Algorithms

Graphs, breadth- and depth-first search

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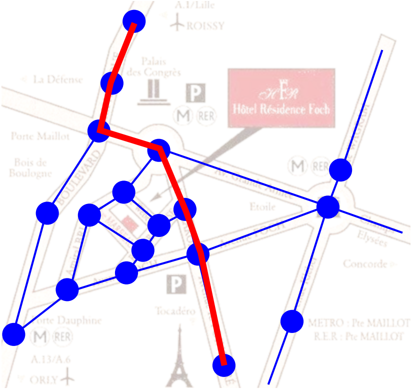
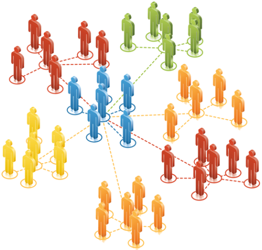
Graphs



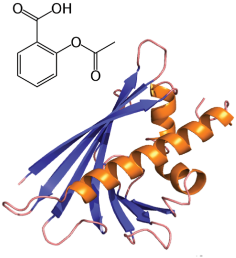
A graph $G = (V, E)$ is made of nodes V and edges E.

Graphs are used pervasively in data sciences.

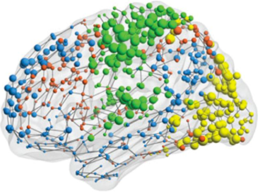
Graphs



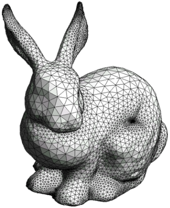
Social networks



Molecules

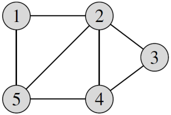


Functional networks



3D shapes

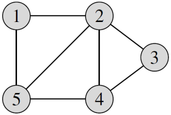
Representation



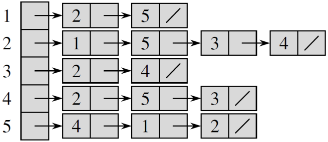
(a)

undirected graph

Representation



(a)

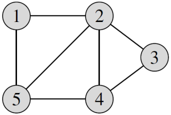


(b)

undirected graph

adjacency list

Representation



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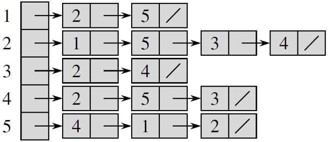
undirected graph



(b)

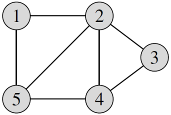
adjacency list

$$
\begin{array}{c|ccccc|}
 & 1 & 2 & 3 & 4 & 5 \\
\hline
1 & 0 & 1 & 0 & 0 & 1 \\
2 & 1 & 0 & 1 & 1 & 1 \\
3 & 0 & 1 & 0 & 1 & 0 \\
4 & 0 & 1 & 1 & 0 & 1 \\
5 & 1 & 1 & 0 & 1 & 0 \\
\hline
\end{array}
$$

(c)

adjacency matrix

Representation



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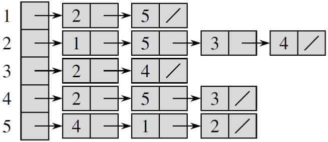
undirected graph



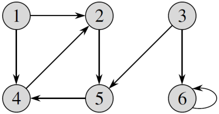
(b)

adjacency list

$$\begin{array}{c|ccccc|} & 1 & 2 & 3 & 4 & 5 \\ \hline 1 & 0 & 1 & 0 & 0 & 1 \\ 2 & 1 & 0 & 1 & 1 & 1 \\ 3 & 0 & 1 & 0 & 1 & 0 \\ 4 & 0 & 1 & 1 & 0 & 1 \\ 5 & 1 & 1 & 0 & 1 & 0 \\ \hline \end{array}$$

(c)

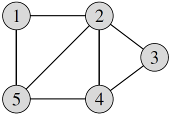
adjacency matrix



(a)

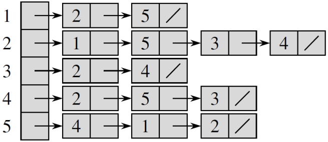
directed graph

Representation



(a)

undirected graph



(b)

adjacency list

$$
\begin{array}{c|ccccc|}
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\hline
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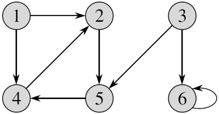
\hline
\end{array}
$$

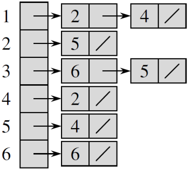
(c)

adjacency matrix



(a)

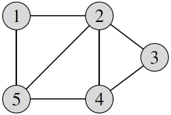
directed graph



(b)

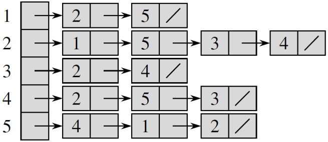
adjacency list

Representation



(a)

undirected graph



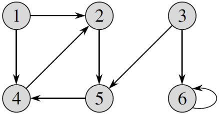
(b)

adjacency list

	1	2	3	4	5
1	0	1	0	0	1
2	1	0	1	1	1
3	0	1	0	1	0
4	0	1	1	0	1
5	1	1	0	1	0

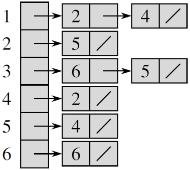
(c)

adjacency matrix



(a)

directed graph



(b)

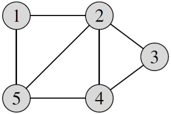
adjacency list

	1	2	3	4	5	6
1	0	1	0	1	0	0
2	0	0	0	0	1	0
3	0	0	0	0	1	1
4	0	1	0	0	0	0
5	0	0	0	1	0	0
6	0	0	0	0	0	1

(c)

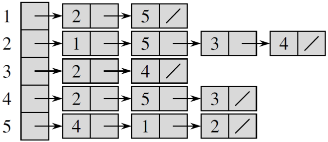
adjacency matrix

Representation efficiency



(a)

undirected graph



(b)

adjacency list

memory: $\Theta(|V| + |E|)$

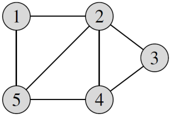
	1	2	3	4	5
1	0	1	0	0	1
2	1	0	1	1	1
3	0	1	0	1	0
4	0	1	1	0	1
5	1	1	0	1	0

(c)

adjacency matrix

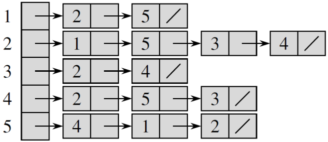
memory: $\Theta(|V|^2)$

Representation efficiency



(a)

undirected graph



(b)

adjacency list

memory: $\Theta(|V| + |E|)$

	1	2	3	4	5
1	0	1	0	0	1
2	1	0	1	1	1
3	0	1	0	1	0
4	0	1	1	0	1
5	1	1	0	1	0

(c)

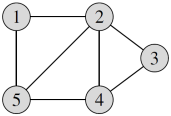
adjacency matrix

memory: $\Theta(|V|^2)$

For undirected graphs, the adjacency matrix is symmetric.

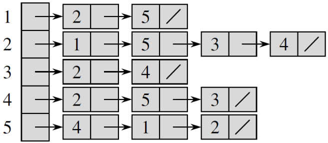
$\Rightarrow$ requires half of the memory.

Representation efficiency



(a)

undirected graph



(b)

adjacency list

memory: $\Theta(|V| + |E|)$

$$\begin{array}{c|ccccc|} & 1 & 2 & 3 & 4 & 5 \\ \hline 1 & 0 & 1 & 0 & 0 & 1 \\ 2 & 1 & 0 & 1 & 1 & 1 \\ 3 & 0 & 1 & 0 & 1 & 0 \\ 4 & 0 & 1 & 1 & 0 & 1 \\ 5 & 1 & 1 & 0 & 1 & 0 \\ \hline \end{array}$$

(c)

adjacency matrix

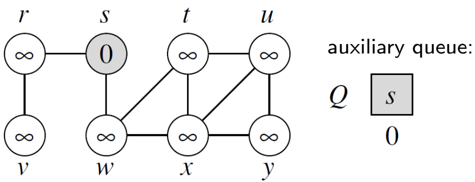
memory: $\Theta(|V|^2)$

For undirected graphs, the adjacency matrix is symmetric.

$\Rightarrow$ requires half of the memory.

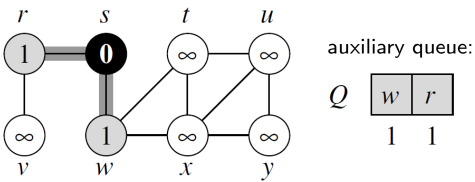
With adjacency matrices, most algorithms are lower bounded as $\Omega(|V|^2)$.

Breadth-first search (BFS)



We start from a source vertex s, and discover all the reachable vertices.

Breadth-first search (BFS)



We start from a source vertex s, and discover all the reachable vertices.

Each discovered vertex has its distance to s (# edges) computed.

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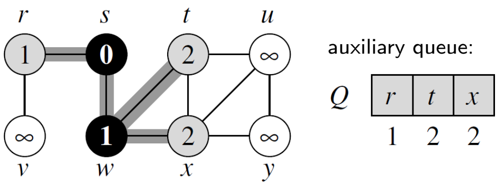

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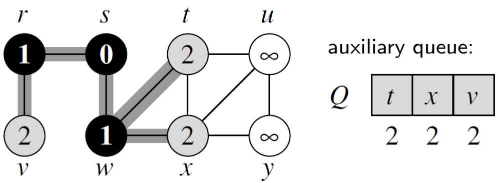
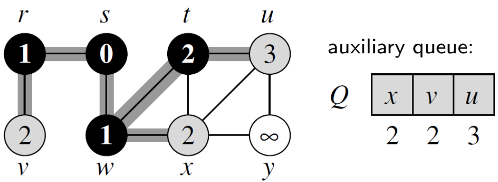


We start from a source vertex s, and discover all the reachable vertices.

Each discovered vertex has its distance to s (# edges) computed.

Breadth-first: nodes at distance k explored before those at distance $k+1$.

Breadth-first search (BFS)



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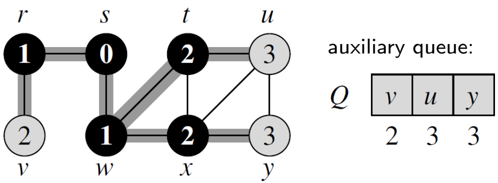

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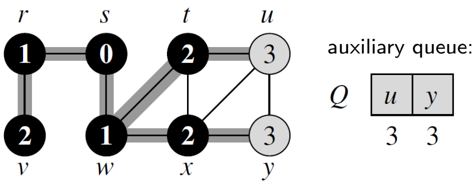

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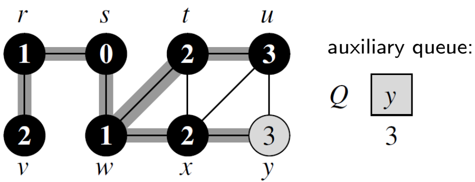

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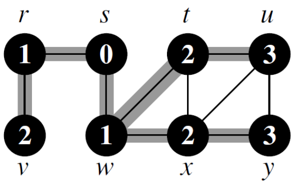


auxiliary queue:

$Q \quad \emptyset$

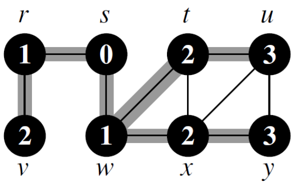
We start from a source vertex s, and discover all the reachable vertices.

Each discovered vertex has its distance to s (# edges) computed.

Breadth-first: nodes at distance k explored before those at distance $k + 1$.

A breadth-first tree (shaded edges) is obtained as a side-product.

Breadth-first search (BFS)



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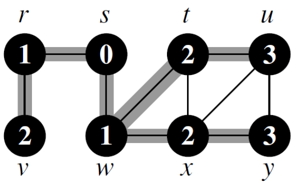
A breadth-first tree (shaded edges) is obtained as a side-product.

- The tree changes if we change the source s (which is the root).

Breadth-first search (BFS)



auxiliary queue:

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We start from a source vertex s, and discover all the reachable vertices.

Each discovered vertex has its distance to s (# edges) computed.

Breadth-first: nodes at distance k explored before those at distance $k + 1$.

A breadth-first tree (shaded edges) is obtained as a side-product.

- The tree changes if we change the source s (which is the root).
- The tree changes if we explore vertex x before vertex t.

Breadth-first search (BFS)

BFS(G, s)

for each vertex $u \in V[G] - \{s\}$
  do $color[u] \leftarrow$ WHITE
    $d[u] \leftarrow \infty$
    $\pi[u] \leftarrow$ NIL

- initialize all distances $d = \infty$
- the parent π of every vertex is NIL; parents constitute the tree
- WHITE vertices are undiscovered

Breadth-first search (BFS)

BFS(G, s)

for each vertex $u \in V[G] - \{s\}$
    do $\mathit{color}[u] \leftarrow \text{WHITE}$
        $d[u] \leftarrow \infty$
        $\pi[u] \leftarrow \text{NIL}$
$\mathit{color}[s] \leftarrow \text{GRAY}$
$d[s] \leftarrow 0$
$\pi[s] \leftarrow \text{NIL}$
$Q \leftarrow \emptyset$
$\text{ENQUEUE}(Q, s)$

$*$ GRAY vertices are discovered, but not yet explored

Breadth-first search (BFS)

```
BFS(G, s)
for each vertex u ∈ V[G] − {s}
      do color[u] ← WHITE
         d[u] ← ∞
         π[u] ← NIL
color[s] ← GRAY
d[s] ← 0
π[s] ← NIL
Q ← ∅
ENQUEUE(Q, s)
while Q ≠ ∅
      do u ← DEQUEUE(Q)
         for each v ∈ Adj[u]
             do if color[v] = WHITE
                   then color[v] ← GRAY
                        d[v] ← d[u] + 1
                        π[v] ← u
                        ENQUEUE(Q, v)
         color[u] ← BLACK
```

Breadth-first search (BFS)

BFS(G, s)

$\Theta(|V|)$

```
for each vertex u ∈ V[G] − {s}
    do color[u] ← WHITE
       d[u] ← ∞
       π[u] ← NIL
```

$\Theta(1)$

```
color[s] ← GRAY
d[s] ← 0
π[s] ← NIL
Q ← ∅
ENQUEUE(Q, s)
while Q ≠ ∅
    do u ← DEQUEUE(Q)
       for each v ∈ Adj[u]
           do if color[v] = WHITE
                 then color[v] ← GRAY
                      d[v] ← d[u] + 1
                      π[v] ← u
                      ENQUEUE(Q, v)
       color[u] ← BLACK
```

Breadth-first search (BFS)

```
           BFS(G, s)
           for each vertex u ∈ V[G] − {s}
Θ(|V|)         do color[u] ← WHITE
                  d[u] ← ∞
                  π[u] ← NIL
           color[s] ← GRAY
           d[s] ← 0
Θ(1)       π[s] ← NIL
           Q ← ∅
           ENQUEUE(Q, s)
O(|V|) →   while Q ≠ ∅
               do u ← DEQUEUE(Q)
                  for each v ∈ Adj[u]
                      do if color[v] = WHITE
                            then color[v] ← GRAY
                                 d[v] ← d[u] + 1
                                 π[v] ← u
                                 ENQUEUE(Q, v)
                  color[u] ← BLACK
```

Breadth-first search (BFS)

```
            BFS(G, s)
         ‖  for each vertex u ∈ V[G] − {s}
Θ(|V|)   ‖        do color[u] ← WHITE
         ‖           d[u] ← ∞
         ‖           π[u] ← NIL
         ‖  color[s] ← GRAY
         ‖  d[s] ← 0
Θ(1)     ‖  π[s] ← NIL
         ‖  Q ← ∅
         ‖  ENQUEUE(Q, s)
O(|V|) →    while Q ≠ ∅
                  do u ← DEQUEUE(Q)
O(|E|) →             for each v ∈ Adj[u]
                          do if color[v] = WHITE
                                then color[v] ← GRAY
                                     d[v] ← d[u] + 1
                                     π[v] ← u
                                     ENQUEUE(Q, v)
                     color[u] ← BLACK
```

Breadth-first search (BFS)

$O(|V| + |E|)$

```
BFS(G, s)
for each vertex u ∈ V[G] − {s}
      do color[u] ← WHITE
         d[u] ← ∞
         π[u] ← NIL
color[s] ← GRAY
d[s] ← 0
π[s] ← NIL
Q ← ∅
ENQUEUE(Q, s)
while Q ≠ ∅
      do u ← DEQUEUE(Q)
         for each v ∈ Adj[u]
             do if color[v] = WHITE
                   then color[v] ← GRAY
                        d[v] ← d[u] + 1
                        π[v] ← u
                        ENQUEUE(Q, v)
         color[u] ← BLACK
```

Exploring a path recursively

Assume a breadth-first tree has already been constructed.

```
PRINT-PATH(G, s, v)
if v = s
    then print s
    else if π[v] = NIL
            then print "no path from" s "to" v "exists"
            else PRINT-PATH(G, s, π[v])
                 print v
```

Exploring a path recursively

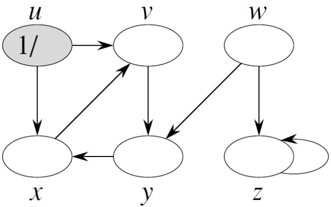
Assume a breadth-first tree has already been constructed.

```
PRINT-PATH(G, s, v)
1  if v = s
2     then print s
3     else  if π[v] = NIL
4              then print "no path from" s "to" v "exists"
5              else  PRINT-PATH(G, s, π[v])
6                    print v
```

Despite this being recursive, the total cost is $O(|V|)$.

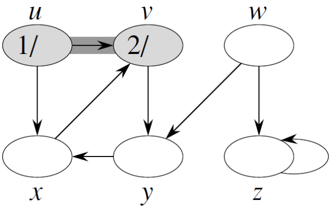
Line (5) is called on a path that is one edge shorter each time.

Depth-first search (DFS)



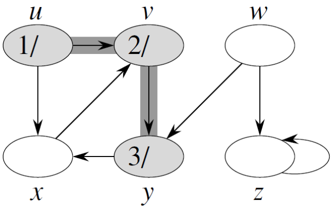
Inside each vertex, we write discovery time / finishing time.

Depth-first search (DFS)



Inside each vertex, we write discovery time / finishing time.

Depth-first search (DFS)



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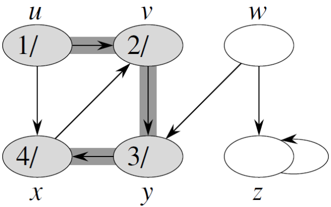

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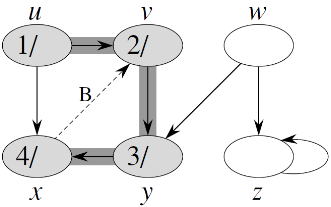
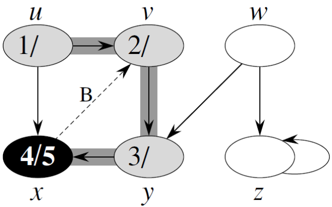
Depth-first search (DFS)



Inside each vertex, we write discovery time / finishing time.

Back edge to an already discovered vertex.

Depth-first search (DFS)

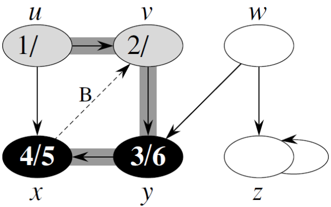


Inside each vertex, we write discovery time / finishing time.

Back edge to an already discovered vertex.

Backtrack to the next available move.

Depth-first search (DFS)



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Backtrack to the next available move.

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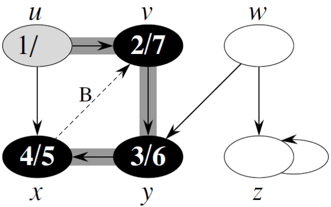

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Back edge to an already discovered vertex.

Backtrack to the next available move.

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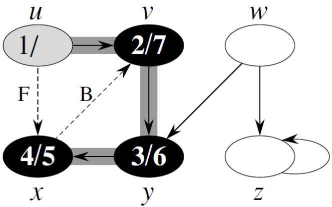

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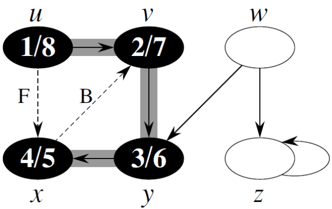

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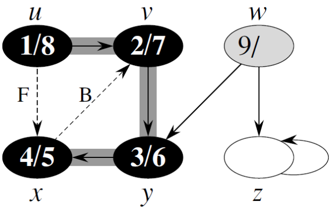
Backtrack to the next available move.

Forward edge to an already discovered vertex.

Depth-first search (DFS)



Inside each vertex, we write discovery time / finishing time.

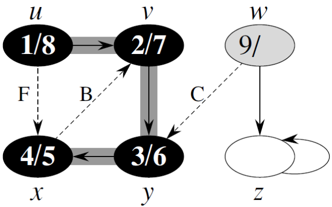
Back edge to an already discovered vertex.

Backtrack to the next available move.

Forward edge to an already discovered vertex.

Select a new source.

Depth-first search (DFS)



Inside each vertex, we write discovery time / finishing time.

Back edge to an already discovered vertex.

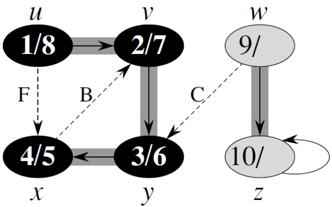
Backtrack to the next available move.

Forward edge to an already discovered vertex.

Select a new source.

Cross edge across two separate trees.

Depth-first search (DFS)



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Cross edge across two separate trees.

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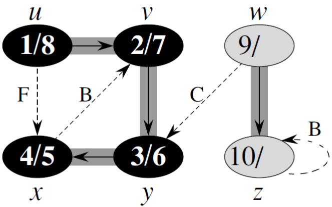

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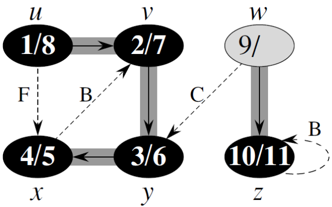

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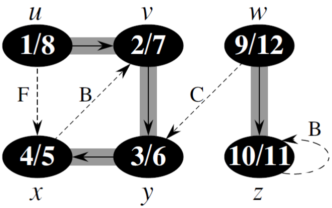

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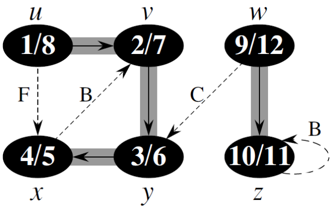
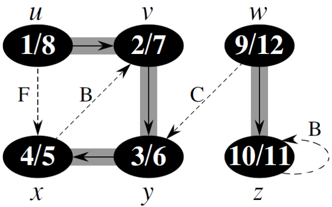


Unlike BFS, we might have many disjoint trees (shaded edges), thus obtaining a depth-first forest.

Depth-first search (DFS)



Unlike BFS, we might have many disjoint trees (shaded edges), thus obtaining a depth-first forest.

Like BFS, the specific forest changes if the order of exploration changes.

Depth-first search (DFS)

```
DFS(G)
for each vertex u ∈ V[G]
      do color[u] ← WHITE
         π[u] ← NIL
time ← 0
for each vertex u ∈ V[G]
      do if color[u] = WHITE
            then DFS-VISIT(u)
```

Depth-first search (DFS)

```
DFS(G)
for each vertex u ∈ V[G]
      do color[u] ← WHITE
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(u will be the root of a new tree in the forest)

Depth-first search (DFS)

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time ← 0
for each vertex u ∈ V[G]
     do if color[u] = WHITE
           then DFS-VISIT(u)     (u will be the root of a new tree in the forest)
```

```
DFS-VISIT(u)
color[u] ← GRAY              ▷ White vertex u has just been discovered.
time ← time + 1
d[u] ← time
for each v ∈ Adj[u]          ▷ Explore edge (u, v).
     do if color[v] = WHITE
           then π[v] ← u
                DFS-VISIT(v)
color[u] ← BLACK             ▷ Blacken u; it is finished.
f[u] ← time ← time + 1
```

Depth-first search (DFS)

DFS(G)

$\Theta(|V|)$
- **for** each vertex $u \in V[G]$
  - **do** $color[u] \leftarrow$ WHITE
  - $\pi[u] \leftarrow$ NIL

$time \leftarrow 0$

$\Theta(|V|)$
- **for** each vertex $u \in V[G]$
  - **do if** $color[u] =$ WHITE
    - **then** DFS-VISIT(u) (u will be the root of a new tree in the forest)

DFS-VISIT(u)

- $color[u] \leftarrow$ GRAY ▷ White vertex u has just been discovered.
- $time \leftarrow time + 1$
- $d[u] \leftarrow time$
- **for** each $v \in Adj[u]$ ▷ Explore edge (u, v).
  - **do if** $color[v] =$ WHITE
    - **then** $\pi[v] \leftarrow u$
    - DFS-VISIT(v)
- $color[u] \leftarrow$ BLACK ▷ Blacken u; it is finished.
- $f[u] \leftarrow time \leftarrow time + 1$

Depth-first search (DFS)

```
DFS(G)
                for each vertex u ∈ V[G]
Θ(|V|)              do color[u] ← WHITE
                       π[u] ← NIL
                time ← 0
                for each vertex u ∈ V[G]
Θ(|V|)              do if color[u] = WHITE
                          then DFS-VISIT(u)
```

(u will be the root of a new tree in the forest)

```
DFS-VISIT(u)
                color[u] ← GRAY              ▷ White vertex u has just been discovered.
                time ← time + 1
                d[u] ← time
                for each v ∈ Adj[u]          ▷ Explore edge (u, v).
Θ(|E|)              do if color[v] = WHITE
                          then π[v] ← u
                               DFS-VISIT(v)
                color[u] ← BLACK             ▷ Blacken u; it is finished.
                f[u] ← time ← time + 1
```

Suggested reading

Chapters 22.1, 22.2 (skip the “Shortest Paths” paragraph), and 22.3 (skip the “Properties of depth-first search” paragraph) of:

“Introduction to Algorithms – 2nd Ed.”, Cormen et al.