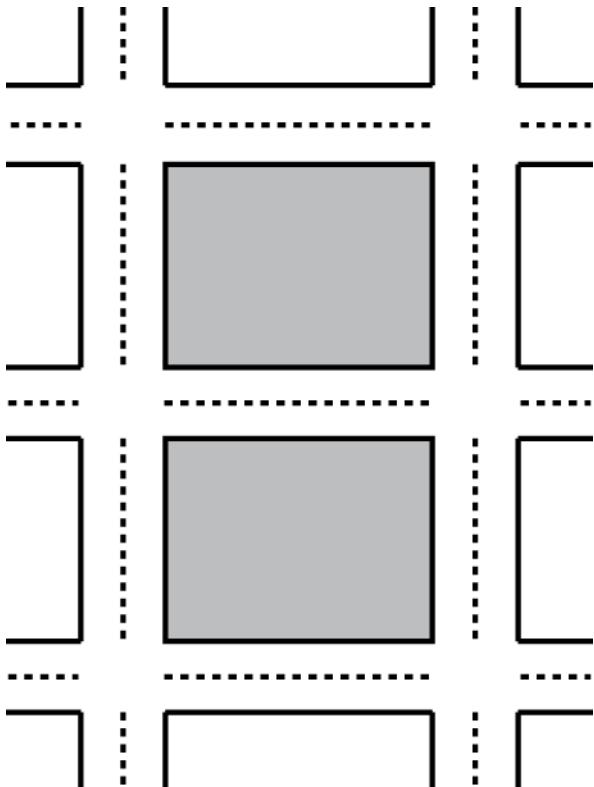
- You want to make sure to plow every lane (notice each street has 2 lanes, so you'll have to drive down each road twice)
- You don't want to retrace your steps unless you have to
- You want to return to your starting point

# Applications of Euler Circuits



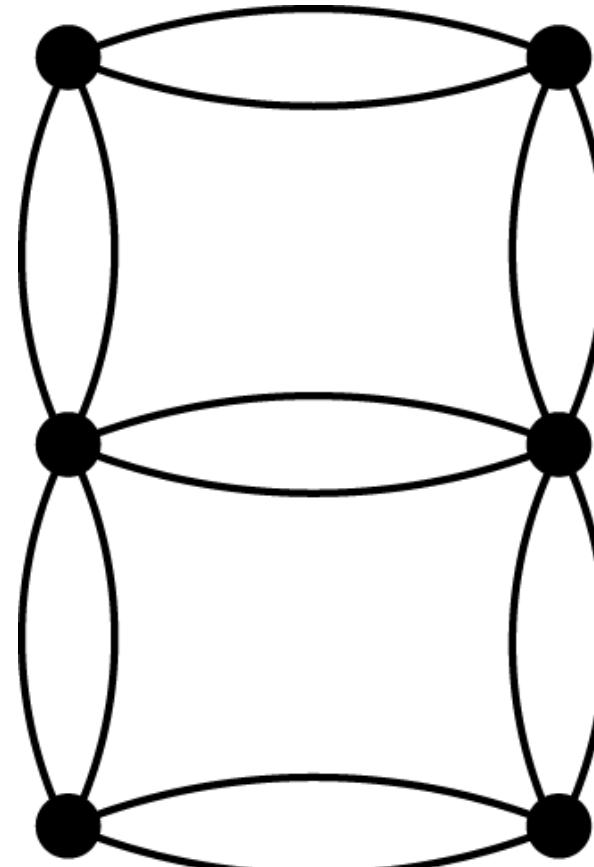
- Let's draw the graph for this problem
- Each intersection will be represented by a vertex
- Each lane will be represented by an edge

# Applications of Euler Circuits



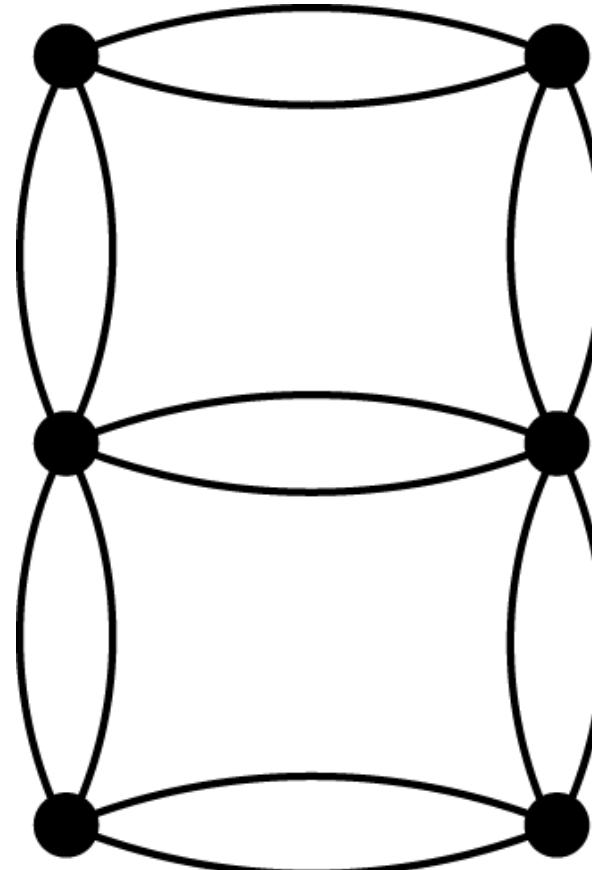
# Applications of Euler Circuits

- Can you solve the problem?
- Pick a starting point and try to find an Euler circuit for this graph

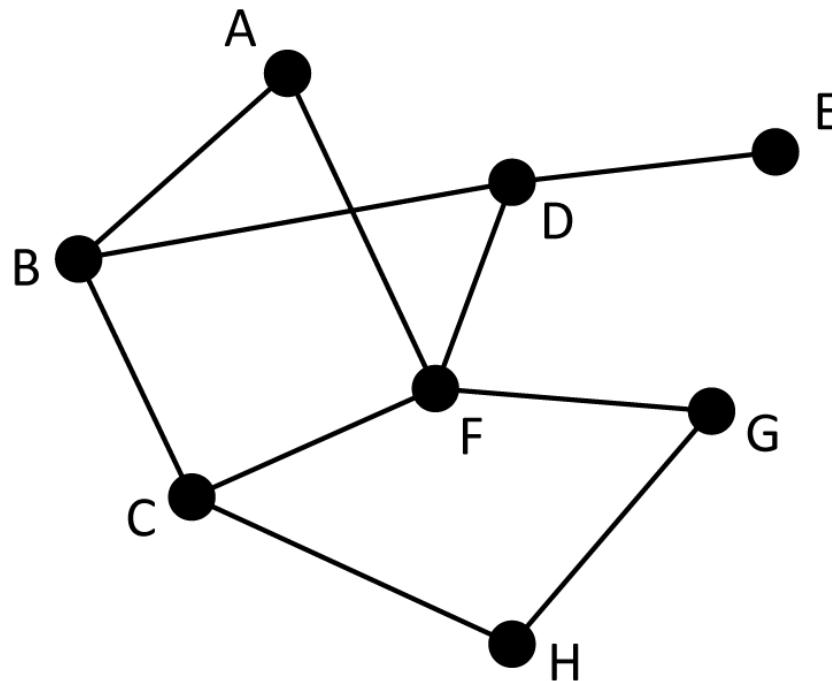


# Applications of Euler Circuits

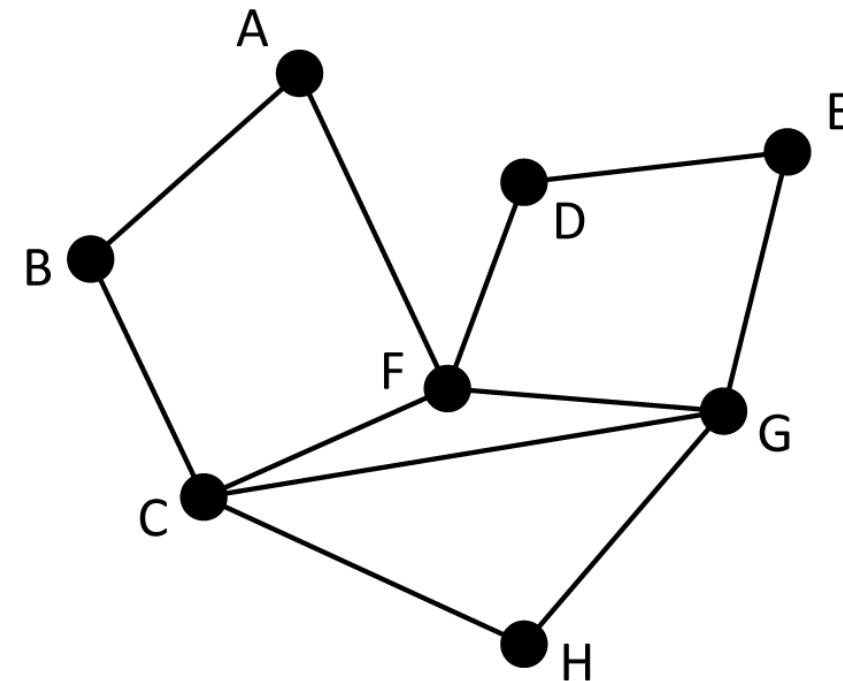
- Can you solve the problem?
- Pick a starting point and try to find an Euler circuit for this graph
- It turns out we *can* find an Euler circuit for this graph (there are lots!)



# When does a graph have an Euler circuit?



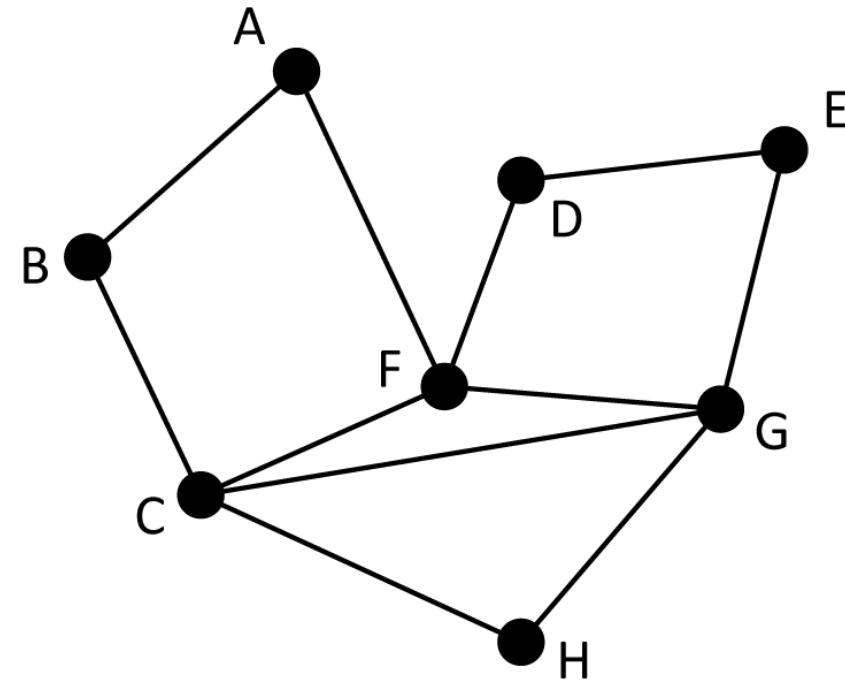
This graph **does not** have an Euler circuit.



This graph **does have** an Euler circuit.

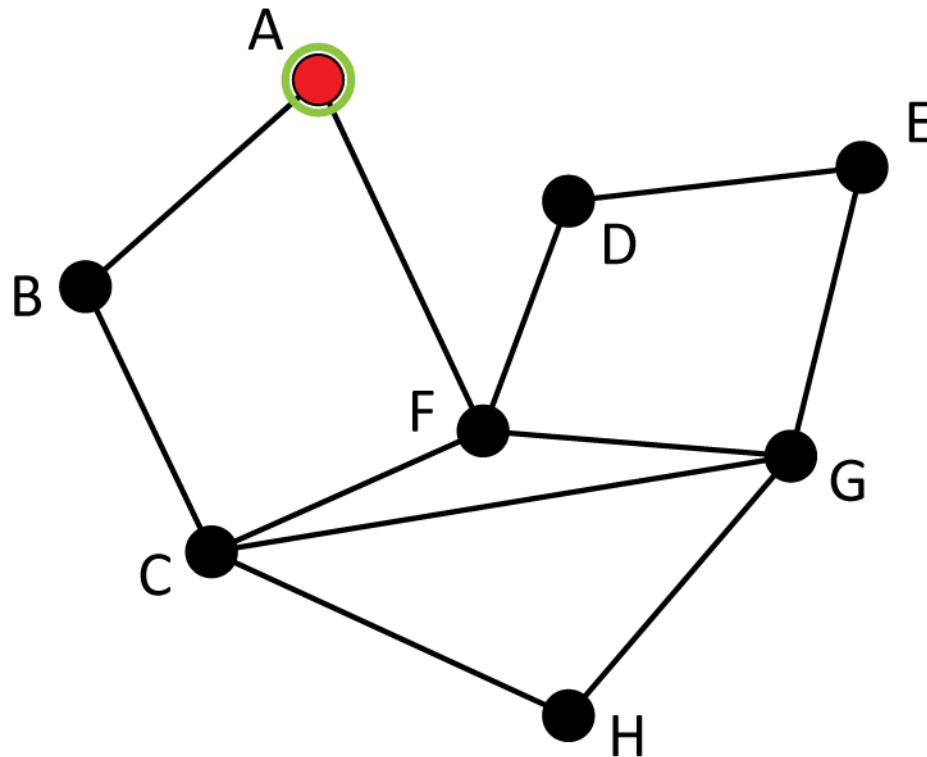
# When does a graph have an Euler circuit?

- How could I convince you that this graph has an Euler circuit?
- I can show it to you!

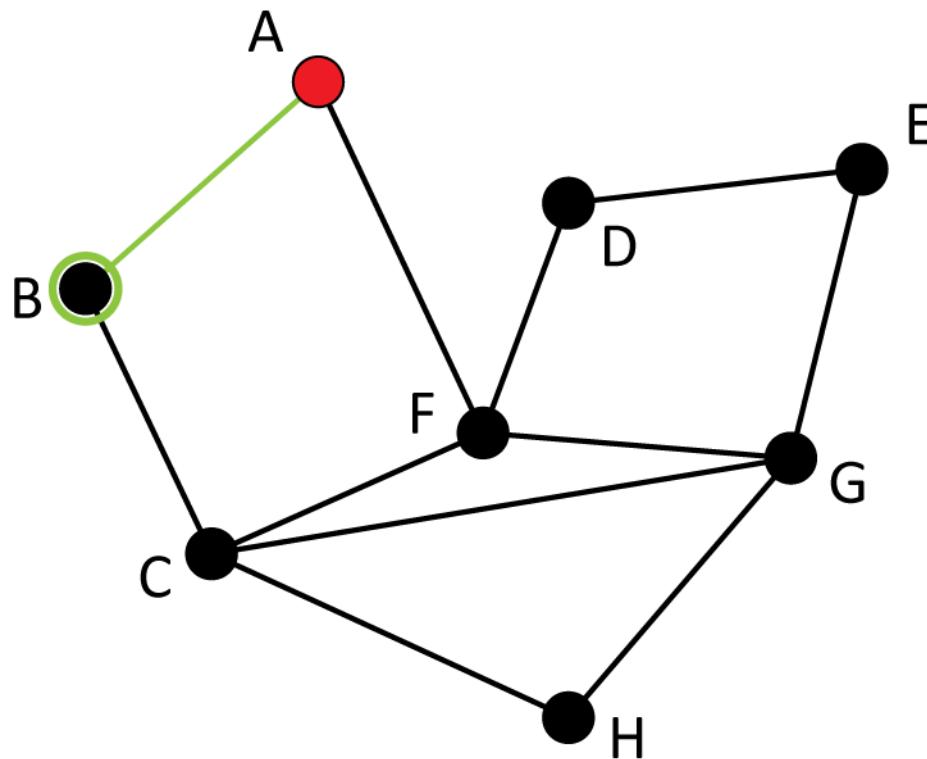


This graph **does** have an Euler circuit.

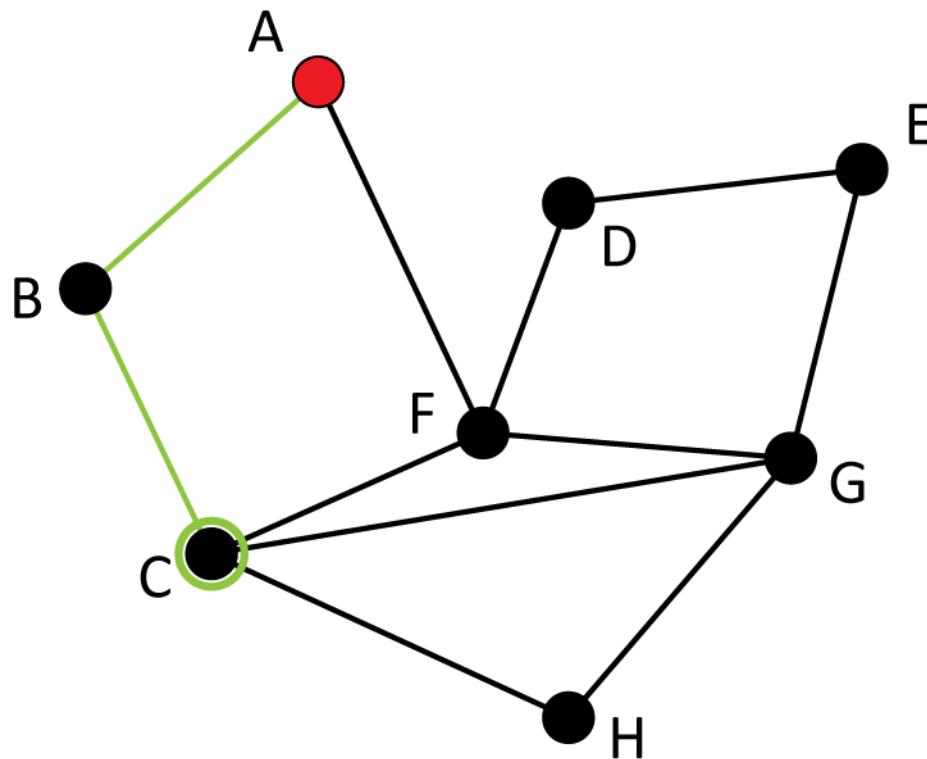
# Finding the Euler Circuit



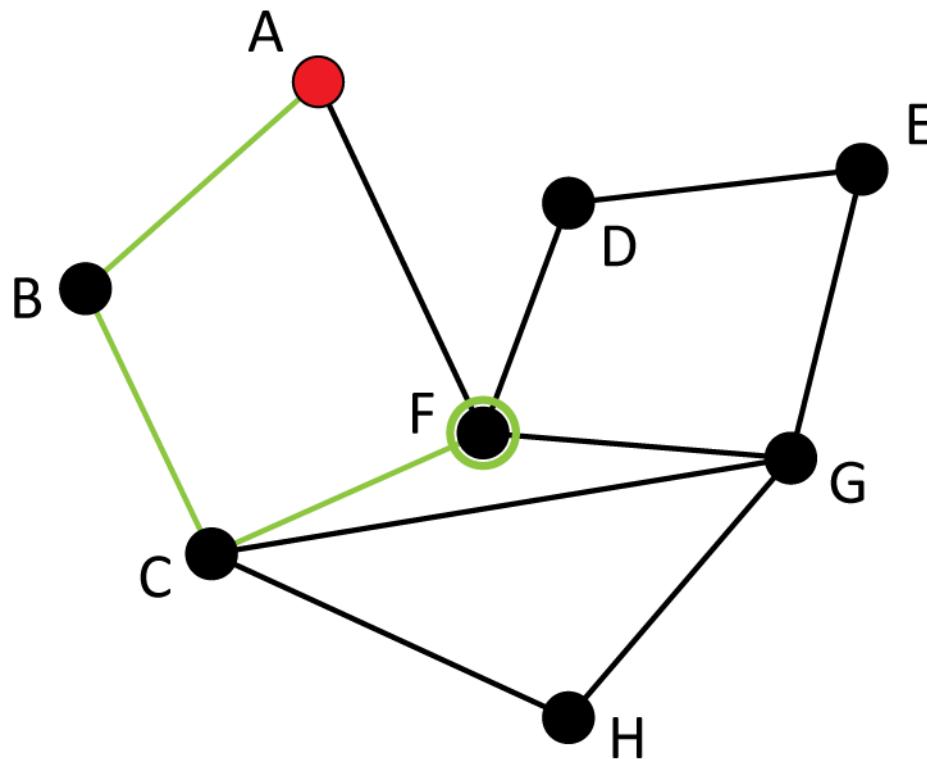
# Finding the Euler Circuit



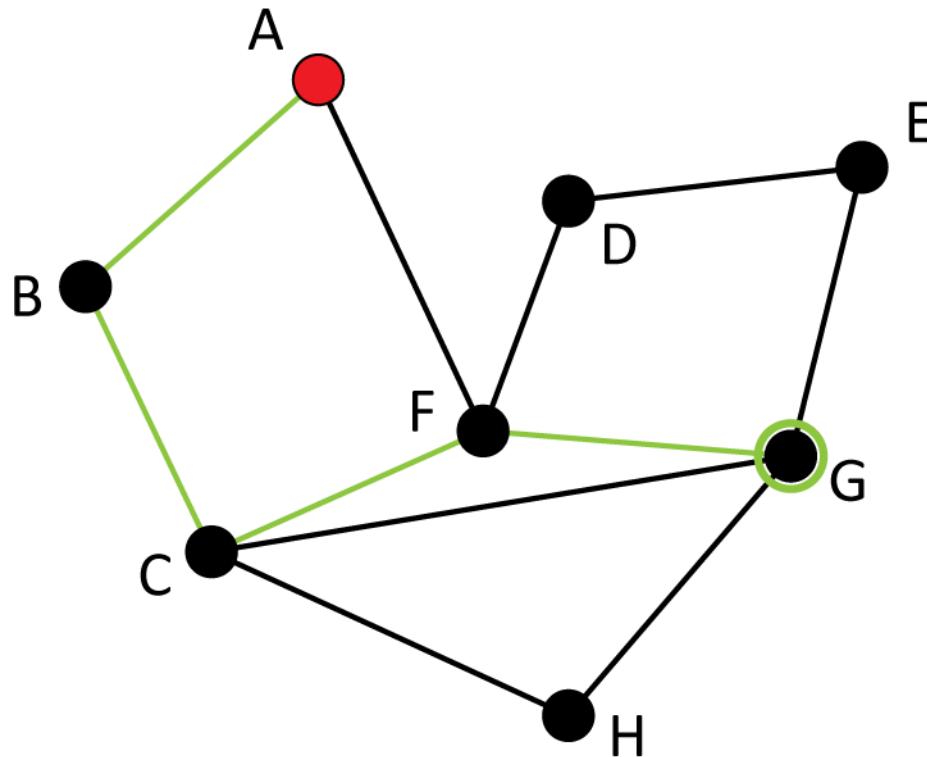
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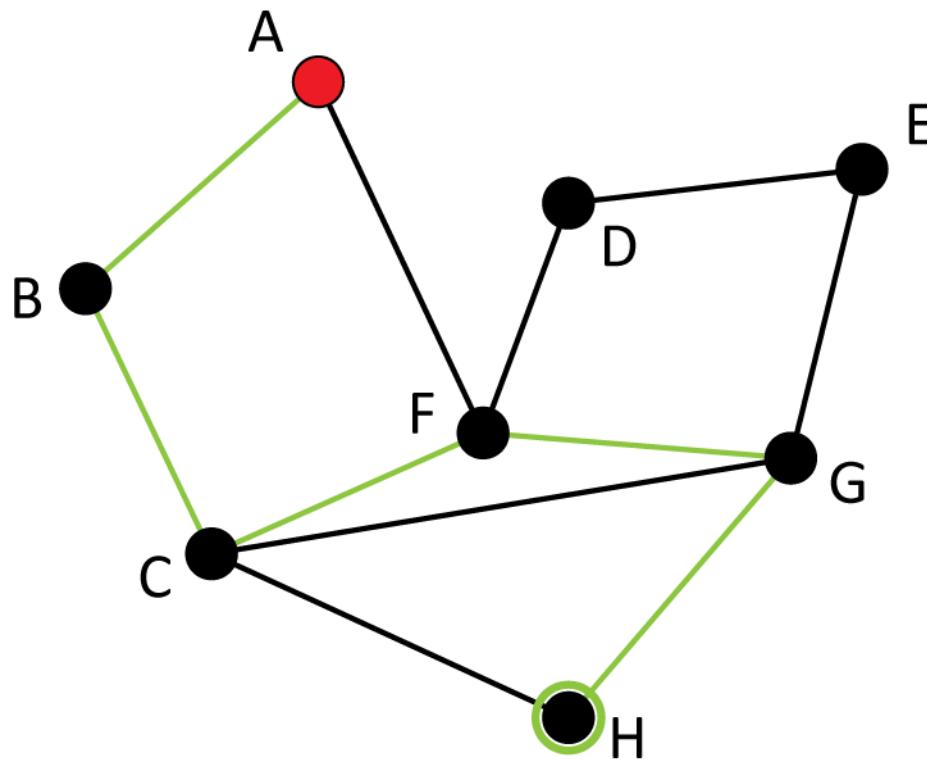
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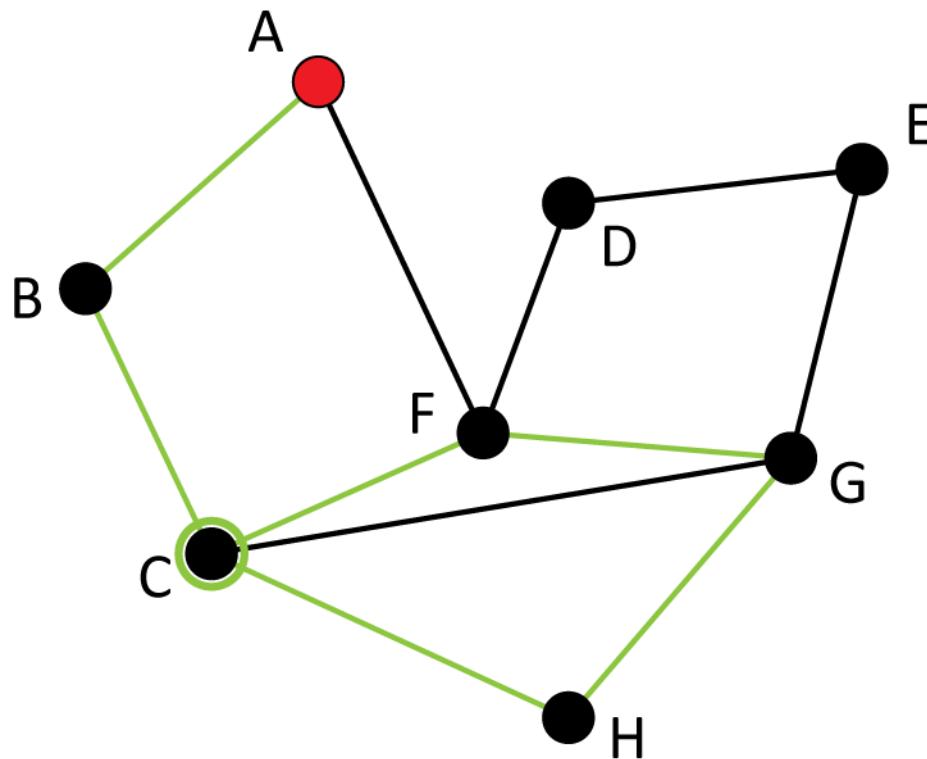
# Finding the Euler Circuit



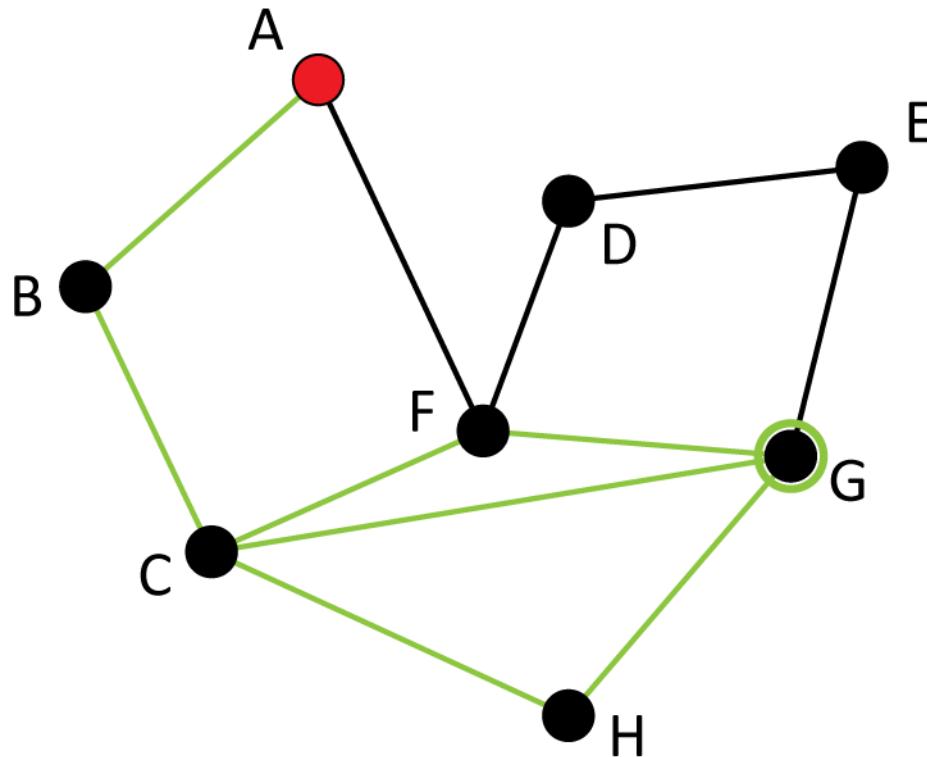
# Finding the Euler Circuit



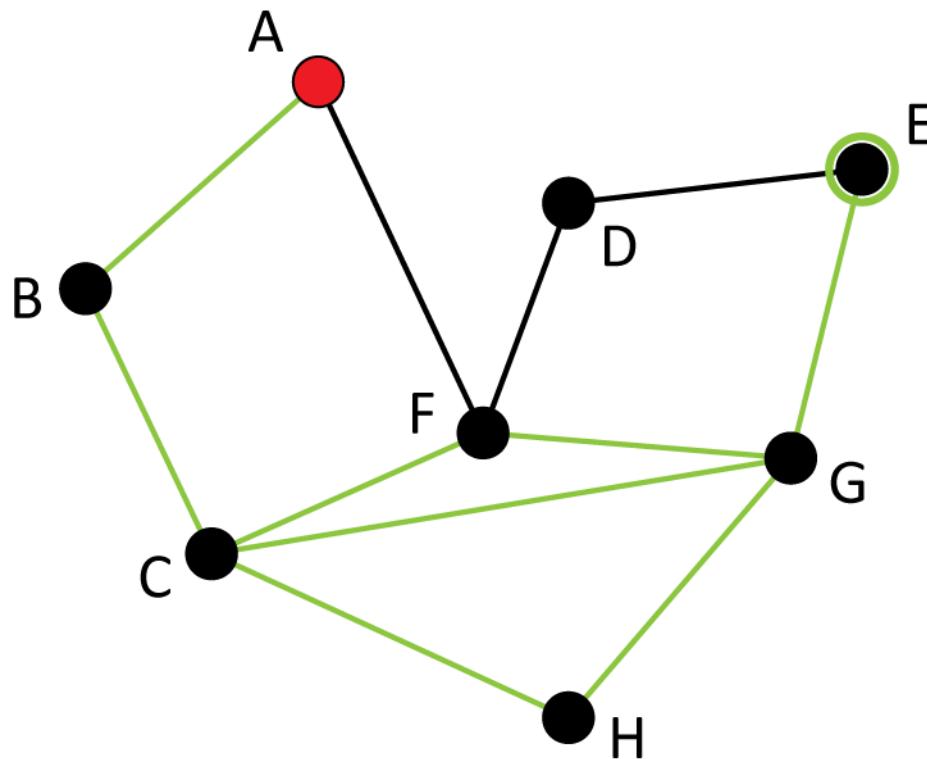
# Finding the Euler Circuit



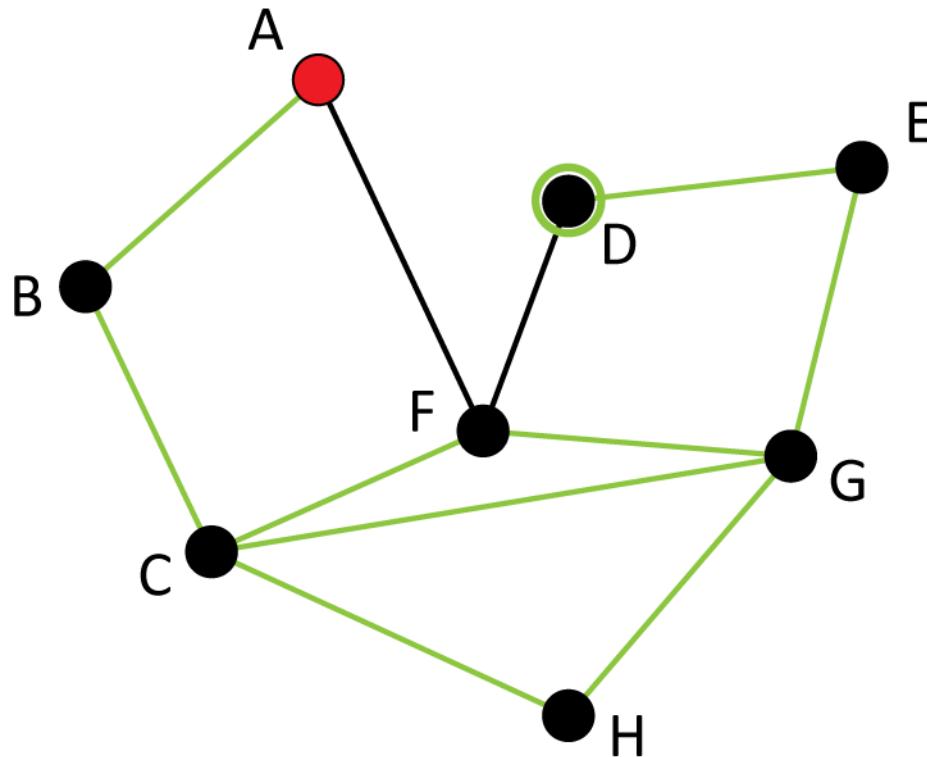
# Finding the Euler Circuit



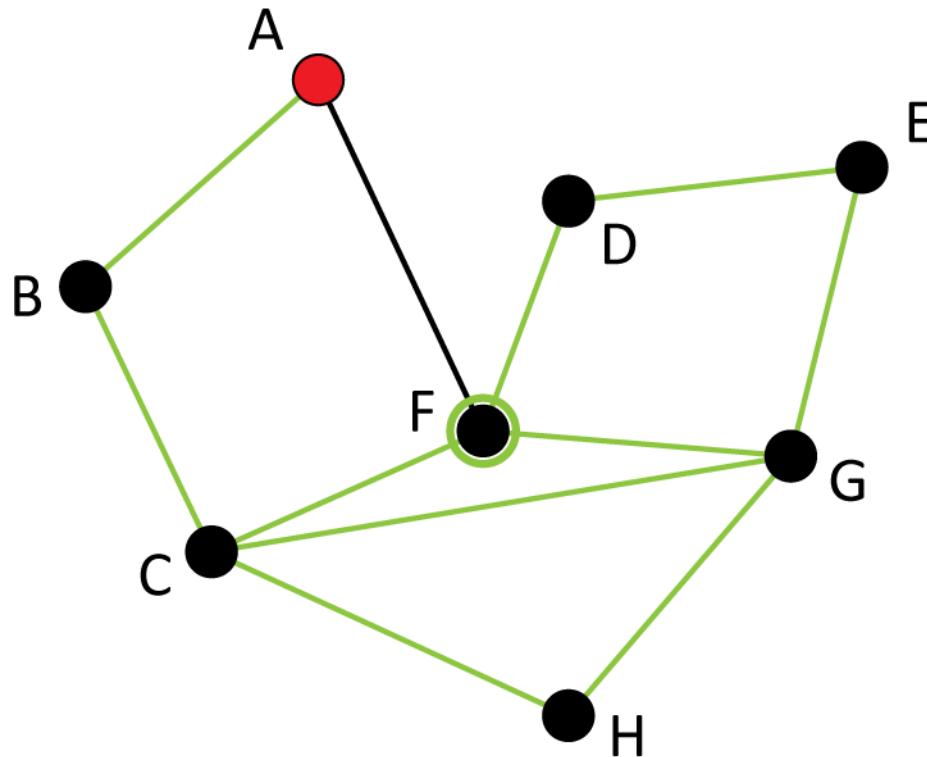
# Finding the Euler Circuit



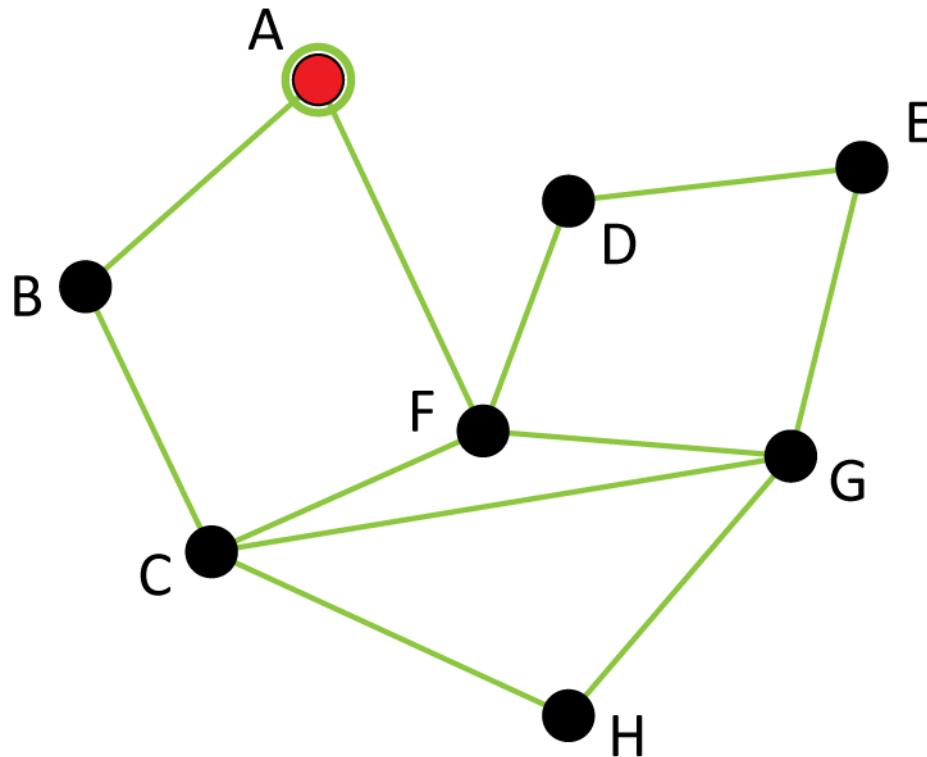
# Finding the Euler Circuit



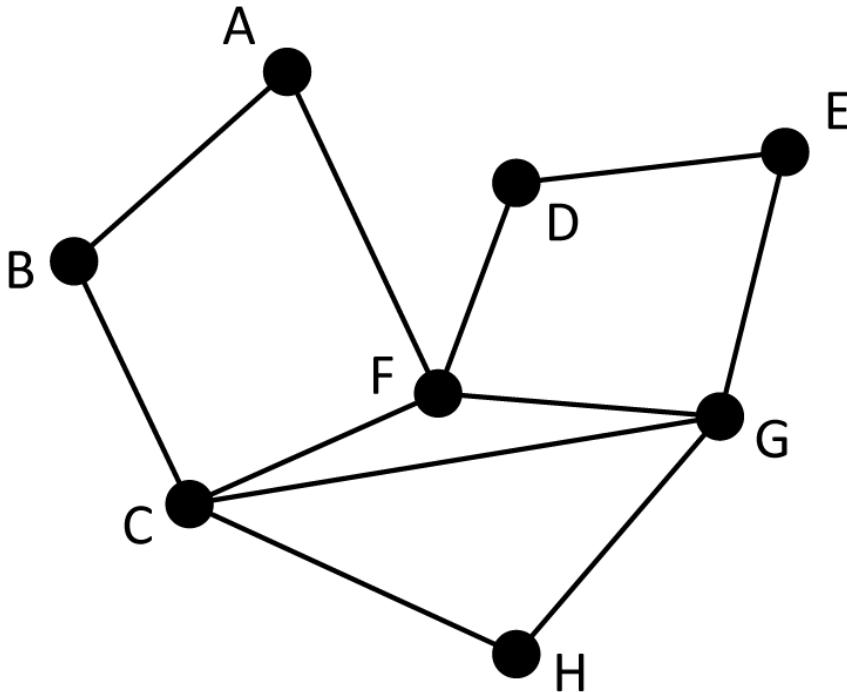
# Finding the Euler Circuit



# Finding the Euler Circuit

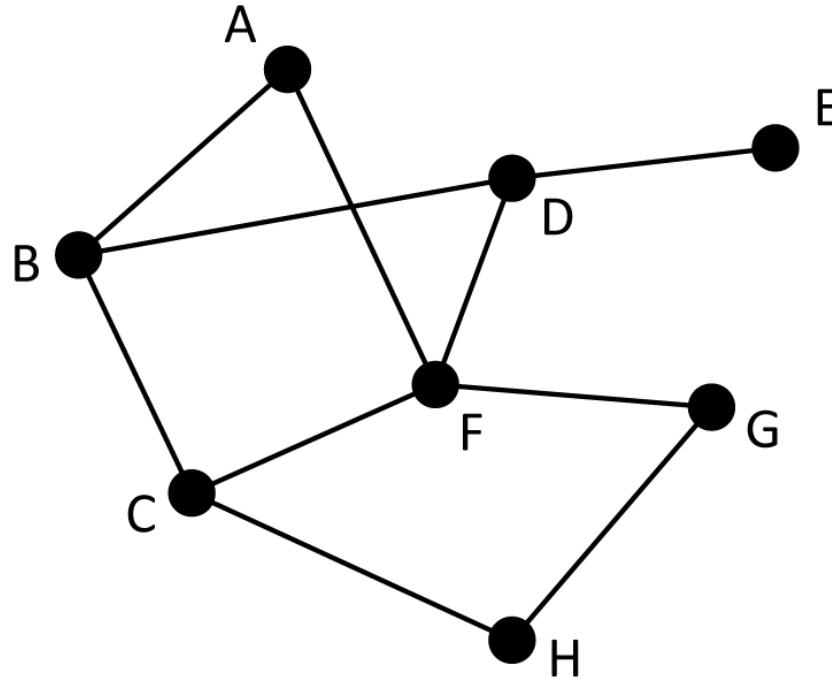


# There are lots of Euler circuits...

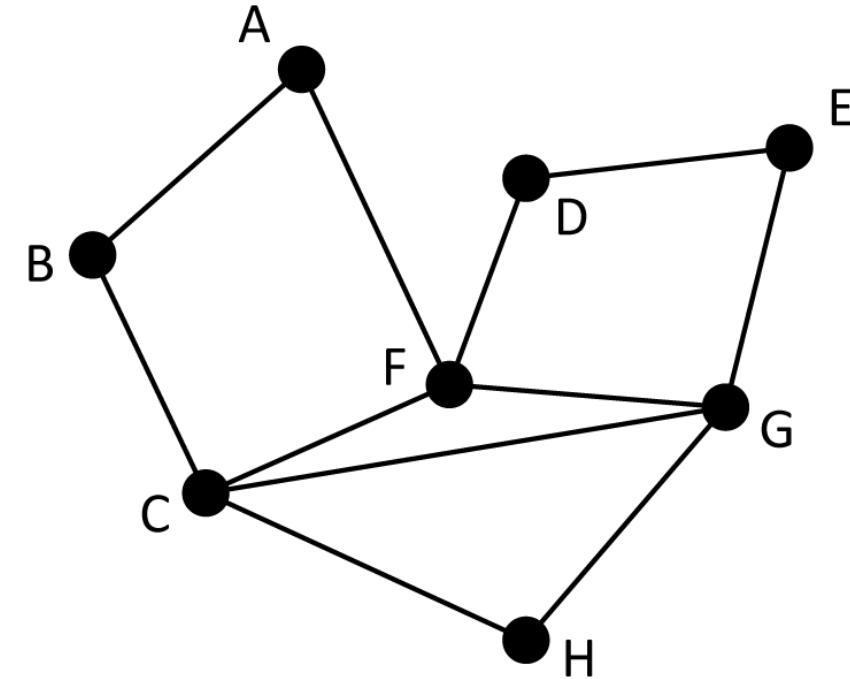


- That was just one of the many Euler circuits this graph has
- Take a moment and try to find one on your own
- You don't have to start at A!

*Why does a graph have an Euler circuit (or not)?*



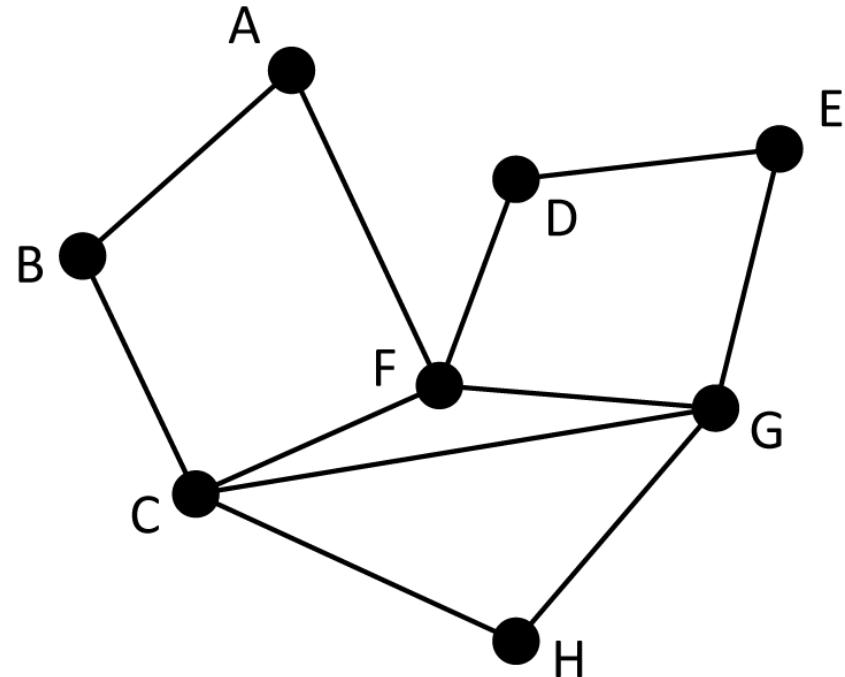
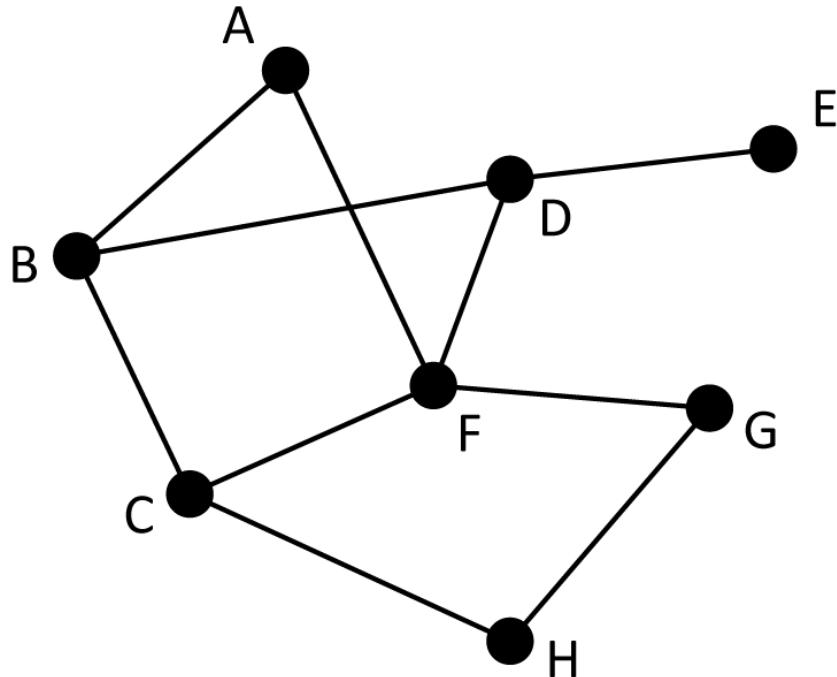
**Why** does this graph not have an Euler circuit?



**Why** does this graph have an Euler circuit?

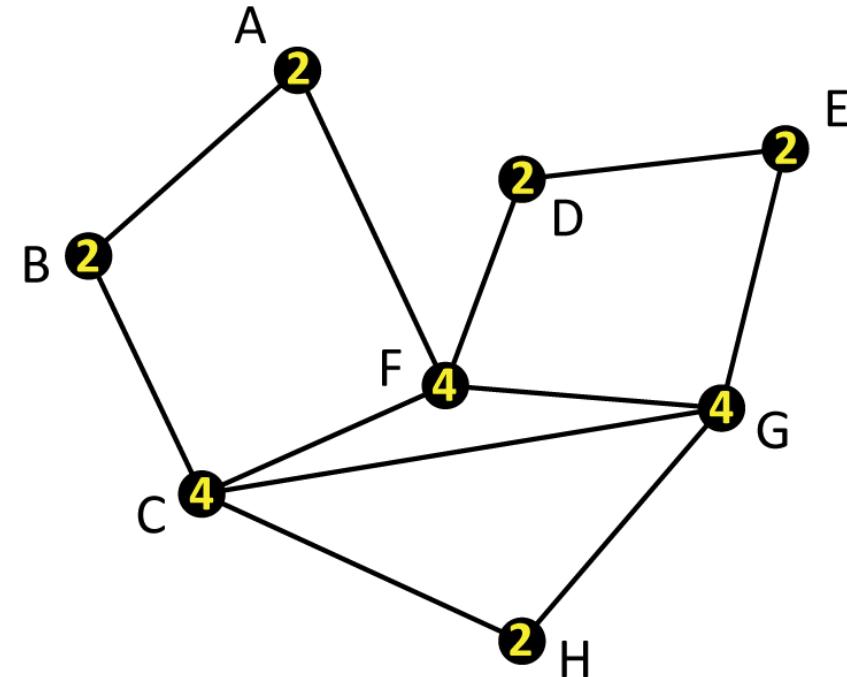
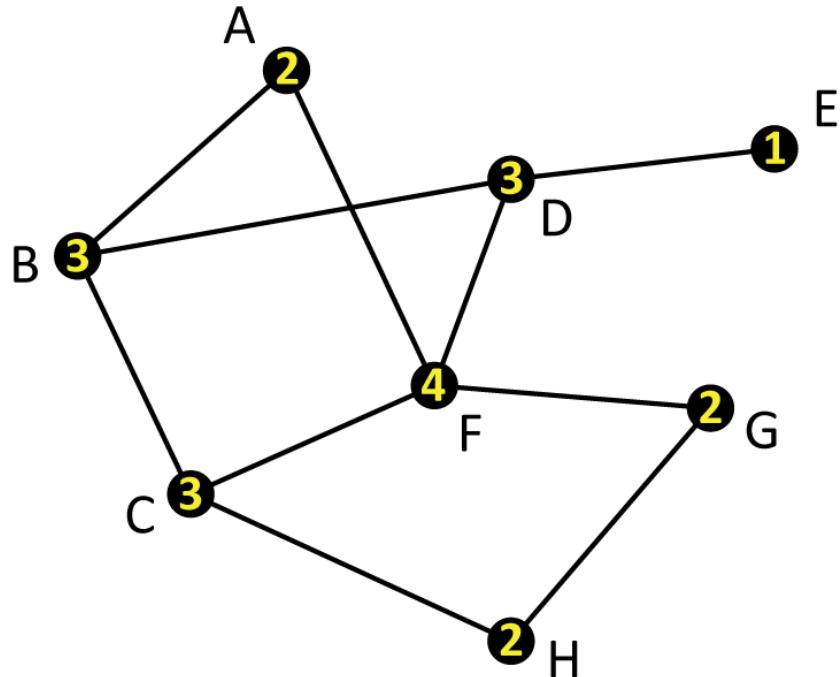
# Degree

- The **degree** of a vertex is the number of edges that meet at that vertex



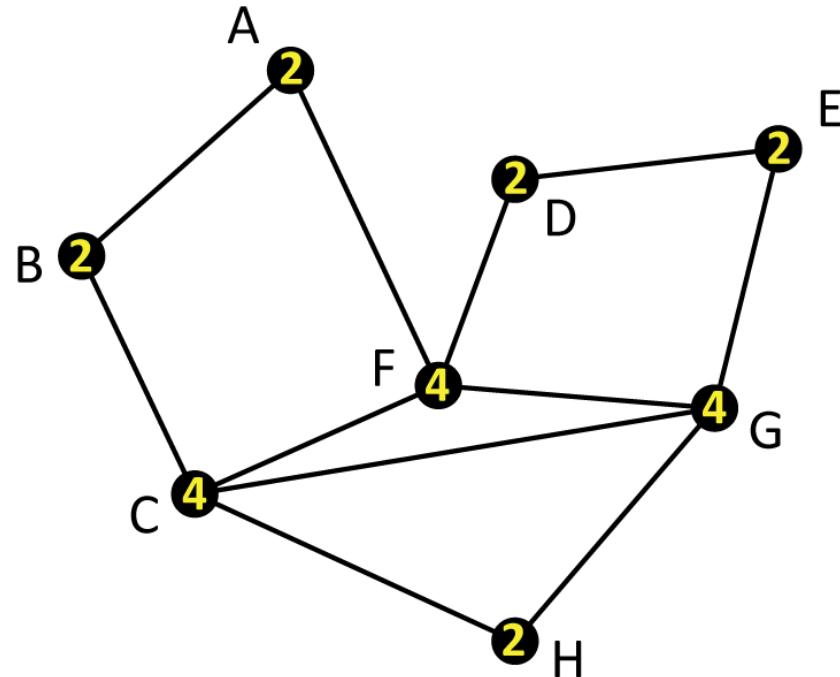
# Degree

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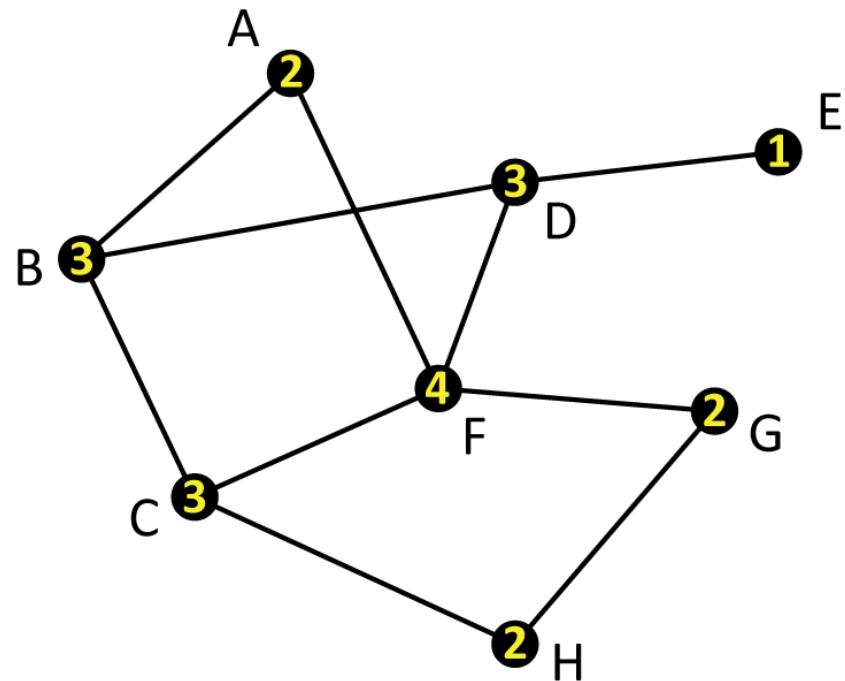
# Degree

- The **degree** of a vertex is the number of edges that meet at that vertex
- For example, in this graph, the degree of C is **4** because there are four edges (to B, to F, to G, and to H) that meet there



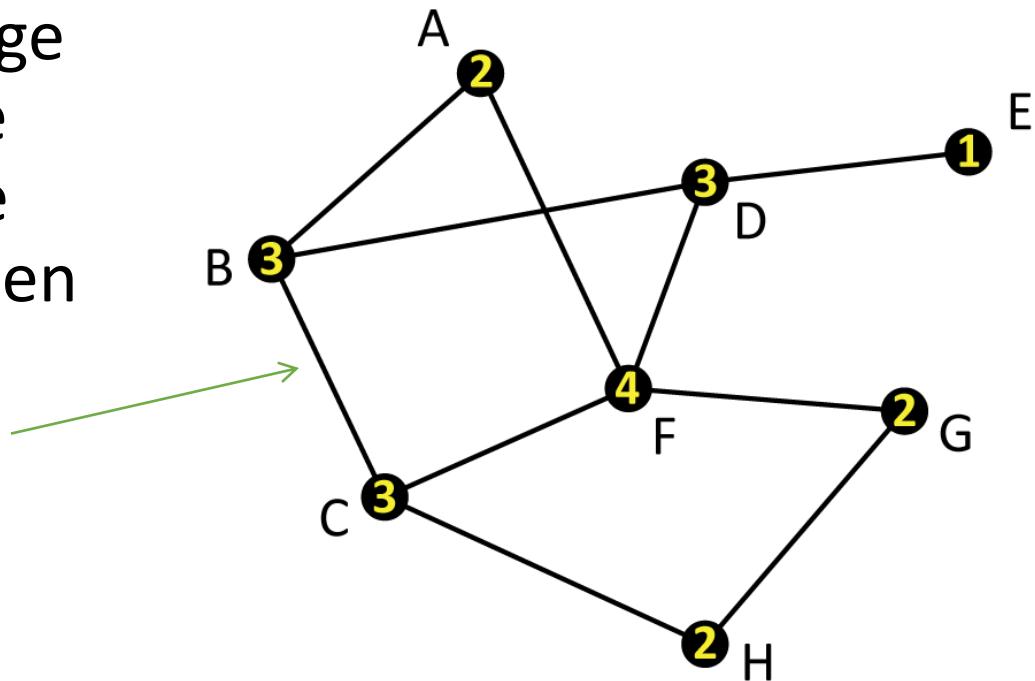
# Fact About Degrees

- Add up all the degrees in this graph
- $2+3+3+3+1+4+2+2 = 20$
- We have counted each edge twice



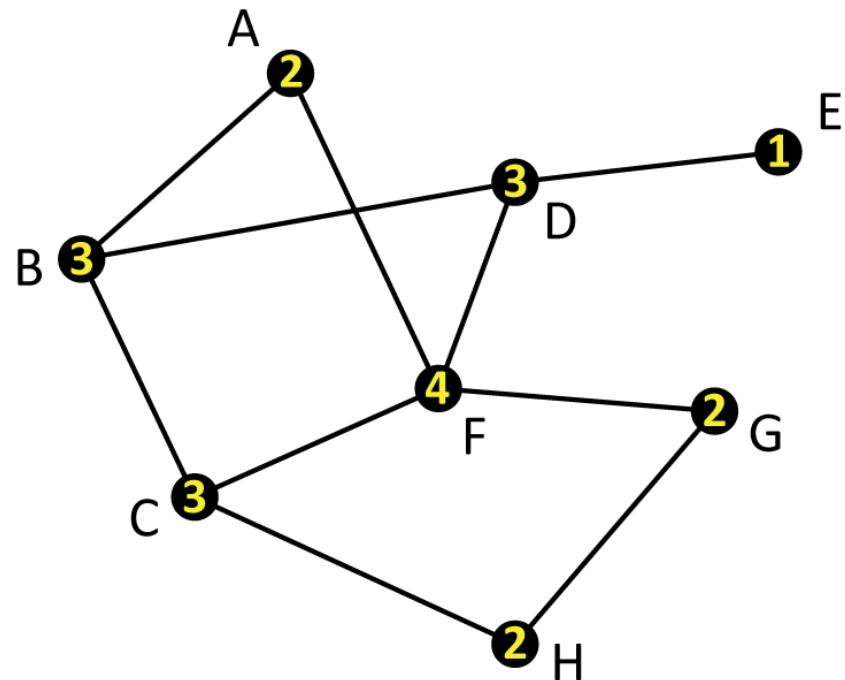
# Fact About Degrees

- We counted this edge when we added the degree of B, and we counted it again when we counted the degree of C



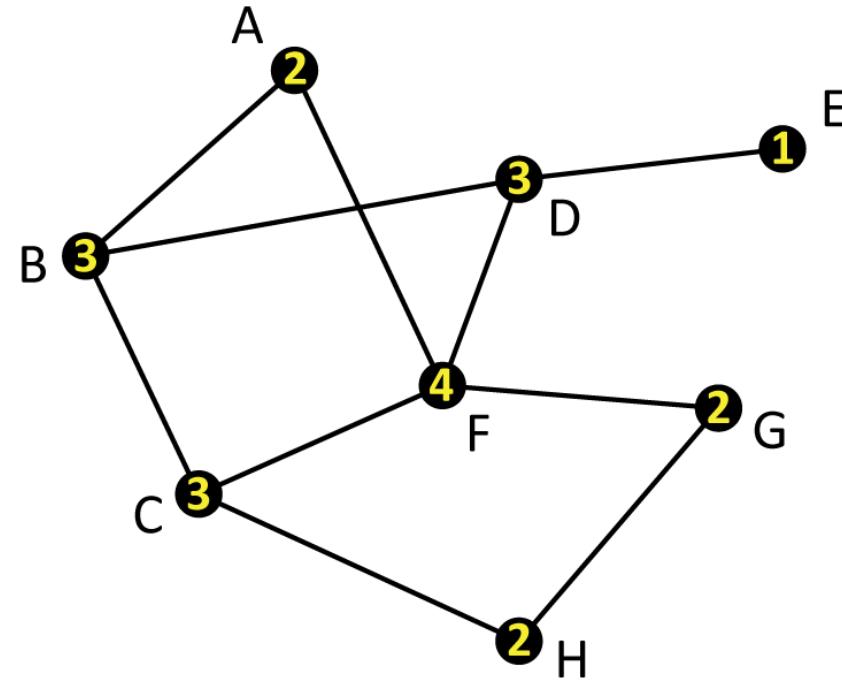
# Fact About Degrees

*The sum of all the degrees in a graph equals two times the total number of edges.*



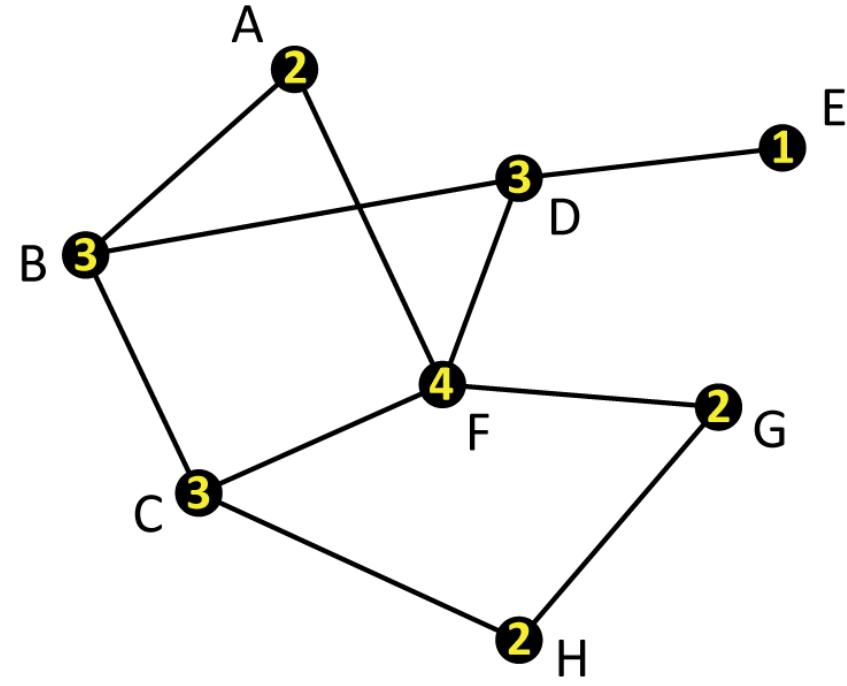
# What does degree have to do with Euler circuits?

- You might be able to tell right away that this graph can't possibly have an Euler circuit
- Why not?



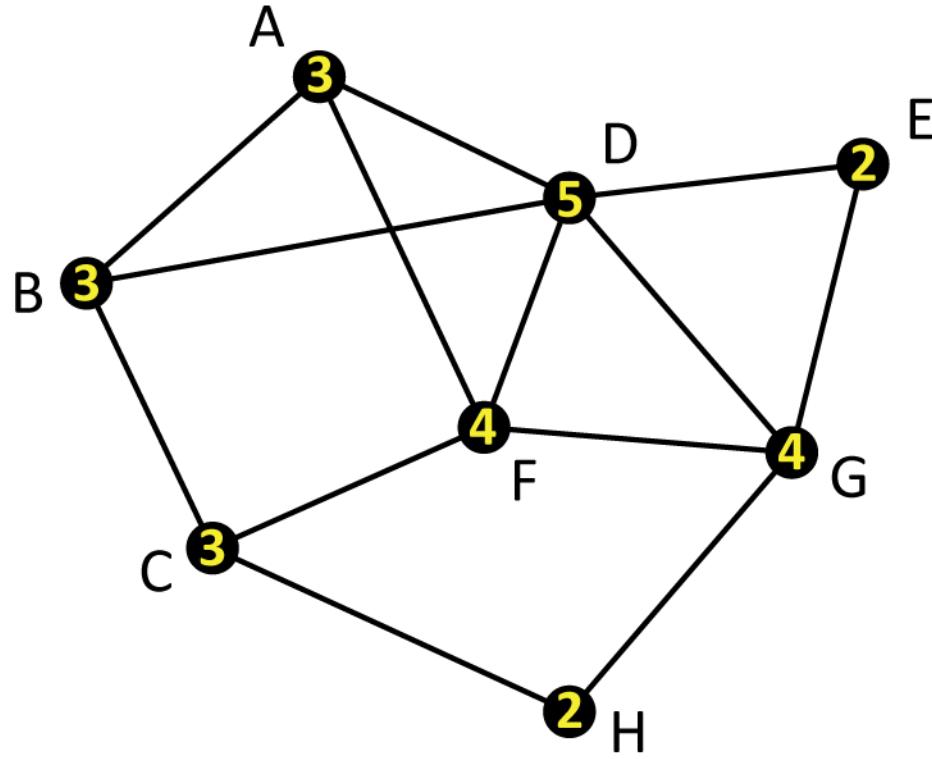
# What does degree have to do with Euler circuits?

- If a graph has a vertex with degree 1, the graph cannot have an Euler circuit
  - If we start at E, we will never be able to return to E without retracing
  - If we don't start at E, we will never be able to go there, since when we leave we will have to retrace



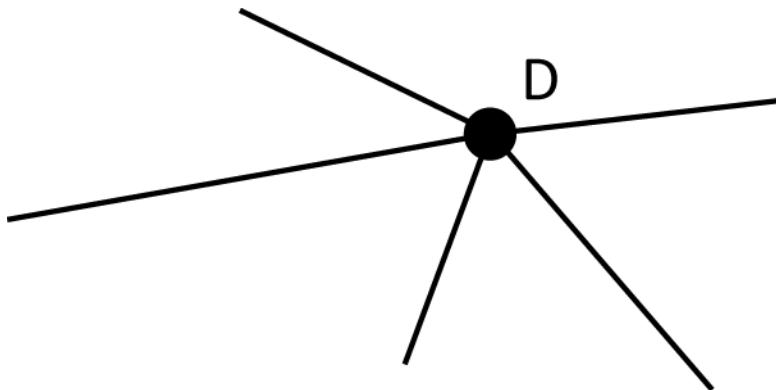
# What does degree have to do with Euler circuits?

- The problem isn't just degree 1
- This graph also doesn't have an Euler circuit
- The problem is that some of the degrees are ***odd numbers***



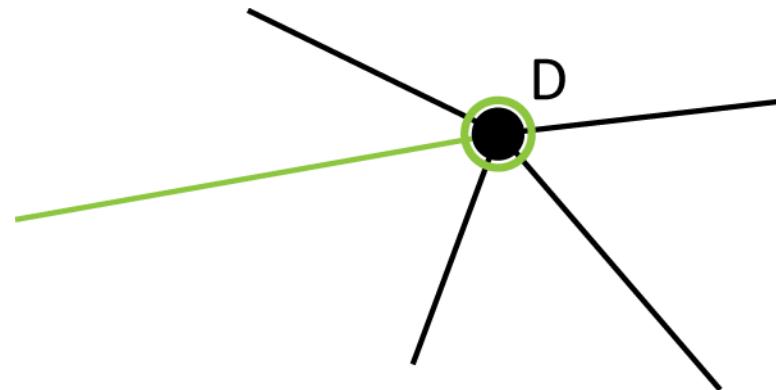
# What does degree have to do with Euler circuits?

- Let's focus on vertex D, which has degree 5
- Suppose we start elsewhere in the graph



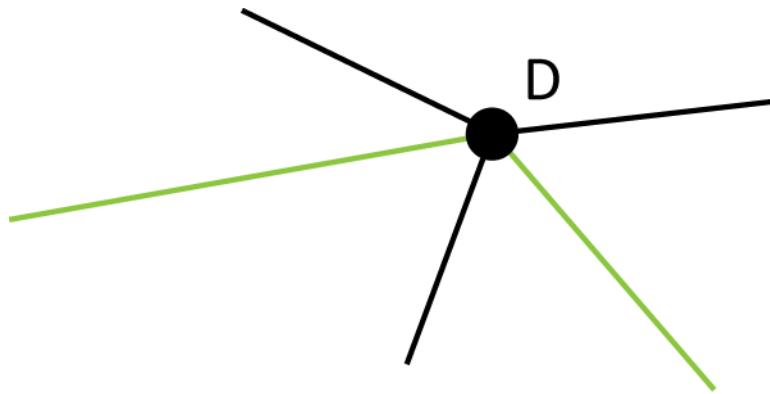
# What does degree have to do with Euler circuits?

- Since we want to cover all edges, we'll have to visit D eventually



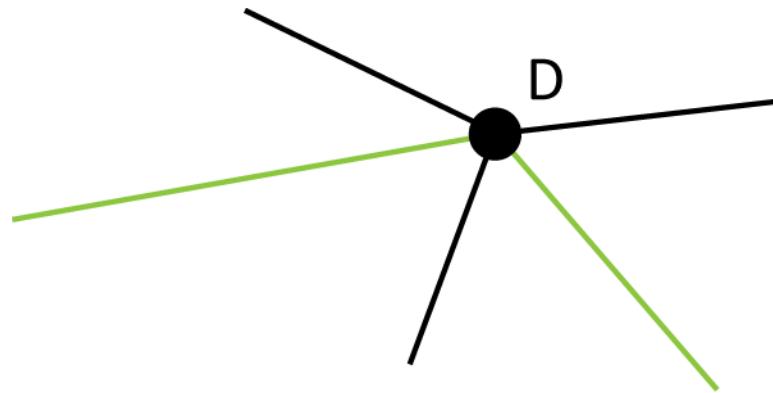
# What does degree have to do with Euler circuits?

- We have several unused edges, so we need to follow one of them and leave D



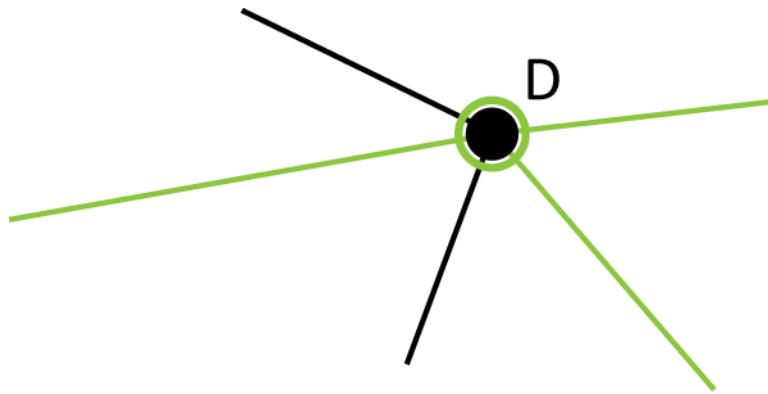
# What does degree have to do with Euler circuits?

- In fact, every time we visit a vertex, we will “use up” **two** of the edges that meet at that vertex



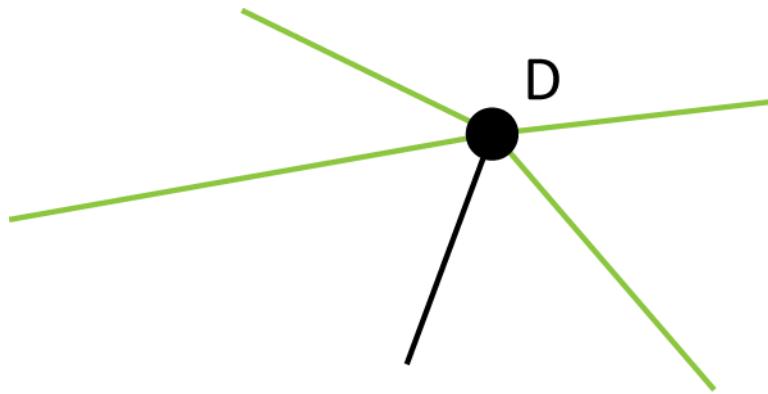
# What does degree have to do with Euler circuits?

- We have unused edges, so we need to visit D again at some point...



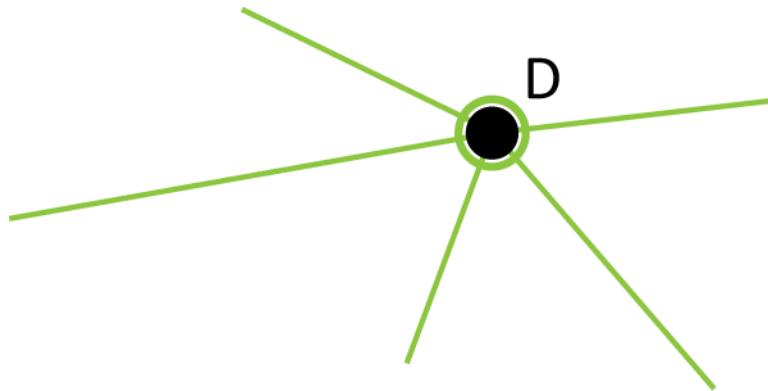
# What does degree have to do with Euler circuits?

- ...and then leave again...



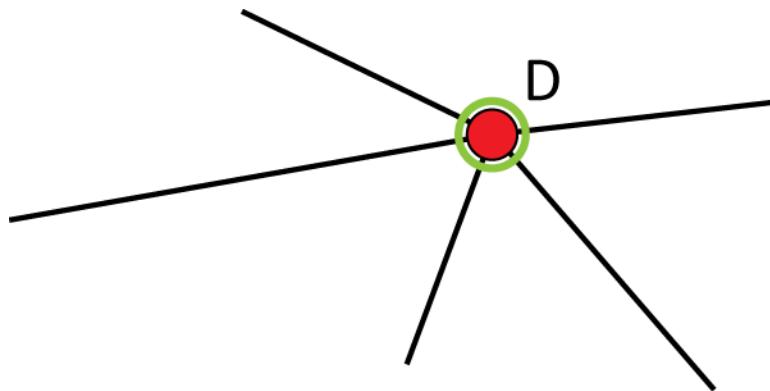
# What does degree have to do with Euler circuits?

- ...and then come back again.
- But now we're stuck, since we can't leave D without retracing, but D wasn't our starting point.



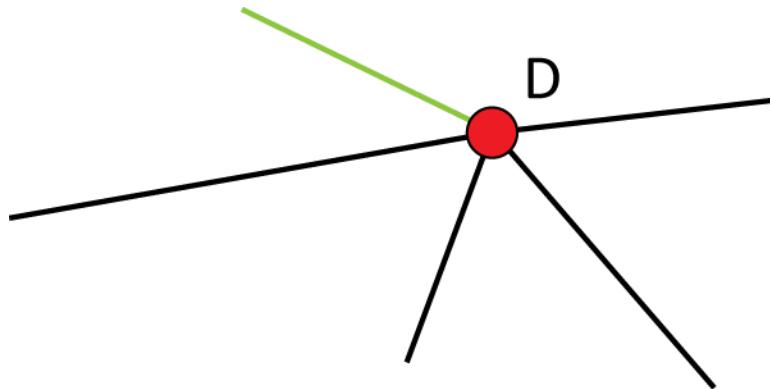
# What does degree have to do with Euler circuits?

- What if we had started at D?



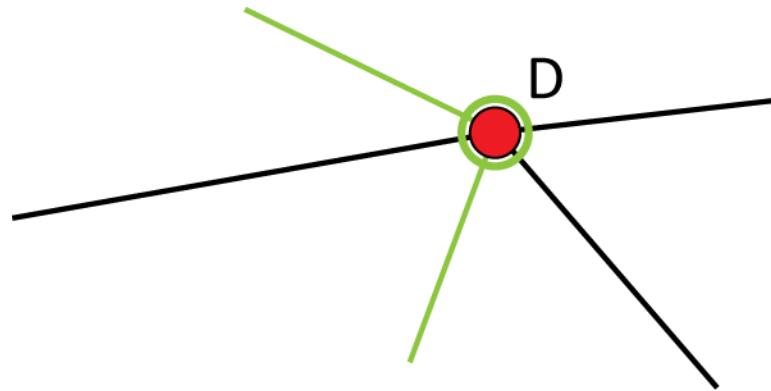
# What does degree have to do with Euler circuits?

- First, we need to leave D...



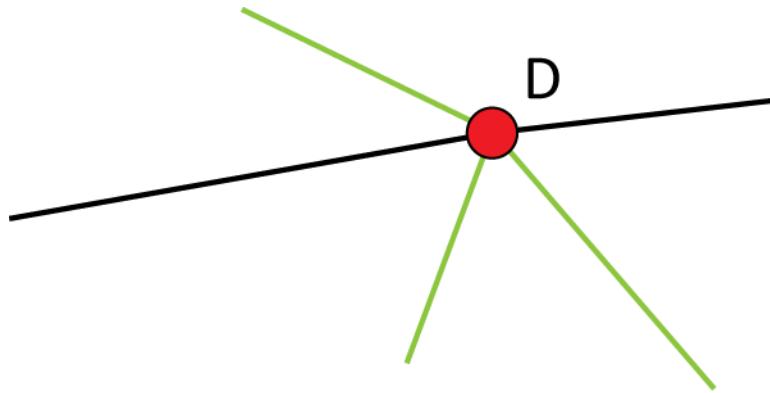
# What does degree have to do with Euler circuits?

- ... then sometime later, we have to come back to D...



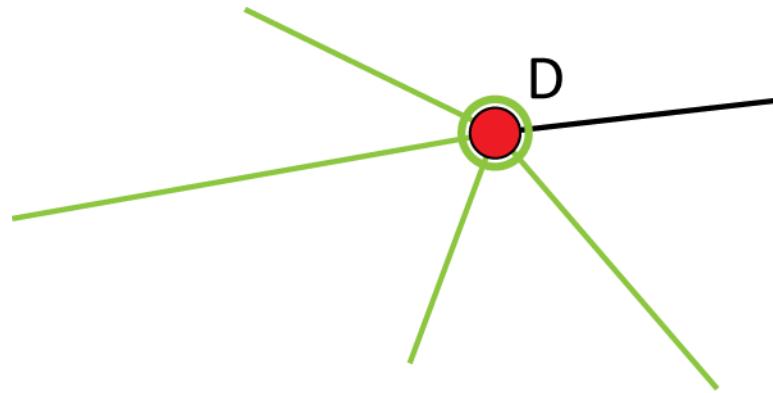
# What does degree have to do with Euler circuits?

- ... and then leave again ...



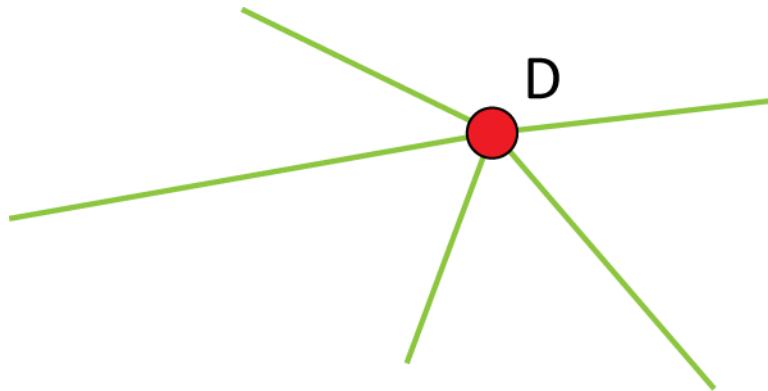
# What does degree have to do with Euler circuits?

- ... and then come back again ...



# What does degree have to do with Euler circuits?

- ... and then leave again.
- But D was our starting point, and we have run out of edges to use to come back to D!



# No Euler Circuits With Odd Degrees

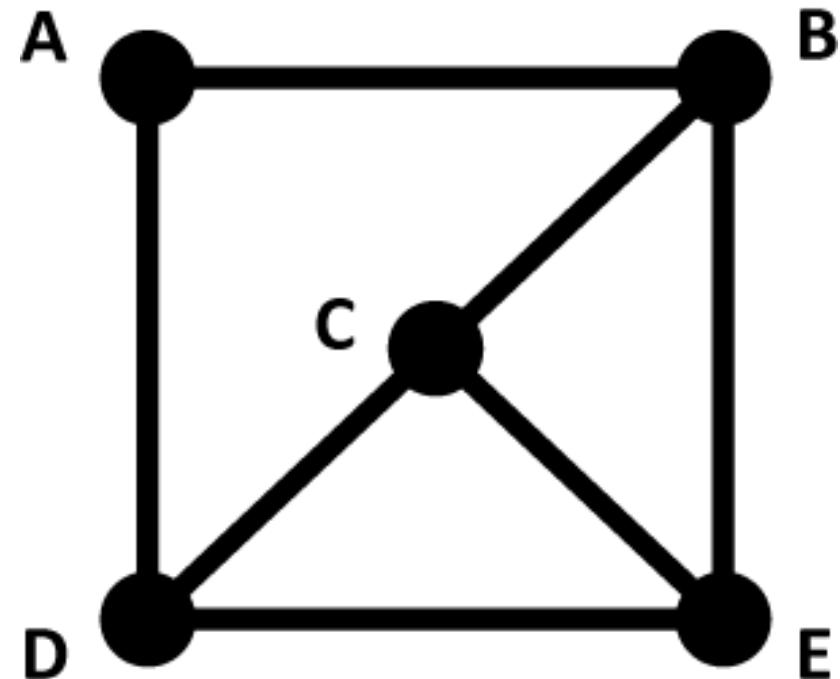
- If a graph has *any* vertex with an odd degree, then the graph does not have an Euler circuit
- The reverse is true as well

# Euler's Theorem

- If a graph has all even degrees, then it has an Euler circuit. If a graph has any vertices with odd degree, then it does not have an Euler circuit.

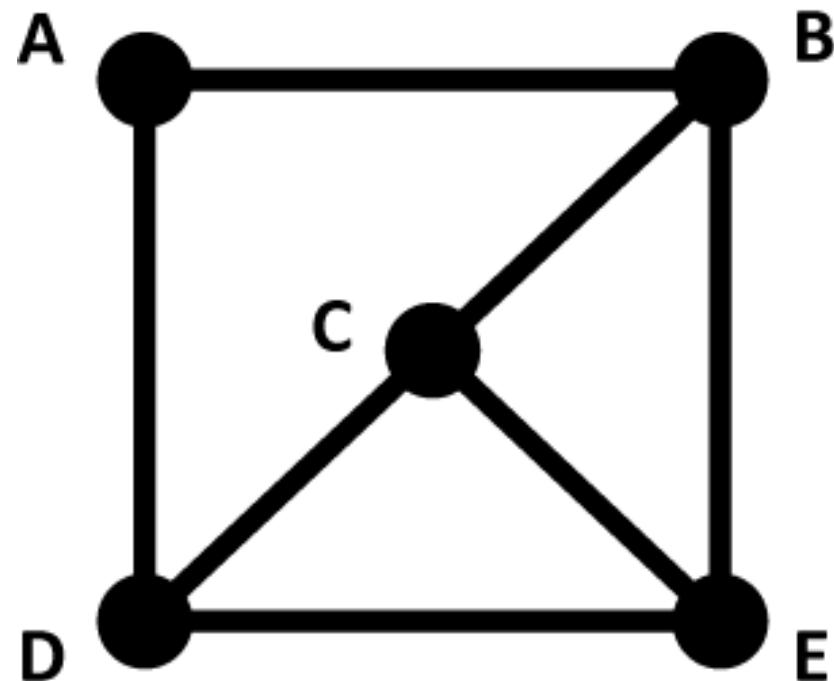
# Practice With Euler's Theorem

- Does this graph have an Euler circuit? If not, explain why. If so, then find one.



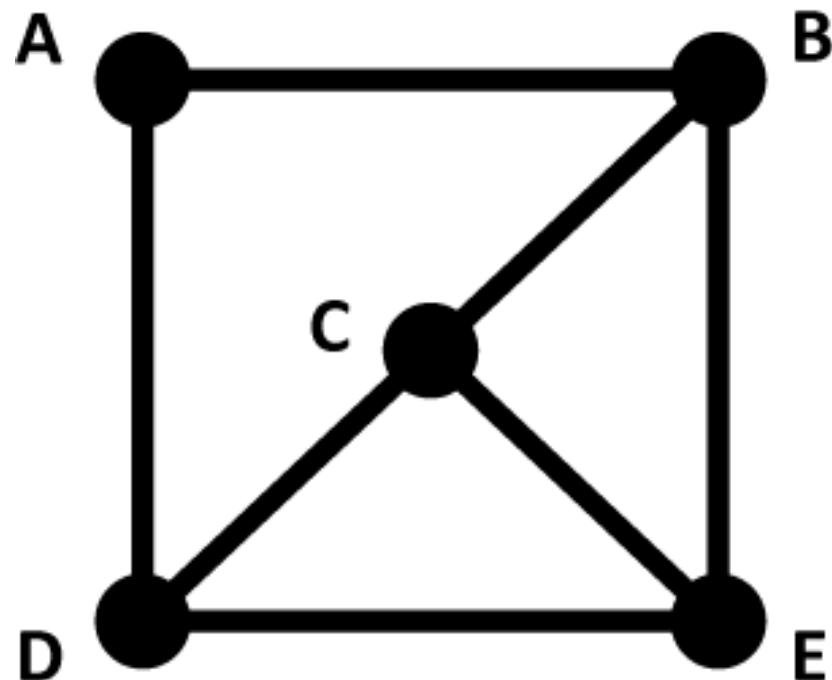
# Practice With Euler's Theorem

- Does this graph have an Euler circuit? If not, explain why. If so, then find one.
- **Answer:** No, since vertex C has an odd degree.



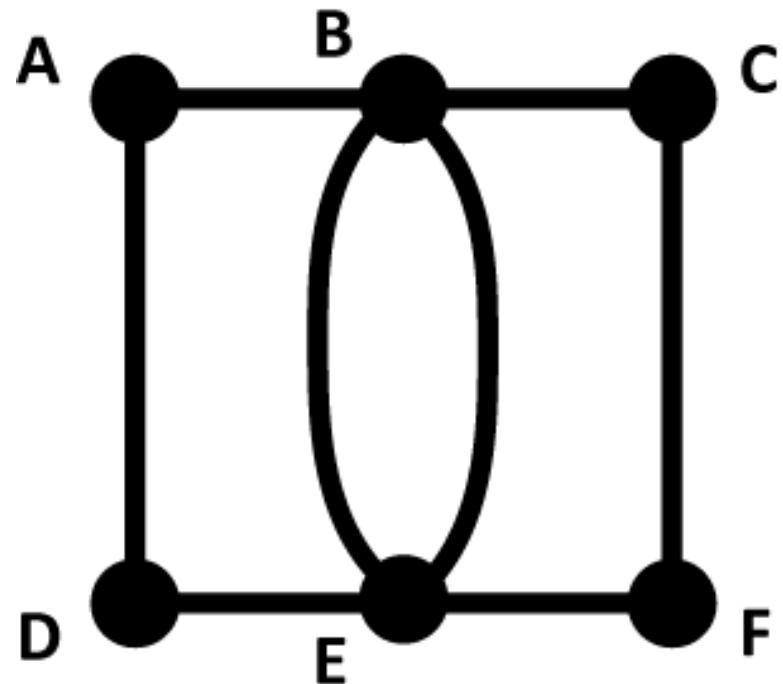
# Practice With Euler's Theorem

- Does this graph have an Euler circuit? If not, explain why. If so, then find one.
- Notice that D and E also have odd degree, but we only need one odd-degree vertex for Euler's Theorem



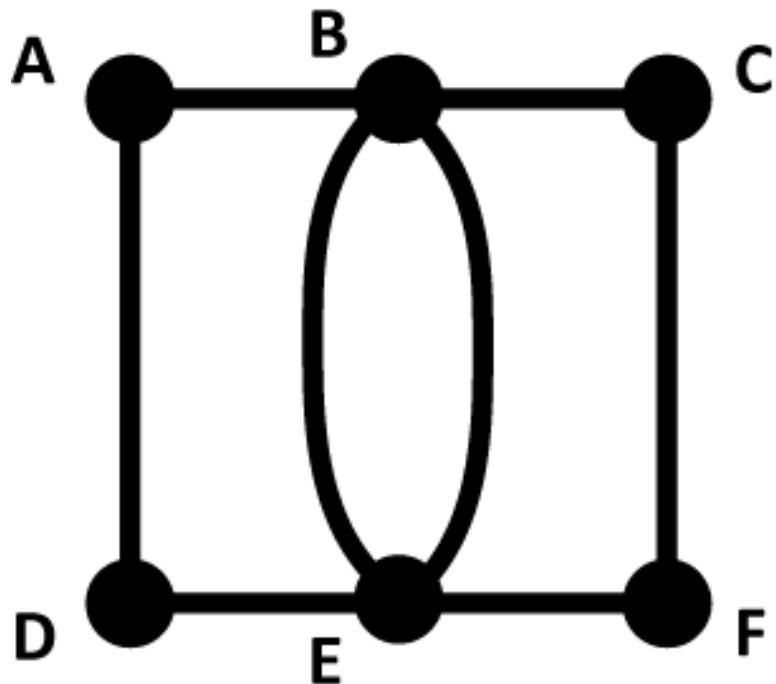
# Practice With Euler's Theorem

- Does this graph have an Euler circuit? If not, explain why. If so, then find one.



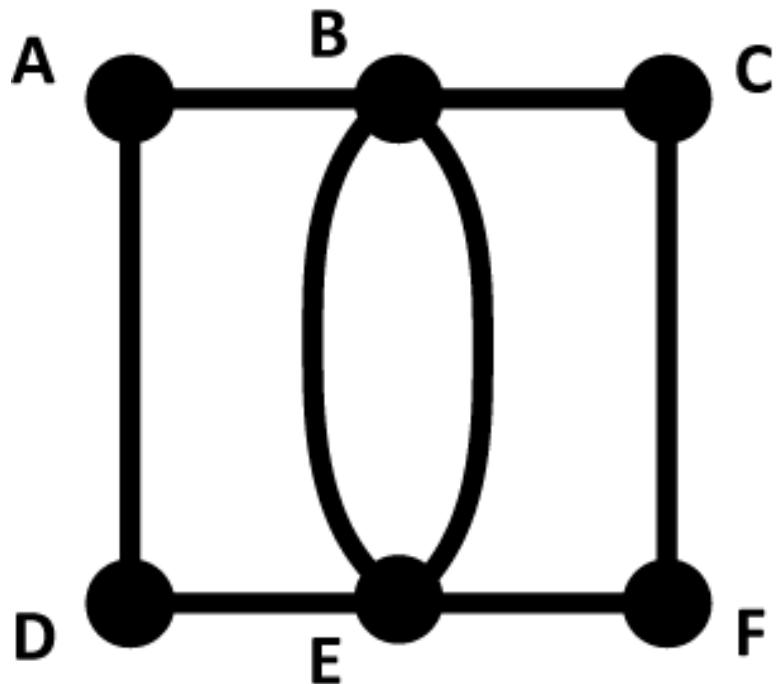
# Practice With Euler's Theorem

- Does this graph have an Euler circuit? If not, explain why. If so, then find one.
- **Answer:** All of the vertices have even degree, so there must be an Euler circuit...



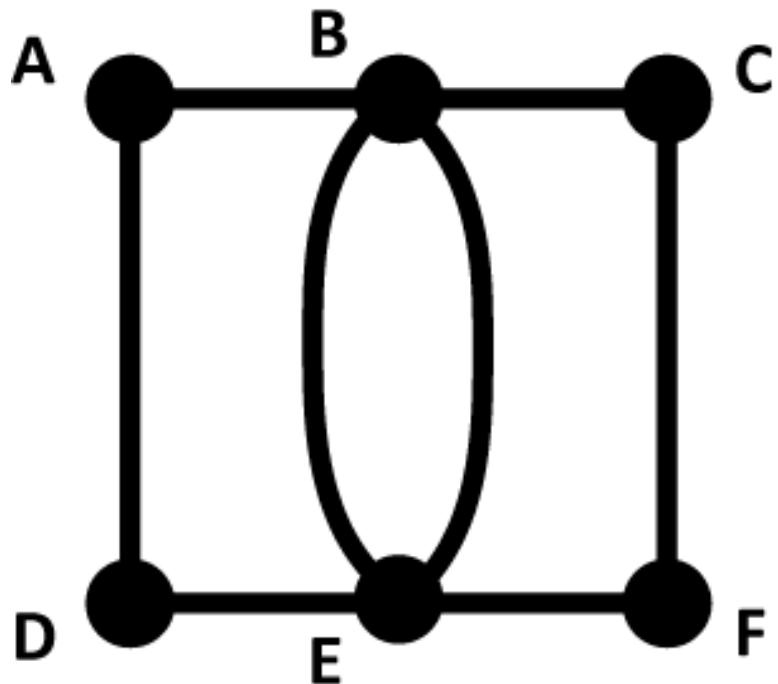
# Practice With Euler's Theorem

- Does this graph have an Euler circuit? If not, explain why. If so, then find one.
- **Answer** (continued):  
With some trial and error, we can find an Euler circuit:  
A,B,C,F,E,B,E,D,A



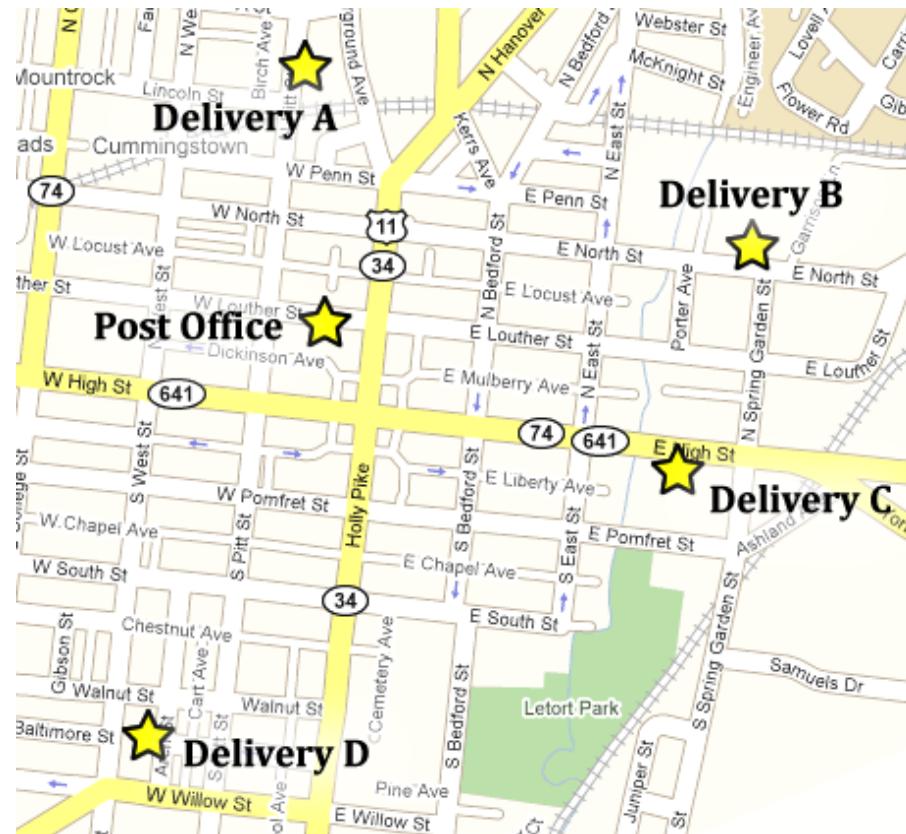
# Practice With Euler's Theorem

- Does this graph have an Euler circuit? If not, explain why. If so, then find one.
- Note there are many different circuits we could have used



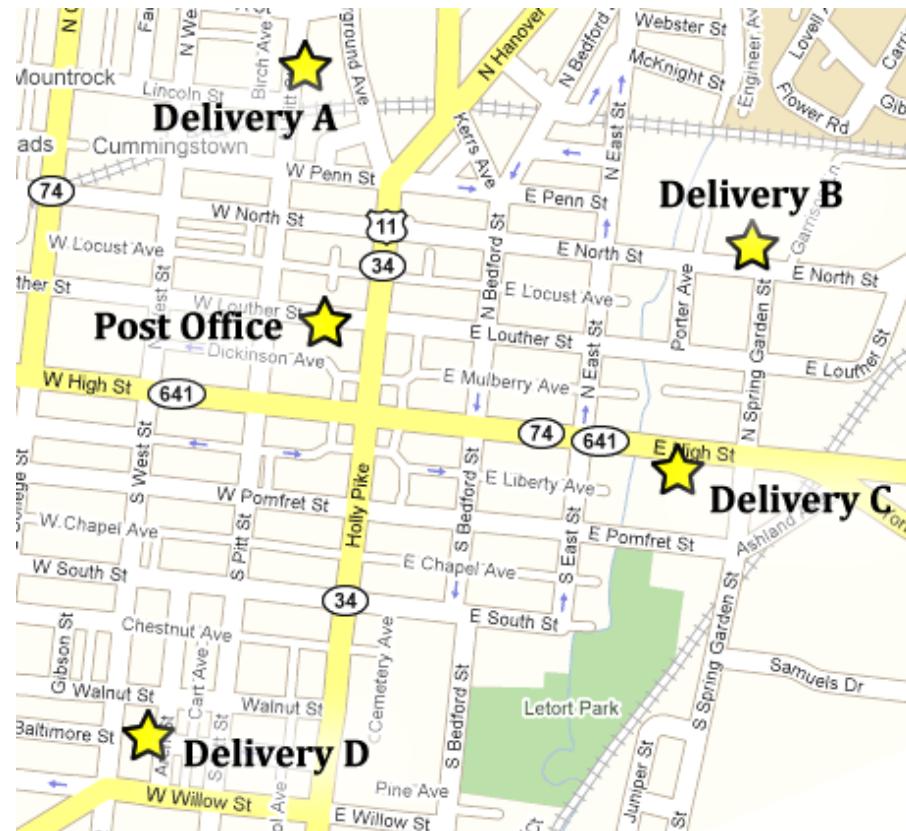
# A New Kind of Problem

- A postal worker needs to take several packages from the post office, deliver them to the four locations shown on the map, and then return to the office

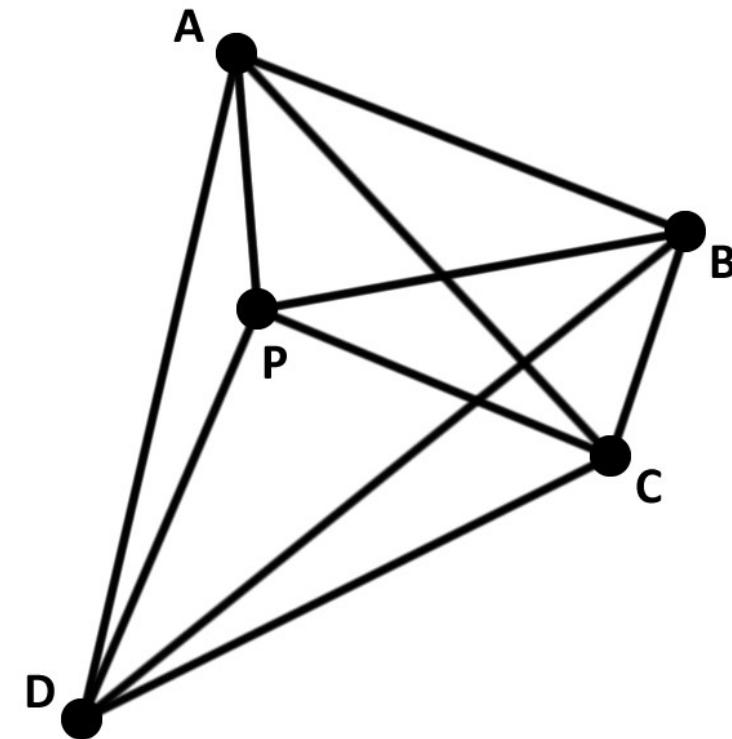
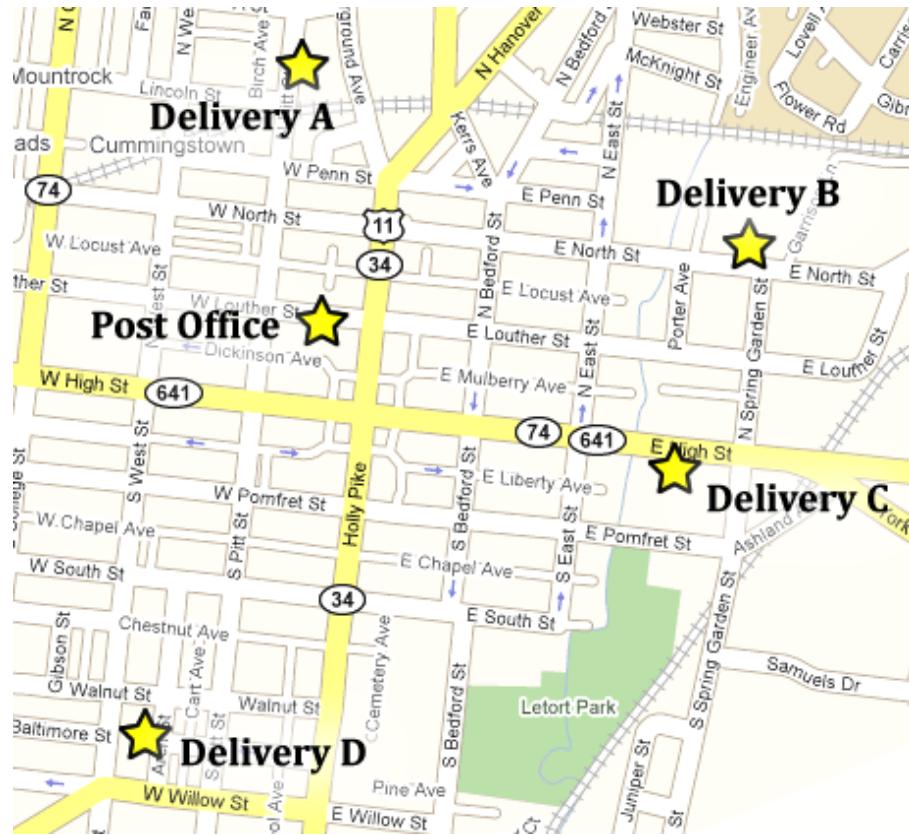


# A New Kind of Problem

- The postal worker wants to know the best route to take to deliver the packages
- Do we want to use Euler circuits to solve this problem?

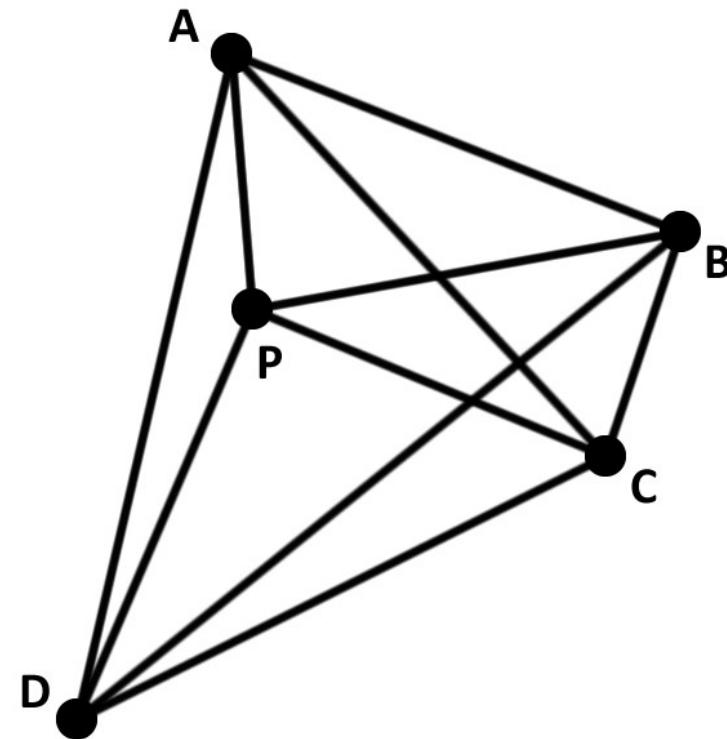


# Modeling this Problem



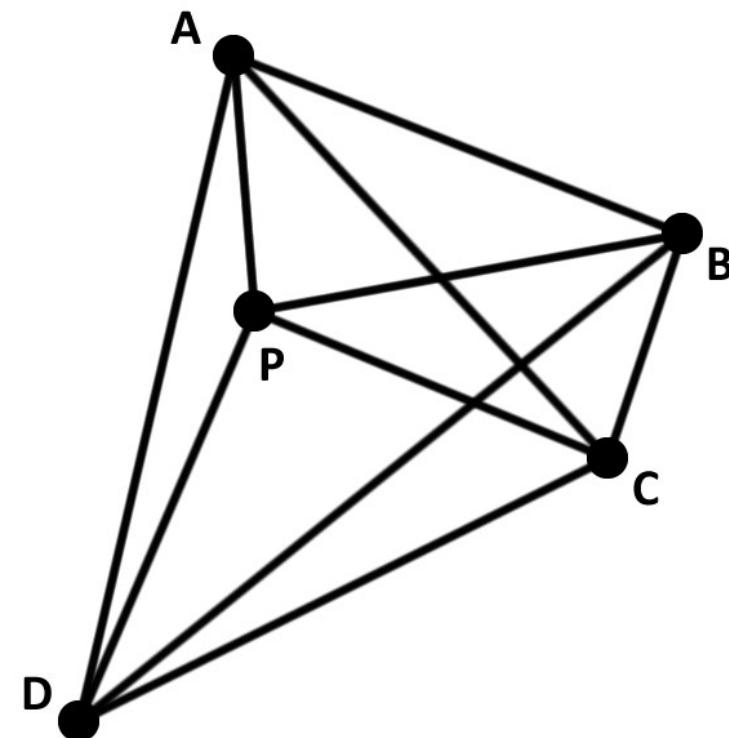
# A New Kind of Graph

- This is called a **complete graph** because every pair of vertices is connected by an edge
- This represents our ability to travel from any point to any other



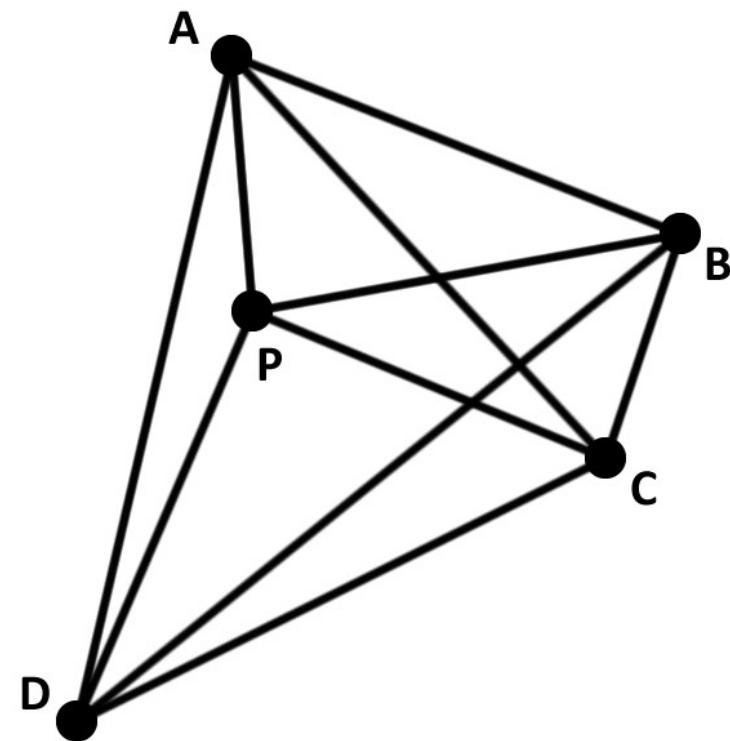
# A New Kind of Circuit

- We don't need an Euler circuit, which would have us travel along each edge
- We just need to visit each **vertex** once and then return to our starting point

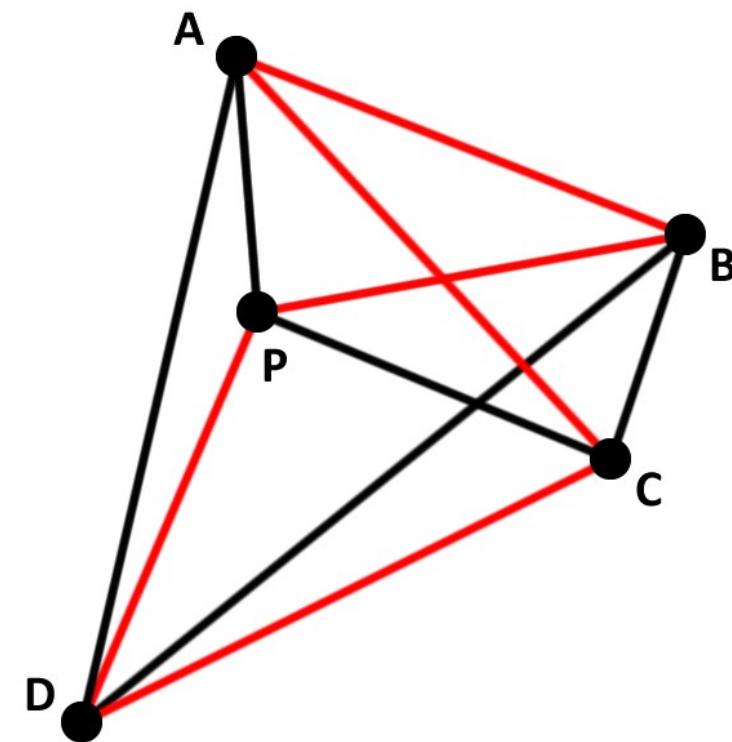
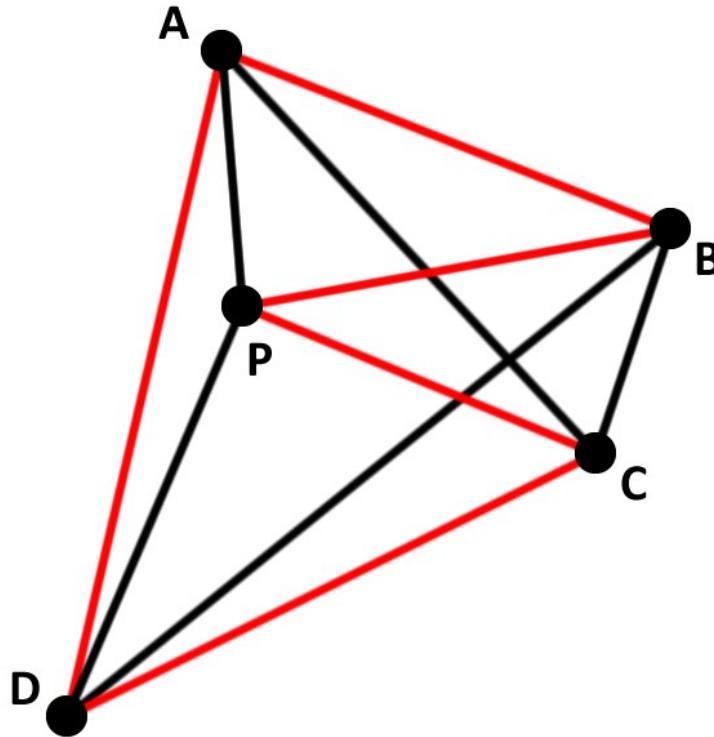


# A New Kind of Circuit

- A **Hamiltonian circuit** is a circuit that visits each vertex exactly once, except for the starting vertex, which is the same as the ending vertex



# Examples of Hamiltonian Circuits



# Finding the “Best” Circuit

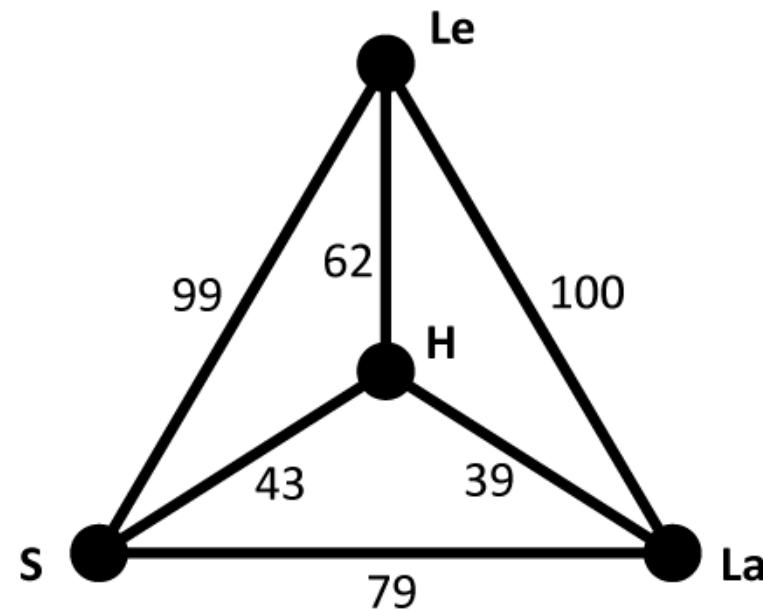
- We want to find the circuit that has the lowest total “cost”
- Here “cost” might mean
  - travel time
  - distance
  - monetary cost
  - etc.

# The Brute-Force Method

1. Examine all possible Hamiltonian circuits
2. Compute the total cost of all of these circuits
3. Choose the circuit with the lowest total cost

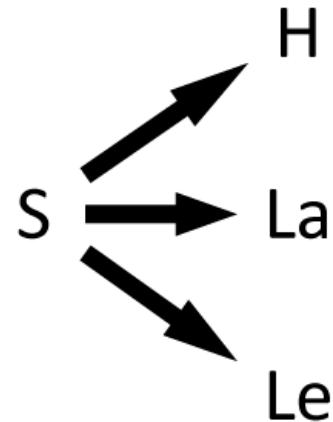
# Example: Road Trip!

- Suppose you want to take a road trip for Spring Break
- You want to start from Shippensburg (S), and visit Harrisburg (H), Lancaster (La), and Lewisburg (Le) in some order before returning to Ship



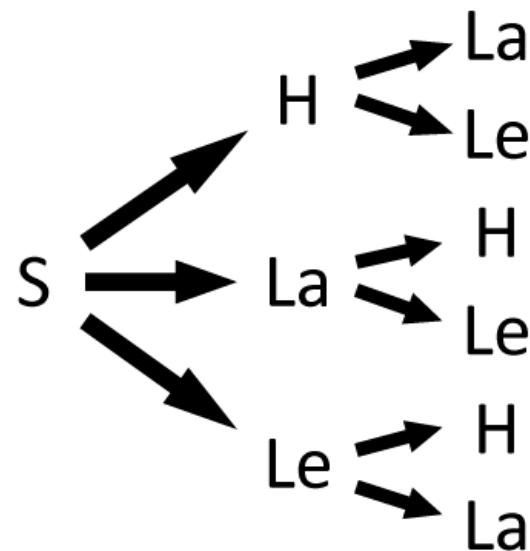
# Step 1: Find All Possible Circuits

- From Shippensburg, we have three choices for our first destination



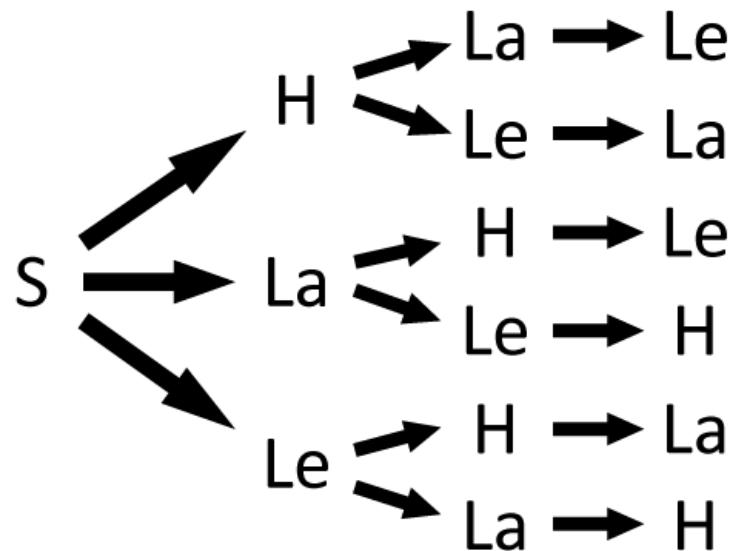
# Step 1: Find All Possible Circuits

- From each of these possibilities, we now have two choices



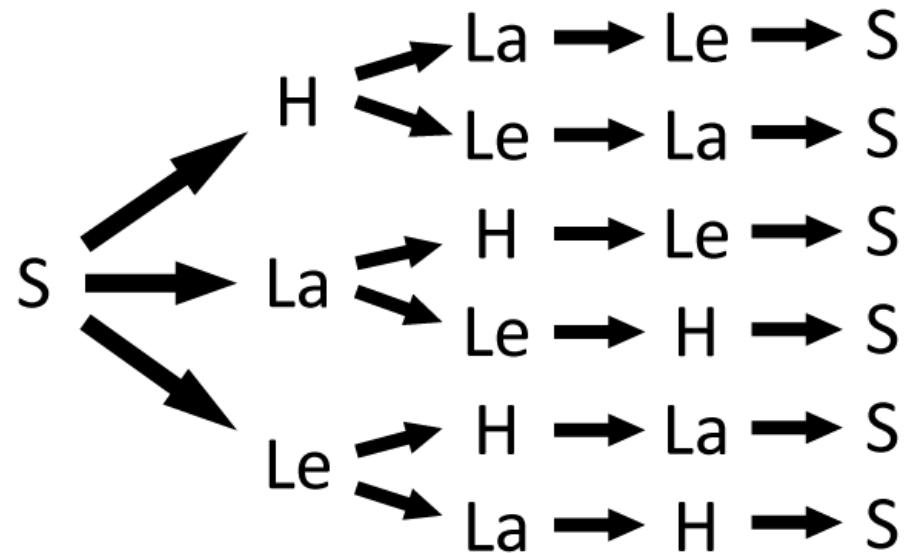
# Step 1: Find All Possible Circuits

- Next, we only have one choice remaining



# Step 1: Find All Possible Circuits

- And finally, we must return to S



## Step 2: Find the Cost of Each Circuit

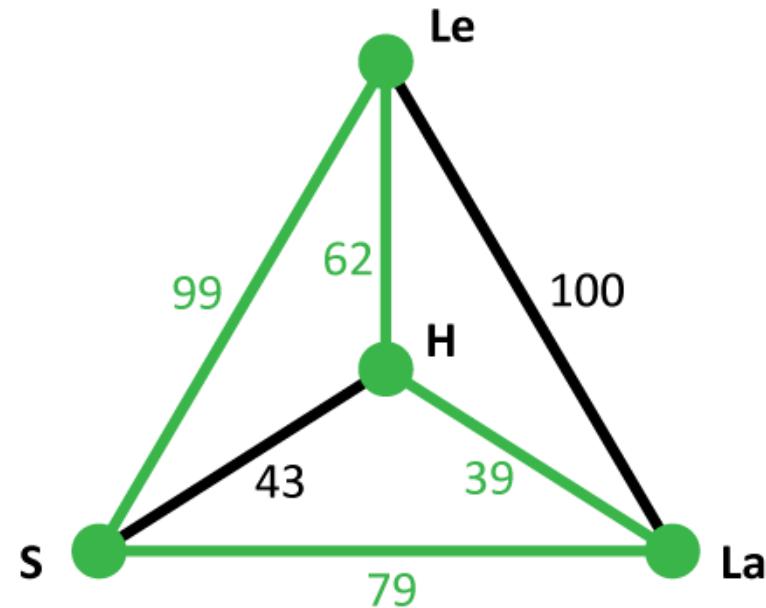
Circuit	Cost
S – H – La – Le – S	$43 + 39 + 100 + 99 = 281$
S – H – Le – La – S	$43 + 62 + 100 + 79 = 284$
S – La – H – Le – S	$79 + 39 + 62 + 99 = 279$
S – La – Le – H – S	$79 + 100 + 62 + 43 = 284$
S – Le – H – La – S	$99 + 62 + 39 + 79 = 279$
S – Le – La – H – S	$99 + 100 + 39 + 43 = 281$

# Step 3: Choose the Lowest Cost Circuit

Circuit	Cost
S – H – La – Le – S	$43 + 39 + 100 + 99 = 281$
S – H – Le – La – S	$43 + 62 + 100 + 79 = 284$
<b>S – La – H – Le – S</b>	<b><math>79 + 39 + 62 + 99 = 279</math></b>
S – La – Le – H – S	$79 + 100 + 62 + 43 = 284$
<b>S – Le – H – La – S</b>	<b><math>99 + 62 + 39 + 79 = 279</math></b>
S – Le – La – H – S	$99 + 100 + 39 + 43 = 281$

# It's a tie! Or is it?

- If we draw these two circuits, we find that in fact they are the same
- One circuit is the reverse of the other, so the total costs are the same
- In fact, while it looked like there were 6 total circuits, really there were only 3



# Pros and Cons

- The brute force method is good because we know for sure we find the best possible answer
- The biggest disadvantage of the brute force method is that the total number of circuits gets very large if we look at graphs with more vertices

# How Many Circuits?

- In our example, we had 4 total vertices
- So from our starting point, we had 3 choices, then we had 2 choices, then 1 choices, then no choice but to go back to the start
- That gave us  $3 \times 2 \times 1 = 6$  total circuits
- But really there were only half that: 3 circuits

# How Many Circuits?

- What if we had 5 total vertices?
- We would have 4 choices, then 3, then 2, then 1, then back to the start
- That gives us  $4 \times 3 \times 2 \times 1 = 24$  total circuits
- And again there would only really be half that: 12 circuits

# How Many Circuits?

- The calculation we are doing is a common one in mathematics, called **factorial**
- The factorial of a whole number  $n$  is the product of all the whole numbers between 1 and  $n$
- Factorial is written with an exclamation point:  
$$n! = n \times (n - 1) \times \dots \times 3 \times 2 \times 1$$
- For example:  $5! = 5 \times 4 \times 3 \times 2 \times 1 = 120$

# How Many Circuits?

- Factorial numbers grow very quickly
- $7! = 5040$
- This means that if we had tried to solve our road trip problem with 8 locations instead of 4, we would have had to consider over five thousand circuits instead of just six

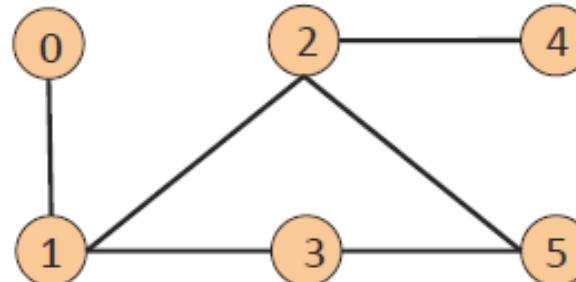
# Weighted Graphs

In a weighted graph, each edge has a **weight** or **cost**

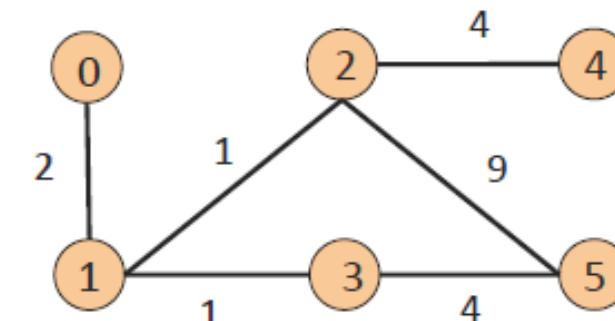
- Typically numeric (ints, decimals, doubles, etc.)
- Some graphs allow negative weights; many do not

## □ Unweighted vs weighted graph

- A weighted graphs has weights on the edges
- Example:
  - how many “likes” in your friend’s post
  - Similarity between a pair of proteins



Unweighted graph

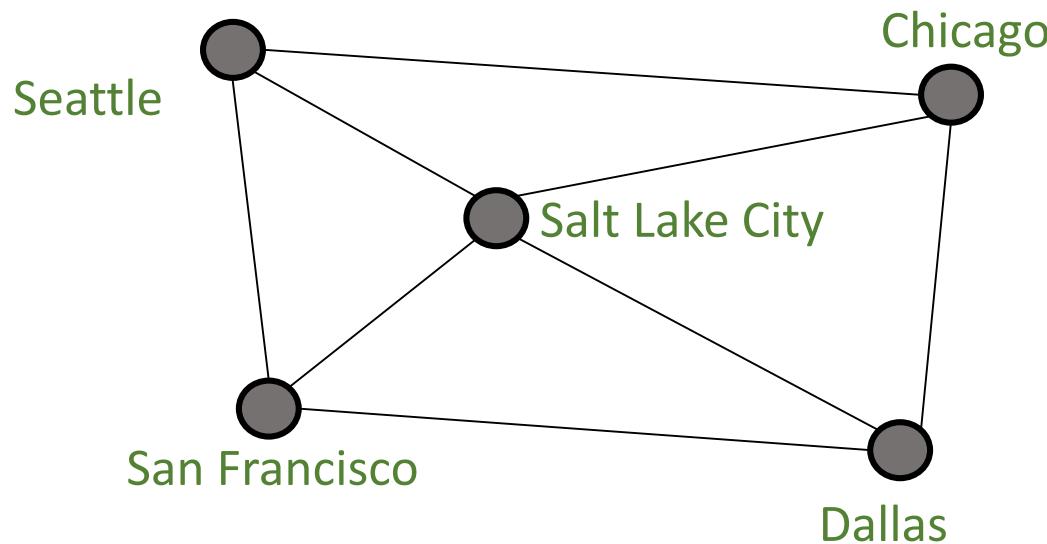


Weighted graph

# Paths and Cycles

We say "a **path** exists from  $v_0$  to  $v_n$ " if there is a list of vertices  $[v_0, v_1, \dots, v_n]$  such that  $(v_i, v_{i+1}) \in E$  for all  $0 \leq i < n$ .

A **cycle** is a path that begins and ends at the same node ( $v_0 == v_n$ )



Example path (that also happens to be a cycle):

[Seattle, Salt Lake City, Chicago, Dallas, San Francisco, Seattle]

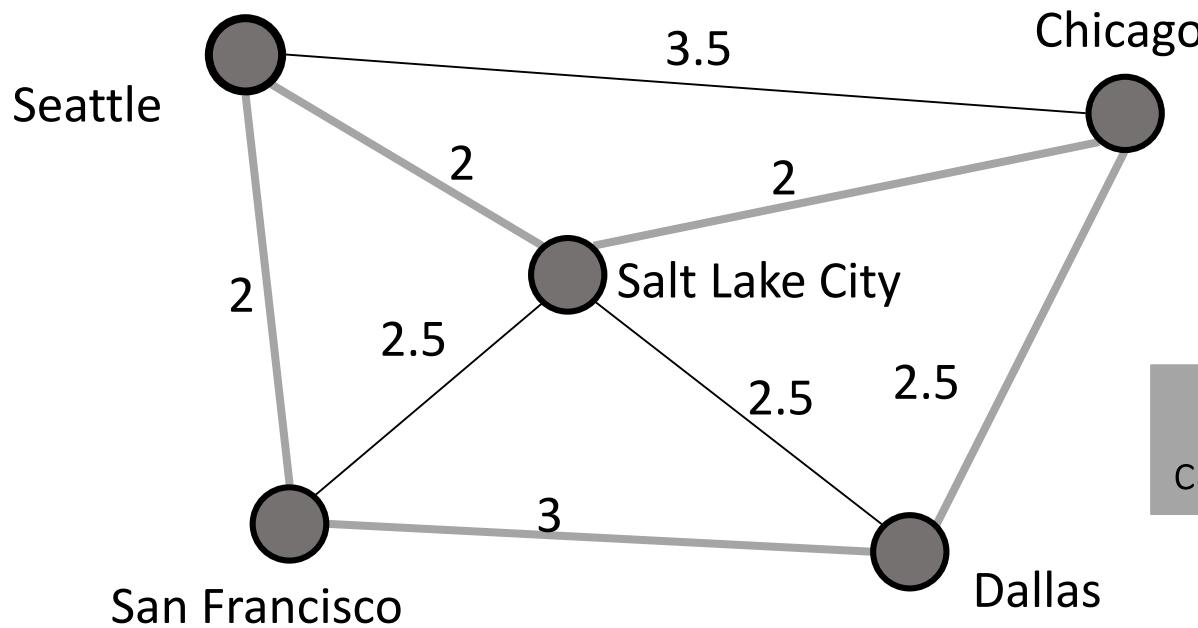
# Path Length and Cost

Path length: Number of edges in a path

Path cost: Sum of the weights of each edge

Example where

$P = [ \text{Seattle}, \text{Salt Lake City}, \text{Chicago}, \text{Dallas}, \text{San Francisco}, \text{Seattle} ]$



$$\begin{aligned}\text{length}(P) &= 5 \\ \text{cost}(P) &= 11.5\end{aligned}$$

Length is sometimes called "unweighted cost"

# Simple Paths and Cycles

A **simple path** repeats no vertices (except the first might be the last):

[Seattle, Salt Lake City, San Francisco, Dallas]

[Seattle, Salt Lake City, San Francisco, Dallas, Seattle]

A **cycle** is a path that ends where it begins:

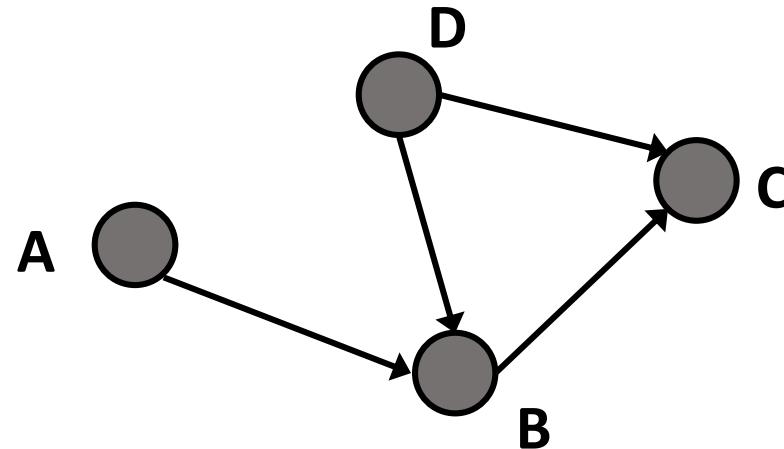
[Seattle, Salt Lake City, Seattle, Dallas, Seattle]

A **simple cycle** is a cycle and a simple path:

[Seattle, Salt Lake City, San Francisco, Dallas, Seattle]

# Paths and Cycles in Directed Graphs

Example:



- Is there a path from A to D?

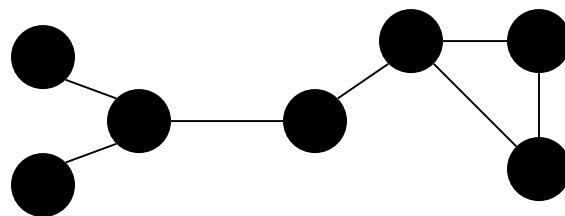
No

- Does the graph contain any cycles?

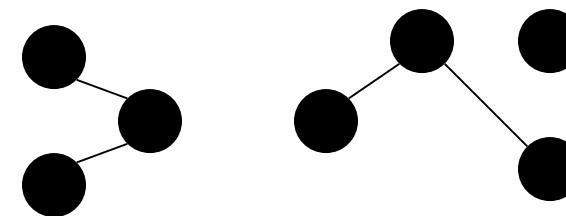
No

# Undirected Graph Connectivity

An undirected graph is **connected** if for all pairs of vertices  $u \neq v$ , there exists a *path* from  $u$  to  $v$

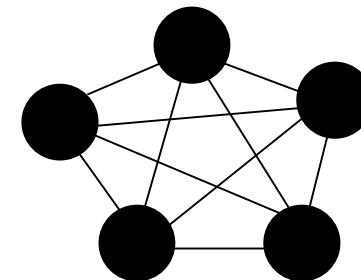


Connected graph



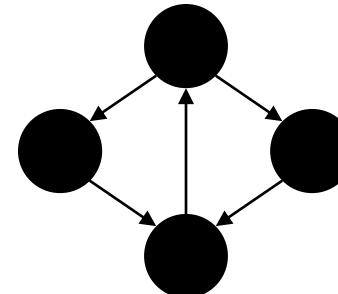
Disconnected graph

An undirected graph is **complete**, or **fully connected**, if for all pairs of vertices  $u \neq v$  there exists an *edge* from  $u$  to  $v$

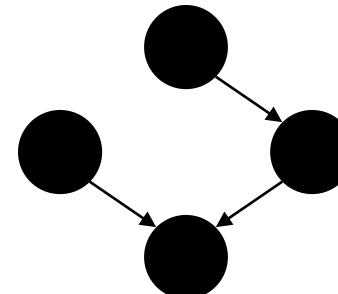


# Directed Graph Connectivity

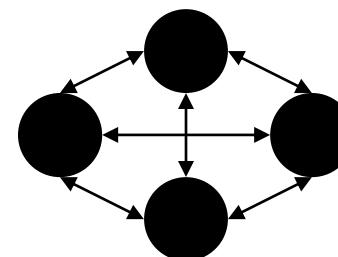
A directed graph is **strongly connected** if there is a path from every vertex to every other vertex



A directed graph is **weakly connected** if there is a path from every vertex to every other vertex  
*ignoring direction of edges*



A direct graph is **complete** or **fully connected**, if for all pairs of vertices  $u \neq v$ , there exists an *edge* from  $u$  to  $v$

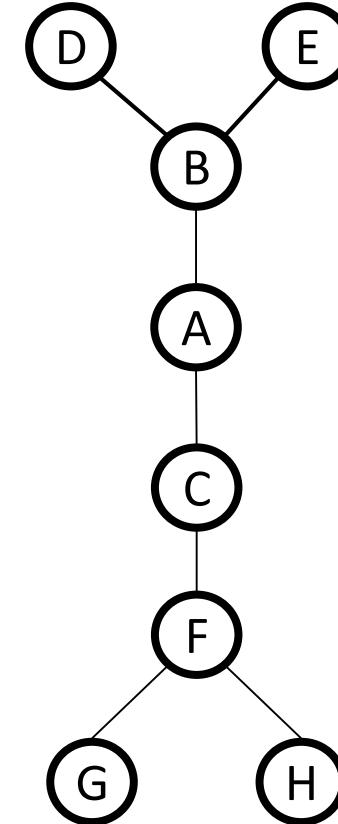


# Trees as Graphs

When talking about graphs, we say a **tree** is a graph that is:

- undirected
- acyclic
- connected

All trees are graphs, but NOT all graphs are trees



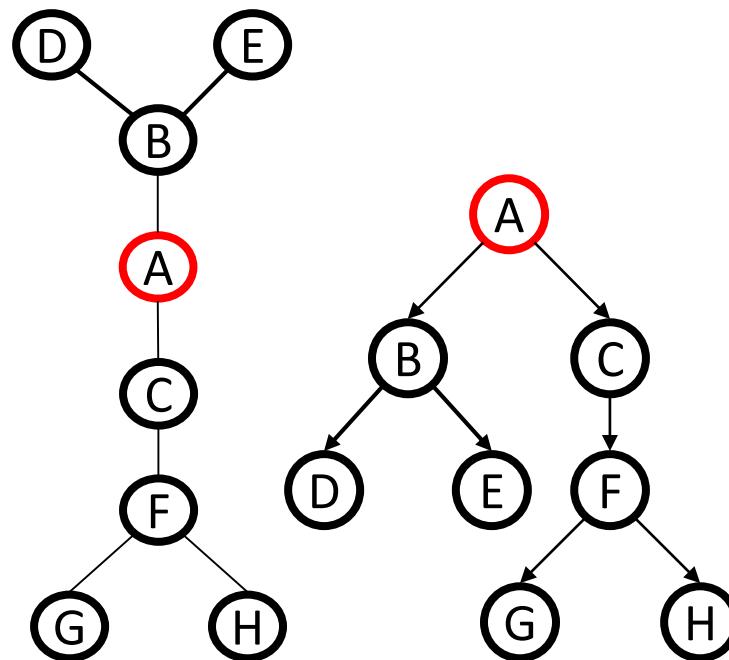
# Rooted Trees

We are more accustomed to **rooted trees** where:

- We identify a unique **root**
- We think of edges as directed: parent to children

Picking a root gives a unique rooted tree

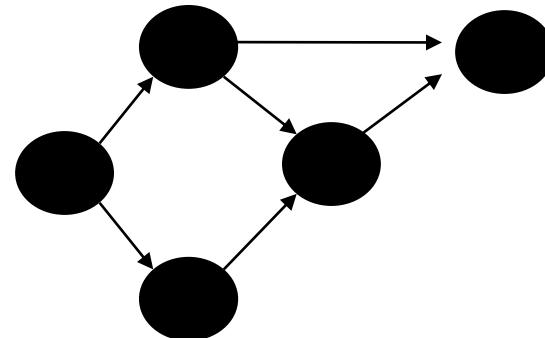
- The tree is simply drawn differently and with undirected edges



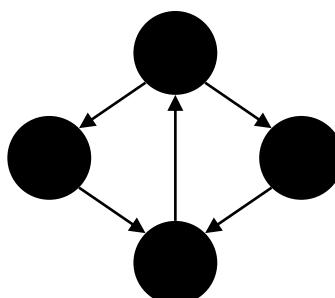
# Directed Acyclic Graphs (DAGs)

A **DAG** is a directed graph with no directed cycles

- Every rooted directed tree is a DAG
- But not every DAG is a rooted directed tree



- Every DAG is a directed graph
- But not every directed graph is a DAG



# Brute Force is Hard!

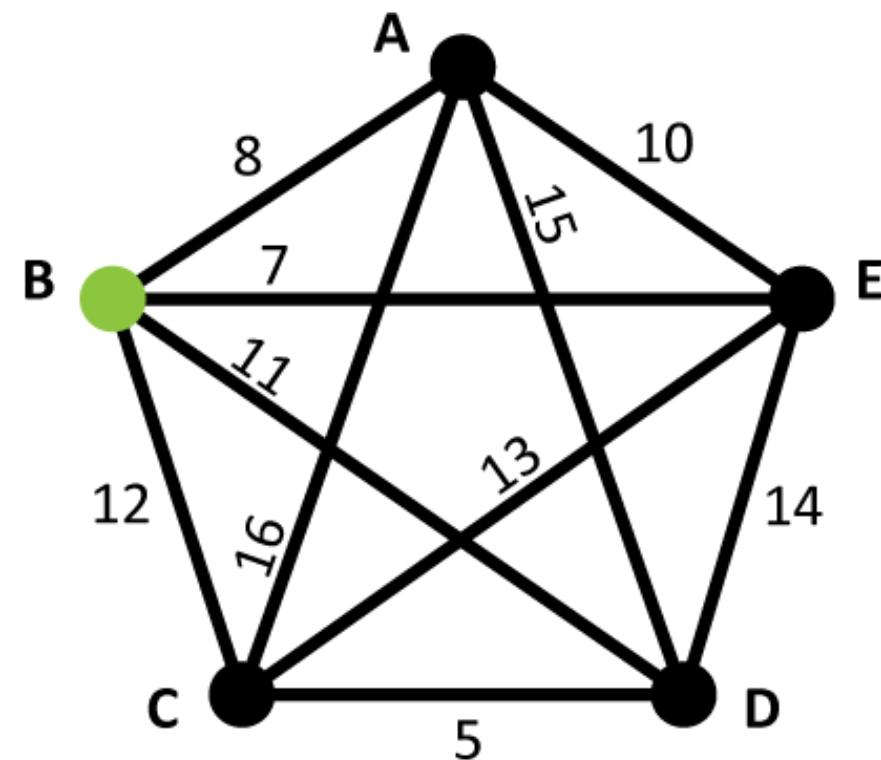
- As we have seen, the brute force method can require us to examine a very large number of circuits
- In this section we will develop *algorithms* for finding an answer much more quickly
- The downside is that we will no longer be guaranteed to have the best possible answer

# Nearest-Neighbor Algorithm

- The first algorithm we will consider is called the nearest-neighbor algorithm
- It's based on a common sense idea: at each vertex, choose the closest vertex that you haven't visited yet

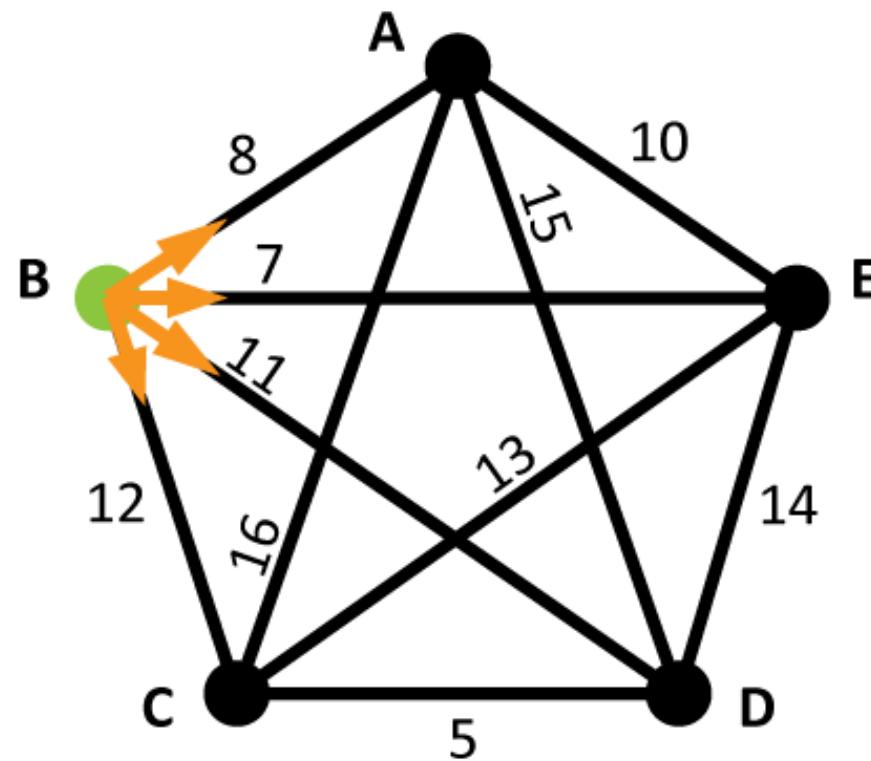
# Nearest-Neighbor Algorithm

- We have to have a starting point
- We will choose our second vertex by finding the “nearest neighbor”



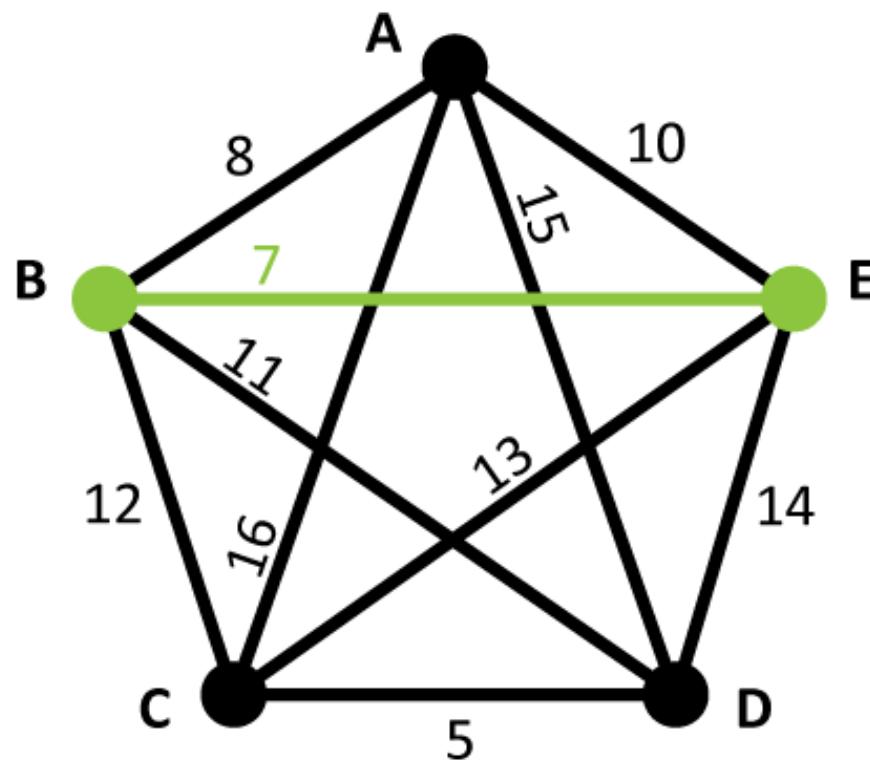
# Nearest-Neighbor Algorithm

- Where do we go first?
- Choose the cheapest edge



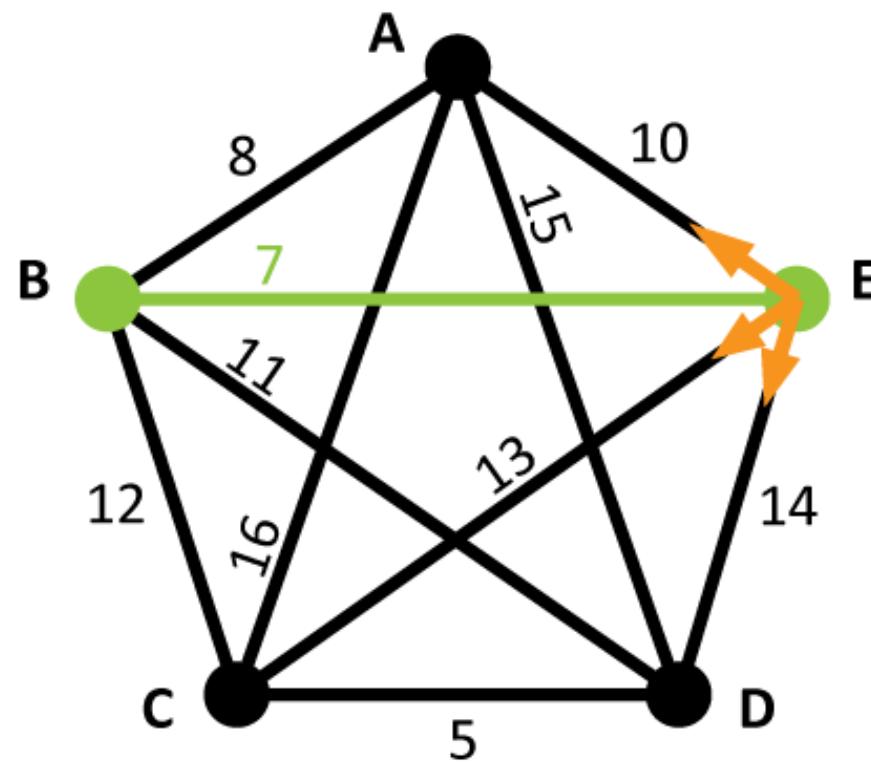
# Nearest-Neighbor Algorithm

- Choose the cheapest edge
- In this case, we go from B to E (7)



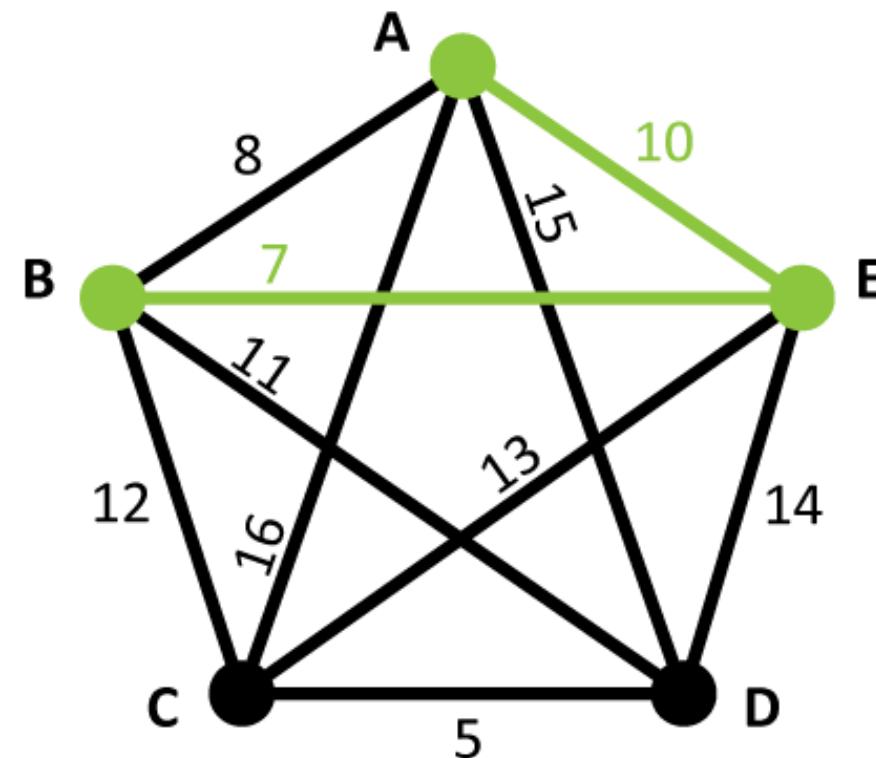
# Nearest-Neighbor Algorithm

- Now where do we go?
- We can't go back to B



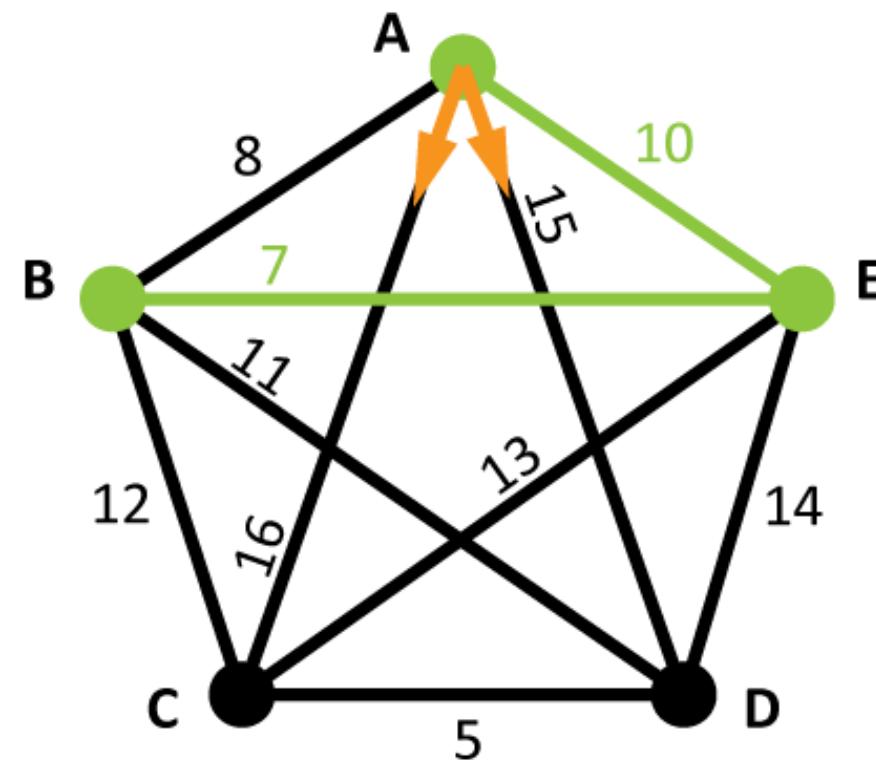
# Nearest-Neighbor Algorithm

- Now where do we go?
- We can't go back to B
- Again choose the cheapest edge



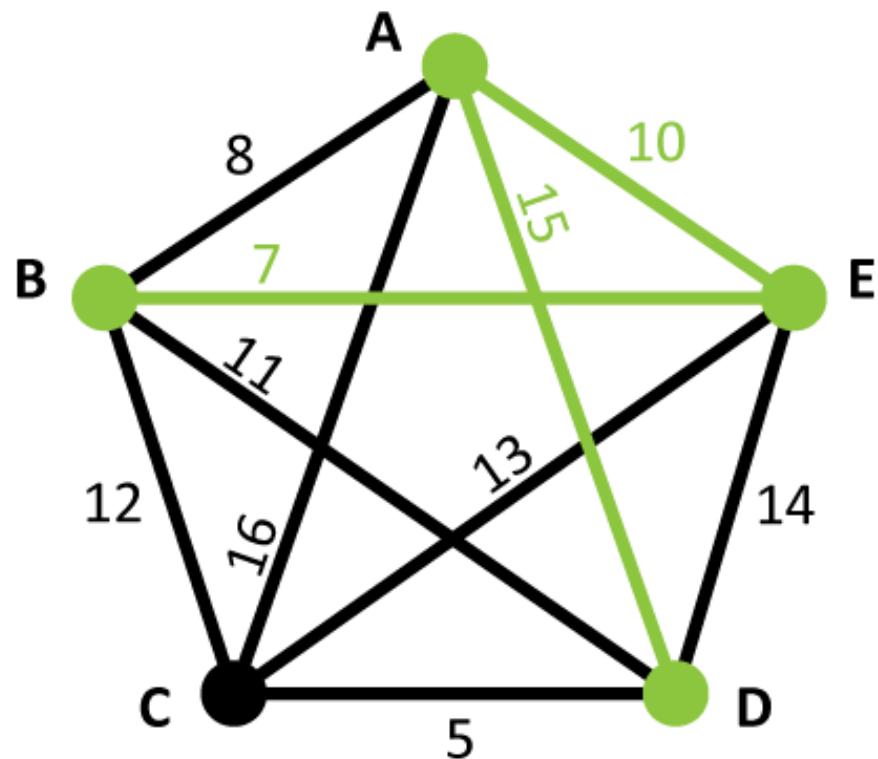
# Nearest-Neighbor Algorithm

- Now where do we go?
- We can't go back to E, but we also can't go to B



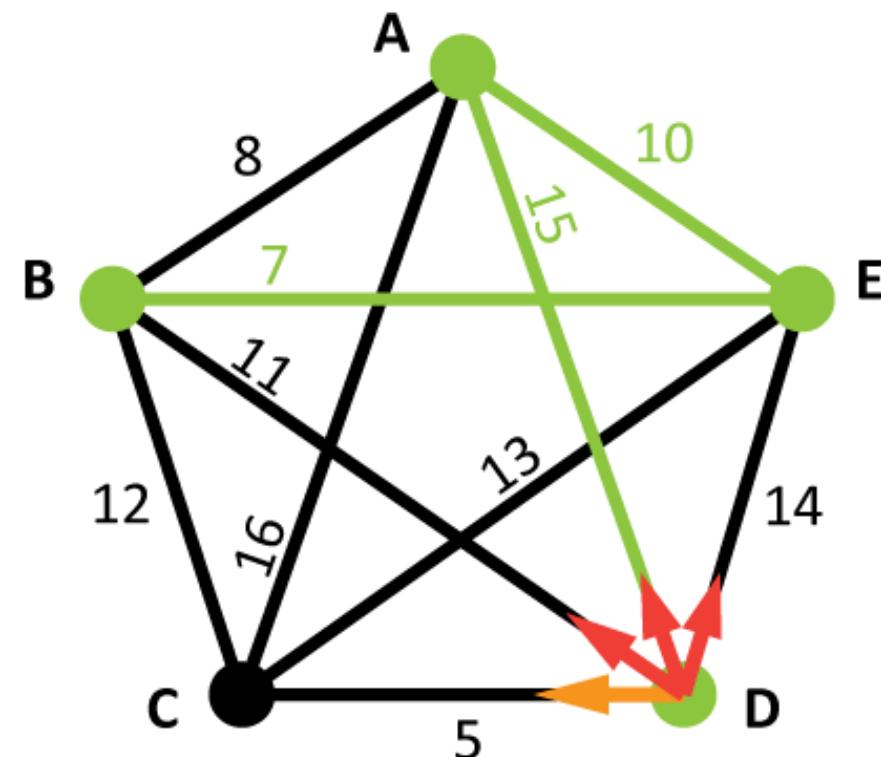
# Nearest-Neighbor Algorithm

- The rule is “nearest neighbor”: always choose the lowest cost edge, unless that would take you back to a vertex you have already been to



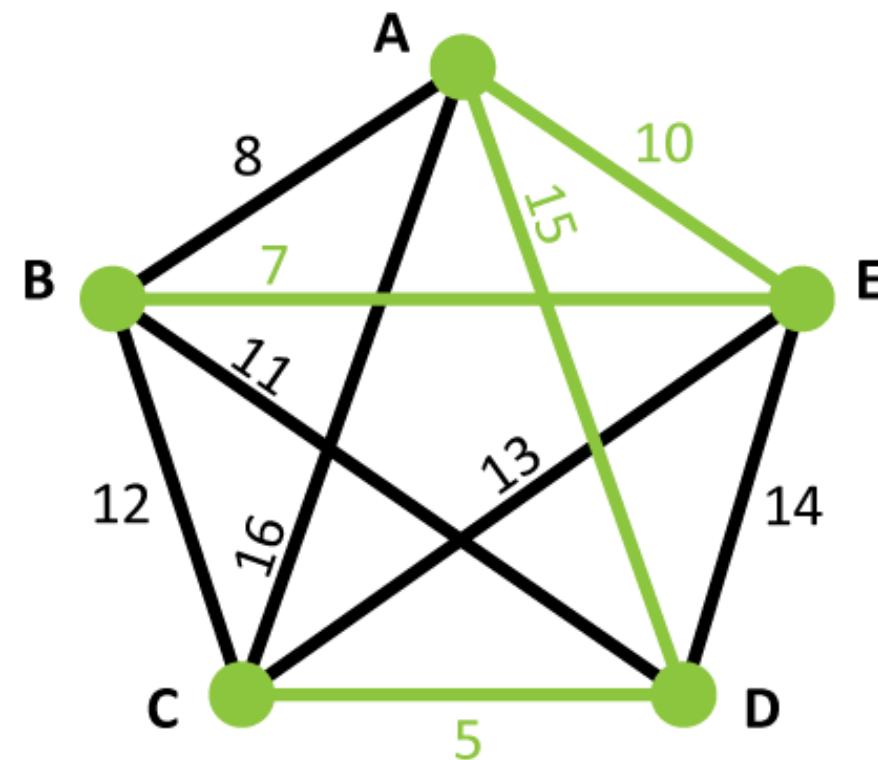
# Nearest-Neighbor Algorithm

- Now we only have one choice
- We can't go back to A or E, and we can't return to B because that would leave out C



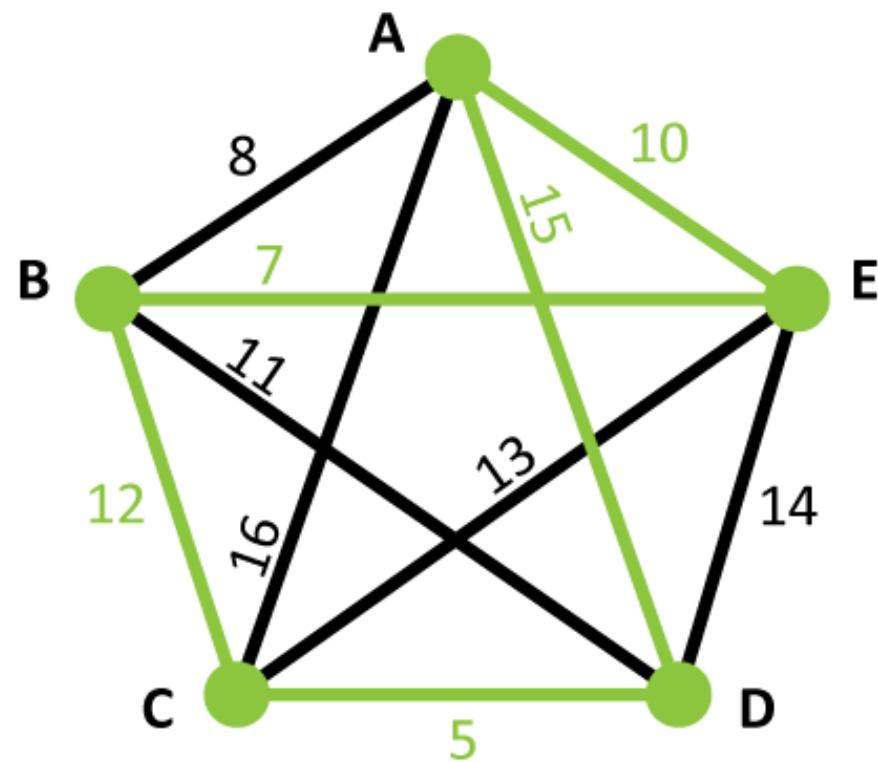
# Nearest-Neighbor Algorithm

- Now we only have one choice
- We can't go back to A or E, and we can't return to B because that would leave out C
- So we must go to C



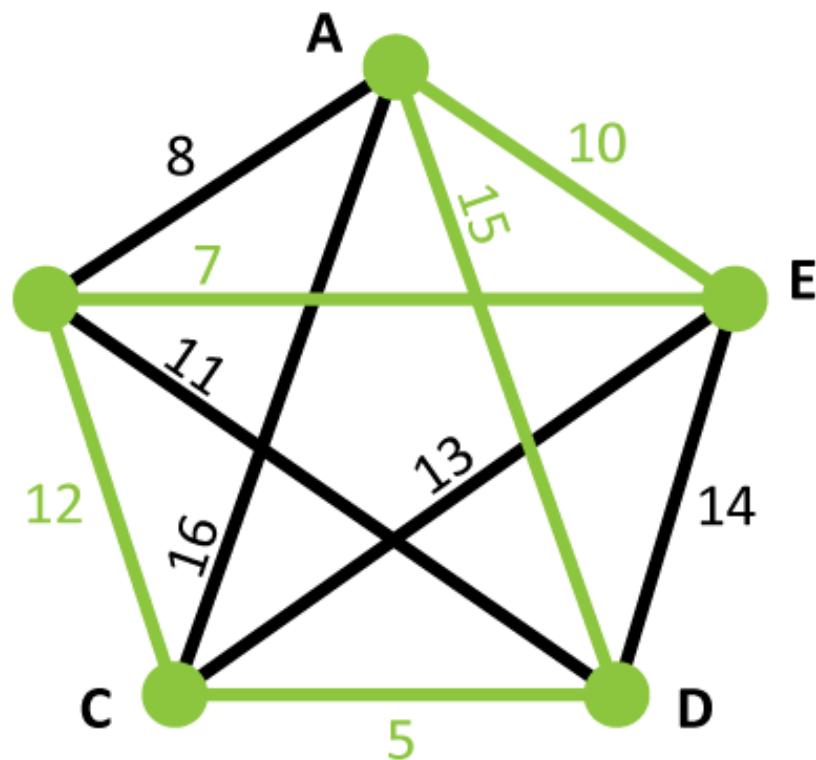
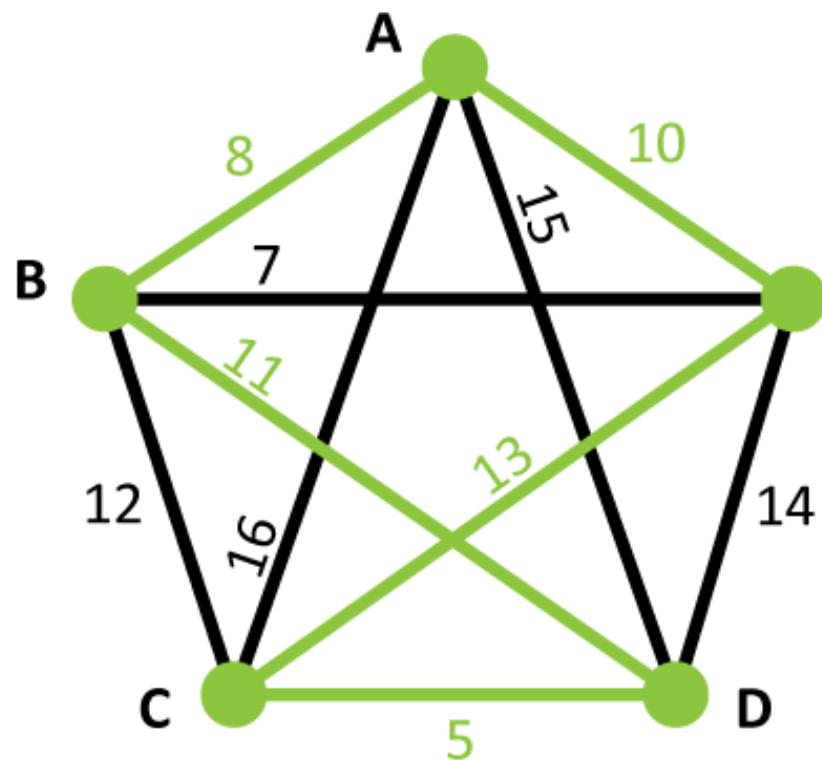
# Nearest-Neighbor Algorithm

- We have now visited all of the vertices, so we finally return to B
- This circuit has a total cost of 49
- Is it the best circuit?



# Nearest-Neighbor Algorithm

- It is *not* the best! The solution on the left has a total cost of 47



# Nearest-Neighbor Algorithm

1. From the starting vertex, choose the edge with the smallest cost and use that as the first edge in your circuit.
2. Continue in this manner, choosing among the edges that connect from the current vertex to vertices you have not yet visited.
3. When you have visited every vertex, return to the starting vertex.

# Nearest-Neighbor Algorithm

- **Advantages:** easy, “heuristic,” and fast
- **Disadvantage:** doesn’t always give you the best possible answer
- “Heuristic” means that this method uses a common-sense idea

# Representation

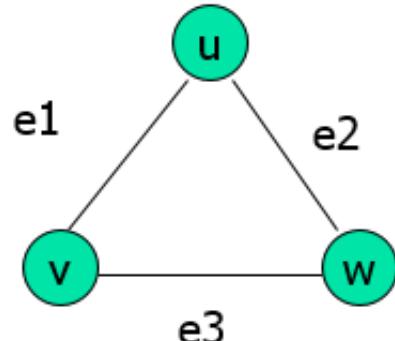
- **Incidence (Matrix):** Most useful when information about edges is more desirable than information about vertices.
- **Adjacency (Matrix/List):** Most useful when information about the vertices is more desirable than information about the edges. These two representations are also most popular since information about the vertices is often more desirable than edges in most applications

# Representing Graphs

The **incidence matrix** of  $G$  with respect to this listing of the vertices and edges is the  $n \times m$  zero-one matrix with 1 as its  $(i, j)$  entry when edge  $e_j$  is incident with  $v_i$ , and 0 otherwise.

- In other words, for an incidence matrix  $M = [m_{ij}]$ ,

$$\begin{array}{ll} m_{ij} = 1 & \text{if edge } e_j \text{ is incident with } v_i \\ m_{ij} = 0 & \text{otherwise.} \end{array}$$



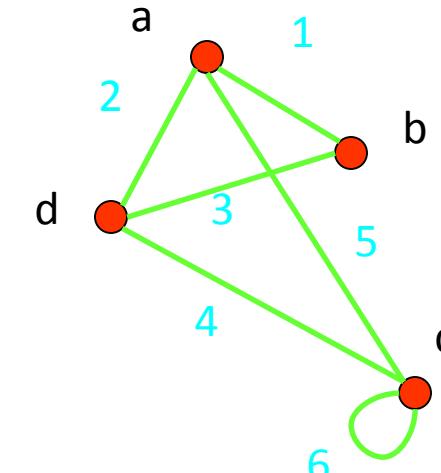
	$e_1$	$e_2$	$e_3$
$v$	1	0	1
$u$	1	1	0
$w$	0	1	1

# Representing Graphs

**Example:** What is the incidence matrix M for the following graph G based on the order of vertices a, b, c, d and edges 1, 2, 3, 4, 5, 6?

**Solution:**

$$M = \begin{bmatrix} 1 & 1 & 0 & 0 & 1 & 0 \\ 1 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 1 & 1 \\ 0 & 1 & 1 & 1 & 0 & 0 \end{bmatrix}$$



**Note:** Incidence matrices of undirected graphs contain two 1s per column for edges connecting two vertices and one 1 per column for loops.

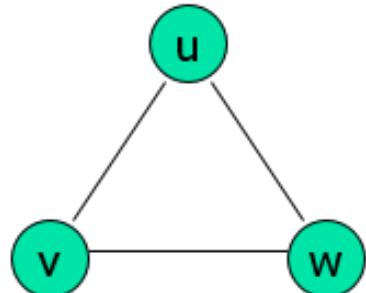
# Representing Graphs

The **adjacency matrix**  $A$  (or  $A_G$ ) of  $G$ , with respect to this listing of the vertices, is the  $n \times n$  zero-one matrix with  $1$  as its  $(i, j)$  entry when  $v_i$  and  $v_j$  are adjacent, and  $0$  otherwise.

- In other words, for an adjacency matrix  $A = [a_{ij}]$ ,

$a_{ij} = 1$  if  $\{v_i, v_j\}$  is an edge of  $G$ ,

$a_{ij} = 0$  otherwise.



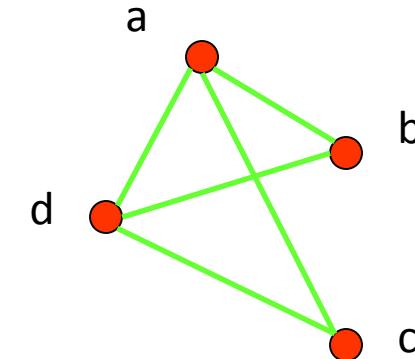
	v	u	w
v	0	1	1
u	1	0	1
w	1	1	0

# Representing Graphs

•**Example:** What is the adjacency matrix  $A_G$  for the following graph  $G$  based on the order of vertices a, b, c, d ?

**Solution:**

$$A_G = \begin{bmatrix} 0 & 1 & 1 & 1 \\ 1 & 0 & 0 & 1 \\ 1 & 0 & 0 & 1 \\ 1 & 1 & 1 & 0 \end{bmatrix}$$



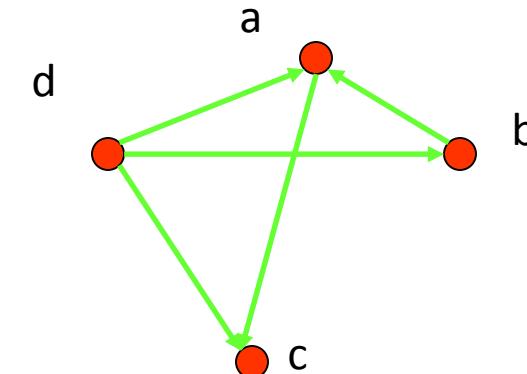
**Note:** Adjacency matrices of undirected graphs are always symmetric.

# Representing Directed Graphs

•**Example:** What is the adjacency matrix  $A_G$  for the following directed graph  $G$  based on the order of vertices a, b, c, d ?

**Solution:**

$$A_G = \begin{bmatrix} 0 & 0 & 1 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 1 & 1 & 1 & 0 \end{bmatrix}$$

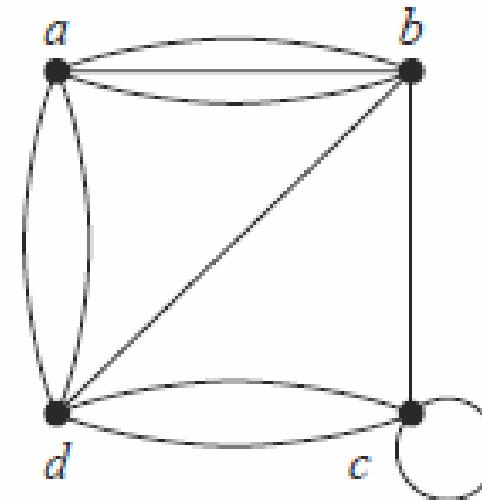


# Representing “Pseudographs”

- Example** What is the adjacency matrix  $A_G$  for the following pseudograph  $G$  based on the order of vertices  $a, b, c, d$  ?

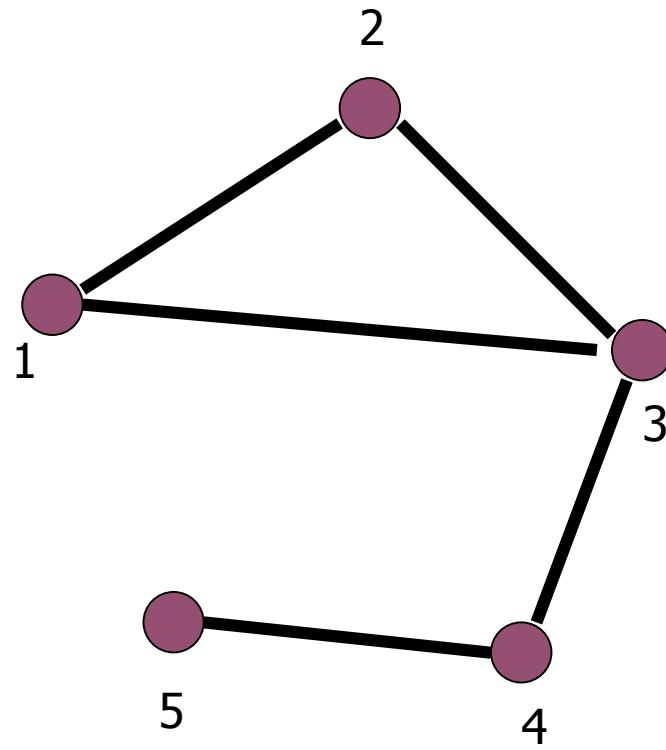
Solution:

$$\begin{bmatrix} 0 & 3 & 0 & 2 \\ 3 & 0 & 1 & 1 \\ 0 & 1 & 1 & 2 \\ 2 & 1 & 2 & 0 \end{bmatrix}$$



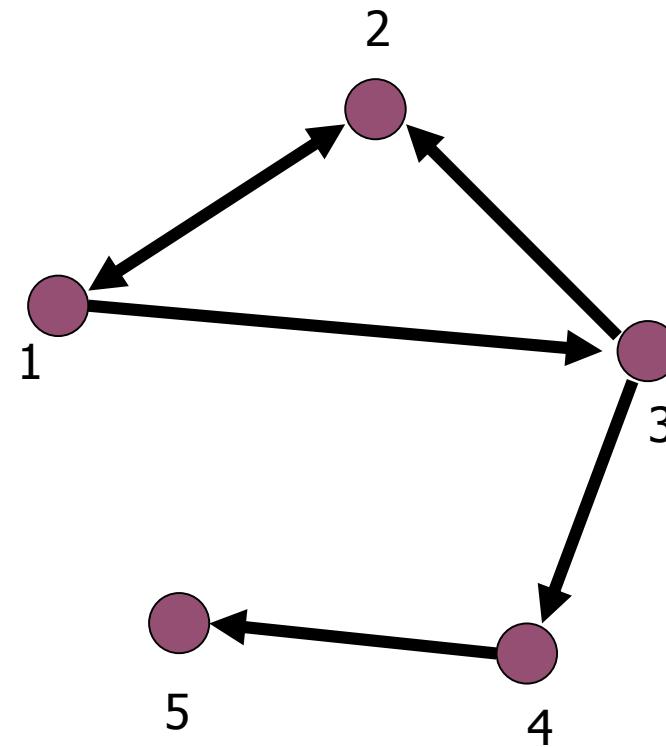
- Adjacency Matrix
  - symmetric matrix for undirected graphs

$$A = \begin{bmatrix} 0 & 1 & 1 & 0 & 0 \\ 1 & 0 & 1 & 0 & 0 \\ 1 & 1 & 0 & 1 & 0 \\ 0 & 0 & 1 & 0 & 1 \\ 0 & 0 & 0 & 1 & 0 \end{bmatrix}$$



- Adjacency Matrix
  - unsymmetric matrix for undirected graphs

$$A = \begin{bmatrix} 0 & 1 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 & 0 \end{bmatrix}$$



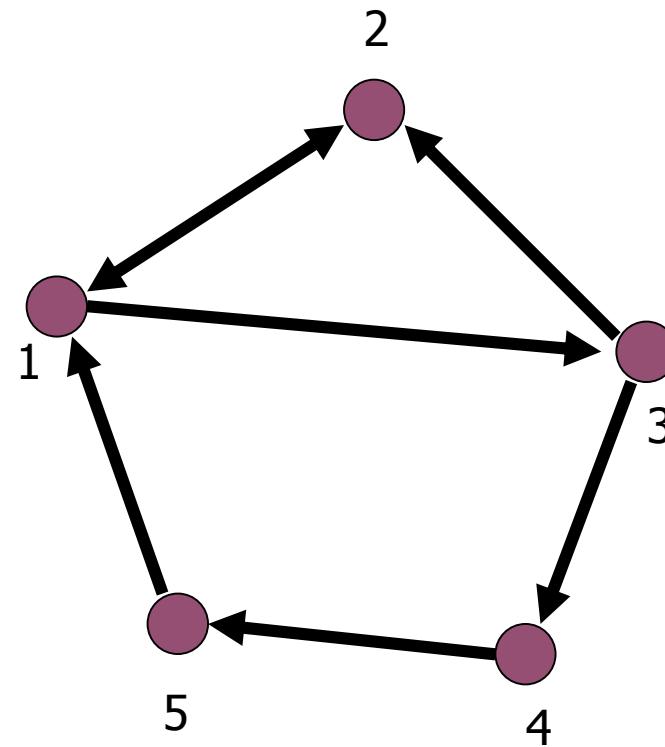
# Example. Random Walks

- Start from a node, and follow links uniformly at random.
- Stationary distribution: The fraction of times that you visit node  $i$ , as the number of steps of the random walk approaches infinity
  - if the graph is strongly connected, the stationary distribution converges to a unique vector.

# Random Walks

- stationary distribution: principal left eigenvector of the normalized adjacency matrix
  - $x = xP$
  - for undirected graphs, the degree distribution

$$P = \begin{bmatrix} 0 & 1/2 & 1/2 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 \\ 0 & 1/2 & 0 & 1/2 & 0 \\ 0 & 0 & 0 & 0 & 1 \\ 1 & 0 & 0 & 0 & 0 \end{bmatrix}$$



## Example. Counting Paths between Vertices

We can use the adjacency matrix of a graph to find the number of paths between two vertices in the graph.

**Theorem:** Let  $G$  be a graph with adjacency matrix  $\mathbf{A}$  with respect to the ordering  $v_1, \dots, v_n$  of vertices (with directed or undirected edges, multiple edges and loops allowed). The number of different paths of length  $r$  from  $v_i$  to  $v_j$  equals the  $(i,j)$ th entry of  $\mathbf{A}^r$ , where  $r > 0$  is a positive integer,

- Note: This is the standard power of matrix  $\mathbf{A}$ , not a Boolean product.

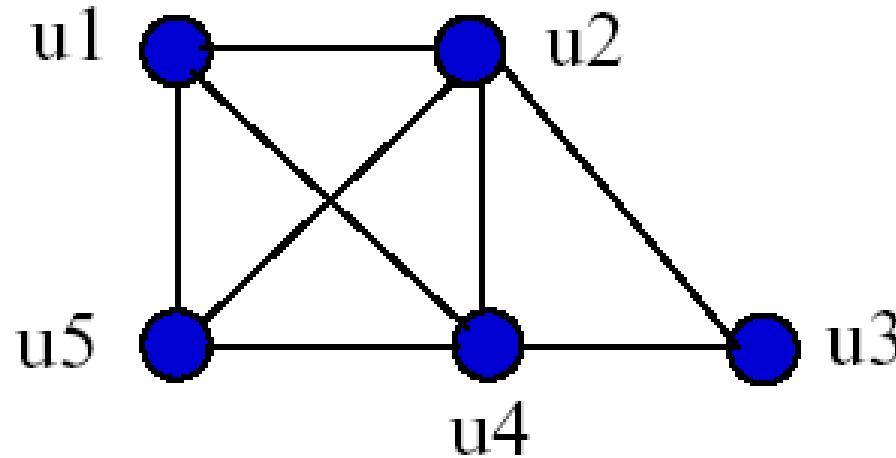
**Example:** How many paths of length four are there from  $a$  to  $d$  in the graph  $G$ .

$$G \quad \begin{array}{ccccc} & a & & b & \\ & \bullet & & \bullet & \\ & | & & \diagdown & \\ & & \text{adjacency} & & \\ & & \text{matrix } A \text{ of } G & & \\ & d & & c & \end{array} \quad \begin{bmatrix} 0 & 1 & 1 & 0 \\ 1 & 0 & 0 & 1 \\ 1 & 0 & 0 & 1 \\ 0 & 1 & 1 & 0 \end{bmatrix} \quad \mathbf{A}^4 = \begin{bmatrix} 8 & 0 & 0 & 8 \\ 0 & 8 & 8 & 0 \\ 0 & 8 & 8 & 0 \\ 8 & 0 & 0 & 8 \end{bmatrix}$$

**Solution:** The adjacency matrix of  $G$  is given above. Hence the number of paths of length four from  $a$  to  $d$  is the  $(1,4)$ th entry of  $\mathbf{A}^4$ . The eight paths are as:

$$\begin{array}{ll} a, b, a, b, d & a, b, a, c, d \\ a, b, d, b, d & a, b, d, c, d \\ a, c, a, b, d & a, c, a, c, d \\ a, c, d, b, d & a, c, d, c, d \end{array}$$

**Example 2**

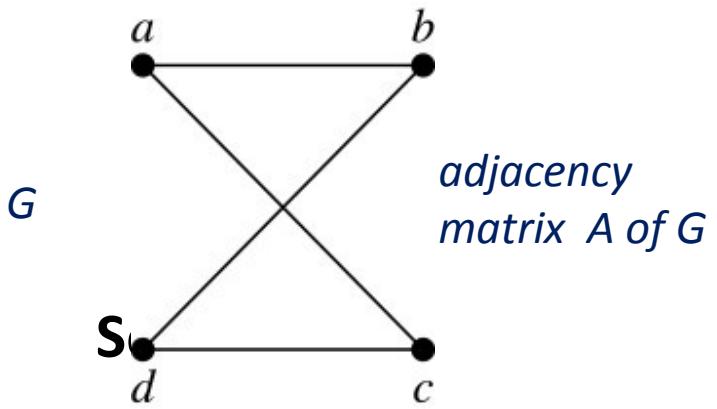


$$M = \begin{bmatrix} 0 & 1 & 0 & 1 & 1 \\ 1 & 0 & 1 & 1 & 1 \\ 0 & 1 & 0 & 1 & 0 \\ 1 & 1 & 1 & 0 & 1 \\ 1 & 1 & 0 & 1 & 0 \end{bmatrix}$$

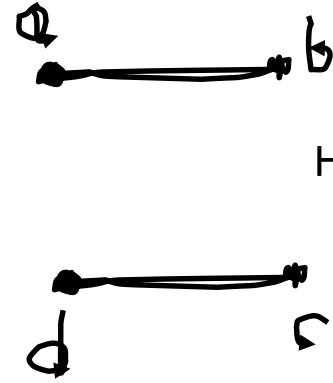
$$M^2 = \begin{bmatrix} 3 & 2 & 2 & 2 & 2 \\ 2 & 4 & 1 & 3 & 2 \\ 2 & 1 & 2 & 1 & 2 \\ 2 & 3 & 1 & 4 & 2 \\ 2 & 2 & 2 & 2 & 3 \end{bmatrix}$$

$$M^3 = \begin{bmatrix} 6 & 9 & 4 & 9 & 7 \\ 9 & 8 & 7 & 9 & 9 \\ 4 & 7 & 2 & 7 & 4 \\ 9 & 9 & 7 & 8 & 9 \\ 7 & 9 & 4 & 9 & 6 \end{bmatrix}$$

**Example:** Use the theorem on the previous slide to show that graph G is connected and graph H is not connected.

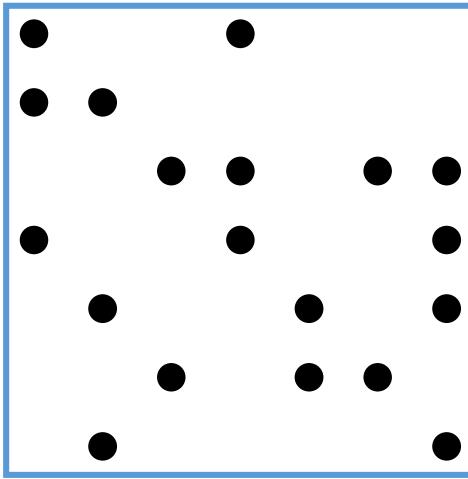


$$\begin{bmatrix} 0 & 1 & 1 & 0 \\ 1 & 0 & 0 & 1 \\ 1 & 0 & 0 & 1 \\ 0 & 1 & 1 & 0 \end{bmatrix}$$

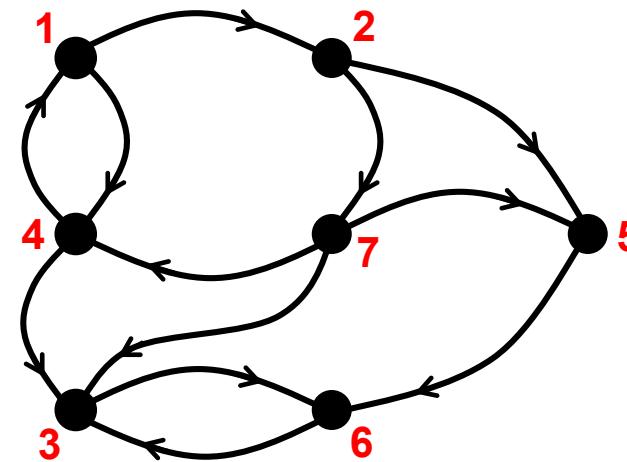


Graph G with  $n$  nodes is connected iff every off-diagonal entry of  $A+A^2+A^3+\cdots+A^n$  is positive, where  $A$  is the adjacency matrix of G.

# Sparse Adjacency Matrix and Graph

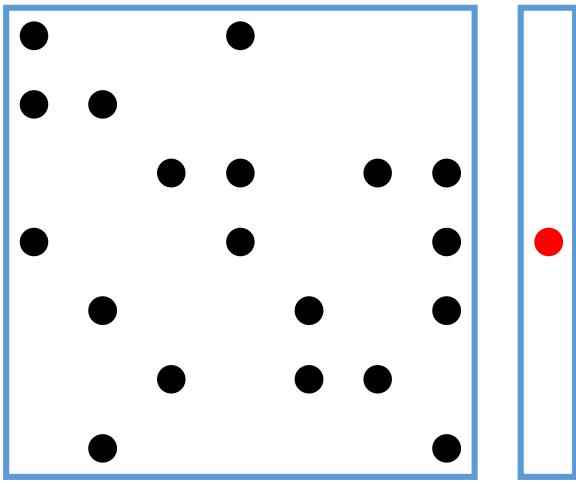


$A^T$



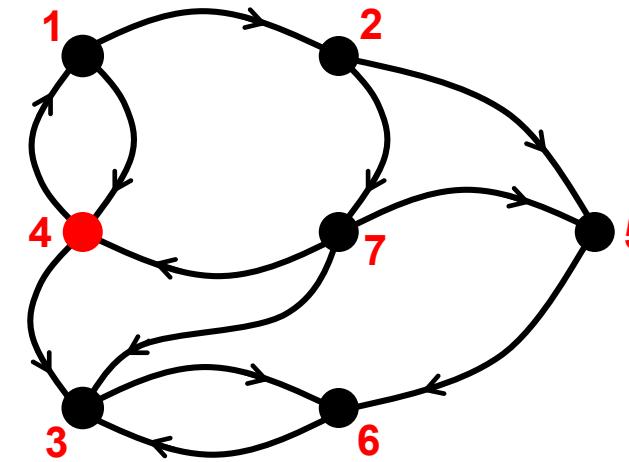
- Adjacency matrix: sparse array, few nonzeros for graph edges
- Storage-efficient implementation from sparse data structures

# Breadth-First Search: sparse mat \* vec



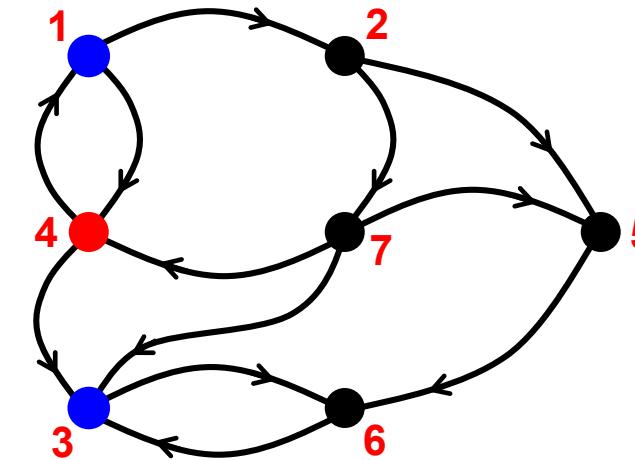
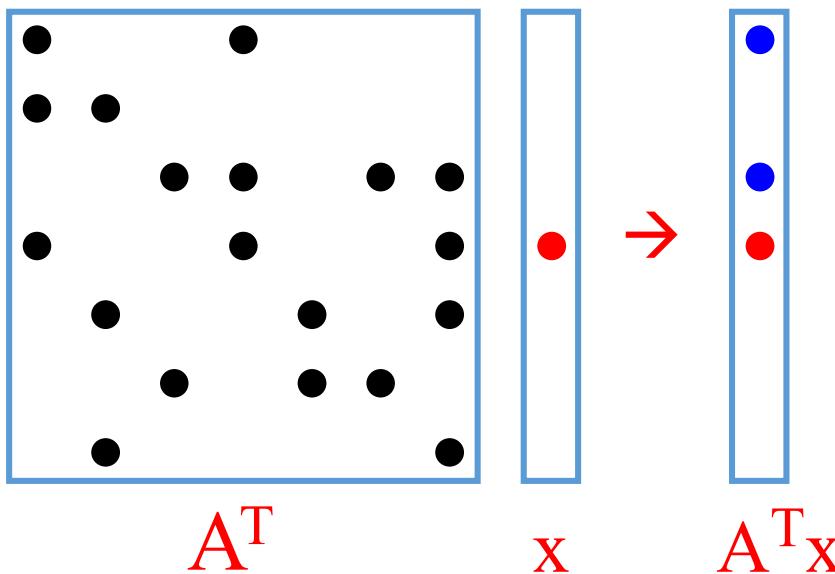
A sparse matrix  $A^T$  represented as a grid of black dots. The matrix has 7 rows and 7 columns. To its right is a vertical vector  $x$  represented by a single red dot.

$$A^T \quad x$$



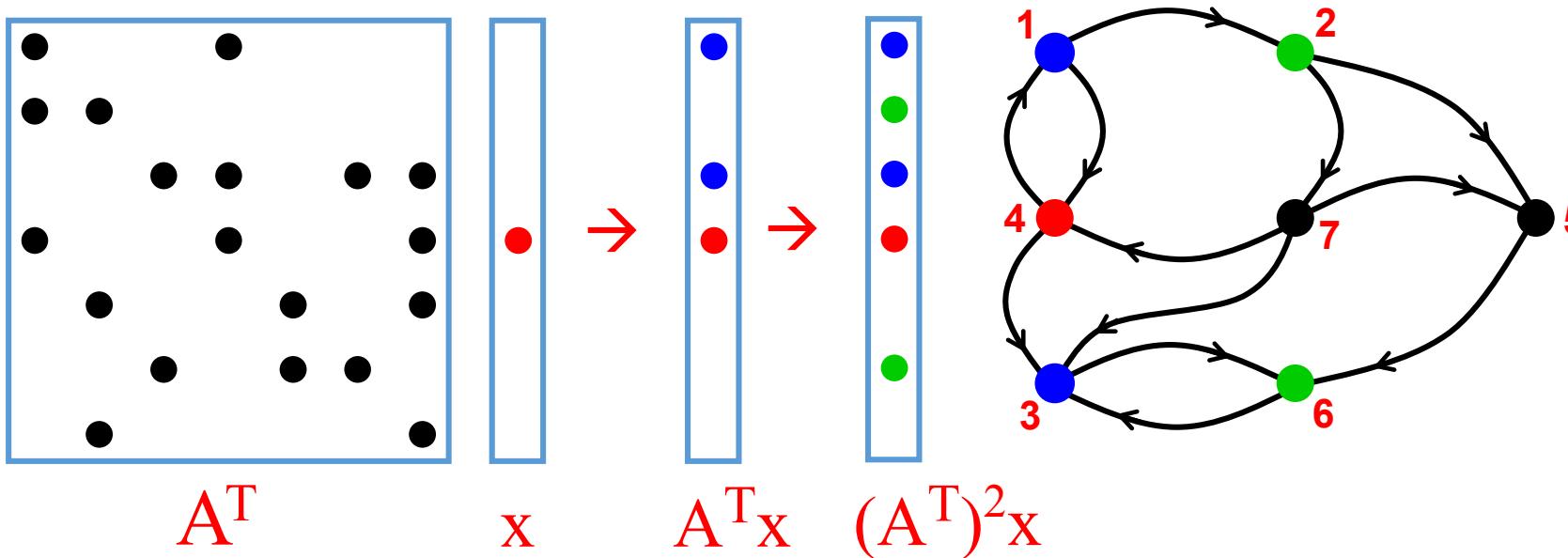
- Multiply by adjacency matrix  $\rightarrow$  step to neighbor vertices
- Work-efficient implementation from sparse data structures

# Breadth-First Search: sparse mat \* vec



- Multiply by adjacency matrix  $\rightarrow$  step to neighbor vertices
- Work-efficient implementation from sparse data structures

# Breadth-First Search: sparse mat \* vec



- Multiply by adjacency matrix → step to neighbor vertices
- Work-efficient implementation from sparse data structures