Algorithms and Data Structures

All Pairs Shortest Paths

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Content of this Lecture

- All-Pairs Shortest Paths
  - Transitive closure: Warshall's algorithm
  - Shortest paths: Floyd's algorithm
- Reachability in Trees

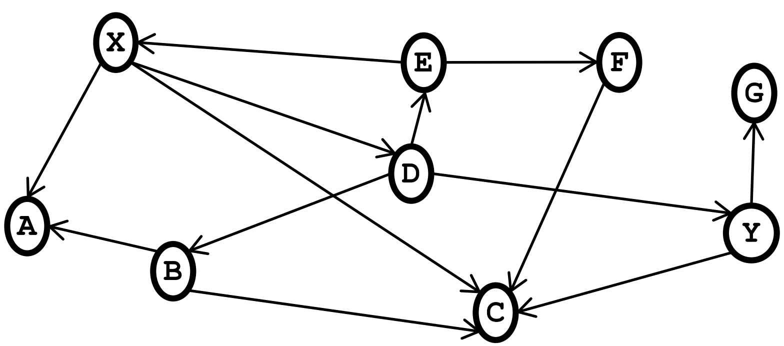
Recall: DFS

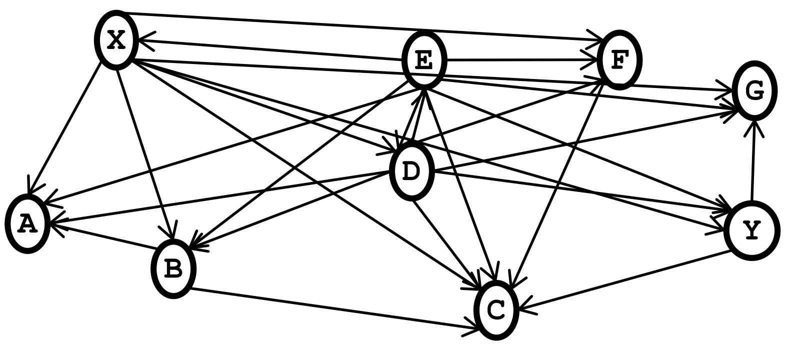
- We put every node exactly once on the stack
  - Once visited, never visited again
- We look at every edge exactly once
  - Outgoing edges of a visited node are never considered again
- U can be implemented as bit-array of size |V|, allowing O(1) operations
  - Add, remove, getNextUnseen
- Altogether: O(n+m)

```
func void traverse (G graph,
                    v node,
                    U set) {
  t := new Stack();
  t.put( v);
  U := U \ {v};
  while not t.isEmpty() do
    n := t.pop();
    print n;
    c := n.outgoingNodes();
    foreach x in c do
      if x∈U then
        U := U \ {x};
        t.push( x);
      end if;
    end for;
  end while;
}
```

Recall: Transitive Closure

- Definition
  Let G=(V,E) be a digraph and $v_i, v_j \in V$. The transitive closure of G is a graph G'=(V, E') where $(v_i, v_j) \in E'$ iff G contains a path from v_i to v_j.
- TC usually is dense and represented as adjacency matrix
- Compact encoding of reachability information

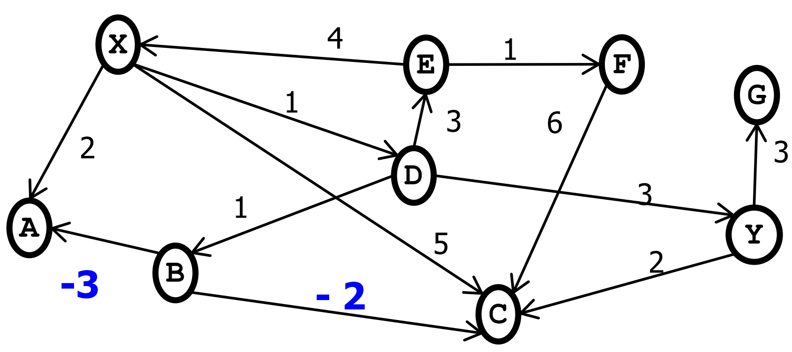




and many more

Shortest Path Problems

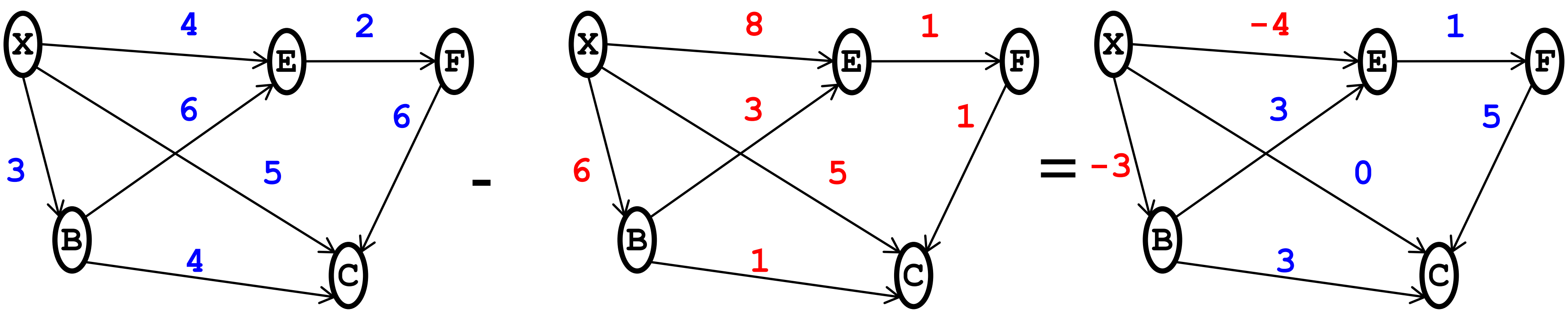
- Dijkstra finds shortest path between a given start node and all other nodes assuming that all edge weights are positive
- All-pairs shortest paths: Given a digraph G with positive or negative edge weights, find the (cycle-free) distance between all pairs of nodes
  - We will interpret "find" as "compute the distance matrix"



→	A	B	C	D	E	F	G	X	Y
A	-	-	-	-	-	-	-	-	-
B	-3	-	-2	-	-	-	-	-	-
C	-	-	-	-	-	-	-	-	-
D	-2	1	-1	-	3	4	6	7	3
E	...	...	...						
F									
G									
X									
Y									

Why Negative Edge Weights?

- One application: Transportation company
  - Every route incurs cost (for fuel, salary, etc.)
  - Every route creates income (for carrying the freight)
- If cost>income, edge weights become negative
  - But still important to find the best route
  - Example: Best tour from X to C



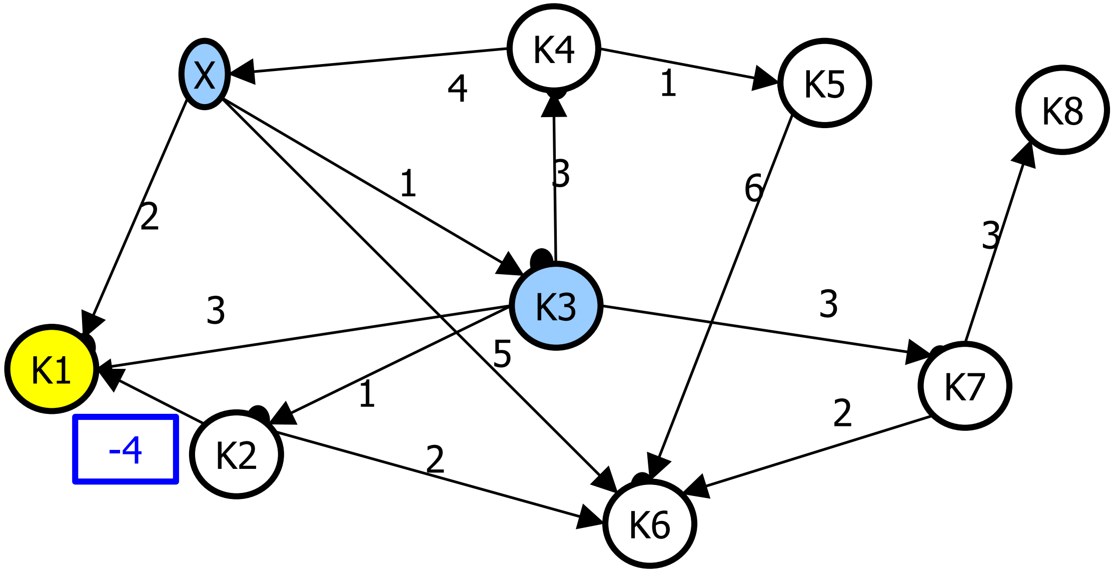
Cost

Incoming

Shortest path = max revenue

No Dijkstra

- Dijkstra's algorithm does not work
  - Recall that Dijkstra enumerates nodes by their shortest paths
  - Now: Adding a subpath to a so-far shortest path may make it "shorter" (by negative edge weights)



X	0
K1	2
K2	2
K3	1
K4	4
K5	
K6	5
K7	4
K8	

No Dijkstra

- Dijkstra's algorithm does not work
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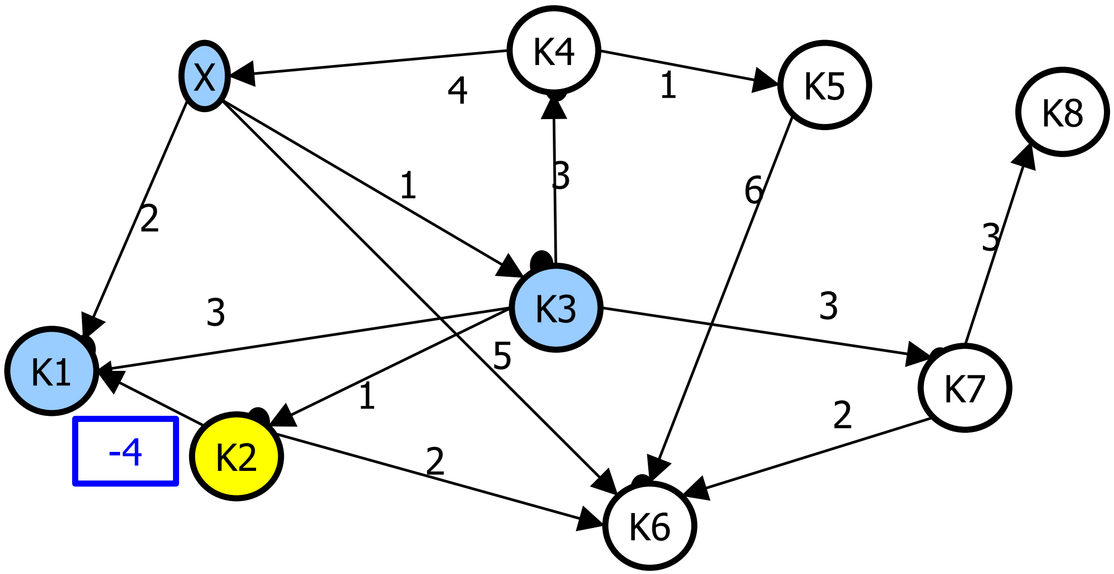

X	0
K1	2
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K3	1
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K5	
K6	5
K7	4
K8	

No Dijkstra

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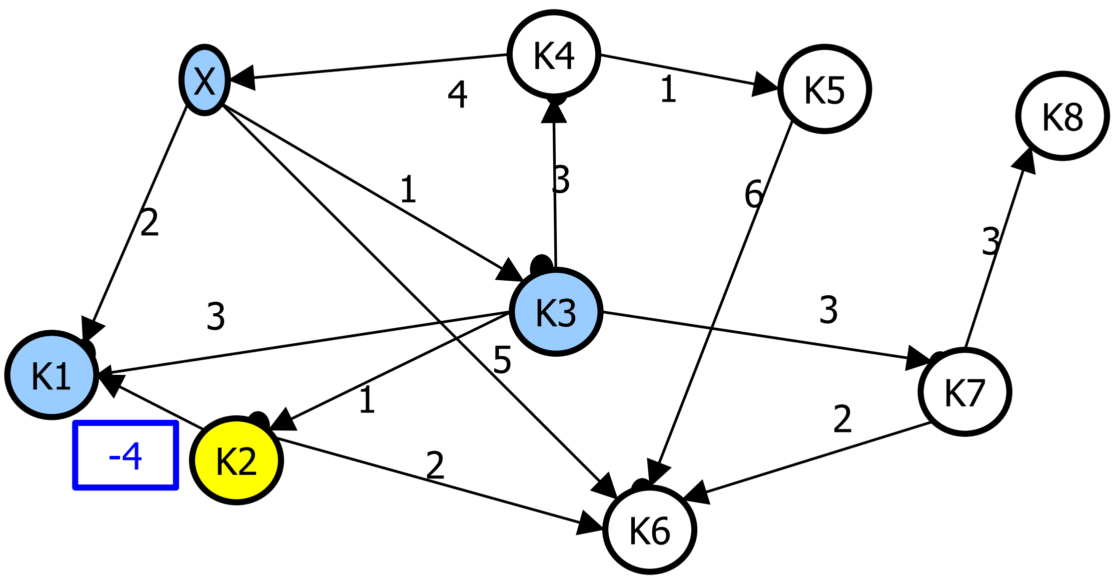
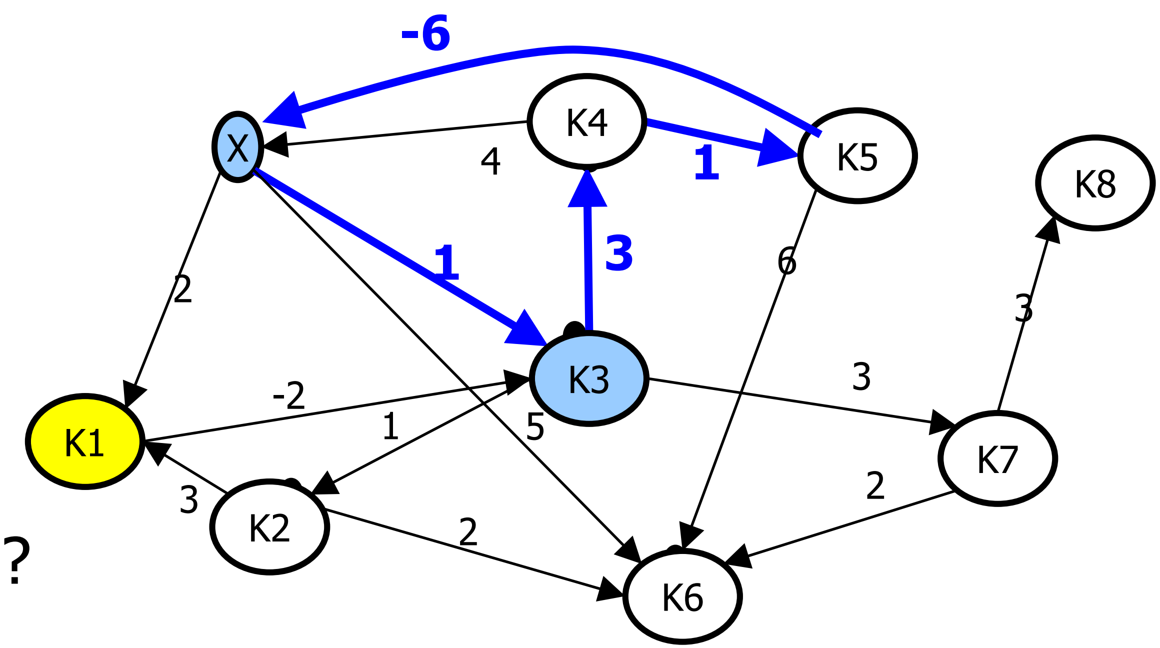


X	0
K1	2
K2	2
K3	1
K4	4
K5	
K6	5
K7	4
K8	

Negative Cycles

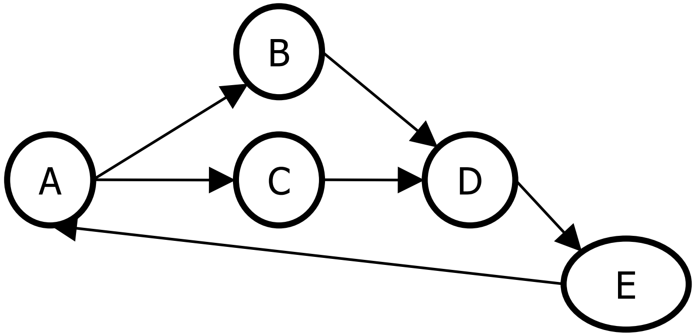


- Shortest path between X and K5?
  - X-K3-K4-K5: 5
  - X-K3-K4-K5-X-K3-K4-K5: 4
  - X-K3-K4-K5-X-K3-K4-K5-X-K3-K4-K5: 3
  - …
- SP-Problem undefined if G contains a negative cycle

All-Pairs: First Approach

- We start with a simpler problem: Computing the transitive closure of a digraph G without edge weights
- First idea
  - Reachability is transitive: $x \overset{p_1}{\rightarrow} y \wedge y \overset{p_2}{\rightarrow} z \Rightarrow x \overset{p_1}{\rightarrow} y \overset{p_2}{\rightarrow} z = x \rightarrow z$
  - We may use this idea to iteratively build longer and longer paths
  - First extend edges with edges – path of length 2
  - Extend paths of length 2 with edges – paths of length 3
  - …
  - No necessary path can be longer then |V|
    - Or it would contain a cycle
- In each step, we store "reachable by a path of length ≤k" in a matrix

Example – After z=1, 2, 3, 4



	A	B	C	D	E
A		1	1		
B				1	
C				1	
D					1
E	1				

	A	B	C	D	E
A		1	1	1	
B				1	1
C				1	1
D	1				1
E	1	1	1		

	A	B	C	D	E
A		1	1	1	1
B	1			1	1
C	1			1	1
D	1	1	1		1
E	1	1	1	1	

	A	B	C	D	E
A	1	1	1	1	1
B	1	1	1	1	1
C	1	1	1	1	1
D	1	1	1	1	1
E	1	1	1	1	1

	A	B	C	D	E
A	1	1	1	1	1
B	1	1	1	1	1
C	1	1	1	1	1
D	1	1	1	1	1
E	1	1	1	1	1

Path length: ≤2 ≤3 ≤4 ≤5

Naïve Algorithm

z appears nowhere; it is there to ensure that we stop when the longest possible shortest paths has been found

```
G = (V, E);
M := adjacency_matrix( G);
M'' := M;
n := |V|;
for z := 1..n-1 do
  M' := M'';
  for i = 1..n do
    for j = 1..n do
      if M'[i,j]=1 then
        for k=1 to n do
          if M[j,k]=1 then
            M''[i,k] := 1;
          end if;
        end for;
      end if;
    end for;
  end for;
end for;
```

- M is the adjacency matrix of G, M″ eventually the TC of G
- M′: Represents paths ≤z
- M″: Represents paths ≤z+1
- Reachability is transitive: $i \overset{p_1}{\rightarrow} j \wedge j \overset{p_2}{\rightarrow} k \Rightarrow i \overset{p_1}{\rightarrow} j \overset{p_2}{\rightarrow} k$
- Loops i and j look at all pairs reachable by a path of length ≤z+1
- Loop k extends path of length ≤z by all outgoing edges
- Obviously $O(n^4)$

Observation

	A	B	C	D	E
A		1	1		
B				1	
C				1	
D					1
E	1				

x

	A	B	C	D	E
A		1	1		
B				1	
C				1	
D					1
E	1				

→

	A	B	C	D	E
A		1	1	1	
B				1	1
C				1	1
D	1				1
E	1	1	1		

- In the first step, we actually compute MxM, and then replace each value ≥1 with 1
  - We only state that there is a path; not how many and not how long
- Computing TC can be described as matrix operations

Paths in the Naïve Algorithm

	A	B	C	D	E
A		1	1		
B				1	
C				1	
D					1
E	1				

	A	B	C	D	E
A		1	1	1	
B				1	1
C				1	1
D	1				1
E	1	1	1		

	A	B	C	D	E
A		1	1	1	1
B	1			1	1
C	1			1	1
D	1	1	1		1
E	1	1	1	1	

	A	B	C	D	E
A	1	1	1	1	1
B	1	1	1	1	1
C	1	1	1	1	1
D	1	1	1	1	1
E	1	1	1	1	1

	A	B	C	D	E
A	1	1	1	1	1
B	1	1	1	1	1
C	1	1	1	1	1
D	1	1	1	1	1
E	1	1	1	1	1

- The naive algorithm always extends paths by one edge
  - Computes MxM, M^2xM, M^3xM, … M^{n-1}xM

Idea for Improvement

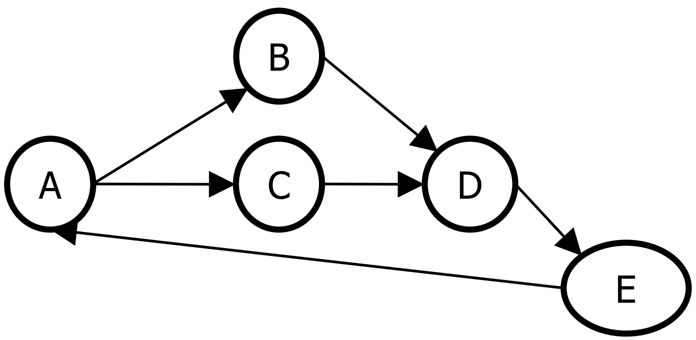
- Why not extend paths by all paths found so-far?
  - We compute
    $M^{2'}=MxM$: Path of length ≤ 2
    $M^{3'}=M^{2'}xM \cup M^{2'}xM^{2'}$: Path of length $\leq 2+1$ and $\leq 2+2$
    $M^{4'}=M^{3'}xM \cup M^{3'}xM^{2'} \cup M^{3'}xM^{3'}$, lengths $\leq 4+1$, $\leq 4+2$, $\leq 4+3/4$
    …
    $M^{n'}= \ldots \cup M^{n-1'}xM^{n-1'}$
  - [We will implement it differently]
- Trick: We can stop much earlier
  - The longest shortest path can have length at most n
  - Thus, it suffices to compute $M^{\log(n)'} = \ldots \cup M^{\log(n)'*}xM^{\log(n)'}$

Algorithm Improved

```
G = (V, E);
M := adjacency_matrix( G);
n := |V|;
for z := 0..ceil(log(n)) do
  for i = 1..n do
    for j = 1..n do
      if M[i,j]=1 then
        for k=1 to n do
          if M[j,k]=1 then
            M[i,k] := 1;
          end if;
        end for;
      end if;
    end for;
 end for;
end for;
```

- We use only one matrix M
- We "add" to M matrices $M^{2'}$, $M^{3'}$ …
- In the extension, we see if a path of length $\leq 2^z$ (stored in M) can be extended by a path of length $\leq 2^z$ (stored in M)
  - Computes all paths $\leq 2^z+2^z=2^{z+1}$
- Analysis: $O(n^3*\log(n))$
- But … we can be even faster

Example – After z=1, 2, 3



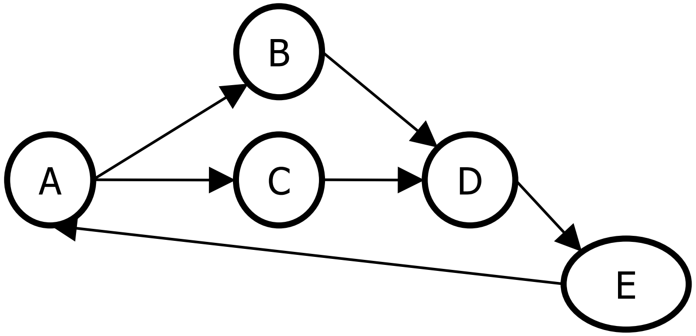
	A	B	C	D	E
A		1	1		
B				1	
C				1	
D					1
E	1				

	A	B	C	D	E
A		1	1	1	
B				1	1
C				1	1
D	1				1
E	1	1	1		

	A	B	C	D	E
A	1	1	1	1	1
B	1	1	1	1	1
C	1	1	1	1	1
D	1	1	1	1	1
E	1	1	1	1	1

Path length: ≤2 ≤4 Done

Further Improvement



	A	B	C	D	E
A		1	1		
B				1	
C				1	
D					1
E	1				

	A	B	C	D	E
A		1	1	1	
B				1	1
C				1	1
D	1				1
E	1	1	1		

- Note: Connection A→D is found twice: A→B→D / A→C→D
- Can we stop "searching" A→D once we found A→B→D?
- Can we enumerate paths such that redundant connections are discovered less often?
  - I.e., less connections are tested

Warshall's Algorithm

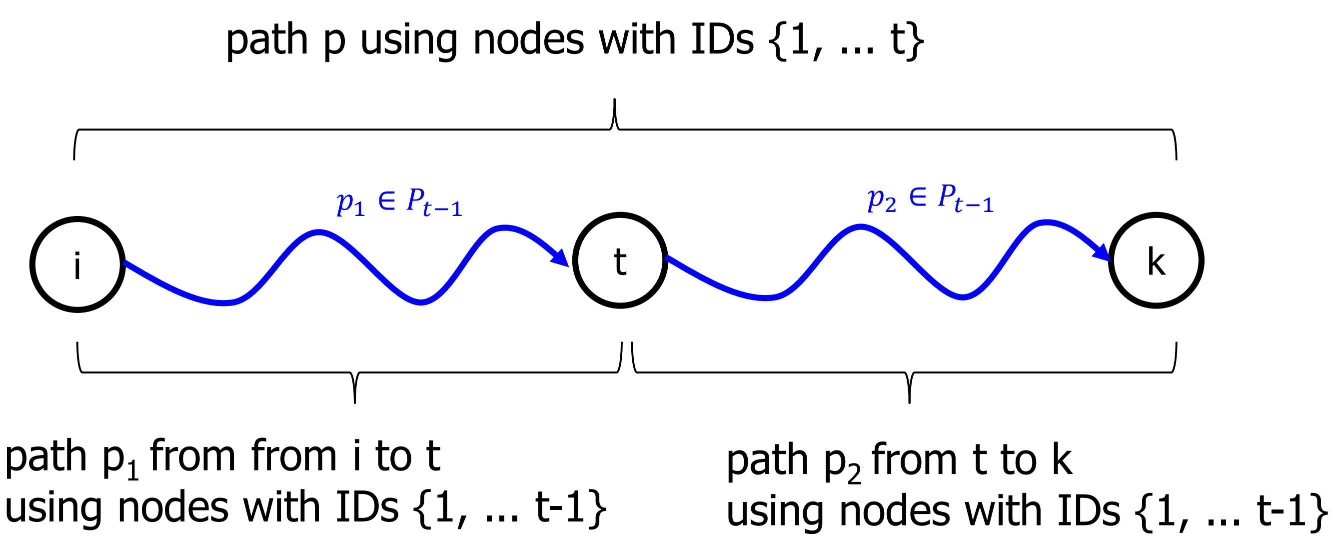
Warshall, S. (1962). A theorem on Boolean matrices. *Journal of the ACM 9(1): 11-12.*

- Preparations
  - Fix an arbitrary order on nodes and assign each node its rank as ID
  - Let P_t be the set of all paths that contain only nodes with ID<t+1
    - Applies to inner nodes of a path, not start and end
  - t gives the highest allowed node ID inside a path
- Idea: Compute P_t inductively
  - We start with P_1
  - Suppose we know P_{t-1}
  - If we increase t by one, we admit one additional node, i.e., ID t
  - Now, every additional path must have the form $i \xrightarrow{p_1 \in P_{t-1}} t \xrightarrow{p_2 \in P_{t-1}} k$
    - All paths with all IDs <t are already known
    - Node t is the only new player, must be in all new paths
  - We are done once t=n
    - This guarantees correctness – all connections found

Warshall's Algorithm

Warshall, S. (1962). A theorem on Boolean matrices. *Journal of the ACM 9(1): 11-12.*

- Enumerate paths by the IDs of the nodes they are allowed to contain
- t gives the highest allowed node ID inside a path



Algorithm

- Enumerate paths by the IDs of the nodes they are allowed to contain
- t gives the highest allowed node ID inside a path
- Thus, node t must be on any new path
- We find all pairs i,k with i→t and t→k
- For every such pair, we set the path i→k to 1

```
G = (V, E);
M := adjacency_matrix( G);
n := |V|;
for t := 1..n do
  for i = 1..n do
    if M[i,t]=1 then
      for k=1 to n do
        if M[t,k]=1 then
          M[i,k] := 1;
        end if;
      end for;
    end if;
  end for;
end for;
```

Example – Warshall's Algorithm

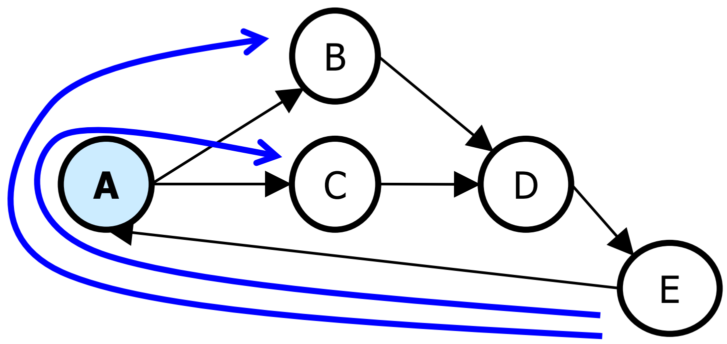
	A	B	C	D	E
A		1	1		
B				1	
C				1	
D					1
E	1				

maxID=t=A

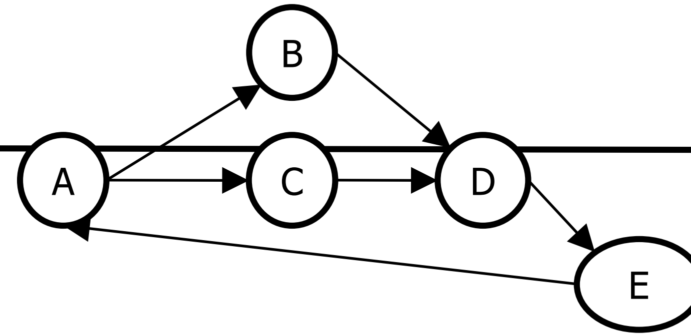
	A	B	C	D	E
A		1	1		
B				1	
C				1	
D					1
E	1	1	1		

A allowed

Connect
E-A with
A-B, A-C



Example – After t=A,B,C,D,E



t=„A"

	A	B	C	D	E
A		1	1		
B				1	
C				1	
D					1
E	1	1	1		

B allowed

Connect A-B/E-B with B-D

t=„B"

	A	B	C	D	E
A		1	1	1	
B				1	
C				1	
D					1
E	1	1	1	1	

C allowed

Connect A-C/E-C with C-D

No news

t=„C"

	A	B	C	D	E
A		1	1	1	
B				1	
C				1	
D					1
E	1	1	1	1	

D allowed

Connect A-D, B-D, C-D,E-D with D-E

	A	B	C	D	E
A		1	1	1	1
B				1	1
C				1	1
D					1
E	1	1	1	1	1

E allowed

Connect everything with everything

	A	B	C	D	E
A	1	1	1	1	1
B	1	1	1	1	1
C	1	1	1	1	1
D	1	1	1	1	1
E	1	1	1	1	1

Little change – Notable Consequences

```
G = (V, E);
M := adjacency_matrix( G);
n := |V|;
for z := 1..n do
  for i = 1..n do
    for j = 1..n do
      if M[i,j]=1 then
        for k=1 to n do
          if M[j,k]=1 then
            M[i,k] := 1;
          end if;
        end for;
      end if;
    end for;
  end for;
end for;
```

$O(n^4)$

Drop z-Loop
Swap i and j loop
Rename j into t

```
G = (V, E);
M := adjacency_matrix( G);
n := |V|;
for t := 1..n do
  for i = 1..n do
    if M[i,t]=1 then
      for k=1 to n do
        if M[t,k]=1 then
          M[i,k] := 1;
        end if;
      end for;
    end if;
  end for;
end for;
```

$O(n^3)$

Content of this Lecture

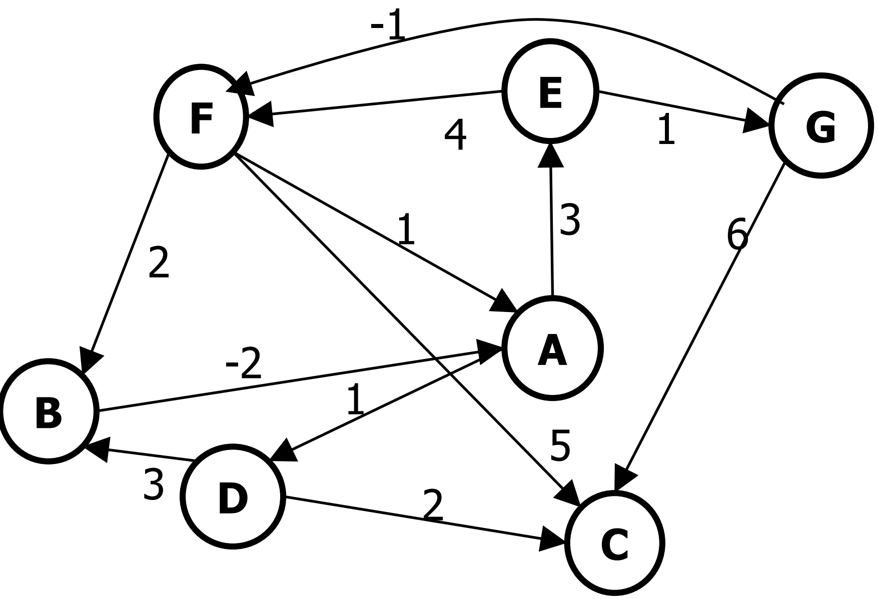
- All-Pairs Shortest Paths
  - Transitive closure: Warshall’s algorithm
  - Shortest paths: Floyd’s algorithm
- Reachability in Trees

Shortest Paths

Floyd, R. W. (1963). Algorithm 97: Shortest Paths. *Communications of the ACM 5(6): 345.*

- Shortest paths: We need to compute the distance between all pairs of reachable nodes
- We use the same idea as Warshall: Enumerate paths using only nodes with IDs smaller than t inside a path
  - Invariant: Before step t, M[i,j] contains the length of the shortest path that uses no node with ID higher than t
  - When increasing t, we find new paths $i \rightarrow t \rightarrow k$ and look at their lengths
  - Thus: $M[i,k] := \min(M[i,k] \cup \{ M[i,t]+M[t,k] \mid i \rightarrow t \wedge t \rightarrow k \})$

Example 1/3



	A	B	C	D	E	F	G
A				1	3		
B	-2						
C							
D		3	2				
E						4	1
F	1	2	5				
G			6			-1	

	A	B	C	D	E	F	G
A				1	3		
B	-2			-1	1		
C							
D		3	2				
E						4	1
F	1	2	5	2	4		
G			6			-1	

	A	B	C	D	E	F	G
A				1	3		
B	-2			-1	1		
C							
D	1	3	2	2	4		
E						4	1
F	0	2	5	1	3		
G			6			-1	

Example 2/3

	A	B	C	D	E	F	G
A				1	3		
B	-2			-1	1		
C							
D	1	3	2	2	4		
E						4	1
F	0	2	5	1	3		
G			6			-1	

	A	B	C	D	E	F	G
A				1	3		
B	-2			-1	1		
C							
D	1	3	2	2	4		
E						4	1
F	0	2	5	1	3		
G			6			-1	

	A	B	C	D	E	F	G
A	2	4	3	1	3		
B	-2	2	1	-1	1		
C							
D	1	3	2	2	4		
E						4	1
F	0	2	3	1	3		
G			6			-1	

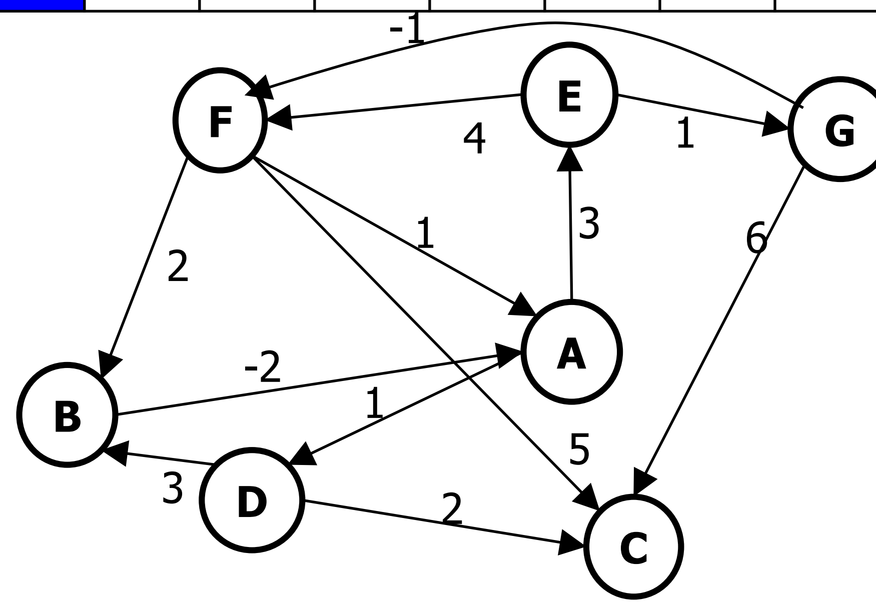
	A	B	C	D	E	F	G
A	2	4	3	1	3	7	4
B	-2	2	1	-1	1	5	2
C							
D	1	3	2	2	4	8	5
E						4	1
F	0	2	3	1	3	7	4
G			6			-1	

Example 3/3

	A	B	C	D	E	F	G
A	2	4	3	1	3	7	4
B	-2	2	1	-1	1	5	2
C							
D	1	3	2	2	4	8	5
E	4	6	7	5	7	4	1
F	0	2	3	1	3	7	4
G	-1	1	2	0	2	-1	3

	A	B	C	D	E	F	G
A	2	4	3	1	3	3	4
B	-2	2	1	-1	1	1	2
C							
D	1	3	2	2	4	4	5
E	0	2	3	1	3	0	1
F	0	2	3	1	3	3	4
G	-1	1	2	0	2	-1	3

	A	B	C	D	E	F	G
A	2	4	3	1	3	7	4
B	-2	2	1	-1	1	5	2
C							
D	1	3	2	2	4	8	5
E						4	1
F	0	2	3	1	3	7	4
G			6			-1	



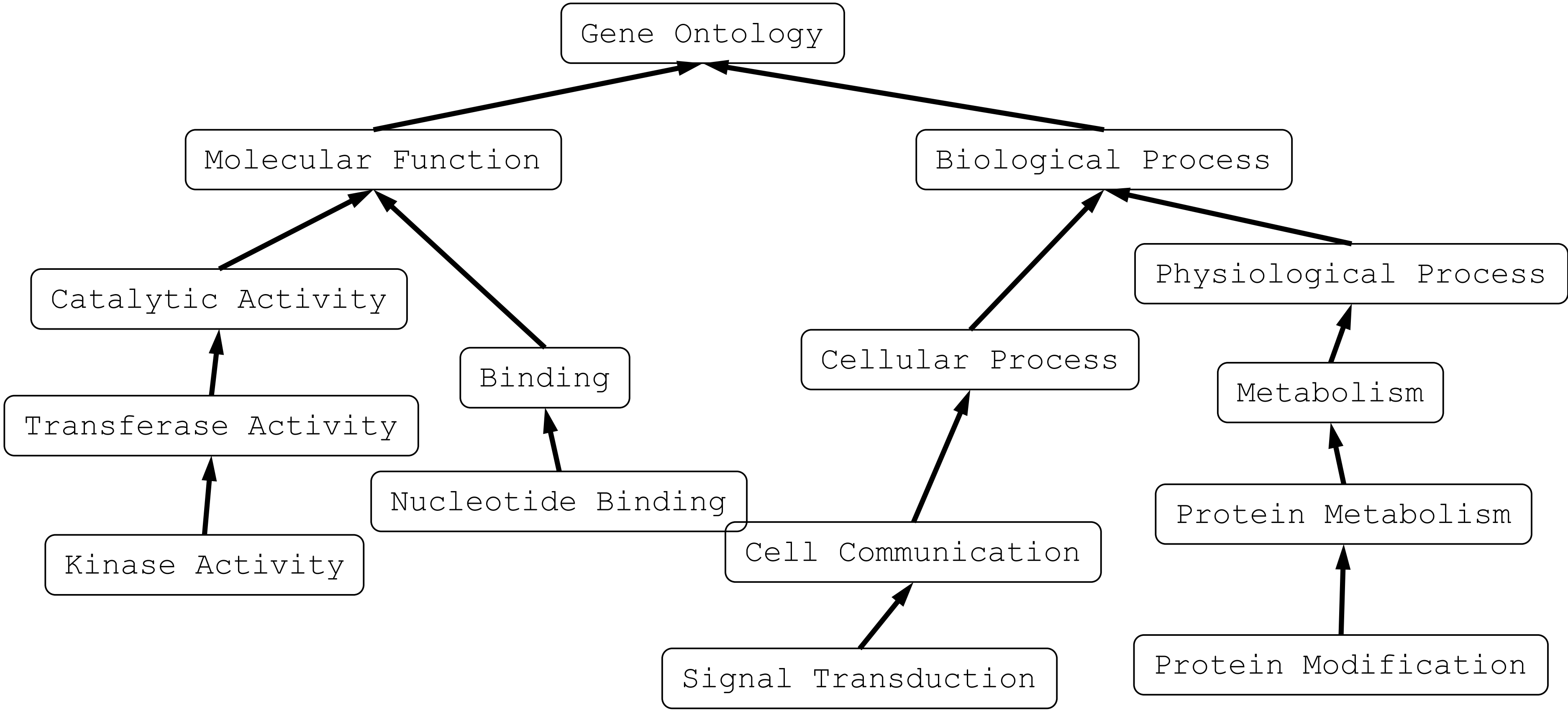
Summary (n=|V|, m=|E|)

- Warshall‘s algorithm computes the transitive closure of any unweighted digraph G in $O(n^3)$
- Floyd‘s algorithm computes the distances between any pair of nodes in a digraph without negative cycles in $O(n^3)$
- Johnson’s alg. solves the problem in $O(n^2*\log(n)+n*m)$
  - Which is faster for sparse graphs
- Storing both information requires $O(n^2)$
- Problem is easier for …
  - Undirected graphs: Connected components
  - Graphs with only positive edge weights: All-pairs Dijkstra
  - Trees: Test for reachability in O(1) after O(n) preprocessing

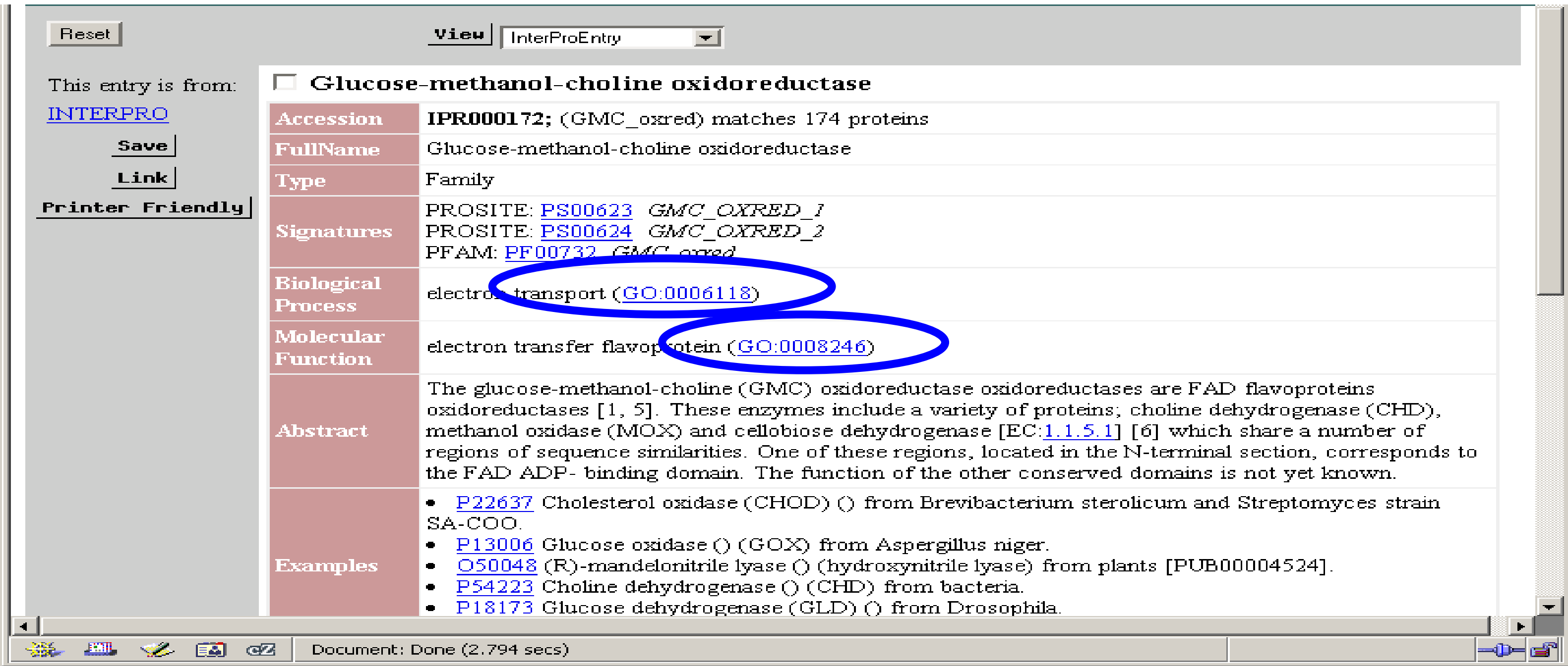
Content of this Lecture

- All-Pairs Shortest Paths
  - Transitive closure: Warshall's algorithm
  - Shortest paths: Floyd's algorithm
- Reachability in Trees

Gene Ontology – Describing Gene Function

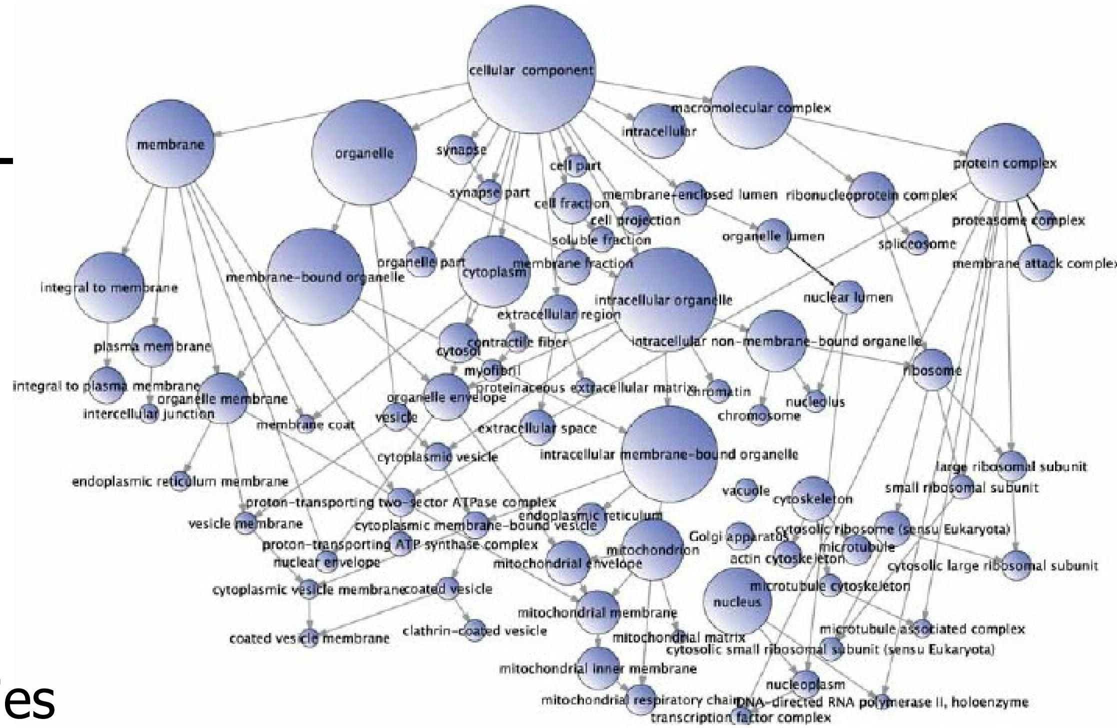


Database Annotation InterPro

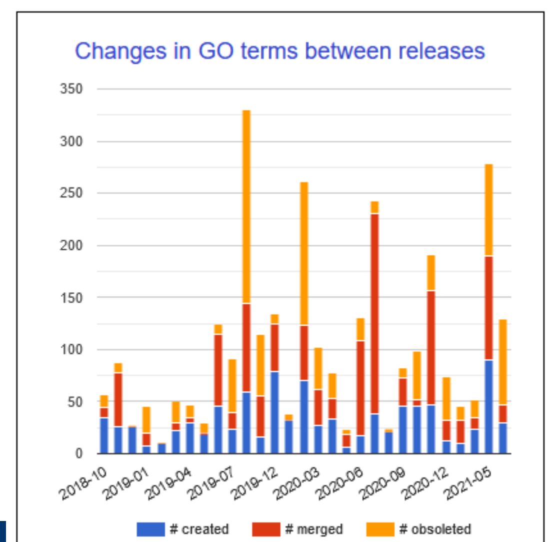


- Used by many databases
- Allows cross-database search
- Provides fixed meaning of terms
  - As informal textual description, not as formal definitions

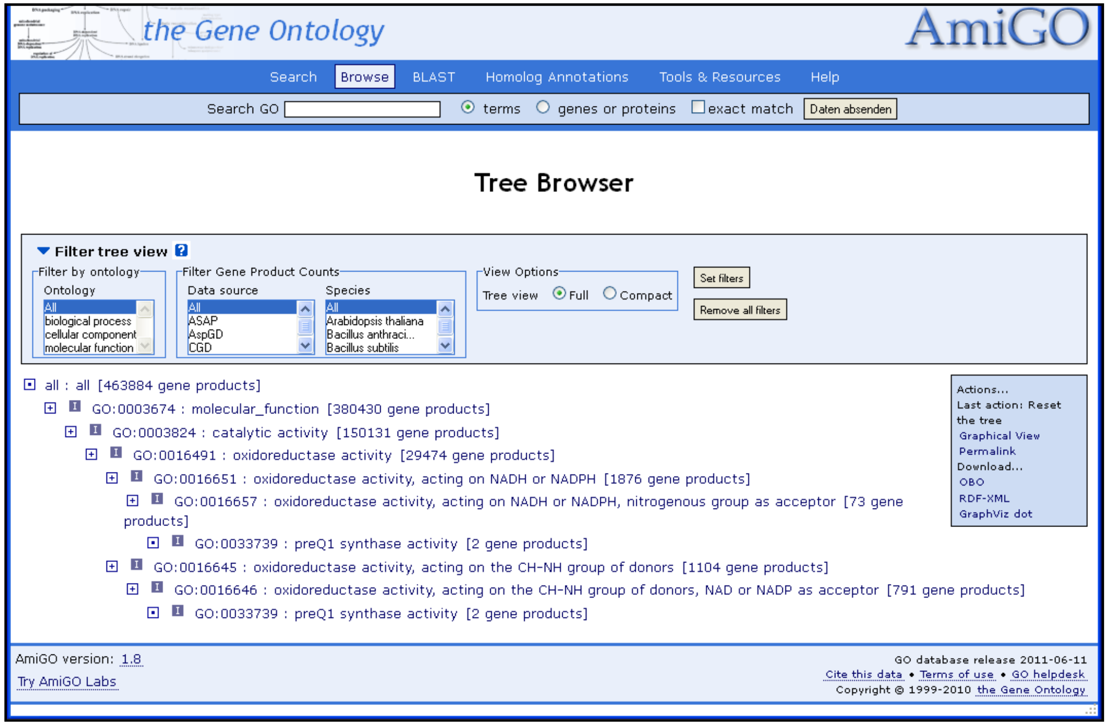
A Large Ontology



- As of 7.7.2021
  - 43917 terms
  - In three subontologies
    - Biological processs
    - Cellular components
    - Molecular functions
  - 3295 obsolete terms
  - Source: http://geneontology.org/stats.html
- Depth: >30



Problem



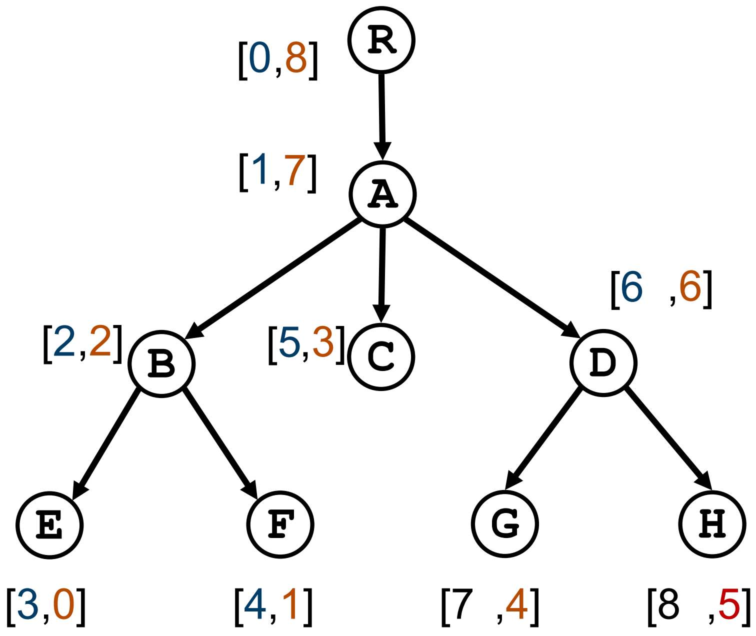
- To see whether a term X IS_A term Y, we need to check whether Y lies on the path from root to X
- Reachability problem

Reachability in Trees

- Let T be a directed tree. A node v is reachable from a node w iff there is a path from w to v
- Testing reachability requires finding paths
  - Which is simple in trees
- Path length is bound by the length of the longest path, i.e., the depth of the tree
- This means O(n) in worst-case
- Let's see whether we can preprocess the data to do this in constant time

Pre-/Postorder Numbers

- Assume a DFS-traversal
- Build an array assigning each node two numbers
- Preorder numbers
  - Keep a counter **`pre`**
  - Whenever a node is entered the first time, assign it the current value of **`pre`** and increment **`pre`**
- Postorder numbers
  - Keep a counter **`post`**
  - Whenever a node is left the last time, assign it the current value of **`post`** and increment **`post`**



Examples from S. Trissl, 2007

Ancestry and Pre-/Postorder Numbers

- Trick: A node v is reachable from a node w iff

  $$pre(v)>pre(w) \wedge post(v)<post(w)$$

- Explanation
  - v can only be reached from w, if w is “higher” in the tree, i.e., v was traversed after w and hence has a higher preorder number
  - v can only be reached from w, if v is “lower” in the tree, i.e., v was left before w and hence has a lower postorder number
- Analysis: Test is O(1)