

# Graph Isomorphism

When are two graphs that may look different when they're drawn, really the same?

Answer:  $G_1(V_1, E_1)$  and  $G_2(V_2, E_2)$  are *isomorphic* if they have the same number of vertices ( $|V_1| = |V_2|$ ) and we can relabel the vertices in  $G_2$  so that the edge sets are identical.

- Formally,  $G_1$  is isomorphic to  $G_2$  if there is a bijection  $f : V_1 \rightarrow V_2$  such that  $\{v, v'\} \in E_1$  iff  $\{f(v), f(v')\} \in E_2$ .
- Note this means that  $|E_1| = |E_2|$

In general, it's very hard to tell if two graphs are isomorphic.

# Reachability

Is there a path in graph  $G$  from vertex  $v$  to  $v'$ ?

- if the vertices in a graph correspond to towns, and  $v$  and  $v'$  are connected by an edge if there's a direct road link from  $v$  to  $v'$ , then  $v$  is reachable from  $v'$  if there's a way of driving from  $v$  to  $v'$
- in a communication network, reachability describes who can (ultimately) communicate with whom.

How can we test if one vertex is reachable from another?

# A Useful Representation of a Graph

How can we represent a graph in a computer.

- You can't draw pictures ...

One obvious way: list the vertices and edges

Anoter way: represent a graph  $G(V, E)$  by its *adjacency matrix*.

If  $V = (v_1, \dots, v_n)$ , then the adjacency matrix is an  $n \times n$  matrix.

- $A = (a_{ij})$ , where  $a_{ij} = 1$  if there is an edge from  $v_i$  to  $v_j$ ; otherwise  $a_{ij} = 0$ .
- in a multigraph,  $a_{ij}$  is the number of edges from  $i$  to  $j$ .

**Example:**

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

## Note:

- an undirected graph will have a symmetric adjacency matrix:  $a_{ij} = a_{ji}$ .
- the indegree of  $v_i =$  sum of entries in column  $i$
- the outdegree of  $v_i =$  sum of entries in row  $i$
- the adjacency matrix is a good way of representing a graph in a computer

# Adjacency Matrices and Reachability

What does the adjacency matrix have to do with reachability?

**Theorem:** Suppose  $A$  is the adjacency matrix of  $G$  and  $A^m = (a_{ij}^{(m)})$ . Then  $a_{ij}^{(m)}$  is the number of paths of length  $m$  from  $v_i$  to  $v_j$ .

**Proof:** By induction on  $m$ . Let  $P(m)$  be the statement of the theorem.  $P(1)$  is immediate from the definition of the adjacency matrix. Assume  $P(m)$ . Suppose  $A^{m+1} = (a_{ij}^{(m+1)})$ . By definition,

$$a_{ij}^{(m+1)} = \sum_{k=1}^n a_{ik}^{(m)} a_{kj}$$

- $a_{ik}^{(m)} = \#$  paths of length  $m$  from  $v_i$  to  $v_k$
- $a_{kj} = \#$  edges (paths of length 1) from  $v_k$  to  $v_j$
- Therefore  $a_{ik}^{(m)} a_{kj} = \#$  paths from  $v_i$  to  $v_j$  of length  $m + 1$  whose second-last vertex (just before  $v_j$ ) is  $v_k$
- Therefore  $a_{ij}^{(m+1)} = \sum_{k=1}^n a_{ik}^{(m)} a_{kj}$  is the total number of paths of length  $m + 1$  from  $v_i$  to  $v_j$

- $v_j$  is reachable from  $v_i$  iff there is a path of length  $\leq n - 1$  from  $v_i$  to  $v_j$  iff the  $ij$  entry in at least one of  $A, A^2, \dots, A^{n-1}$  is 1 (where  $n = |V|$ ).
- The  $ij$  entry of  $A + A^2 + \dots + A^n$  gives the total number of paths of length  $\leq n$  from  $v_i$  to  $v_j$ .

**Example:**

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

$$A^2 = AA = \begin{bmatrix} 0 & 0 & 2 & 0 & 0 \\ 0 & 1 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 & 0 \\ 1 & 1 & 0 & 0 & 1 \\ 0 & 1 & 0 & 0 & 0 \end{bmatrix} \times \begin{bmatrix} 0 & 0 & 2 & 0 & 0 \\ 0 & 1 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 & 0 \\ 1 & 1 & 0 & 0 & 1 \\ 0 & 1 & 0 & 0 & 0 \end{bmatrix} = \begin{bmatrix} 0 & 0 & 0 & 0 & 0 \\ 0 & 2 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 2 & 2 & 0 & 1 \\ 0 & 1 & 0 & 0 & 1 \end{bmatrix}$$

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

## A Better Algorithm

Each time we multiply two  $n \times n$  matrices, we need  $n$  multiplications to compute the  $ij$  entry, and thus  $n^3$  multiplications altogether

- There are theoretically better algorithms for matrix multiplication that take roughly  $n^{2.5}$  multiplications

Thus, to compute  $A^1, \dots, A^n$ , requires roughly  $n^4$  multiplications

- Could cut this down to  $n^3 \log(n)$

*Warshall's algorithm* gives an even better approach to computing reachability.

- I won't cover Warshall's algorithm in class. You can read about it in the text if you want, but it won't be on the prelim/final.
- You can also use Dijkstra's algorithm (which I will cover) to compute reachability efficiently.

# Transitive Closure

Recall that the *transitive closure* of a relation  $R$  is the least relation  $R^*$  such that

1.  $R \subset R^*$
2.  $R^*$  is transitive (so that if  $(u, v), (v, w) \in R^*$ , then so is  $(u, w)$ ).

How are the graphs  $G(V, E)$  and  $G^*(V, E^*)$  corresponding to  $R$  and  $R^*$  related?

- $G^*$  is the result of putting an edge between  $u$  and  $v$  if there's a path from  $u$  to  $v$  in  $G$

How do we prove this?

- Let  $G_k(V, E_k)$  be such that there is an edge  $(v, v') \in E_k$  iff there is a path of length  $\leq k$  in the original graph  $G$ .
- Let  $R_k$  be the relation corresponding to  $G_k$ .
- Note that  $R_1 = R$ . Prove by induction that  $R_k \subseteq R^*$  for all  $k$ . Then show that  $R_{n-1}$  is transitively closed, so  $R_{n-1} = R^*$ .

# Tentative Prelim Coverage

- Chapter 0:
  - Sets
    - \* Set builder notation
    - \* Operations: union, intersection, complementation, set difference
  - Relations:
    - \* reflexive, symmetric, transitive, equivalence relations
  - Functions
    - \* Injective, surjective, bijective
  - Important functions and how to manipulate them:
    - \* exponent, logarithms, ceiling, floor, mod, polynomials
  - Summation and product notation
  - Matrices (especially how to multiply them)
  - Proof and logic concepts
    - \* logical notions ( $\Rightarrow$ ,  $\equiv$ ,  $\neg$ )
    - \* Proofs by contradiction

- Chapter 1
  - You do not have to write algorithms in their notation
  - You must be able to *read* algorithms in their notation
  - Procedures, recursion, recursive calls
  - Loop invariants
  - Analysis of algorithms
    - \* Relative ordering ( $n^2$  vs.  $n \log n$ )
- Chapter 2
  - induction vs. strong induction
  - guessing the right inductive hypothesis
  - inductive (recursive) definitions
- Chapter 3
  - terminology: bipartite, complete, degree, path, tree, clique (number)
  - adjacency matrix
    - \* three representations of a relation
  - reachability and transitive closure

# Shortest Paths

Suppose you have a graph with weights on the edges. (Think of the weights as driving times.) You want to find the minimum length path.

- if there are no weights on the edges, think of this as the special case where all the weights are 1.
- let  $len(u, v)$  be the weight of the edge  $(u, v)$  ( $len(u, v) = \infty$  if there is no edge from  $u$  to  $v$ ).

Could do it by *brute force*:

- If there are  $n$  vertices, find all paths with no repeated vertices, and compute their weight.
- There could be as many as  $(n - 2)!$  paths!

Can we do better?

## Dijkstra's Algorithm: Key Idea

Suppose we want to find the shortest path from  $v_0$  to  $v_n$ .

Generalize: Find the shortest path from  $v_0$  to *every* other vertex.

How?

- First find the closest vertex and the path to it, then the next closest, and so on.
- Sooner or later  $v_n$  will be the next vertex added.

Why does this help?

- Can compute the next closest vertex recursively.

How do we find the vertex closest to  $v_0$ ?

- Easy: just look

If  $U = \{u_0, u_1, \dots, u_k\}$  are the  $k$  closest vertices to  $v_0$  (listed in order, with  $u_0 = v_0$ ), how do we find  $u_{k+1}$ ?

Suppose  $v$  is the next-closest vertex:

- The shortest path from  $v_0$  to  $v$  must go through  $\{u_1, \dots, u_k\}$ 
  - If it got to  $v$  through some other vertex, that vertex would be closer to  $v_0$  than  $v$ !
- That means the minimum length path from  $v_0$  to  $v$  must have length

$$d(v) = \min_{j=0}^k (d(u_j) + \text{len}(u_j, v)) \quad (*)$$

$\text{len}(u_j, v)$  is the weight of the edge from  $u_j$  to  $v$

- Compute  $(*)$  for each vertex not in  $U$ , and pick the shortest.

## Dijkstra's Algorithm: Outline

At  $k$ th step of the algorithm, assume (inductively) we have:

- $u_1, \dots, u_k$ , the  $k$  closest vertices to  $v_0$  (not counting  $v_0$  itself)
- $d(u_j)$  (the minimum distance from  $v_0$  to  $u_j$ )
- the minimum distance  $d_k(v)$  from  $v_0$  to any vertex  $v$ , going on path that involve only  $u_1, \dots, u_k$

At the  $(k + 1)$ st step:

- for every vertex  $v$  connected to  $u_k$ , compute

$$d(u_k) + \text{len}(u_k, v)$$

- If this is better than  $d_k(v)$ , then let this be  $d_{k+1}(v)$ ; otherwise  $d_{k+1}(v) = d_k(v)$
- pick the  $(k + 1)$ st closest vertex

# Dijkstra's Algorithm: Example

$k$	$d(v_1)$	$d(v_2)$	$d(v_3)$	$d(v_4)$	$d(v_5)$	$d(v_6)$	$d(v_7)$	New
0	$\infty$	$\infty$	$\infty$	$\infty$	$\infty$	$\infty$	$\infty$	$v_0$
1	2	4	$\infty$	$\infty$	$\infty$	$\infty$	$\infty$	$v_1$
2	2	4	5	6	$\infty$	$\infty$	$\infty$	$v_2$
3	2	4	5	5	$\infty$	$\infty$	$\infty$	$v_3$
4	2	4	5	5	6	10	10	$v_4$
5	2	4	5	5	6	8	9	$v_5$
6	2	4	5	5	6	7	9	$v_6$
7	2	4	5	5	6	7	8	$v_7$

# Dijkstra's Algorithm

**Input**  $G(V, E)$  [a graph]  
 $v_0, v_n$  [start and end]

## Algorithm Shortest Path

```
 $d(v_0) \leftarrow 0$  [Initialize distance from  $v_0$ ]  
for  $i = 1$  to  $n$  [  $n = |V|$  ]  
     $d(v_i) \leftarrow \infty$   
endfor  
 $U \leftarrow \{v_0\}$  [Initialize closest vertices]  
 $u \leftarrow v_0$  [  $u$  is most recent entry into  $U$  ]  
repeat until  $u = v_n$   
    for  $i = 1$  to  $n$   
        if  $(u, v_i) \in E$  and  $v_i \notin U$ , then  
             $d(v_i) \leftarrow \min(d(v_i), d(u) + \text{len}(u, v_i))$   
        endif  
         $\text{mindist} \leftarrow \infty$  [find next closest vertex]  
        for  $i = 1$  to  $n$   
            if  $v_i \notin U$  and  $d(v_i) < \text{mindist}$  then  
                 $\text{mindist} \leftarrow d(v_i); u \leftarrow v_i$   
            endif  
        endfor  
         $U \leftarrow U \cup \{u\}$   
    endrepeat
```

# Dijkstra's Algorithm: Correctness

Why is this right? Getting the right loop invariant is hard.

- What does  $d(v_i)$  correspond to if  $v_i \notin U$ ?

Loop invariant. For all  $k \geq 0$ , after the  $k$ th iteration of the loop:

- $U$  consists of  $v_0$  and the  $k$  vertices closest to  $v_0$
- $u$  is the  $k$ th closest vertex to  $v_0$
- if  $v \in U$ , then  $d(v)$  is the length of the shortest path from  $v_0$  to  $v$ .
- if  $v \notin U$ , then  $d(v)$  is the length of the shortest path from  $v_0$  to  $v$  that has only vertices in  $U - \{u\}$  as intermediate points.
  - if there is no such path, then  $d(v) = \infty$
- $u$  is the most recently added vertex.

Once we get the right loop invariant, it's not hard to prove that it is maintained ... by induction (of course):

*Basis:*  $P(0)$  is obvious.

*Inductive step:* ...