Algorithms, Data Structures, and Problem Solving

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Dynamic programming (DP) turns recursion into iteration. It can turn exponential problems into polynomial ones. You have to "rethink the problem" to achieve this benefit.

DP can be used when:

- subproblems overlap
- subproblems are slightly smaller than the original
- subproblems have optimal structure
    - *an optimal solution consists of optimal sub-solutions*

Today's Lecture

- Principle of Optimality
- Bellman Equation
- *coin change*
- discussion of the coin change problem and its DP solution
- Another Example
  - sequence alignment
  - Needleman-Wunsch algorithm

Principle of Optimality

this is why dynamic programming works

- formulate the problem as a **series of decisions**
- ingredients:
  - **state** variables describe all we need to know in order to make decisions
  - **actions** describe the available choices
  - **transitions** define the next state
  - **payoffs** (or costs) define if we get closer or farther from optimality
  - the **value function** tracks the best sub-solution

Principle of Optimality

$$V(x_0) = \max_{a_0, a_1, \cdots, a_N} \sum_{n=0}^{N} F(x_n, a_n)$$

$$x_n \in X$$

$$a_n \in A(x_n)$$

$$x_{n+1} = T(x_n, a_n)$$

value function

accumulates the payoff (or cost)

payoff (or cost)

measures progress towards the optimum

$$V(x_0) = \max_{a_0, a_1, \cdots, a_N} \sum_{n=0}^{N} F(x_n, a_n)$$

stage

which decision are we at?

$$x_n \in X$$

state

describes the system

$$a_n \in A(x_n)$$

action

depends on state (and stage)

$$x_{n+1} = T(x_n, a_n)$$

transition

captures the effect of actions

Principle of Optimality

$$V(x_0) = \max_{a_0, a_1, \cdots, a_N} \sum_{n=0}^{N} F(x_n, a_n)$$

intuition: ***V(x)*** is the best possible cumulated payoff at ***x***

Principle of Optimality

$$V(x_0) = \max_{\boxed{a_0, a_1, \cdots, a_N}} \sum_{n=0}^{N} F(x_n, a_n)$$

quite a few choices!

$$x_n \in X$$

$$a_n \in A(x_n)$$

$$x_{n+1} = T(x_n, a_n)$$

can be simplified into a recursion

Bellman Equation

$$V(x_0) = \max_{a_0}\Big(F(x_0, a_0) + V(x_1)\Big)$$

$$x_1 = T(x_0, a_0)$$

if we know $V(x_1)$
then we just need to maximize a ***single*** choice: a_0
instead of N+1 combinations of choices

$$V(x_0) = \max_{a_0, a_1, \cdots, a_N} \sum_{n=0}^{N} F(x_n, a_n)$$

Bellman Equation

$$V(x_0) = \max_{a_0}\big(F(x_0, a_0) + V(x_1)\big)$$

$$x_1 = T(x_0, a_0)$$

if we know $V(x_1)$
then we just need to maximize a ***single*** choice: a_0
instead of N+1 combinations of choices

the tricky part: find a smart way to ***construct V(x)***
➠ that's the essence of dynamic programming!

Group Activity

Coin Change

First steps with dynamic programming.

Discussion of the Coin Change Problem

- Can you identify any subproblem?
    1. what are the subproblems?
    2. do they overlap?
- are subproblems only slightly smaller than the original?
- do subproblems have optimal structure?
- is it exponential if we don’t use DP?

Discussion of the Coin Change Solution

Can you identify the

- state
- action
- transition
- payoff
- value function

in this example?

Sequence Alignment

- minimize the number of edits required to change one string into another
- used in many real applications
  - file comparison
  - computational biology
  - spellchecking
  - ...

The **Needleman–Wunsch** Algorithm for Sequence Alignment

- given:
  - a table of match scores
  - a gap penalty
  - two strings A and B
- compute:
  - the alignment with maximum score
    - *(same as "lowest cost")*
  - there can be more than one solution

The **Needleman–Wunsch** Algorithm for Sequence Alignment

for example:

- perfect match: +10
- vowel to vowel: -2
- consonant to consonant: -4
- vowel to consonant: -10
- gap penalty: -5

b	e	e	r	_	_
c	o	f	f	e	e
-4	-2	-10	-4	-5	-5

score: -30

b	e	_	_	e	r
c	o	f	f	e	e
-4	-2	-5	-5	10	-10

score: -16

The **Needleman–Wunsch** Algorithm for Sequence Alignment

1. *match b with c*
2. *match e with o*
3. *match e with f*
4. *match r with f*
5. *insert e*
6. *insert e*

b	e	e	r	_	_
c	o	f	f	e	e
-4	-2	-10	-4	-5	-5

score: -30

1. *match b with c*
2. *match e with o*
3. *insert f*
4. *insert f*
5. *perfect match for e*
6. *match r with e*

b	e	_	_	e	r
c	o	f	f	e	e
-4	-2	-5	-5	10	-10

score: -16

Condensed representation of possible actions and their effects:

	_	c	o	f	f	e	e
_	**0**	*insert c*					
b	*delete b*		*match b with c*				
e							
e							
r							

Condensed representation of possible actions and their effects:

	_	c	o	f	f	e	e
_	0	-5					
b	-5	-4					
e							
e							
r							

- perfect match: +10
- vowel to vowel: -2
- consonant to consonant: -4
- vowel to consonant: -10
- gap penalty: -5

Condensed representation of possible actions and their effects:

	_	c	o	f	f	e	e
_	0	-5					
b	-5	-4					
e							
e							
r							

insert

delete

match

Condensed representation of possible actions and their effects:

	_	c	o	f	f	e	e
_	**0**	**-5**					
b	**-5**	**-4**					
e							
e							
r							

-5

-5

-2

Condensed representation of possible actions and their effects:

	_	c	o	f	f	e	e
_	0	-5					
b	-5	-4	-9				
e		-9	-6				
e							
r							

Condensed representation of possible actions and their effects:

	_	c	o	f	f	e	e
_	**0**	**-5**					
b	**-5**	**-4**	**-9**				
e		**-9**	**-6**				
e							
r							

insert

delete

match

Problem: more than one way to reach a cell!

	_	c	o	f	f	e	e
_							
b							
e				???			
e							
r							

_	_	b	e		
c	o	f	_		
-5	-5	-4	-5		

_	b	e			
c	o	f			
-5	-10	-10			

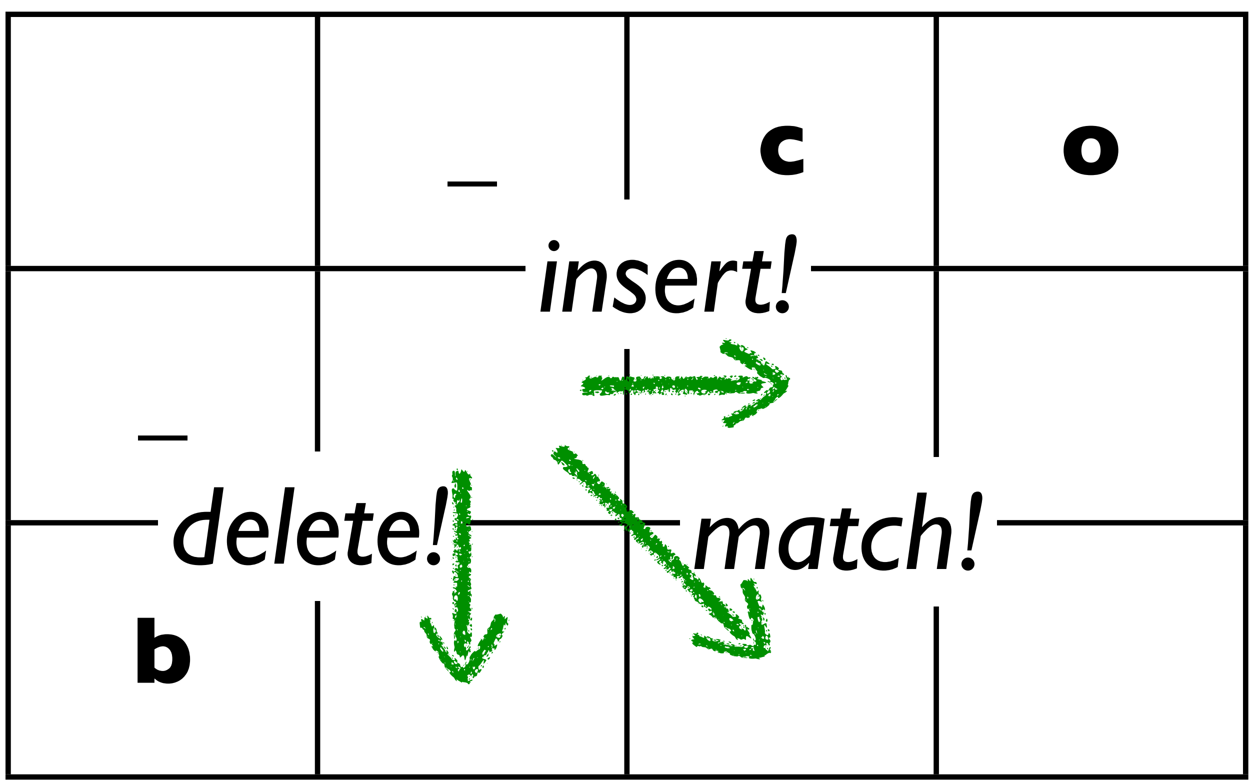
b	e	_			
c	o	f			
-4	-2	-5			

Apply Dynamic Programming

- check optimal subproblem structure
  an optimal solution to the overall problem is composed of optimal solutions to the subproblems

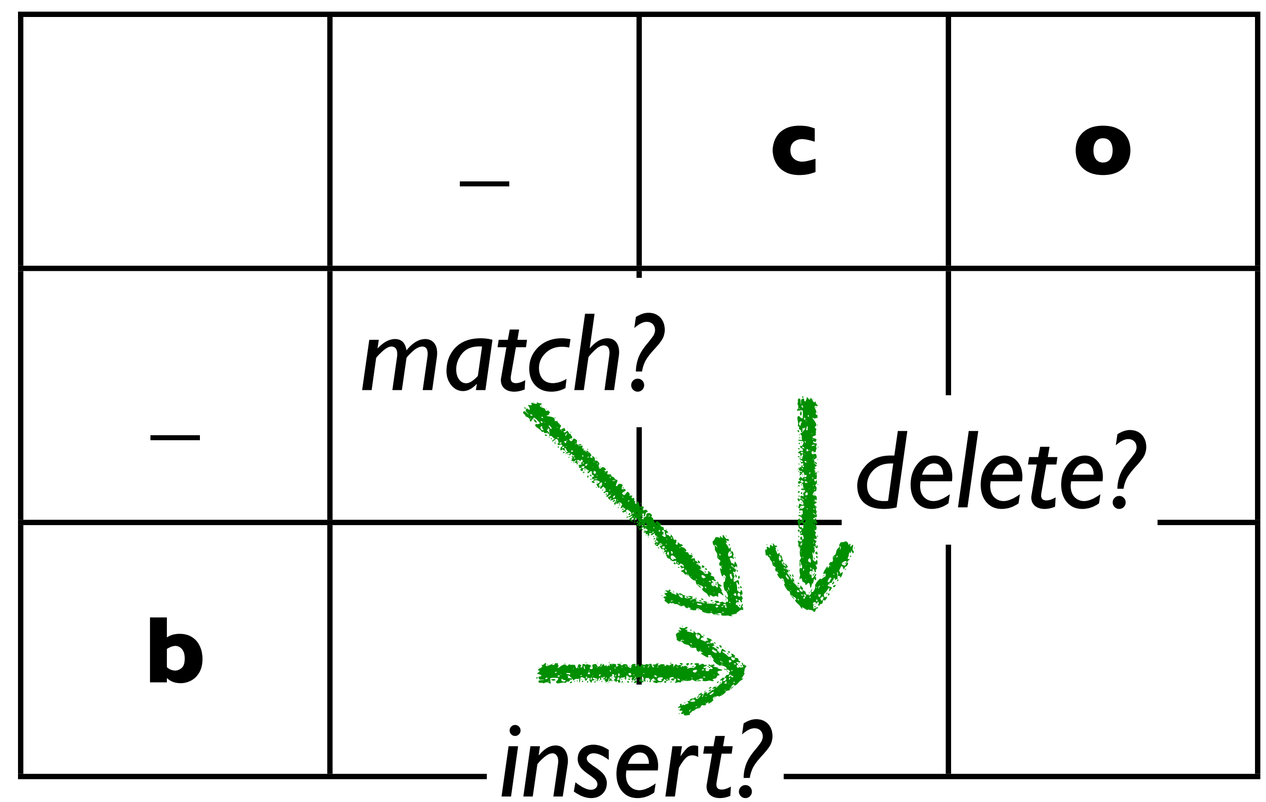
- formulate terms for the Bellman equation
  - state, action, transition
  - payoff and value function
  - order of computation

From tree exploration to local a sequence of local optimizations.



problematic

you need some way of keeping track of all the different ways of combining choices



much better

once a choice is made, it is known to be optimal and does not need to be revisited

Needleman–Wunsch Algorithm

	_	c	o	f	f	e	e
_	0	-5	-10	-15	-20	-25	-30
b	-5						
e	-10						
e	-15						
r	-20						

match?

delete?

insert?

Needleman–Wunsch Algorithm

	_	**c**	**o**	**f**	**f**	**e**	**e**
_	0 0-4?	-5	-5-5? 10	-15	-20	-25	-30
b	-5 -5-5?	-4					
e	-10						
e	-15						
r	-20						

Needleman–Wunsch Algorithm

	_	c	o	f	f	e	e
_	0	-5	-10	-15	-20	-25	-30
b	-5	-4	-9				
e							
e							
r							

-5-10?

-10-5?

-4-5?

Needleman–Wunsch Algorithm

	_	c	o	f	f	e	e
_	0	-5	-10	-15	-20	-25	-30
b	-5	-4	-9	-14			
e	-10						
e	-15						
r	-20						

Needleman–Wunsch Algorithm

	_	**c**	**o**	**f**	**f**	**e**	**e**
_	0	-5	-10	-15	-20	-25	-30
b	-5	-4	-9	-14	-19		
e	-10						
e	-15						
r	-20						

Needleman–Wunsch Algorithm

	_	**c**	**o**	**f**	**f**	**e**	**e**
_	0	-5	-10	-15	-20	-25	-30
b	-5	-4	-9	-14	-19	-24	-29
e	-10	-9	-6	-11	-16	-9	-14
e	-15	-14	-11	-16	-21	-6	+1
r	-20	-19	-16	-15	-20	-11	-4

Needleman–Wunsch Algorithm

	_	c	o	f	f	e	e
_	0	-5	-10	-15	-20	-25	-30
b	-5	-4	-9	-14	-19	-24	-29
						-9	-14
						-6	+1
						-11	-4

how to extract the solution:

1. compute / maintain backpointers
   - *(what was the optimal choice at each cell?)*
2. trace back one of the optimal paths
3. read off the action sequence

Needleman–Wunsch Algorithm

	_	c	o	f	f	e	e
_	0						
b							
e							
e							
r							-4

b	_	_	_	*e*	*e*	*r*
c	*o*	*f*	*f*	*e*	*e*	_

Sequence Alignment

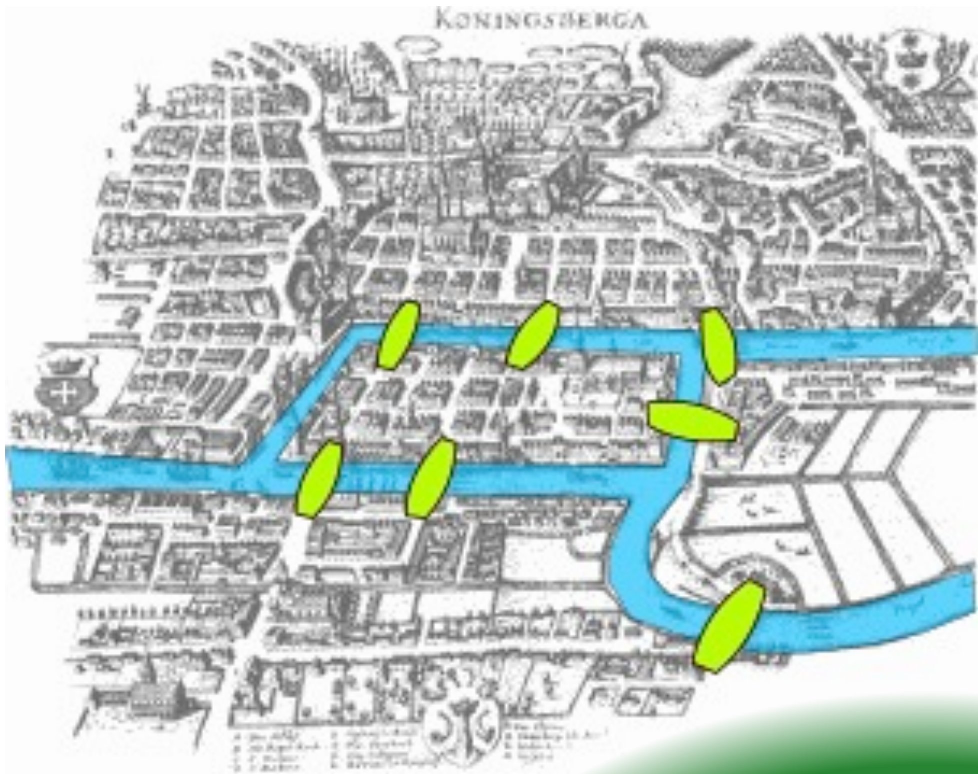
- given a table of costs *(similarity matrix)*
- given a gap cost d
- given two strings A and B
- create table of optimal sub-alignment costs F(i,j)
    - init: F(0,i) = d*i and F(j,0) = d*j
    - F(i,j) = maximum of
        - match: F(i-1,j-1) + cost(A[i], B[j])
        - delete: F(i-1,j) + d
        - insert: F(i,j-1) + d
    - keep (or compute) backpointers
- trace back the result starting from the last cell
- *note: table indices 0...strlen(A) and 0...strlen(B) !*

DP: Take-Home Message

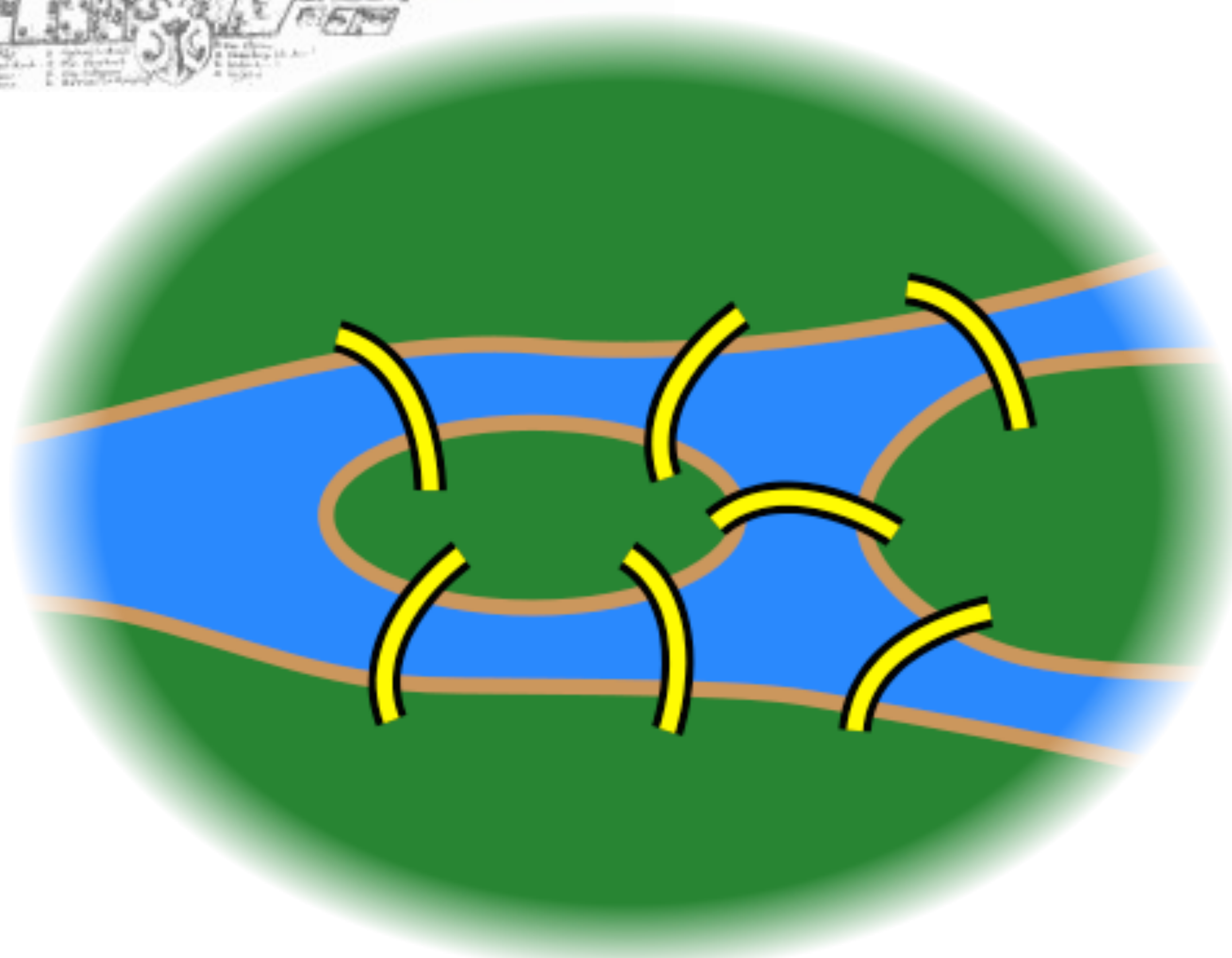
1. divide the problem into <u>steps</u> *(or stages)*
2. store the <u>state</u> *(information)* required in each step
3. an <u>action</u> *(or decision)* is taken at each step to transform the state and accumulate payoff *(or pay cost)*
4. the <u>value function</u> captures the cumulated best action sequence to arrive at a given state
5. <u>trace back</u> the solution after you have reached the goal *(or the start, depending on propagation order)*

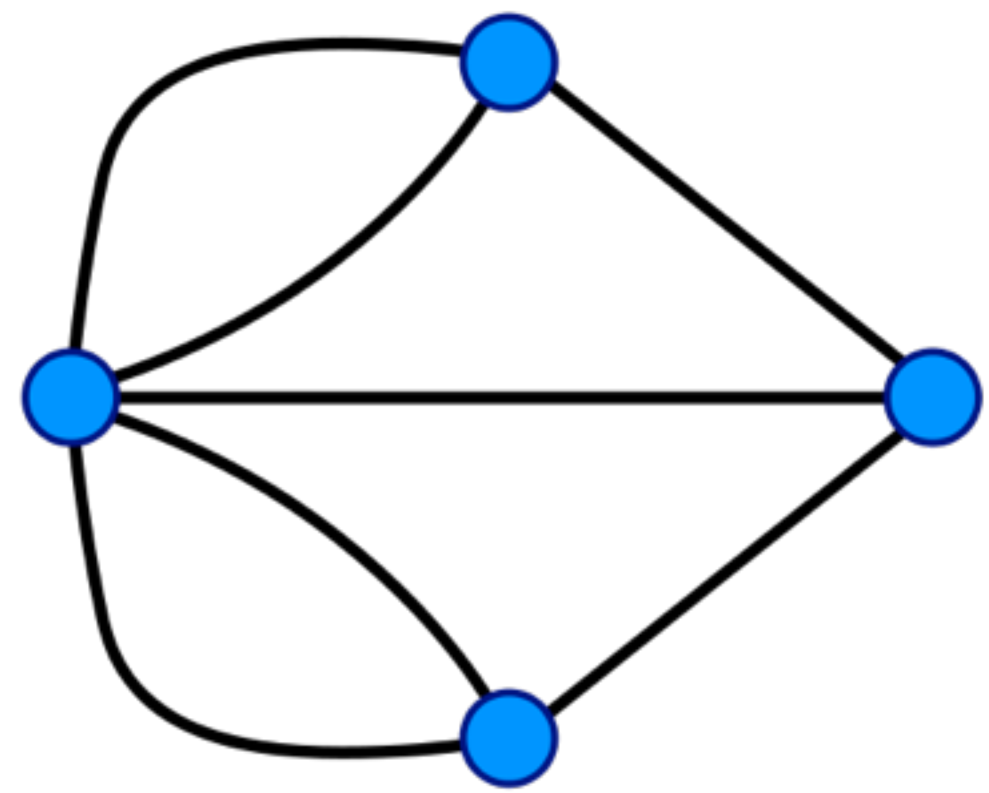
Graphs

- graphs
- *graph representations*
- *graph traversals*
- directed acyclic graphs
- *topological ordering*



- a set of vertices
- a set of edges (connections)





http://en.wikipedia.org/wiki/Seven_Bridges_of_K%C3%B6nigsberg

Why are Graphs Important?

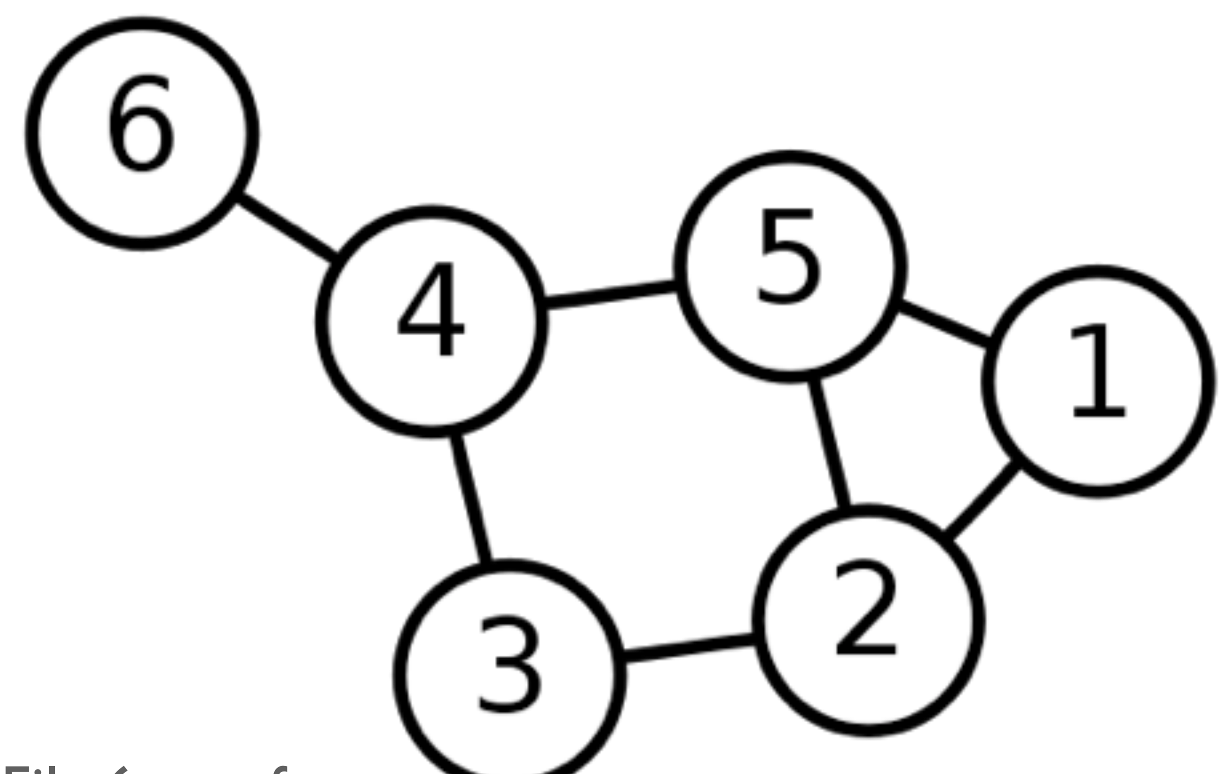
...whenever we model relations between entities...

- **computer science:** communication networks, computation flow, dependency tracking, ...
- **linguistics:** semantic networks (meaning in terms of related words), ...
- **chemistry:** molecule models (atoms and bonds), ...
- **physics:** particle interactions, electromagnetic circuits, ...
- **sociology:** measure prestige, diffusion in social networks, ...
- **biology:** habitats and migration paths, breeding patterns, spread of disease, ...
- **robotics:** path planning, dynamical system models, mapping and localization, ...
- **artificial intelligence:** task planning, scene understanding, ...

Graphs

- a set of vertices
  often just use natural numbers
- a set of edges
- each edge connects two vertices with each other

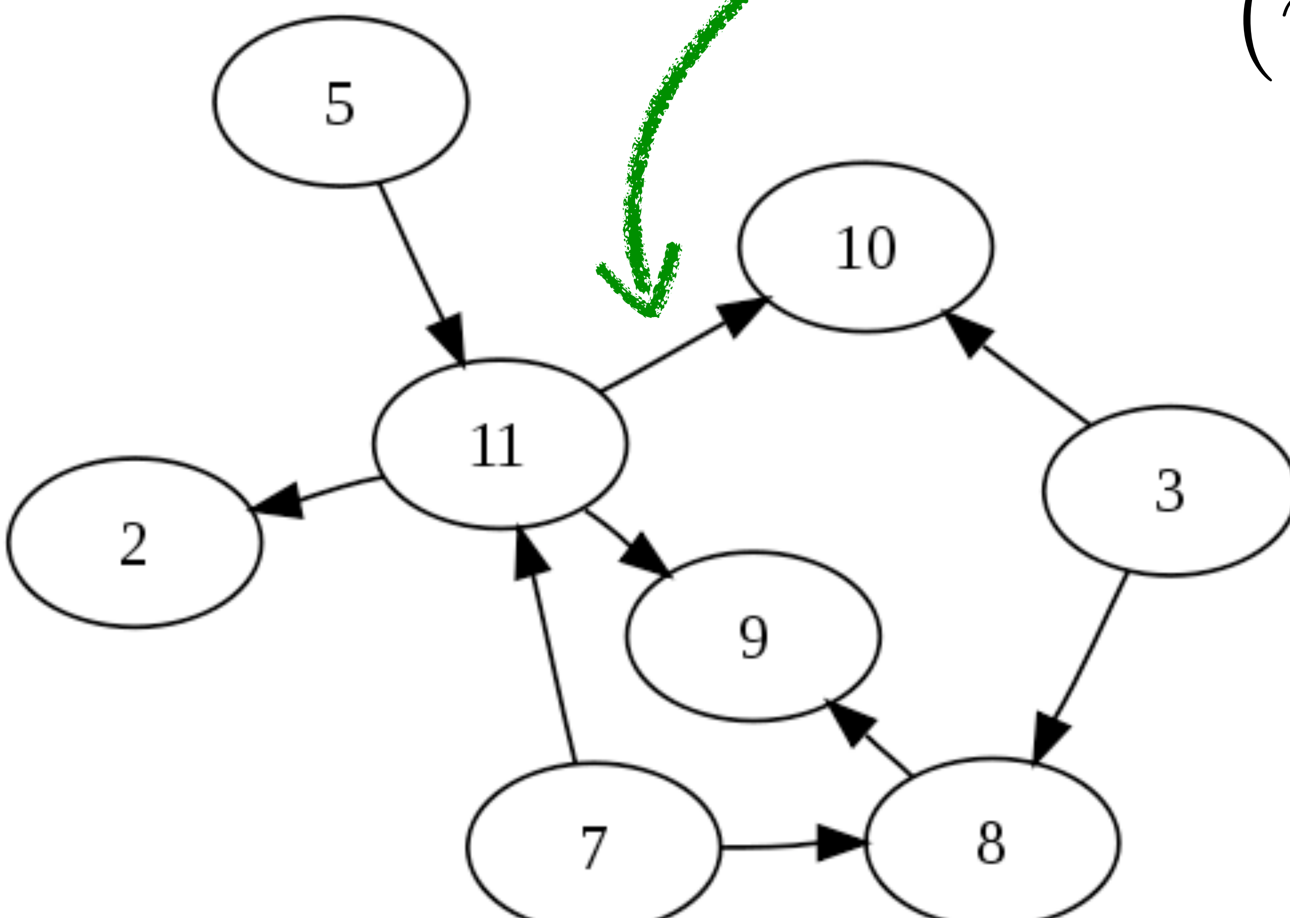
$$G = (V, E)$$
$$V = \{v\}$$
$$E = \{e\}$$
$$e = (v, w) : v, w \in V$$



http://en.wikipedia.org/wiki/File:6n-graf.svg

Edge Variations

- edges can be directed or undirected



$$(v, w) \in E \Leftrightarrow (w, v) \in E$$

http://en.wikipedia.org/wiki/File:Directed_acyclic_graph_3.svg

Edge Variations

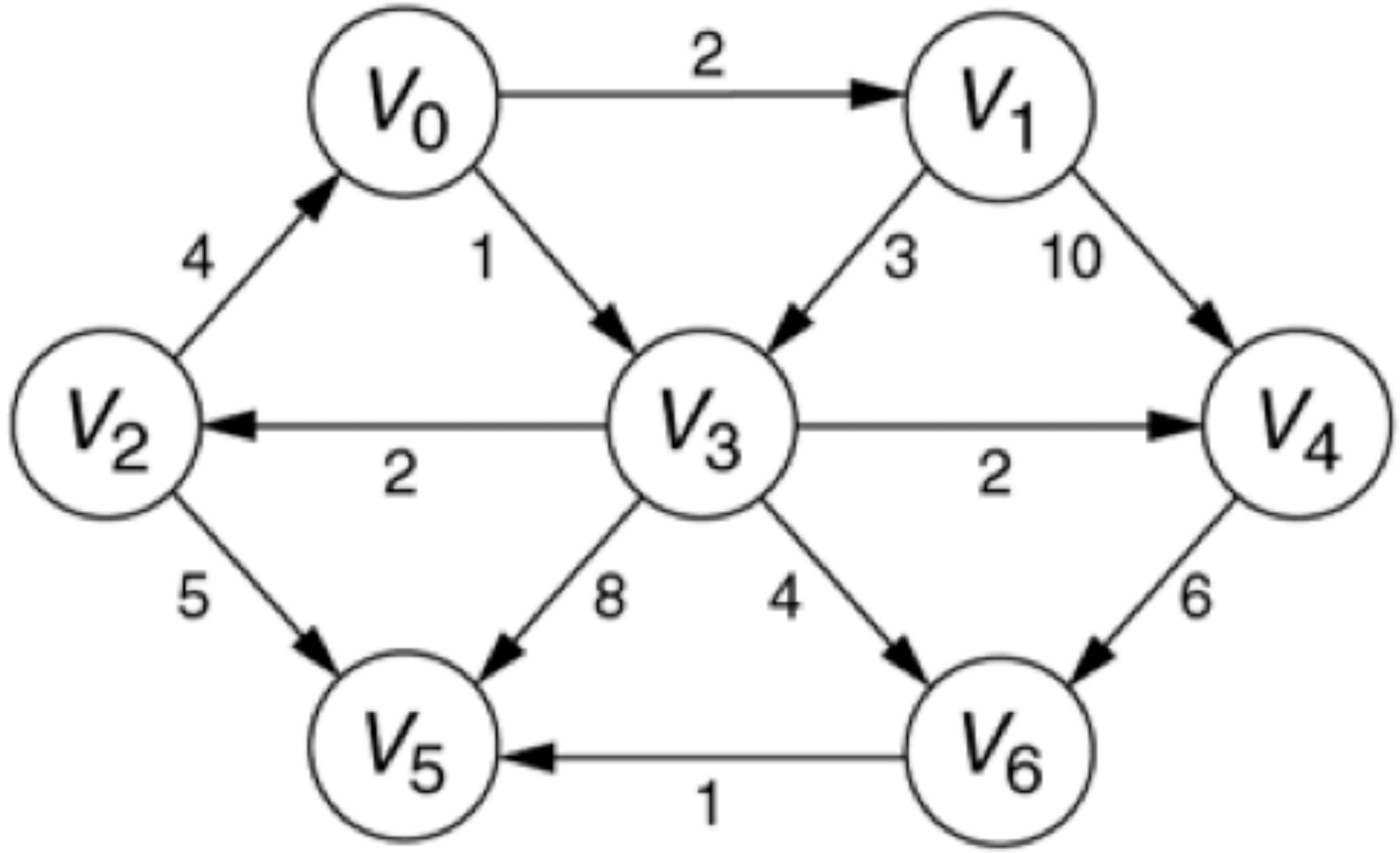
- edges can have extra data, such as ***cost***
- two formalizations are common:

cost "inside" $\quad e = (v, w, c) : v, w \in V, c \in \mathbb{R}$

separate mapping $\quad c = c(e) = c(v, w)$

- *...similarly, vertices can have extra info*

Positive-Weighted Edges



very common, for example:

- roads between cities
- connections between airports
- computer networks
- flow models (information, money, ...)

Paths

- paths are sequences of connected vertices

$$P = (v_1, v_2, \cdots v_N)$$

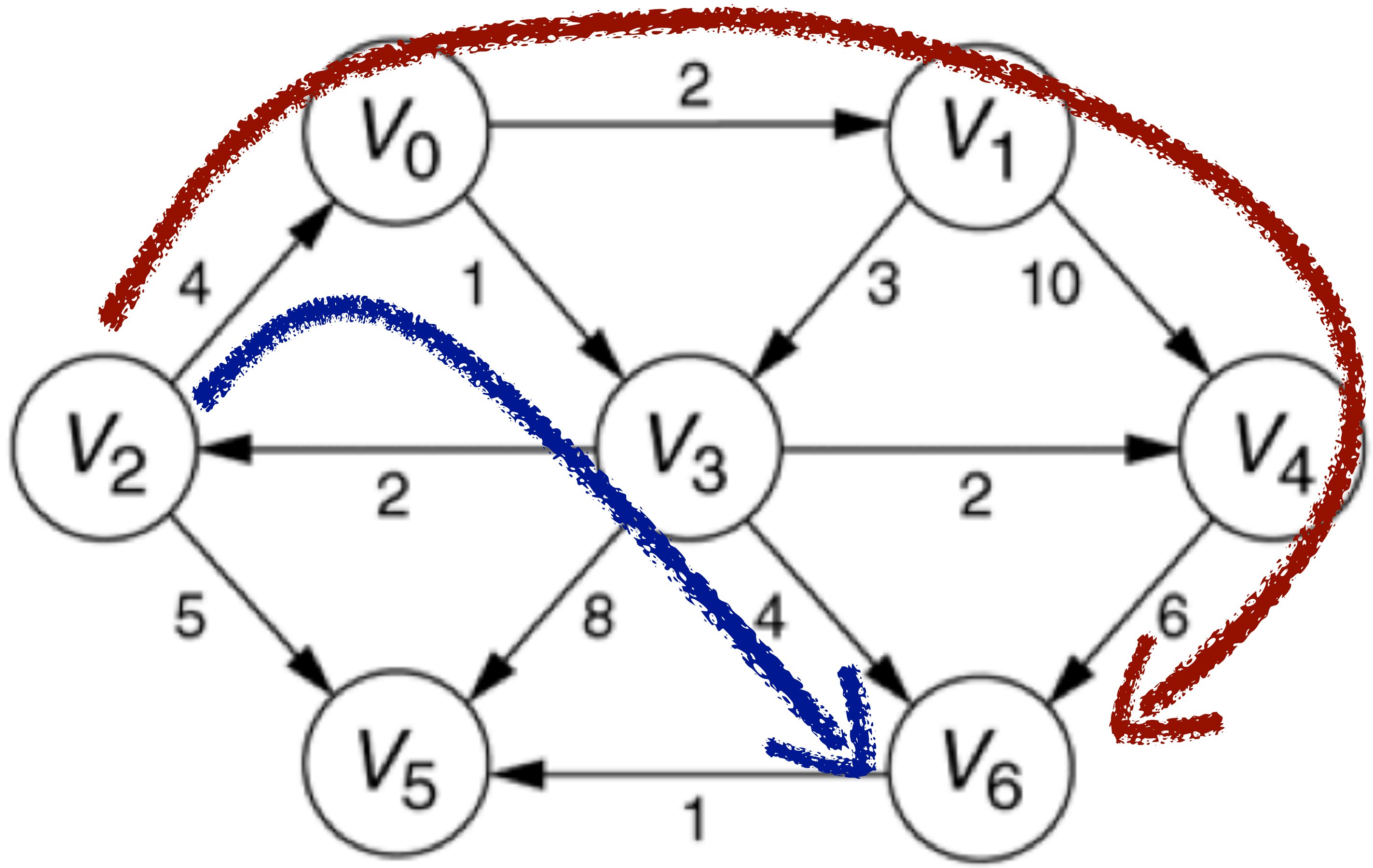
$$(v_i, v_{i+i}) \in E \; \forall \; 1 \leq i < N$$

- path length can be unweighted or weighted

$$|P| = \begin{cases} N - 1 & \text{number of edges} \\ \sum_{1 \leq i < N} c(v_i, v_{i+i}) & \text{sum of costs} \end{cases}$$

Paths

$$P_1 = (2, 0, 3, 6)$$
$$P_2 = (2, 0, 1, 4, 6)$$



- **weighted:** $|P_1| = 4 + 1 + 4 = 9$

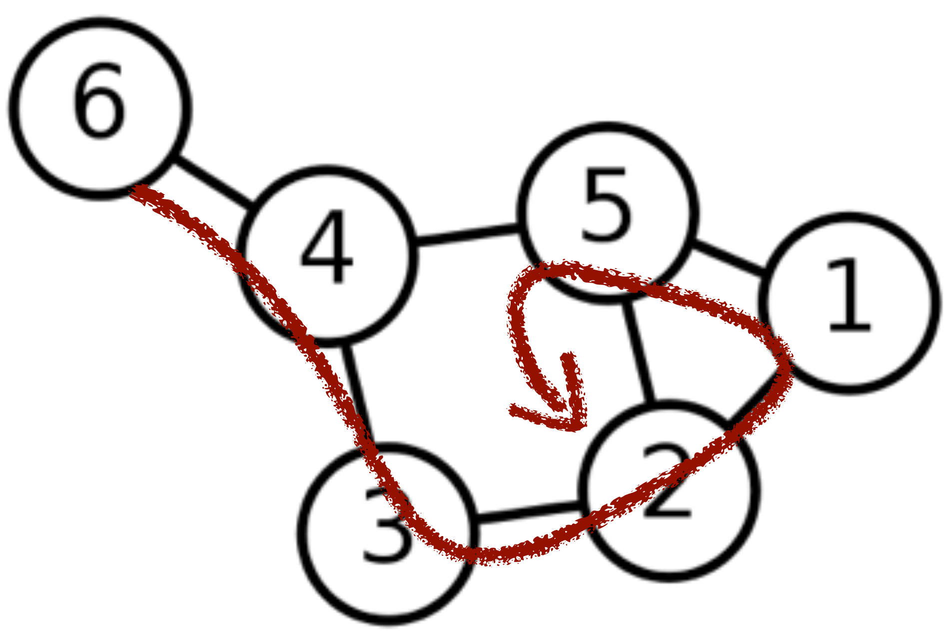
  $|P_2| = 4 + 2 + 10 + 6 = 22$

- **unweighted:** $|P_1| = 3$

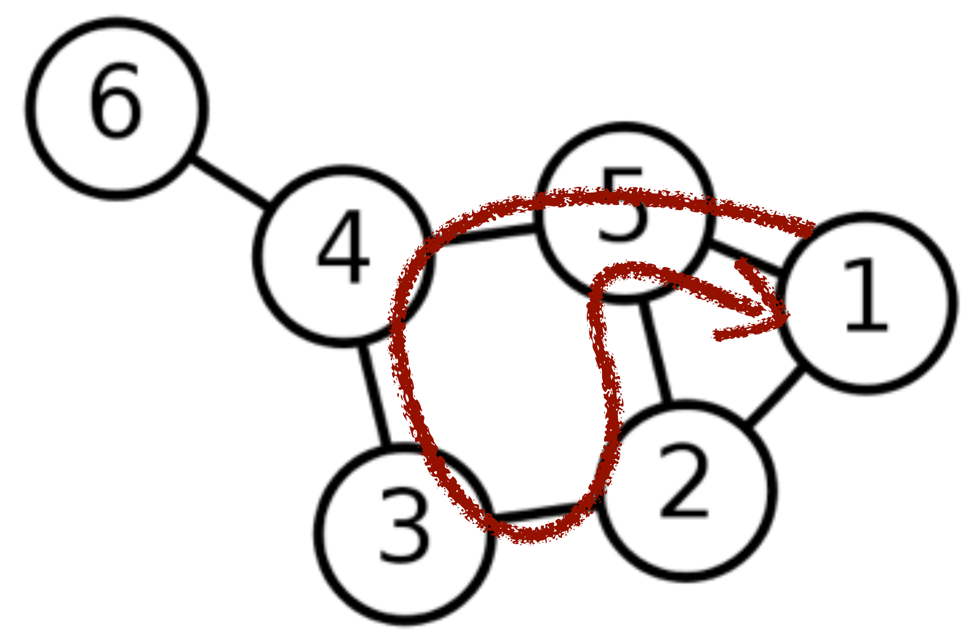
  $|P_2| = 5$

Simple Paths, Cycles

- paths can be cycles: $|P| \geq 1 \cap v_i = v_N$
- paths can be simple: no duplicate vertices
  - exception: start/end of simple cycles
- *important type:* directed acyclic graphs *(DAG)*



non-simple path



non-simple cycle

Implementing Graphs

- adjacency matrix
  - simple, immediate, but can waste space
- adjacency list
  - more appropriate use of space
- storing extra info
  - internally in vertex and edge objects
  - externally in separate maps

Group Activity

Graph Representations

a good exam question...

Graph Traversals

- many possibilities
- two fundamental methods:
    - depth-first search
    - breadth-first search
- another very important method:
    - best-first search (Dijkstra)
- *many advanced and specialized methods, such as heuristic search (A*)*

Group Activity

Graph Traversals

another good exam question...

Directed Acyclic Graphs

- directed graph, but from any vertex ***v***, there is no path that goes back to ***v***
- useful for...
  - scheduling courses, tasks, computations
  - revision control systems
  - Bayesian Networks
    - machine learning
    - probabilistic reasoning

Group Activity

Topological Ordering

yet another good exam question...

Graphs: Take-Home Message

- graphs are extremely versatile
- all the other data structures we've seen are "just" special cases of graphs
    - the specialization brings benefits, such as faster algorithms
- much more can be found on the Web *(which, by the way, can be modeled as a graph)* http://en.wikipedia.org/wiki/Graph_theory