Algorithms for Data Science

CSOR W4246

Eleni Drinea
Computer Science Department

Columbia University

Shortest paths in weighted graphs (Bellman-Ford, Floyd-Warshall)

Outline

1. Shortest paths in graphs with non-negative edge weights (Dijkstra's algorithm)
   - Implementations
   - Graphs with **negative** edge weights: why Dijkstra fails
2. Single-source shortest paths (negative edges): Bellman-Ford
   - A DP solution
   - An alternative formulation of Bellman-Ford
3. All-pairs shortest paths (negative edges): Floyd-Warshall

Today

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Graphs with **non-negative** weights

Input

- a weighted, directed graph $G = (V, E, w)$; function $w : E \to R^+$ assigns non-negative real-valued weights to edges;
- a source (origin) vertex $s \in V$.

Output: for every vertex $v \in V$

1. the length of a shortest s-v path;
2. a shortest s-v path.

Dijkstra's algorithm (Input: $G = (V, E, w), s \in V$)

Output: arrays $dist$, $prev$ with n entries such that

1. $dist(v)$ stores the length of the shortest s-v path
2. $prev(v)$ stores the node before v in the shortest s-v path

At all times, maintain a set S of nodes for which the distance from s has been determined.

- Initially, $dist(s) = 0$, $S = \{s\}$.
- Each time, add to S the node $v \in V - S$ that
  1. has an edge from some node in S;
  2. minimizes the following quantity among all nodes $v \in V - S$

$$d(v) = \min_{u \in S : (u,v) \in E} \{dist(u) + w(u, v)\}$$

- Set $prev(v) = u$.

Implementation

```
Dijkstra-v1(G = (V, E, w), s ∈ V)
   Initialize(G, s)
   S = {s}
   while S ≠ V do
      Select a node v ∈ V − S with at least one edge from S so that
            d(v) = min_{u∈S,(u,v)∈E} {dist[u] + w(u, v)}
      S = S ∪ {v}
      dist[v] = d(v)
      prev[v] = u
   end while

Initialize(G, s)
   for v ∈ V do
      dist[v] = ∞
      prev[v] = NIL
   end for
   dist[s] = 0
```

Improved implementation (I)

Idea: Keep a conservative overestimate of the true length of the shortest s-v path in $dist[v]$ as follows: when u is added to S, update $dist[v]$ for all v with $(u, v) \in E$.

```
Dijkstra-v2(G = (V, E, w), s ∈ V)
   Initialize(G, s)
   S = ∅
   while S ≠ V  do
      Pick u so that dist[u] is minimum among all nodes in V − S
      S = S ∪ {u}
      for (u, v) ∈ E do
         Update(u, v)
      end for
   end while

Update(u, v)
   if dist[v] > dist[u] + w(u, v) then
      dist[v] = dist[u] + w(u, v)
      prev[v] = u
   end if
```

Improved implementation (II): binary min-heap

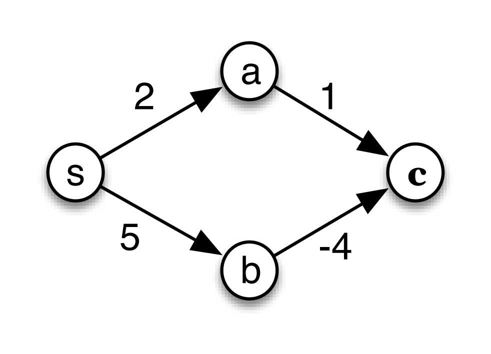
Idea: Use a priority queue implemented as a binary min-heap: store vertex u with key $dist[u]$. Required operations: `Insert`, `ExtractMin`; `DecreaseKey` for `Update`; each takes $O(\log n)$ time.

```
Dijkstra-v3(G = (V, E, w), s ∈ V)
   Initialize(G, s)
   Q = {V; dist}
   S = ∅
   while Q ≠ ∅ do
      u = ExtractMin(Q)
      S = S ∪ {u}
      for (u, v) ∈ E do
         Update(u, v)
      end for
   end while
```

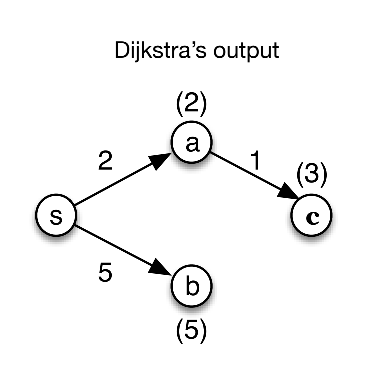
Running time: $O(n \log n + m \log n) = O(m \log n)$

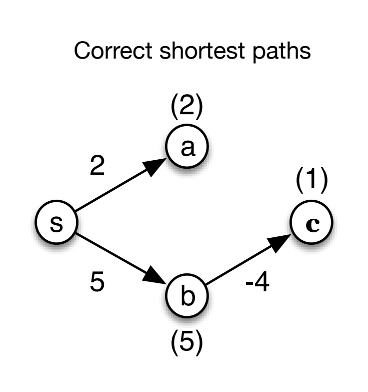
When is `Dijkstra-v3()` *better than* `Dijkstra-v2()`*?*

Example graph with **negative** edge weights



Dijkstra's output and correct output for example graph



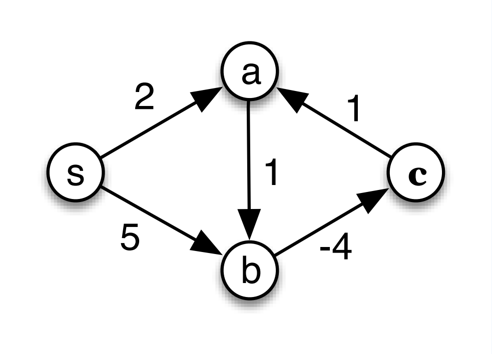


Dijkstra's algorithm will first include a to S and then c, thus missing the shorter path from s to b to c.

Negative edge weights: why Dijkstra's algorithm fails

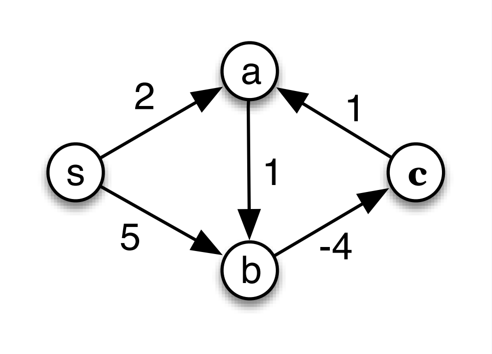
- Intuitively, a path may start on long edges but then compensate along the way with short edges.
- Formally, in the proof of correctness of the algorithm, the last statement about P does not hold anymore: even if the length of path P_v is smaller than the length of the subpath $s \to x \to y$, negative edges on the subpath $y \to v$ may now result in P being *shorter* than P_v.

Bigger problems in graphs with negative edges?



$dist(a) = ?$

Bigger problems in graphs with negative edges?



1. $dist(v)$ goes to $-\infty$ for every v on the cycle (a, b, c, a)
2. **no** solution to shortest paths when negative cycles

$\Rightarrow$ need to detect negative cycles

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Single-source shortest paths, negative edge weights

Input: weighted directed graph $G = (V, E, w)$ with $w : E \to R$; a source (origin) vertex $s \in V$.

Output:

1. If G has a negative cycle reachable from s, answer **"negative cycle in G"**.
2. Else, compute for every $v \in V$
   2.1 the length of a shortest s-v path;
   2.2 a shortest s-v path.

Properties of shortest paths

Suppose the problem **has** a solution for an input graph.

- *Can there be negative cycles in the graph?*
- *Can there be positive cycles in the graph?*
- *Can the shortest paths contain positive cycles?*
- *Consider a shortest s-t path; are its subpaths shortest? In other words, does the problem exhibit optimal substructure?*

Towards a DP solution

Key observation: if there are no negative cycles, a path cannot become shorter by traversing a cycle.

Fact 1.

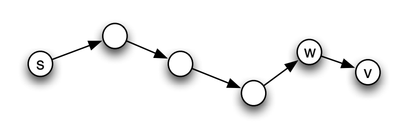
If G has no negative cycles, then there is a shortest s-v path that is simple, thus has at most $n-1$ edges.

Fact 2.

The shortest paths problem exhibits optimal substructure.

Facts 1 and 2 suggest a DP solution.

Subproblems



Let

$$OPT(i, v) = \text{cost of a shortest } s\text{-}v \text{ path with } \textit{at most } i \text{ edges}$$

Consider a shortest s-v path using at most i edges.

- If the path uses at most $i - 1$ edges, then

$$OPT(i, v) = OPT(i - 1, v).$$

- If the path uses i edges, then

$$OPT(i, v) = \min_{x:(x,v)\in E} \{OPT(i - 1, x) + w(x, v)\}.$$

Recurrence

Let

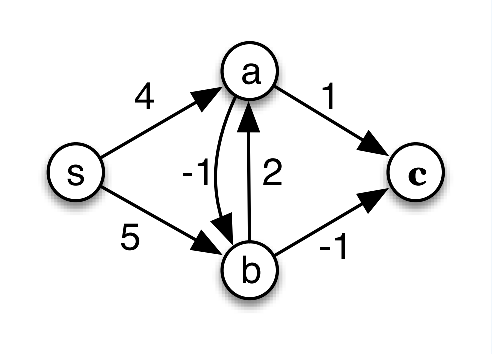
$$OPT(i, v) = \text{cost of a shortest } s\text{-}v \text{ path using } \textit{at most } i \text{ edges}$$

Then

$$OPT(i,v) = \begin{cases} 0 & \text{, if } i = 0, v = s \\ \infty & \text{, if } i = 0, v \neq s \\ \min \begin{cases} OPT(i-1, v) \\ \min\limits_{x:(x,v) \in E} \{OPT(i-1, x) + w(x, v)\} \end{cases} & \text{, if } i > 0 \end{cases}$$

Example of Bellman-Ford

Compute shortest s-v paths in the graph below, for all $v \in V$.



Pseudocode

$n \times n$ dynamic programming table M such that $M[i, v] = OPT(i, v)$.

```
Bellman-Ford(G = (V, E, w), s ∈ V)
   for v ∈ V do
       M[0, v] = ∞
   end for
   M[0, s] = 0
   for i = 1, ..., n − 1 do
       for v ∈ V (in any order) do
```

$$M[i, v] = \min \begin{cases} M[i-1, v] \\ \min\limits_{x:(x,v)\in E} \left\{ M[i-1, x] + w(x, v) \right\} \end{cases}$$

```
       end for
   end for
```

Running time & Space

- **Running time:** $O(nm)$
- **Space:** $\Theta(n^2)$ —can be improved (*coming up*)
- To reconstruct actual shortest paths, also keep array $prev$ of size n such that

$$prev[v] = \text{predecessor of } v \text{ in current shortest } s\text{-}v \text{ path.}$$

Improving space requirements

Only need two rows of M at all times.

$\triangle$ Actually, only need one (see Remark 1)! Thus drop the index i from $M[i, v]$ and only use it as a counter for #repetitions.

$$M[v] = \min\left\{M[v], \min_{x:(x,v)\in E}\left\{M[x] + w(x, v)\right\}\right\}$$

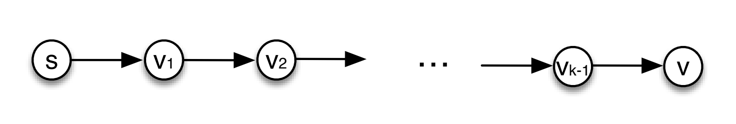
Remark 1.

Throughout the algorithm, $M[v]$ is the length of some s-v path. After i repetitions, $M[v]$ is no larger than the length of the current shortest s-v path with at most i edges.

Early termination condition: if at some iteration i **no** value in M changed, then stop (*why?*)

$*$ This allows us to detect negative cycles!

An alternative way to view Bellman-Ford



- Let $P = (s = v_0, v_1, v_2, \ldots, v_k = v)$ be a shortest s-v path.
- Then P can contain at most $n - 1$ edges.
- *How can we correctly compute* $dist(v)$ *on this path?*

Key observations about subroutine `Update`(u, v)

Recall subroutine `Update` from Dijkstra's algorithm:

$$\texttt{Update}(u, v) : dist(v) = \min\{dist(v), dist(u) + w(u, v)\}$$

Fact 3.

Suppose u is the last node before v on the shortest s-v path, and suppose $dist(u)$ has been correctly set. The call `Update`(u, v) *returns the correct value for $dist(v)$.*

Fact 4.

No matter how many times `Update`(u, v) *is performed, it will never make $dist(v)$ too small. That is,* `Update` *is a safe operation: performing few extra updates can't hurt.*

Performing the correct sequence of updates

Suppose we update the edges on the shortest path P in the order they appear on the path (though not necessarily consecutively). Hence we update

$$(s, v_1), (v_1, v_2), (v_2, v_3), \ldots, (v_{k-1}, v).$$

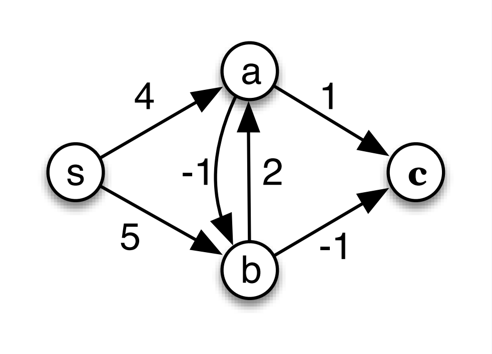
This sequence of updates correctly computes $dist(v_1)$, $dist(v_2)$, …, $dist(v)$ (by induction and Fact 3).

How can we guarantee that this specific sequence of updates occurs?

A concrete example

Consider the shortest s-b path, which uses edges $(s, a), (a, b)$.

How can we guarantee that our algorithm will update these two edges **in this order**? *(More updates in between are allowed.)*



Bellman-Ford algorithm

Update all m edges in the graph, $n-1$ times in a row!

- By Fact 4, it is ok to update an edge several times in between.
- All we need is to update the edges on the path in this particular order. This is guaranteed if we update all edges $n-1$ times in a row.

Pseudocode

We will use `Initialize` and `Update` from Dijkstra's algorithm.

`Initialize`(G, s)

for $v \in V$ **do**

$dist[v] = \infty$

$prev[v] = NIL$

end for

$dist[s] = 0$

`Update`(u, v)

if $dist[v] > dist[u] + w(u, v)$ **then**

$dist[v] = dist[u] + w(u, v)$

$prev[v] = u$

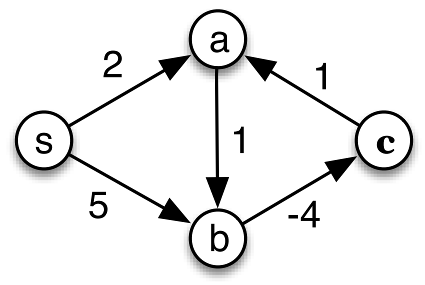
end if

Bellman-Ford

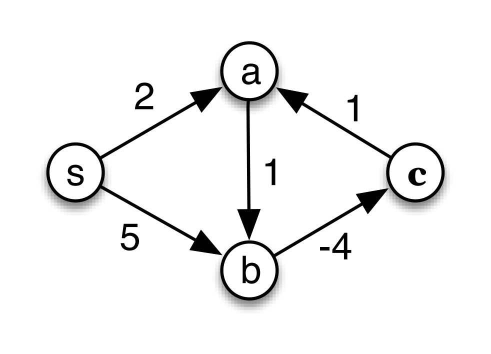
```
Bellman-Ford(G = (V, E, w), s)
  Initialize(G, s)
  for i = 1, ..., n − 1 do
      for (u, v) ∈ E do
          Update(u, v)
      end for
  end for
```

Running time? Space?

Detecting negative cycles



Detecting negative cycles



1. $dist(v)$ goes to $-\infty$ for every v on the cycle.
2. Any shortest s-v path can have at most $n-1$ edges.
3. Update all edges n times (instead of $n-1$): if $dist(v)$ changes **for any** $v \in V$, then there is a negative cycle.

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All pairs shortest-paths

- **Input:** a directed, weighted graph $G = (V, E, w)$ with real edge weights
- **Output:** an $n \times n$ matrix D such that

$$D[i, j] = \text{length of shortest path from } i \text{ to } j$$

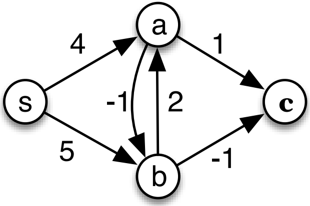
Solving all pairs shortest-paths

1. Straightforward solution: run Bellman–Ford once for every vertex ($O(n^2 m)$ time).
2. Improved solution: Floyd-Warshall's dynamic programming algorithm ($O(n^3)$ time).

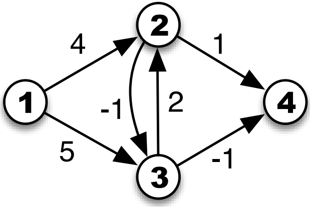
Towards a DP formulation

- Consider a shortest s-t path P.
- This path uses some intermediate vertices: that is, if $P = (s, v_1, v_2, \ldots, v_k, t)$, then $v_1, \ldots, v_k$ are intermediate vertices.
- For simplicity, relabel the vertices in V as $\{1, 2, 3, \ldots, n\}$ and consider a shortest i-j path where intermediate vertices may only be from $\{1, 2, \ldots, k\}$.
- **Goal:** compute the length of a shortest i-j path for every pair of vertices (i, j), using $\{1, 2, \ldots, n\}$ as intermediate vertices.

Example

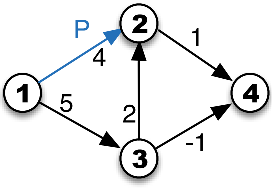


Rename {s, a, b, c} as {**1, 2, 3, 4**}

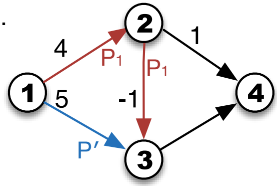


Examples of shortest paths

Shortest (**1, 2**)-path using {} or {1} is P.
Shortest (**1, 2**)-path using {1,2,3,4} is P.

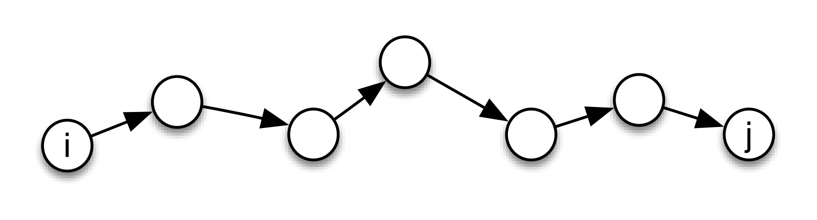


Shortest (**1, 3**)-path using {} or {1} is P′.
Shortest (**1, 3**)-path using {1,2} or {1,2,3} is P_1.
Shortest (**1, 3**)-path using {1,2,3,4} is P_1 .



A shortest i-j path using nodes from $\{1, \ldots, k\}$

Consider a shortest i-j path P where intermediate nodes may only be from the set of nodes $\{1, 2, \ldots, k\}$.



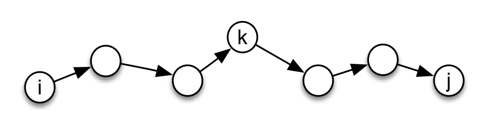
Fact: any subpath of P must be shortest itself.

A useful observation

Focus on the last node k from the set $\{1, 2, \ldots, k\}$. Either

1. P completely avoids k: then a shortest i-j path with intermediate nodes from $\{1, \ldots, k\}$ is the same as a shortest i-j path with intermediate nodes from $\{1, \ldots, k-1\}$.

2. Or, k is an intermediate node of P.



Decompose P into an i-k subpath P_1 and a k-j subpath P_2.

i. P_1, P_2 are shortest subpaths themselves.
ii. All intermediate nodes of P_1, P_2 are from $\{1, \ldots, k-1\}$.

Subproblems

Let

$$OPT_k(i,j) \;=\; \text{cost of shortest } i-j \text{ path } P \text{ using } \{1,\ldots,k\} \text{ as intermediate vertices}$$

1. Either k does not appear in P, hence

$$OPT_k(i,j) = OPT_{k-1}(i,j)$$

2. Or, k appears in P, hence

$$OPT_k(i,j) = OPT_{k-1}(i,k) + OPT_{k-1}(k,j)$$

Recurrence

Hence

$$OPT_k(i,j) = \begin{cases} w(i,j) & \text{, if } k = 0 \\ \\ \min \begin{cases} OPT_{k-1}(i,j) \\ OPT_{k-1}(i,k) + OPT_{k-1}(k,j) \end{cases} & \text{, if } k \geq 1 \end{cases}$$

We want $OPT_n(i,j)$.

Time/space requirements?

Floyd-Warshall on example graph

Let $D_k[i,j] = OPT_k(i,j)$.

$D_0 =$

0	4	5	∞
∞	0	-1	1
∞	2	0	-1
∞	∞	∞	0

$D_1 =$

0	4	5	∞
∞	0	-1	1
∞	2	0	-1
∞	∞	∞	0

$D_2 =$

0	4	3	5
∞	0	-1	1
∞	2	0	-1
∞	∞	∞	0

$D_3 =$

0	4	3	2
∞	0	-1	-2
∞	2	0	-1
∞	∞	∞	0

Space requirements

- A single $n \times n$ dynamic programming table D, initialized to $w(i, j)$ (the adjacency matrix of G).
- Let $\{1, \ldots, k\}$ be the set of intermediate nodes that may be used for the shortest i-j path.
- After the k-th iteration, $D[i, j]$ contains the length of some i-j path that is no larger than the length of the shortest i-j path using $\{1, \ldots, k\}$ as intermediate nodes.

The Floyd-Warshall algorithm

`Floyd-Warshall`$(G = (V, E, w))$

for $k = 1$ to n **do**
  for $i = 1$ to n **do**
    for $j = 1$ to n **do**
      $D[i, j] = \min(D[i, j], D[i, k] + D[k, j])$
    end for
  end for
end for

- Running time: $O(n^3)$
- Space: $\Theta(n^2)$