DSC40B: Theoretical Foundations of Data Science II

Lecture 14: Shortest Path in Weighted Graphs – part I

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Prelude

Previously

- Basics of graphs, representations, graph search strategies
- ▶ BFS: also leads to shortest path distance in input graph
 - Note: graph is unweighted!

► Today:

- Weighted graphs
 - where each edge has an edge weight
- Properties of shortest paths in weighted graphs
- Bellman-Ford algorithm for computing single-source shortest path for any weighted graphs



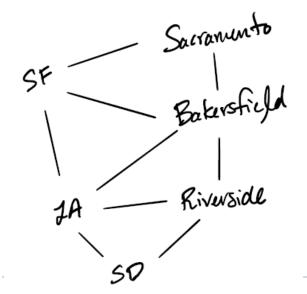
Weighted graphs, and shortest paths in them

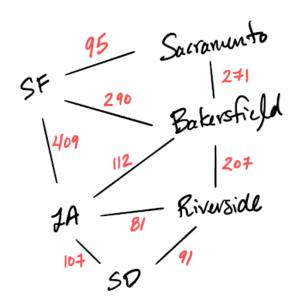


Unweighted graph:

$$G = (V, E)$$

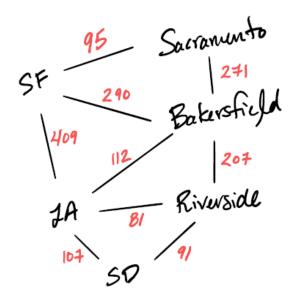
- Nodes and edges can carry meaning, and thus can carry weights as well.
- ► Example: transportation network





Weighted Graph

- ▶ (Edge) weighted graph $G = (V, E; \omega)$
 - \blacktriangleright is a graph G=(V,E) together with an edge weight assignment map: $\omega:E\to R$
 - i.e., a graph where each edge e has a weight (real value) $\omega(e)$



can be directed / undirected

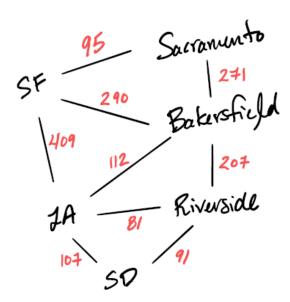
- weights can be positive/negative
- useful in many applications
 - strength of connection in a social network
 - distance in a transportation network
 - probability that two nodes interact in a proteinprotein interaction network

Path lengths

• Given a path in a weighted graph, its length is the total weights of all edges in the path.

Examples:

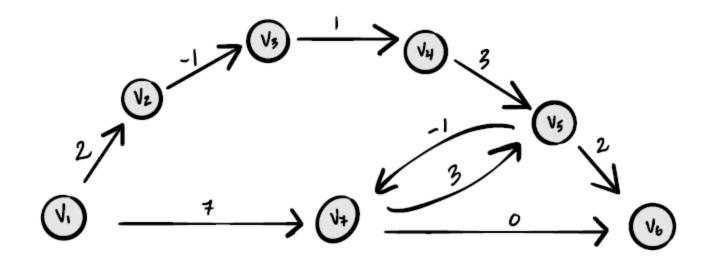
- > SF, LA, Bakersfield, Riverside
 - ▶ length = 728
- > SF, LA, Riverside
 - ▶ length = **490**
- LA, SD, Riverside, LA, SF
 - ▶ length = 688
- ▶ LA, SF
 - ▶ length = 409
- LA, Bakerfield, SF
 - ▶ length = 402





Shortest Paths

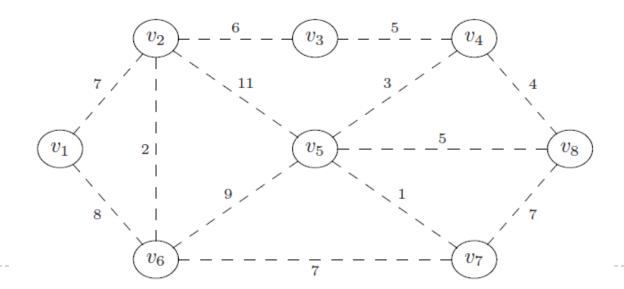
 \blacktriangleright A shortest path from u to v is a path from u to v with minimum length.



▶ Shortest path from v_1 to v_6 ?

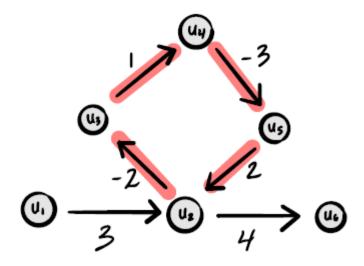
Shortest Paths

- lacktriangle A shortest path from u to v is a path from u to v with minimum length.
- The (shortest-path) distance from u to v is the length of the shortest path from u to v
- lacktriangle A shortest path from u to v may not be unique
 - but all shortest paths from u to v have same length



Properties of shortest paths

- Shortest path is not well-defined if the input graph has "negative cycles"
 - A negative cycle is a cycle whose length is negative

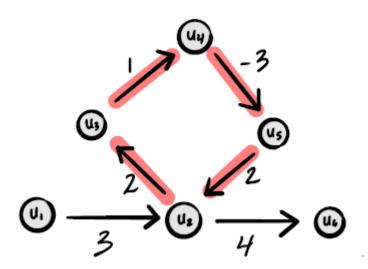


Negative weights are usually okay. Negative cycles make shortest path not well-defined.



Properties of shortest paths

- Shortest path is not well-defined if the input graph has "negative cycles"
 - A negative cycle is a cycle whose length is negative
- Assume we have a graph with no negative cycle
 - ▶ Then for any pair $u, v \in V$, there is always a shortest path that is simple.
 - If a path is not simple, there is a cycle inside, then removing this cycle can only make the path length shorter





Properties of shortest paths

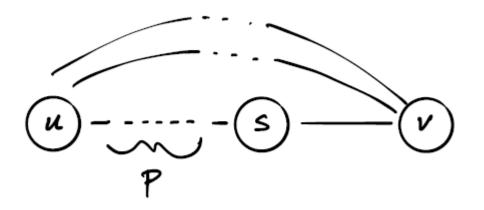
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 - ▶ Then for any pair $u, v \in V$, there is always a shortest path that is simple.
 - If a path is not simple, there is a cycle inside, then removing this cycle can only make the path length shorter
- ▶ Hence from now on, when we can assume that shortest paths are simple.



Properties of shortest path

Optimal Substructure Property (Theorem):

If $(u_1, u_2, ..., u_m)$ is a shortest path from u_1 to u_m , then any sub-path $(u_i, ..., u_i)$ is also a shortest path.





Property of shortest paths

From now on, let $\delta(u, v)$ denote the (shortest path) distance from u to v

Triangle inequality:

- Suppose (z, v) is an edge. Then $\delta(s, v) \leq \delta(s, z) + \omega(z, v)$
- One can view $\delta(s,z) + \omega(z,v)$ as the shortest path from s to v using edge (z,v) as last edge
- If $\delta(s,v)=\delta(s,z)+\omega(z,v)$, then z is the predecessor of v along a shortest path from s to v
 - ightharpoonup that is, (z, v) is the last edge along a shortest path from s to v
 - \blacktriangleright that is, z is the predecessor of v along the shortest path from s to v



Single-source shortest paths (SSSP) and Does BFS work for weighted graphs?



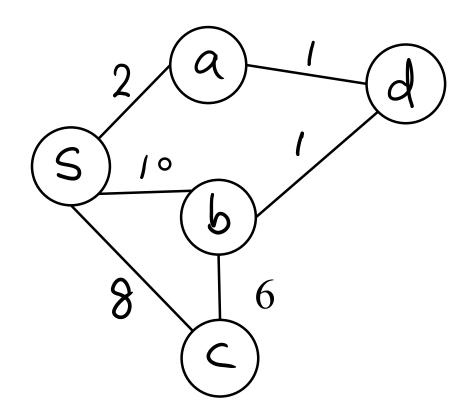
- Single-source shortest path (SSSP) problem:
 - Given a weighted graph $G = (V, E; \omega)$, and a source node s, compute the shortest path distance from s to all other nodes in V
 - ▶ i.e, compute $\delta(s, u)$ for all $u \in V$
- Once we have an algorithm for SSSP, we can use it to solve for all-pairs shortest path problem (where we compute shortest path distance among all pairs of nodes in V)
 - by simply running SSSP once using each node as source



- An unweighted graph G = (V, E)
 - can be thought of as a weighted graph where all edges have the same unit weight, i.e, $\omega(e)=1$ for any edge $e\in E$
- Hence,
 - ▶ BFS can compute the shortest path lengths (to the source) for an unweighted graph, or equivalently, a graph where all edges have the same positive edge weights!

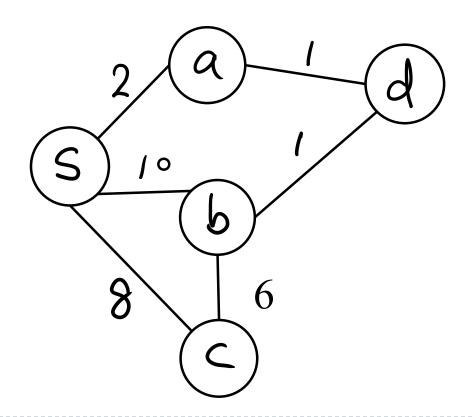
Can BFS idea work in general?

- Not really
- **Example:**



Can BFS idea work?

- Not really
- **Example:**



Intuitively, what went wrong?

- Recall BFS is a greedy algorithm and keeps exploring nodes in increasing distance to the source.
- In BFS, at the time we explore a node u, we have found its correct distance to the source s already.
- This however fails when edges have non-equal weights.



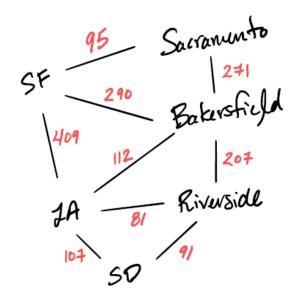
Can we use BFS to solve SSSP?

- Suppose edge weights are all positive integers
- ▶ Then here is an idea to compute SSSP:
- ► Input:
 - ▶ $G = (V, E; \omega)$ where $\omega: E \to \mathbb{Z}$ gives integer weights, and a source node $s \in V$
- Output:
 - lacktriangle The shortest path distance from s to all nodes in V
- ► Approach #0:
 - Step I: For each edge with weight k, replace it by a path with k edges, each of which has weight 1. Call the new graph $\hat{G} = (\hat{V}, \hat{E})$.
 - Step 2: Use BFS on the new graph \hat{G}



Problem with Approach #0

- Only works when edges have positive integer weights
- Even for integer-weighted graphs, it can be highly inefficient.



We need better algorithms for SSSP.



Key operation for SSSP: Edge Update



Two algorithms for SSSP

Bellman-Ford algorithm

- Morks for any weighted graph G = (V, E)
- ▶ Has time complexity $\Theta(V \cdot E)$

Dijkstra algorithm

- Works for graphs with positive edge weights
- More efficient! Has time complexity $\Theta((V+E)\lg V)$ (which we will discuss in class), and can be made to run in $\Theta(V\lg V+E)$ time.

Both algorithms

- use an update() operation to keep track of shortest path estimates
- perform it repeatedly till all shortest path distances to source are round

From now on, for simplicity, we use V and E to denote |V| and |E| in time complexity.



Estimated shortest path

- Fix the source node to be s
- ▶ Both algorithms keep track of the shortest path found so far,
 - we call these estimated shortest paths
 - \triangleright set u.est = the length of estimated shortest path source s to u

- ▶ At the beginning, u.est = ∞ for all nodes other than the source s
- \blacktriangleright And s. est = 0
- Then the algorithm will iteratively update shortest path estimates u.est when it finds better (shorter) path to reach it.



Estimated shortest path so far

- Fix the source node to be s
- ▶ Both algorithms keep track of the shortest path found so far,
 - we call these estimated shortest paths
 - \blacktriangleright set u.est = the length of estimated shortest path source s to u
- ▶ Key: during the update process, at any moment,
 - the estimated shortest path can only improve,
 - is at least as long as the true shortest path (i.e, u.est $\geq \delta(s, u)$),
 - and once it finds shortest distances, it will stay that way.
- \blacktriangleright For each node u, we will remember u's
 - ightharpoonup predecessor along the estimated shortest path from s to u
 - \triangleright u.est, the current estimated distance from s to u



Updating edges

- The way we update the estimates is via repeatedly performing "update(u, v)" operation over an edge $(u, v) \in E$
 - ν has current predecessor
 - \triangleright is u a better predecessor for v?
 - if yes, then we should update v.est and v's predecessor!

▶ In particular:

Is the current shortest path from

source
$$s \rightsquigarrow u \rightarrow v$$

shorter than the current shortest path from

source
$$s \rightsquigarrow v$$
's current predecessor $\rightarrow v$?

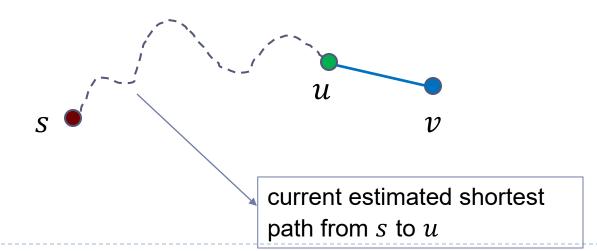
If yes, then we have discovered a shorter path to v, and we change v's predecessor and estimated distance.



Updating edges

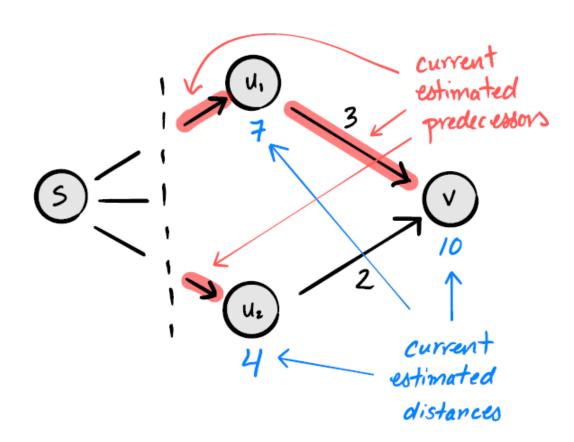
update(u, v) // where $(u, v) \in E$ is an edge in graph

- If $v.est > u.est + \omega(u, v)$
 - \blacktriangleright Then we found a better path from s to v
 - \square by first going from s to u, and then go to v through edge (u, v)
 - ▶ So we update $v.est = u.est + \omega(u, v)$ and set u to be v's predecessor
- Dtherwise, we do nothing.



Example

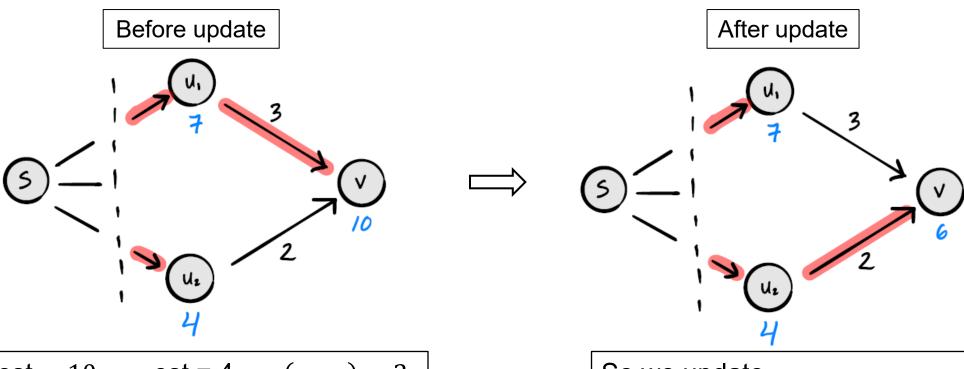
 \blacktriangleright Before update(u_2, v)





Example

ightharpoonup update (u_2, v)



$$v.est = 10, \ u_2.est = 4, \ \omega(u_2, v) = 2$$

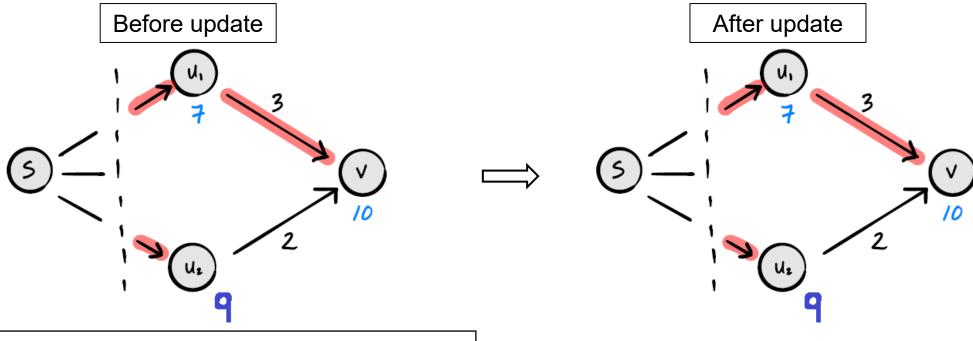
- $\Rightarrow v.\text{est} > u_2.\text{est} + \omega(u_2, v)$
- \Rightarrow find a shorter path from s to v!

 \Longrightarrow

So we update $v.\text{est} = u_2.\text{est} + \omega(u_2, v) = 6$ and set v's predecessor to u_2

Another Example

 \rightarrow update(u_2, v)



v.est = 10, $u_2.est = 9$, $\omega(u_2, v) = 2$

- \Rightarrow v.est $< u_2$.est $+\omega(u_2, v)$
- \Rightarrow The path from s to u_2 then to v is not

shorter than what already discovered for v!

Do Nothing!

Implementing update() in python

- ► To implement update(u,v) in python, let
 - est be a dictionary of estimated shortest path distances
 - predecessor be a dictionary of estimated shortest path predecessors
 - weights be a function which returns edge weights



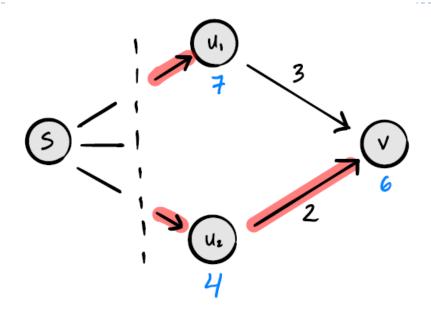
Implementing update() in python

```
def update(u, v, weights, est, predecessor):
    """Update edge (u,v)."""
    if est[v] > est[u] + weights(u,v):
        est[v] = est[u] + weights(u,v)
        predecessor[v] = u
        return True
    else:
        return False
```

Time complexity: $\Theta(1)$



When does an update discover a shortest path?



- lacktriangle So update (u_2,v) discovered a new estimated shortest path from s to v
- Is this the shortest path?
- Not necessarily: We might discover a shorter path, say, reaching v through u_1



When does an update discover a shortest path?

[Theorem Update]

Let u and v be graph nodes

Suppose:

- \triangleright (a) current shortest path distance estimate u.est is correct
 - \rightarrow i.e, u.est = $\delta(s, u)$
- \blacktriangleright (b) there is a shortest path from s to v with u being v's predecessor

Then, after update(u, v), the estimated shortest path distance to v is correct

• i.e., after update, $v.est = \delta(s, v)$

Bellman-Ford shortest path algorithm



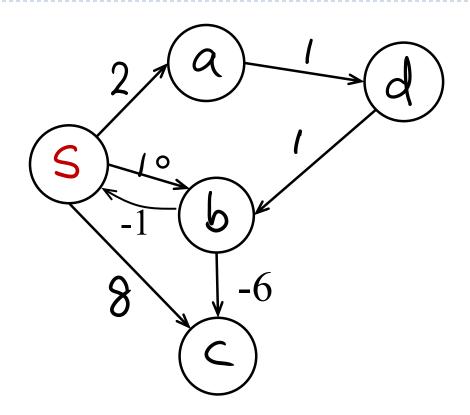
- ▶ [Theorem Update] implies that if we have already computed the shortest path distance from source s for those nodes whose shortest paths from s have k hops, then we can compute those shortest paths with k+1 hops via the update() operations.
 - In particular, let u be the predecessor of v along some shortest path from s to v, and assume u.est is already correct (i.e, u.est = $\delta(s, u)$)
 - then performing update(u,v) will render v.est = $\delta(s, v)$

▶ [Observation]:

Any any moment, if v.est is already correct, then performing further update() on any edge will not change v.est.



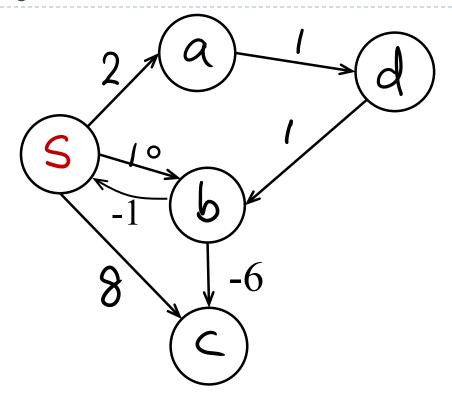
More specifically



- \blacktriangleright At the beginning, we only know that s. est = 0
- ▶ For all other nodes $v \in V$, we set v.est = ∞



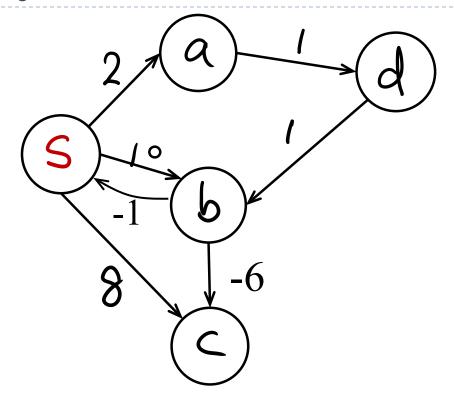
More specifically



- \blacktriangleright Now perform update for all edges in E
- Afterwards, all nodes whose shortest path from s has only one edge are now guaranteed to be estimated correctly!



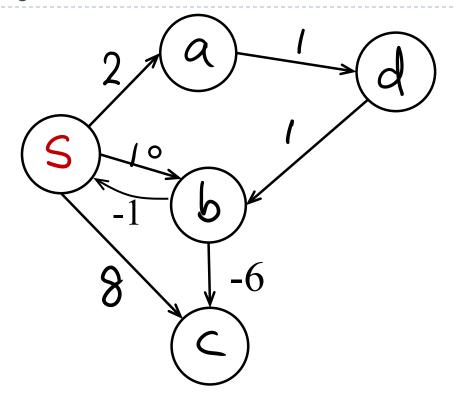
More specifically



- ▶ Now perform update for all edges in E again
- Afterwards, all nodes whose shortest path from s has at most two edges are now guaranteed to be estimated correctly!



More specifically



- ▶ Now perform update for all edges in E repeatedly ...
- Afterwards, all nodes whose shortest path from s has at most more and more edges will be now guaranteed to be estimated correctly



Loop Invariant

- Suppose we perform "update all edges" k times
- Loop invariant:
 - Then all nodes whose shortest path from source s has $\leq k$ edges are guaranteed to be estimated correctly.
- Note that it is possible that some nodes whose shortest path has > k edges are also estimated correctly.



- How many times should we perform "update all edges"
 - in order to guarantee that we find shortest path for all nodes?
- ▶ Note that shortest paths are simple
 - ▶ Hence a shortest path has at most V-1 edges in it
- ▶ Hence after r = V 1 rounds of "update all edges",
 - we can guarantee that the shortest path distances to all nodes in V are estimated correctly.

This is the idea behind Bellman-Ford Algorithm!



Bellman-Ford Algorithm in Python

```
def bellman_ford(graph, weights, source):
    """Assume graph is directed."""
    est = {node: float('inf') for node in graph.nodes}
    est[source] = 0
    predecessor = {node: None for node in graph.nodes}

for i in range(len(graph.nodes) - 1):
    for (u, v) in graph.edges:
        update(u, v, weights, est, predecessor)

return est, predecessor
```

- Setup takes _____ time
- ► Each update takes _____ time
- There are _____ numbers of updates
- Total time complexity is ______

Bellman-Ford Algorithm in Python

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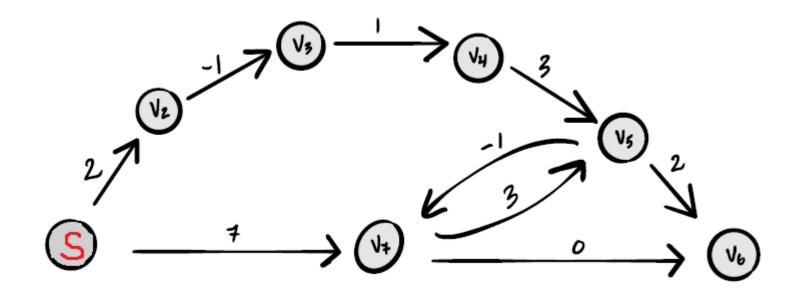
for i in range(len(graph.nodes) - 1):
    for (u, v) in graph.edges:
        update(u, v, weights, est, predecessor)

return est, predecessor
```

- Setup takes $\Theta(V)$ time
- \bullet Each update takes $\underline{\Theta(1)}$ time
- ▶ There are $E \cdot (V-1)$ numbers of updates
- ▶ Total time complexity is $\Theta(V \cdot E)$

Example

- Suppose graph.edges returns edges in the following order:
 - $(v_3, v_4), (s, v_2), (v_2, v_3), (v_7, v_6), (v_5, v_7), (v_7, v_5), (v_4, v_5), (v_5, v_6), (v_5, v_4), (s, v_7)$





Early-stopping and negative cycles



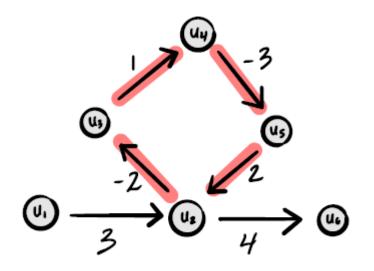
Early-stopping

- ▶ Bellman-Ford may not need to run V-1 iterations
- If there is no distance change after a round, we can stop (called early-stopping)

```
def bellman_ford(graph, weights, source):
    """Early stopping version."""
    est = {node: float('inf') for node in graph.nodes}
    est[source] = 0
    predecessor = {node: None for node in graph.nodes}
    for i in range(len(graph.nodes) - 1):
        any changes = False
        for (u, v) in graph edges:
            changed = update(u, v, weights, est, predecessor)
            any_changes = changed or any_changes
        if not any_changes:
            break
    return est, predecessor
```

Negative Cycles

Recall: if a graph has negative cycle(s), then the shortest paths are not well-defined

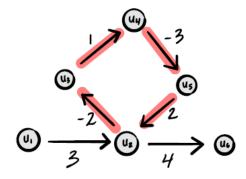




Negative Cycles

Recall: if a graph has negative cycle(s), then the shortest paths are not welldefined

- If a graph does not have any negative cycle, then the estimated distances stop changing after V-1 iterations
 - Why?
- \blacktriangleright But if a graph has negative cycle(s), then some estimated distances continue to decrease even after V iterations





Negative Cycles

- If a graph does not have any negative cycle, then the estimated distances stop changing after V-1 iterations
- \blacktriangleright But if a graph has negative cycle(s), then some estimated distances continue to decrease even after V iterations

- Hence Bellman-Ford can be modified to also detect negative cycles
 - ▶ Run a V iteration of "update all edges"
 - If any estimated distance is still decreasing, a negative cycle exists



Modified Bellman-Ford with early stopping and negative cycle detection

```
def bellman_ford(graph, weights, source):
    """Early stopping version, detects negative cycles."""
    est = {node: float('inf') for node in graph.nodes}
    est[source] = 0
    predecessor = {node: None for node in graph.nodes}
    for i in range(len(graph.nodes)):
        any_changes = False
        for (u, v) in graph.edges:
            changed = update(u, v, weights, est, predecessor)
            any_changes = changed or any_changes
        if not any_changes:
            break
    # this will be True if negative cycles exist
    contains negative cycles = any changes
    return est, predecessor, contains_negative_cycles
```

FIN

