Lecture 13

Dynamic programming III

Chinmay Nirkhe | CSE 421 Spring 2025

Previously in CSE 421…

General dynamic programming algorithm

- **Iterate through subproblems:** Starting from the “smallest” and building up to the “biggest.” For each one:
    - Find the optimal value, using the previously-computed optimal values to smaller subproblems.
    - Record the choices made to obtain this optimal value. (If many smaller subproblems were considered as candidates, record which one was chosen.)
- **Compute the solution:** We have the value of the optimal solution to this optimization problem but we don’t have the actual solution itself. Use the recorded information to actually reconstruct the optimal solution.

General dynamic programming runtime

$$\text{Runtime} = (\text{Total number of subproblems}) \times \begin{pmatrix} \text{Time it takes to solve problems} \\ \text{given solutions to subproblems} \end{pmatrix}$$

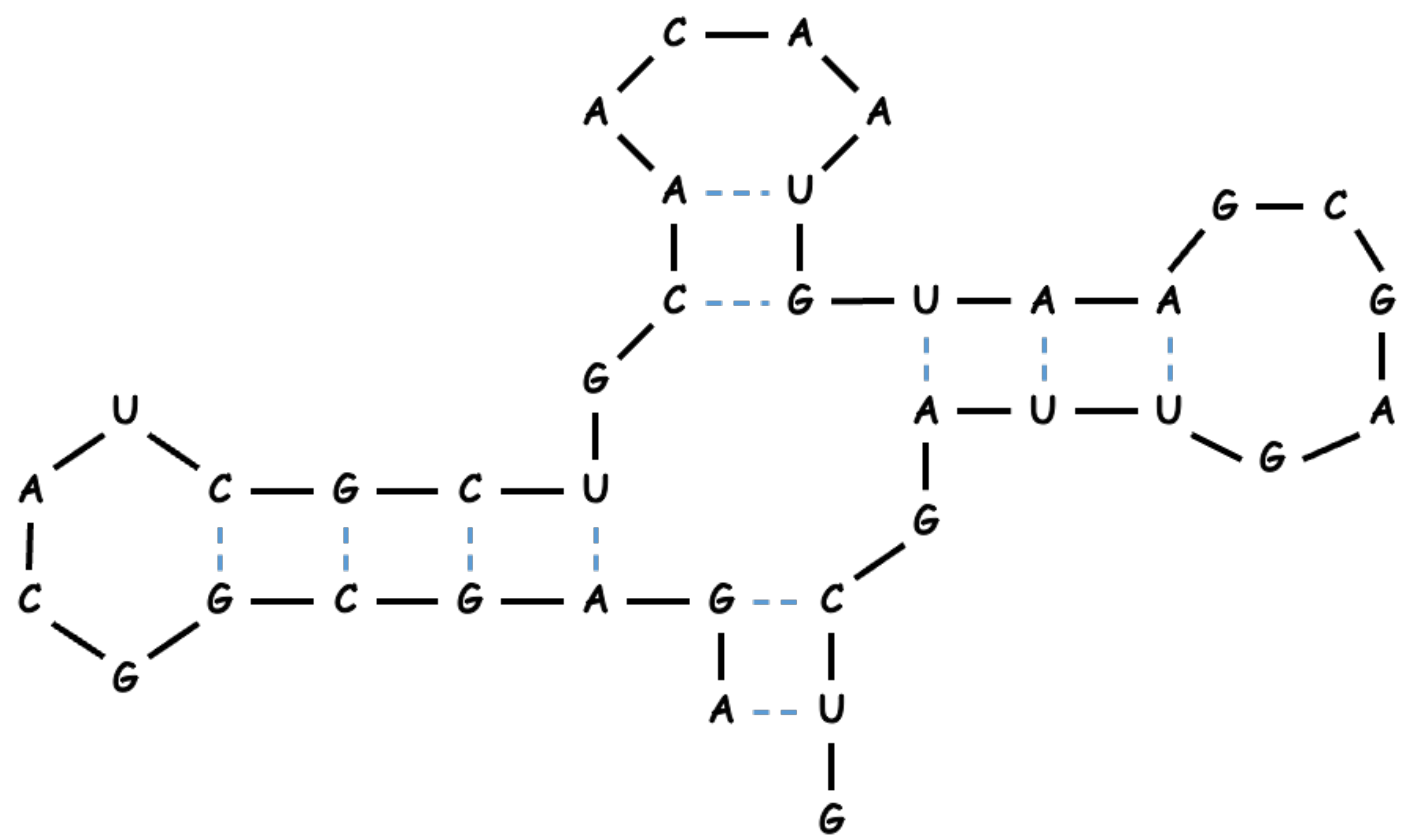
Knapsack overview

- **Input:** n items of integer values v_i and weights w_i and weight threshold W.
- **Input length:** $O(n \log VW)$
- **Output:** optimal $S \subseteq [n]$ maximizing $\text{value}(S)$ s.t. $\text{weight}(S) \leq W$
- **Various algorithms:**
  - Brute force alg: Runtime of $O(n2^n \log VW)$
  - DP alg: Runtime $O(nW \log VW)$ or $O(nV \log VW)$
  - ϵ-approx. alg: Runtime $O\left(\dfrac{n^3 \log VW}{\epsilon}\right)$

Today

RNA secondary structure

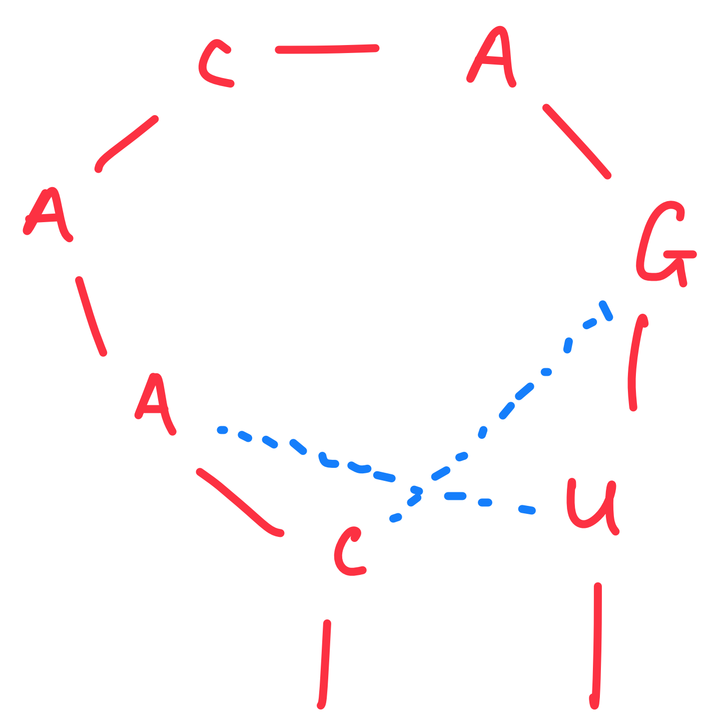
- RNA is expressed as a sequence of nucleotides: a string $B = b_1 \ldots b_n$ where each $b_i \in \{A, C, G, U\}$ for adenine, cytosine, guanine, and uracil.
- RNA tends to not be linear in a molecule and forms **secondary structures**
    - Secondary structures cause the molecule to loop back and forth
    - These are bonds between the base pairs

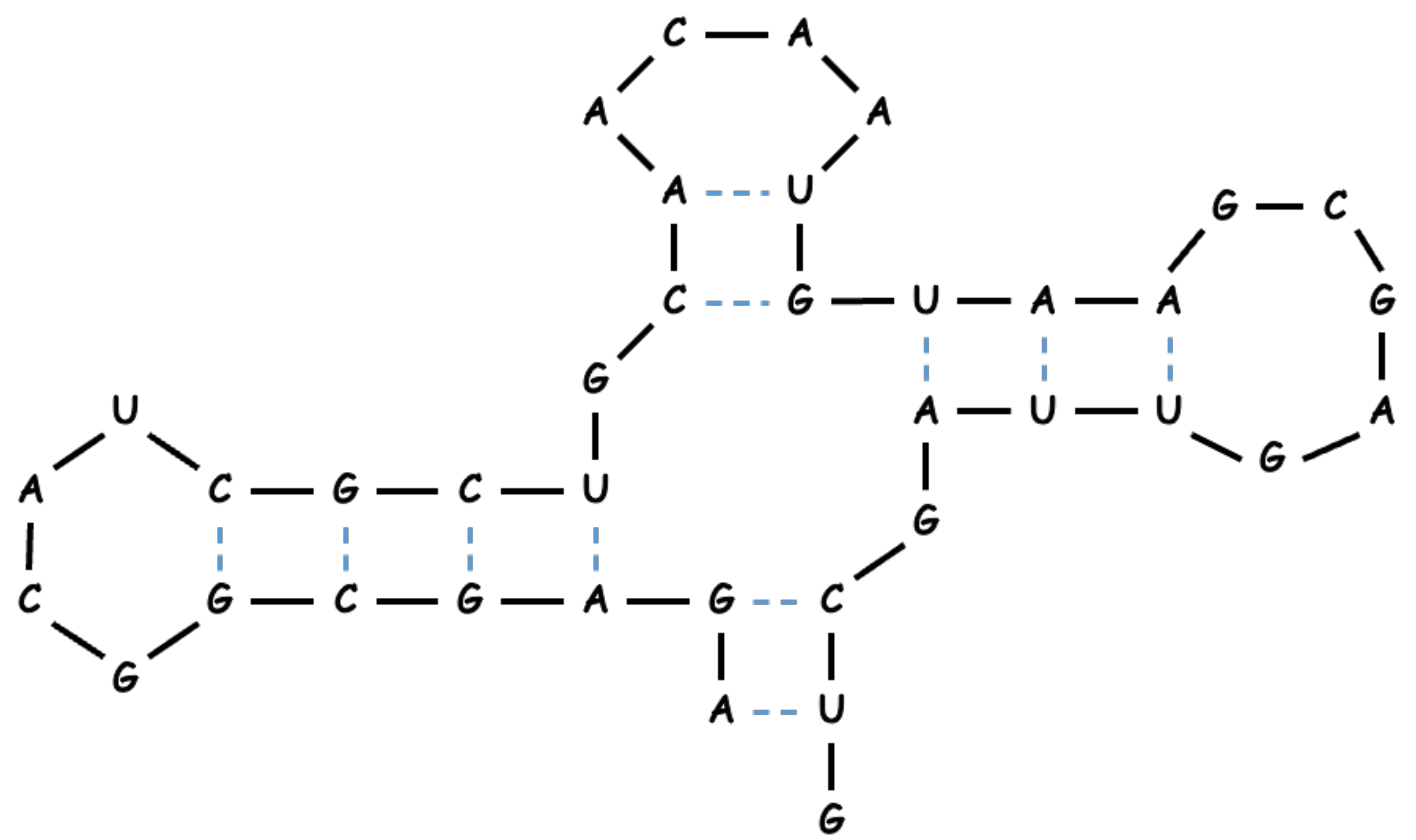


RNA secondary structure hypothesis

- **Definition.** A *secondary structure* for an RNA seq. $B = b_1 \ldots b_n$ is a set of pairs $S = \{(b_i, b_j)\}$ such that
  - WC condition: S is a matching and pairs are Watson-Crick complements i.e. $(b_i, b_j) \in WC := \{(A, U), (U, A), (G, C), (C, G)\}$
  - No sharp bends: $(b_i, b_j) \in S$ only if $4 < |i - j|$
  - Non-crossing: If (b_i, b_j) and (b_k, b_ℓ) then the intervals $[i, j]$ and $[k, \ell]$ are either disjoint or one contains the other.

not allowed:





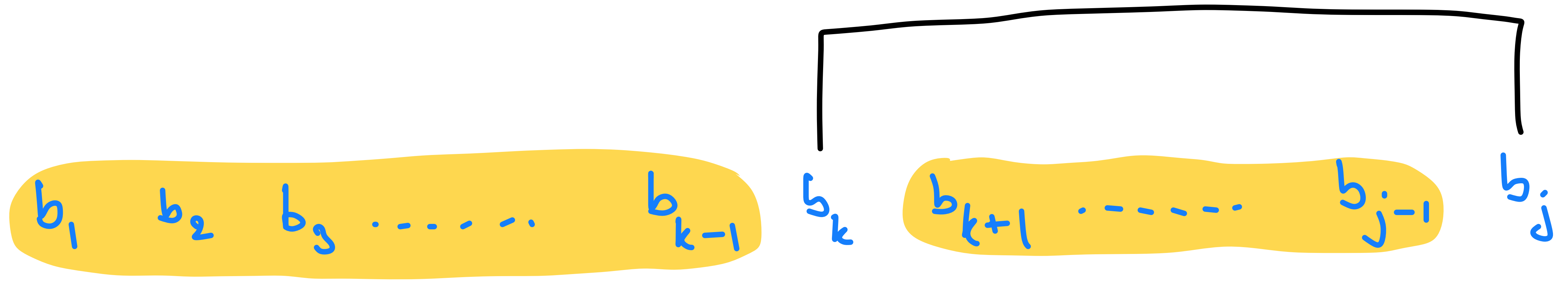
RNA secondary structure problem

- **Input:** an RNA seq. $B = b_1 \ldots b_n$
- **Output:** a secondary structure S of maximal size for B.

- **Dynamic programming attempt 1:** For $1 \leq i \leq j \leq n$ define $S(j)$ as the maximal secondary structure using bases only $b_1, b_2, \ldots, b_j$. Let $f(j) = |S(j)|$.

RNA secondary structure problem

- Consider if in the optimal solution $(b_k, b_j) \in S$



- Splits problem into smaller problems but they aren't subproblems.
- **Problem:** Our choice of subproblem was not expressive enough.

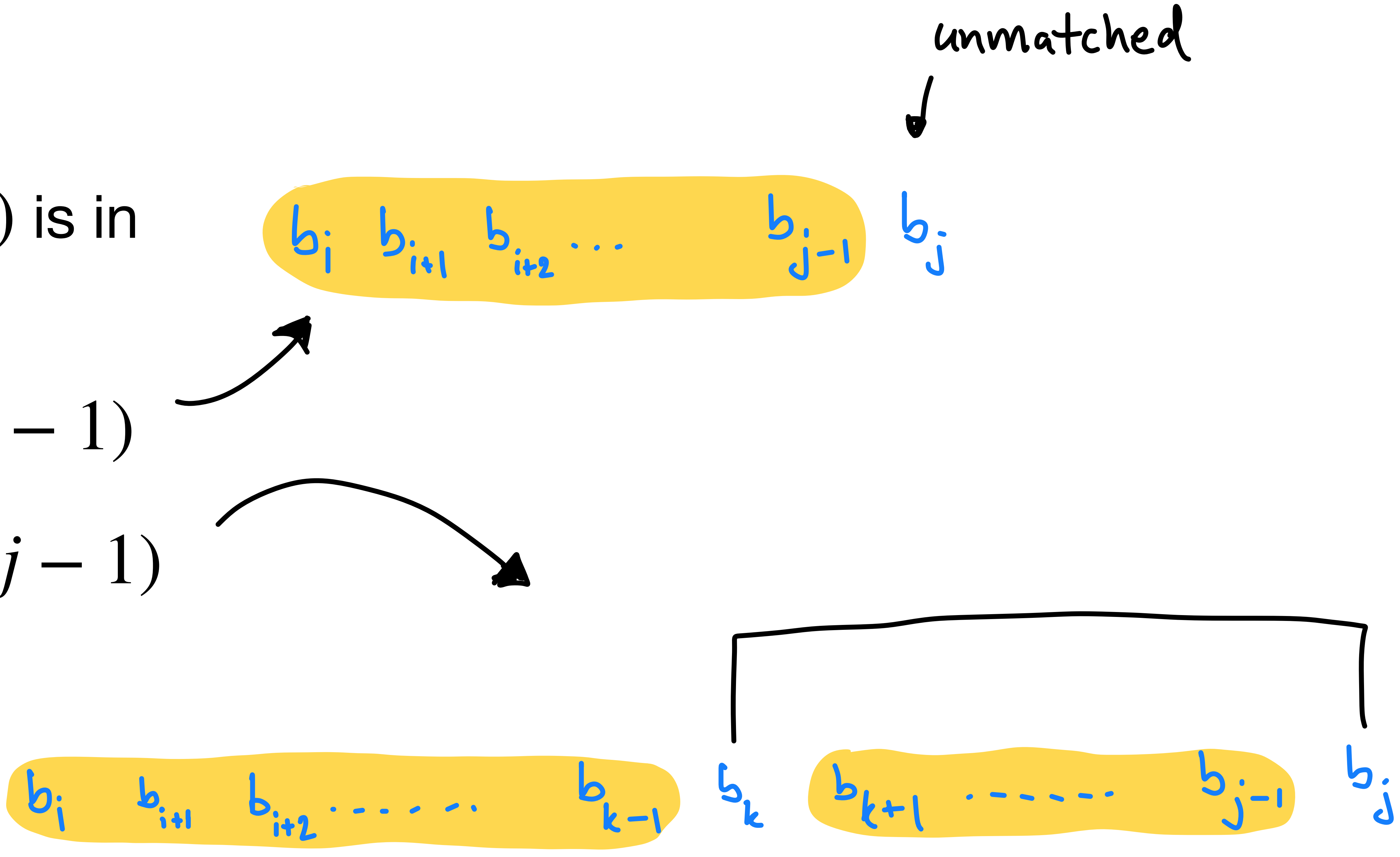
RNA secondary structure problem

- **Input:** an RNA seq. $B = b_1 \ldots b_n$
- **Output:** a secondary structure S of maximal size for B.

- **Dynamic programming intuition:** For $1 \leq i \leq j \leq n$ define $S(i,j)$ as the maximal secondary structure using bases only $b_i, b_{i+1}, \ldots, b_j$. Let $f(i,j) = |S(i,j)|$.

RNA secondary structure DP algorithm

- **Dynamic programming intuition:** For $1 \leq i \leq j \leq n$ define $S(i, j)$ as the maximal secondary structure using bases only $b_i, b_{i+1}, \ldots, b_j$. Let $f(i, j) = |S(i, j)|$.
- **Recursive definition**:
  - In optimal solution, either b_j is not in a SS or (b_k, b_j) is in the SS
  - In first case, $f(i, j) = f(i, j-1)$ and $S(i, j) = S(i, j-1)$
  - In second case, $f(i, j) = 1 + f(i, k-1) + f(k+1, j-1)$
  - Optimal solution can be calculated as a recursive minimization



RNA secondary structure DP algorithm

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  - In second case, $f(i,j) = 1 + f(i,k-1) + f(k+1,j-1)$
- **Observation:** The recursive definition of $f(i,j)$ only depends on $f(i',j')$ for $|j'-i'| < |j-i|$.
  - Therefore, we fill memo from bottom-to-top w.r.t $|j-i|$.

RNA secondary structure DP algorithm

- **Filling memoization tables:**
  - Construct $n \times n$ tables M and f initialized as $\perp$
  - Set $f(i,i) \leftarrow 0$ for all i.
  - For $i \leftarrow 1$ to n and $z \leftarrow 1 \leftarrow n - i$ iterate over length of interval z
    - Let $j \leftarrow i + z$
    - valid partner k w.r.t. WC and sharp corner conditions
    - Compute $V \leftarrow \min_{k \in \{i,\ldots,j-5\} \wedge (b_j,b_k) \in WC} 1 + f(i,k-1) + f(k+1,j-1)$ and let k be its argmin.
    - If $V > f(i,j-1)$, set $f(i,j) \leftarrow V$ and set $\underbrace{M(i,j) \leftarrow k}$
    - Else, set $f(i,j) \leftarrow V$ and keep $\underbrace{M(i,j) = \perp}$.

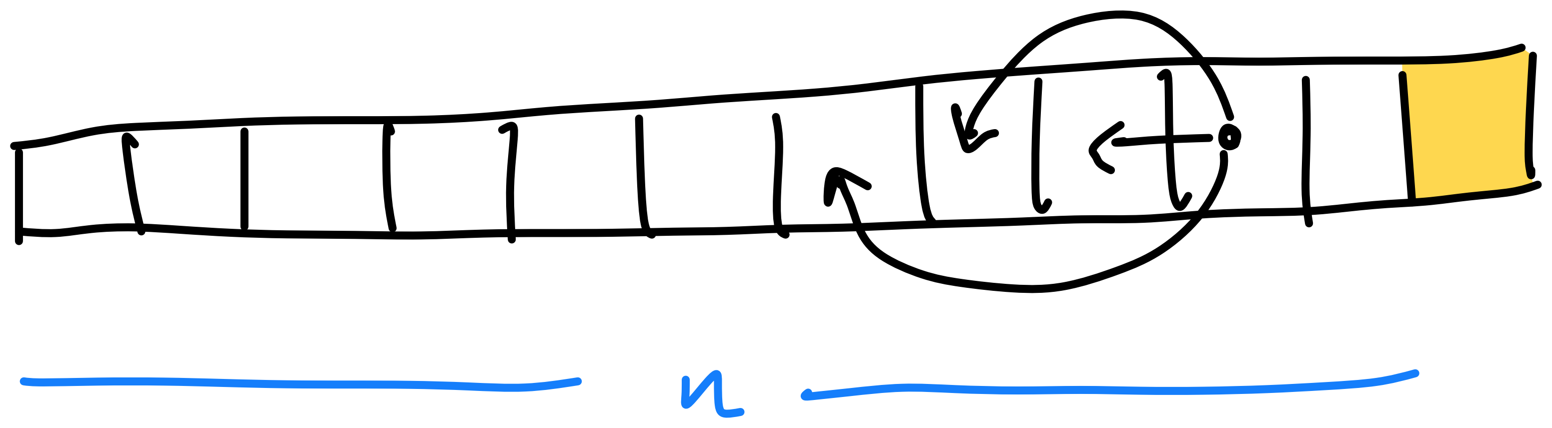
record secondary structure in optimal sol.

RNA secondary structure DP algorithm

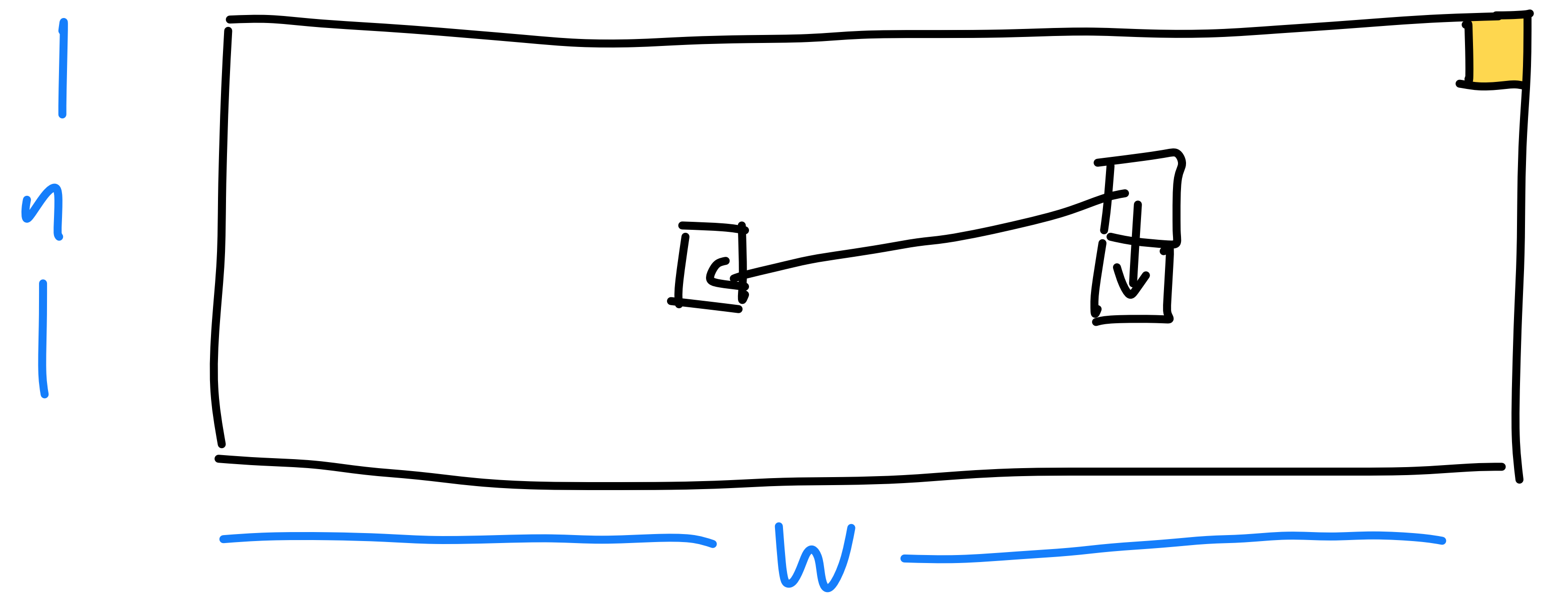
- **Computing optimal secondary structure:**
- If $M(i,j) = k$ this means that $(b_k, b_j) \in S$. Else j is not included in S.
- To calculate optimal secondary structure run $\text{Print}(1,n)$ where
- $\text{Print}(i,j)$**:**
  - If $M(i,j) \leftarrow k$ output $(k,j) \cup \text{Print}(i,k-1) \cup \text{Print}(k+1,j-1)$
  - Else, output $\text{Print}(i,j-1)$
- Can be made to run faster in practice using DFS or BFS instead of recursion
- **Runtime:** $O(n^2)$ sized table with each recursive computation taking $O(n)$ time. Print runs in $O(n)$ time after the table is computed. Total runtime: $O(n^3)$.

Dynamic programming patterns

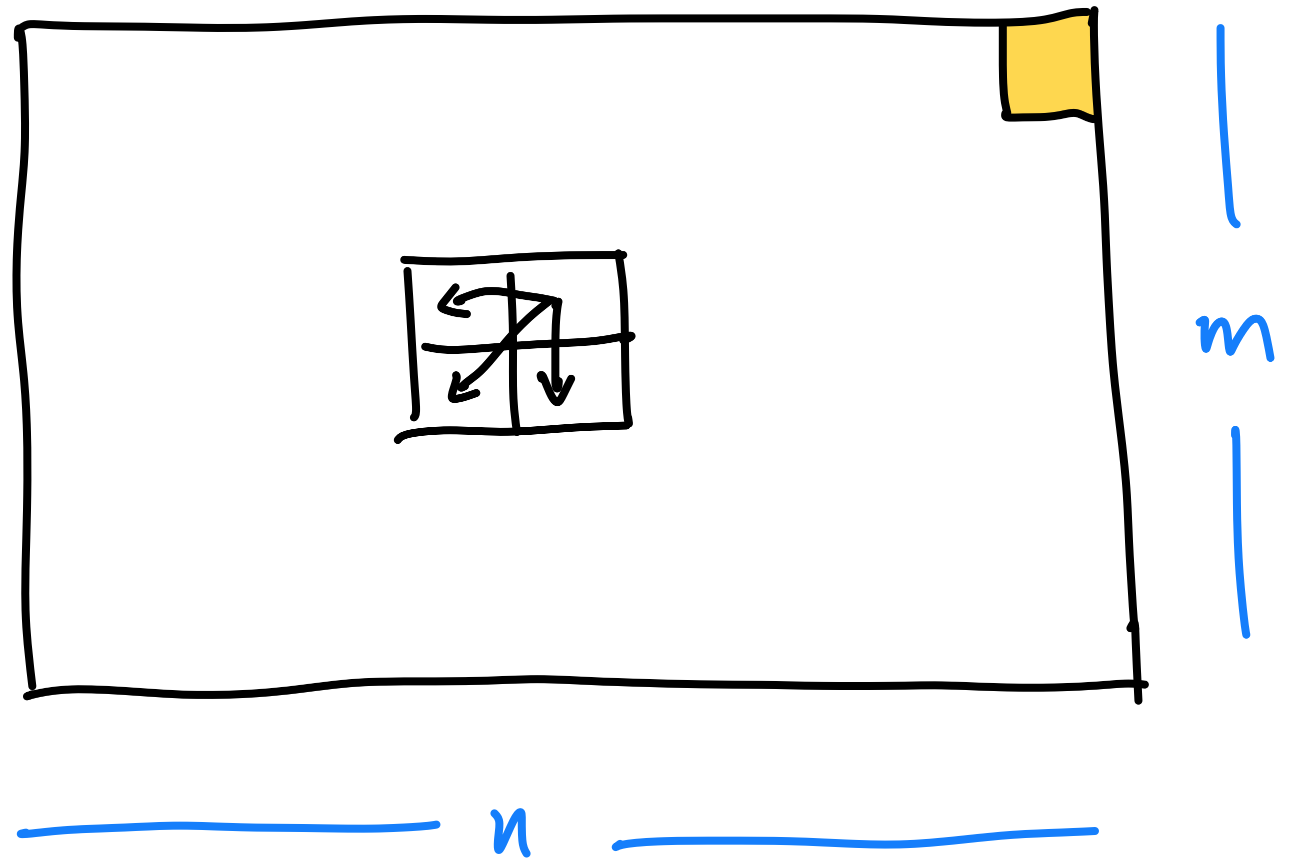
Tribonacci



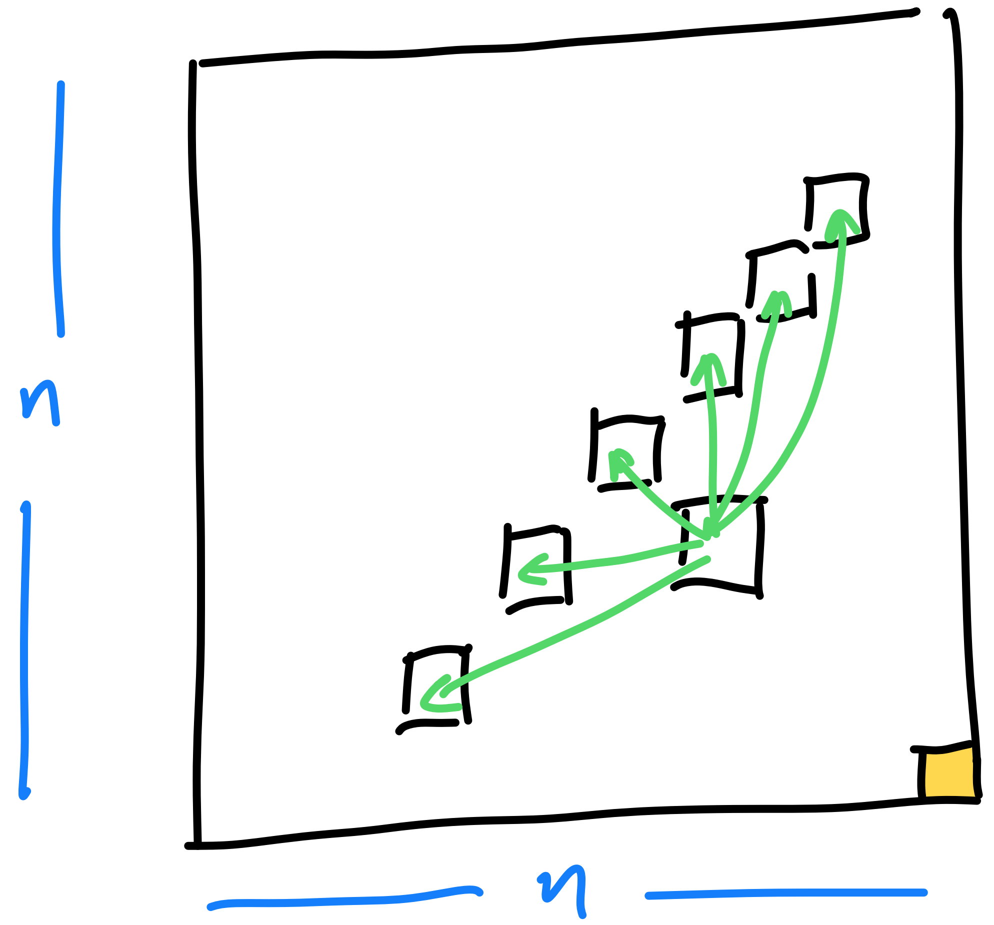
Knapsack



Edit distance



RNA second sequence



O(n) recursive calls per entry

Top-down vs bottom-up DP algorithms

- So far we have seen that the recursive subproblems in DP algorithms are always smaller. Examples
  - Knapsack: $f(n, W')$ depends on $f(n-1, W'')$ for $W'' \leq W'$
  - RNA SS: $f(i, j)$ depends on $f(i', j')$ where $|j' - i'| < |j - i|$
- Yields a "bottom-up" ordering for filling the memoization table
- Instead we could fill up the table "top-down"

Top-down vs bottom-up DP algorithms

- In a “top-down” DP algorithm $f(x)$
  - Conclude that $f(x)$ can be defined recursively based on $f(y_1), f(y_2), \ldots f(y_k)$
  - For each y_j, check if $f(y_j)$ has been previously calculated
    - If yes, use the value of $f(y_j)$
    - If not, recursive compute $f(y_j)$
- Overall, runtime is asymptotically the same! Each square of the memo is only computed once.

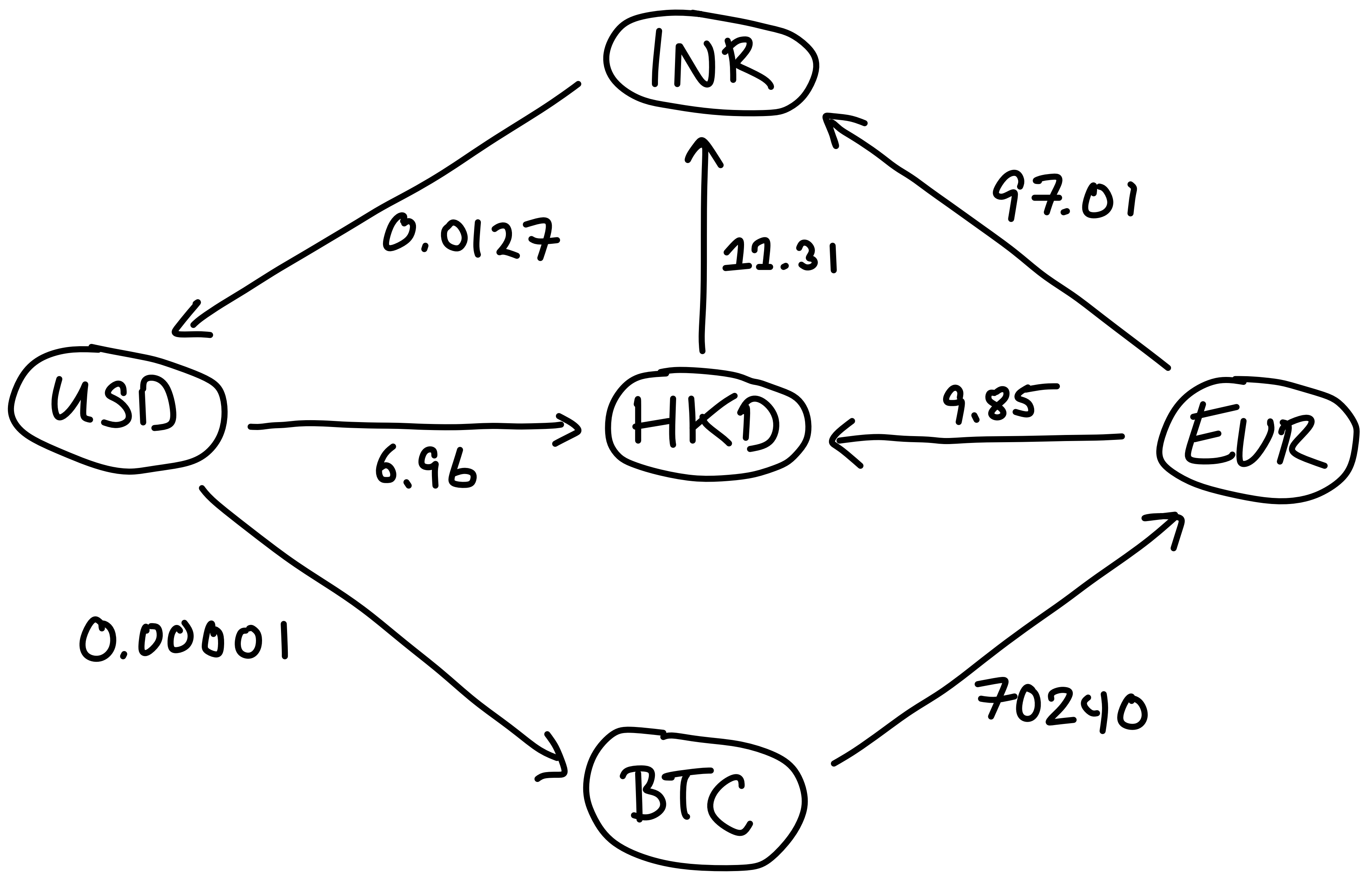
Top-down vs bottom-up DP tradeoffs

- In top-down approaches, not all squares may get calculated
  - Can yield constant factor savings in terms of runtime
- However, the recursion stack usually scales poorly in top-down approaches
  - For example, in Tribonacci, recursion stack would be $\Omega(n)$ in depth
  - Recursion stack is often in computer's memory while data being manipulated is expressed on the hard drive
  - Can yield memory overflow errors if not carefully programmed
- Top-down is better when the order of filling out squares isn't well defined
  - Occurs in graph DP algorithms like Bellman-Ford which we see soon
  - In such cases, a more sophisticated analysis is needed to argue that recursive defs. are not cyclical

Graph dynamic programming

Currency exchange

- USD to BTC: 0.00001
- BTC to EUR: 70,240
- INR to USD: 0.0127
- EUR to INR: 97.01
- EUR to HKD: 9.85
- HKD to INR: 11.31
- USD to HKD: 6.96



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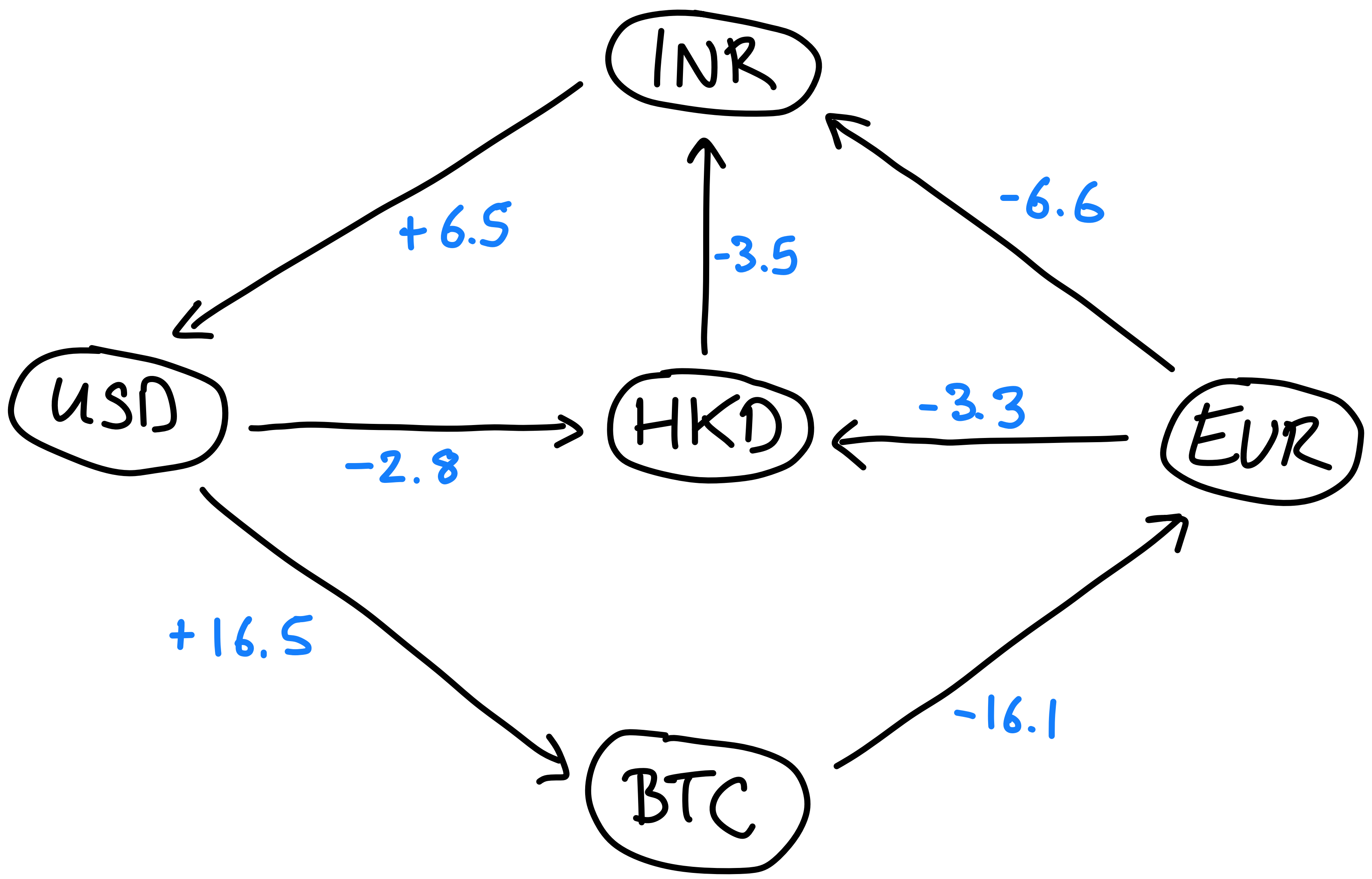
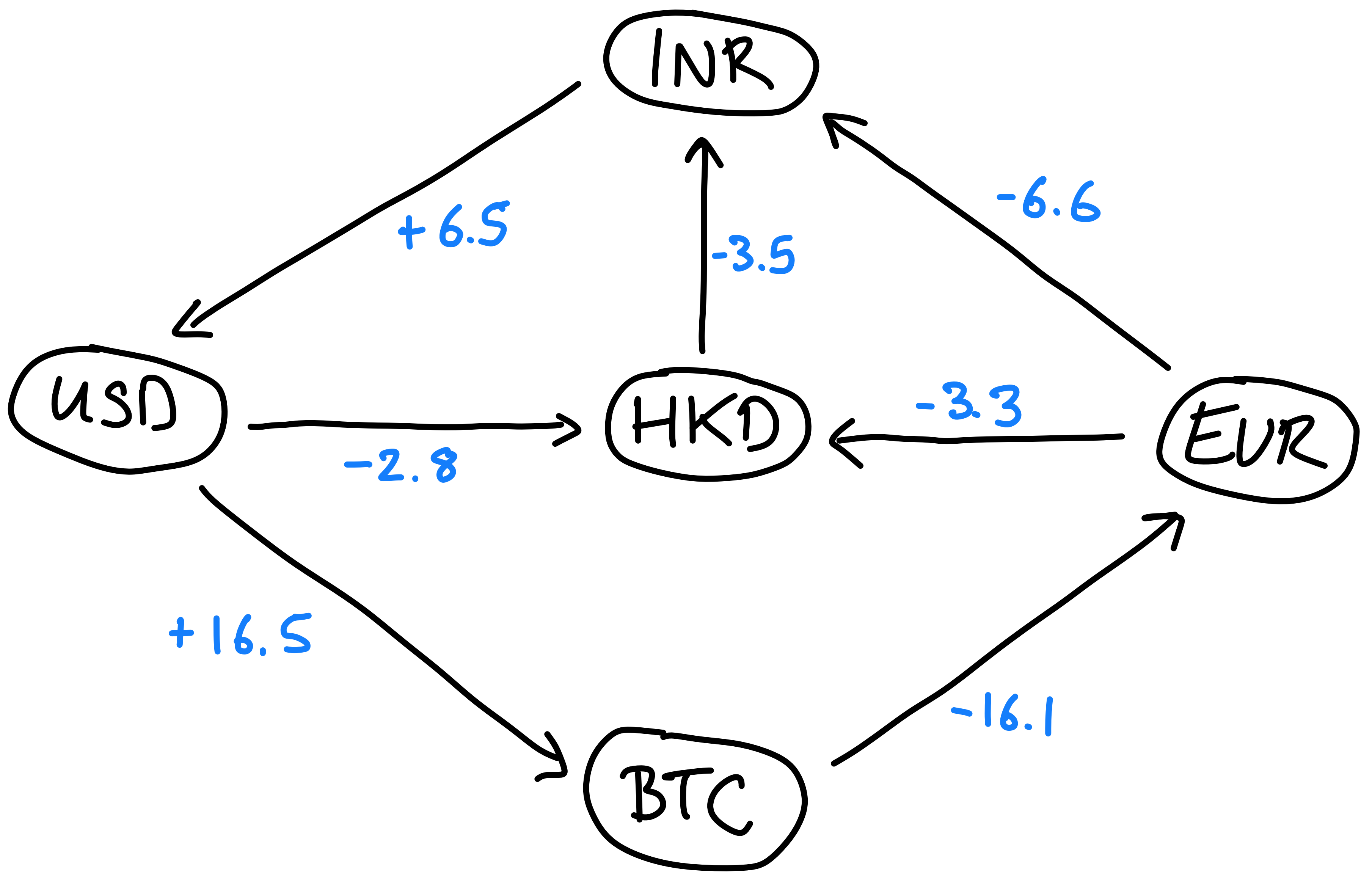
Set edge weight to $\log_2(1/r) = -\log_2(r)$



Currency exchange

Set edge weight to $\log_2(1/r) = -\log_2(r)$

- A path $p : u \rightsquigarrow v$ of net weight w implies a currency conversion from 1 unit of u to 2^{-w} units of v
- Finding a path of least weight from u to v yields the best seq. of currency exchanges
- Direct conversion of USD to HKD yields $2^{2.8}$ HKD per USD



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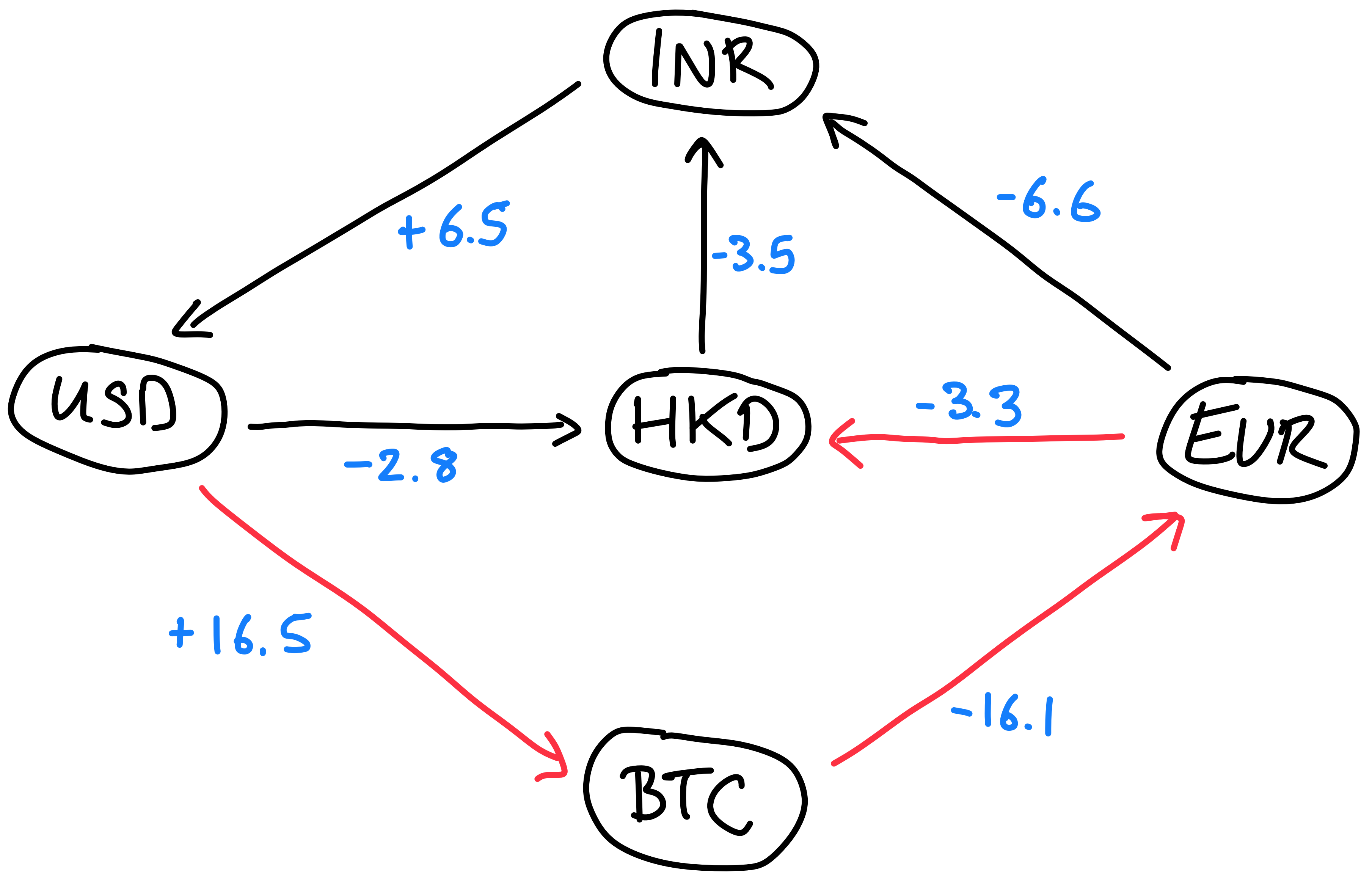
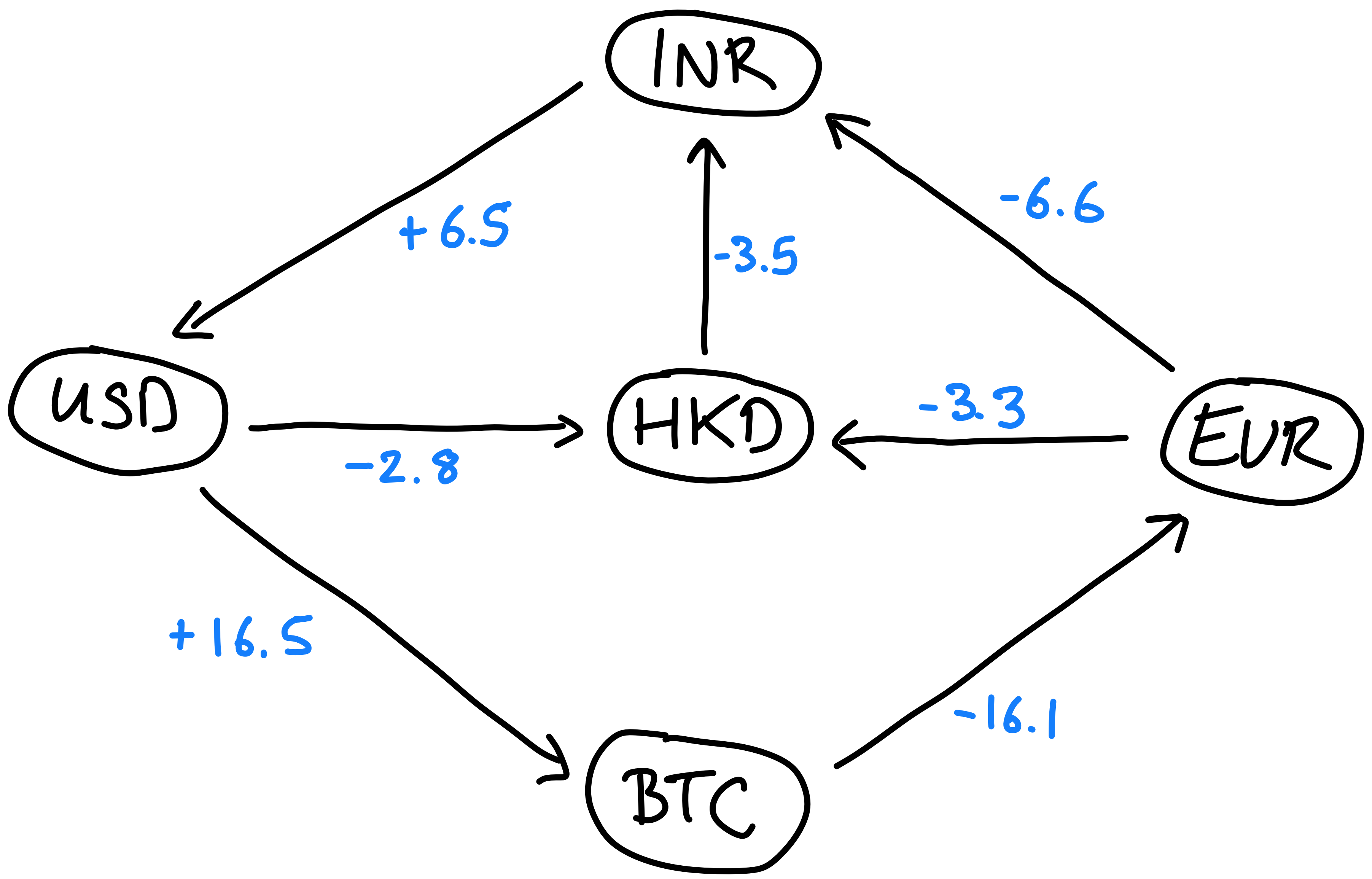
- USD→BTC→EUR→HKD yields $2^{-(16.5-16.1-3.3)} = 2^{2.9}$ HKD per USD



Currency exchange

Set edge weight to $\log_2(1/r) = -\log_2(r)$

- What happens if HKD to INR rate changes from $2^{3.5}$ to $2^{4.0}$?



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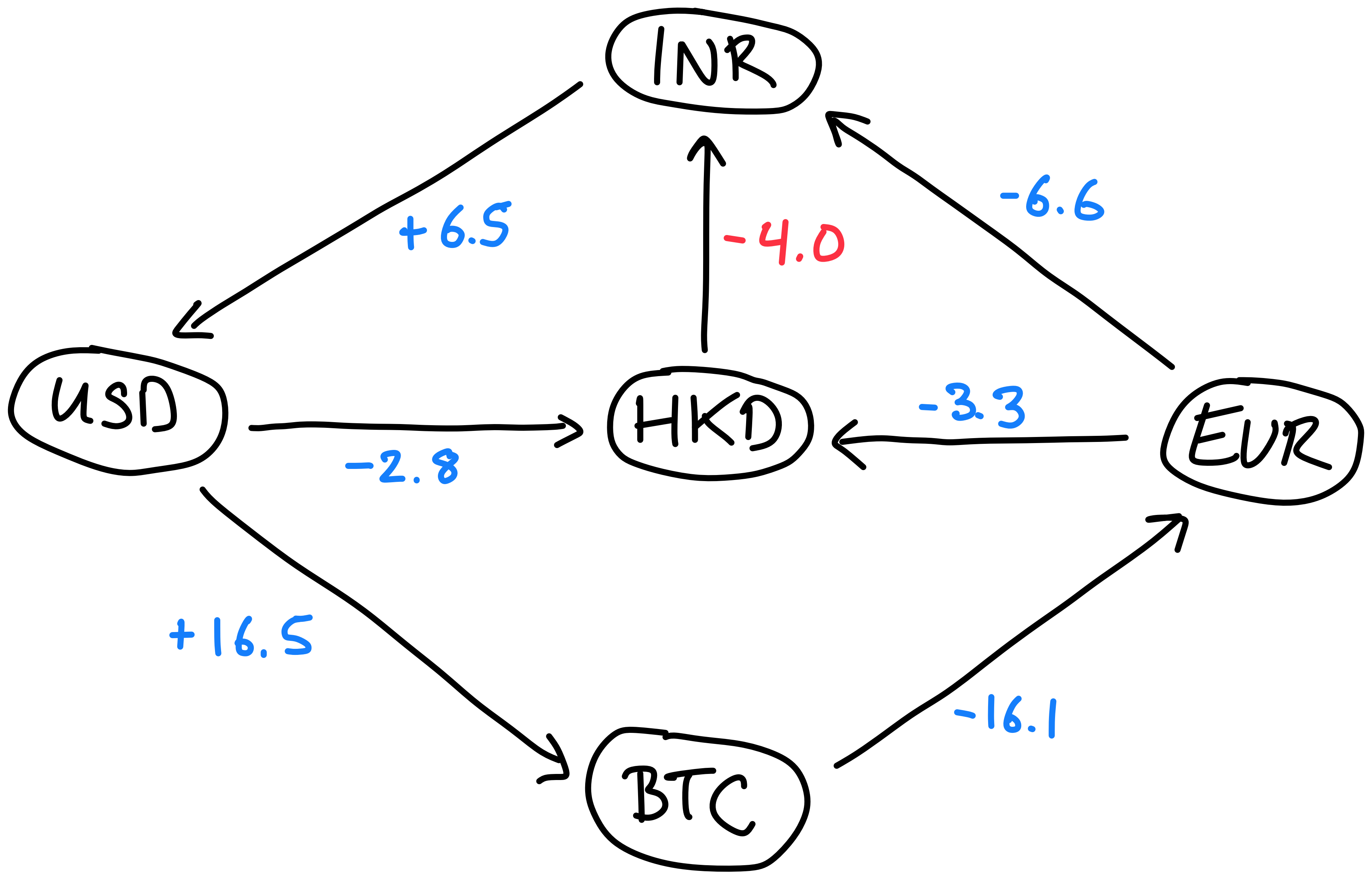
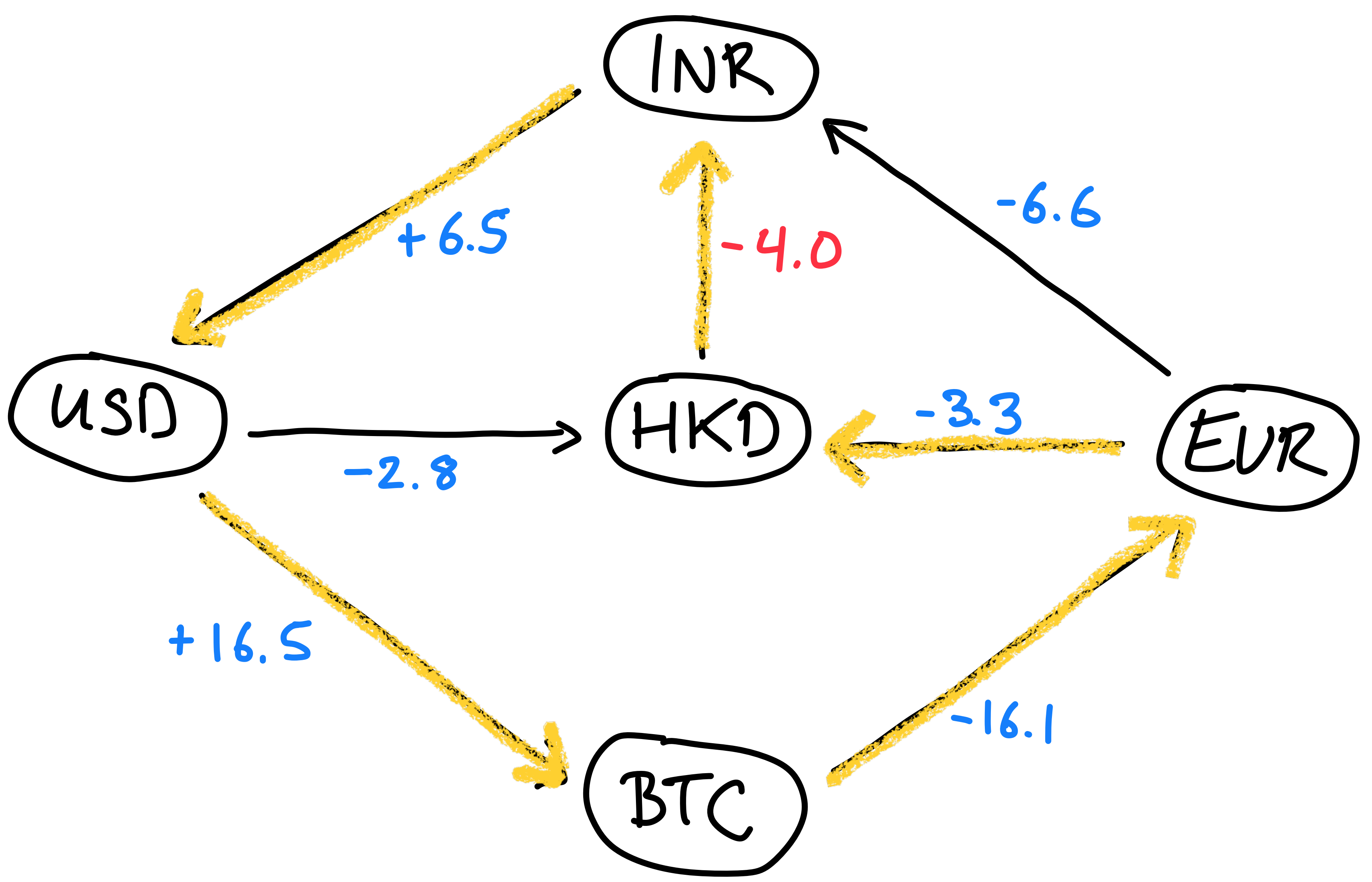


Currency exchange

Set edge weight to $\log_2(1/r) = -\log_2(r)$

- Consider the highlighted path from USD to USD:
- Converts 1 USD to $2^{0.8} > 1$ USD
- Constitutes a **negative cycle** in the graph
- In the currency exchange problem, negative cycles represent **arbitrage**
- Since there is a negative cycle, any currency can be converted into any other for arbitrarily cheap as the graph is strongly connected



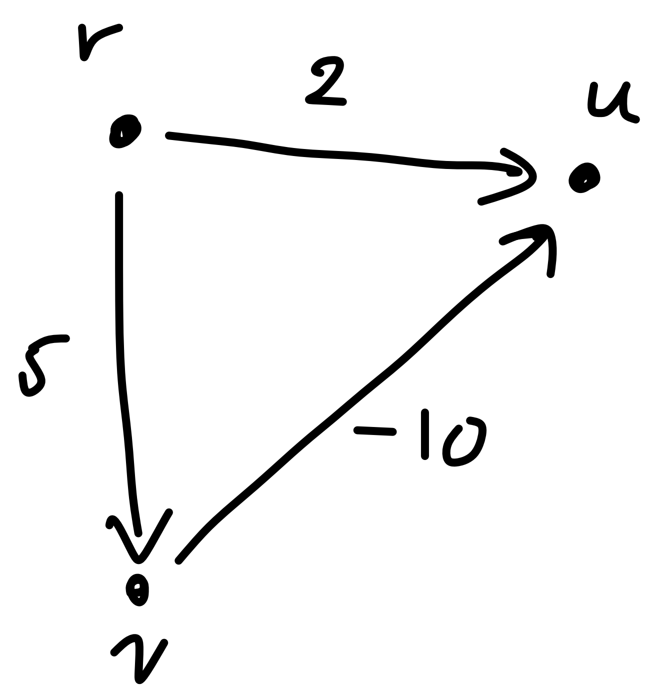
Negative weights shortest paths

- **Input**: A directed graph $G = (V, E)$ with weights $w : E \to \mathbb{R}$ and a vertex r
- **Output**: For every vertex v, the distance of the **lightest** directed path $r \rightsquigarrow v$ where a path's weight is the sum of its weights

- Why not just run Dijkstra's?
- Dijkstra's will incorrectly calculate distances when negative weights are involved

Negative weights shortest paths

- **Dijkstra's property:** Once a vertex v is visited, the distance $d(r, v)$ never needs updating again
    - This does not hold with negative weights
    - Need a slower but more careful algorithm that accounts for negative weights
- In this example,
    - Dijkstra's would set distance of u as 2 with path $r \to v$ in its first step
    - However, need to update the distance of u to -5 after v is visited.



Negative weights shortest paths

Applications

- Trade routes: each vertex is a commodity and edge $x \to y$ of weight w means 1 unit of x can be exchanged for 2^{-w} units of y
  - Multiplicative gains can be converted to linear gains by taking logarithms
  - Negative weights imply multiplicative losses
- Chemical networks: cost represent the excess energy required or **released** when a transformation is made
- Subsidies offered by governments for certain trades being performed
  - Example, US Govt. subsides flights from Portland, Oreg. to Pendleton, Oreg. to incentive airlines to fly to this market. (Annually, about $4 million for just this route)
  - How can an airline design its route network to maximize revenue in light of subsidies?

The Bellman-Ford algorithm

- Dijkstra's is a **greedy** algorithm and suffices to calculate shortest/lightest paths when all weights are non-negative
  - Distances will never need to be recalculated once set
- Bellman-Ford is a **dynamic programming** algorithm for computing shortest path in directed graphs
  - Will run slower than Dijkstra's: $O(mn)$ time versus $O(n+m)$ time
  - Will involve "resetting" distances as the algorithm goes along
  - Bellman-Ford will detect **negative cycles** as shortest paths are undefined if there are negative cycles

Failed attempt #1

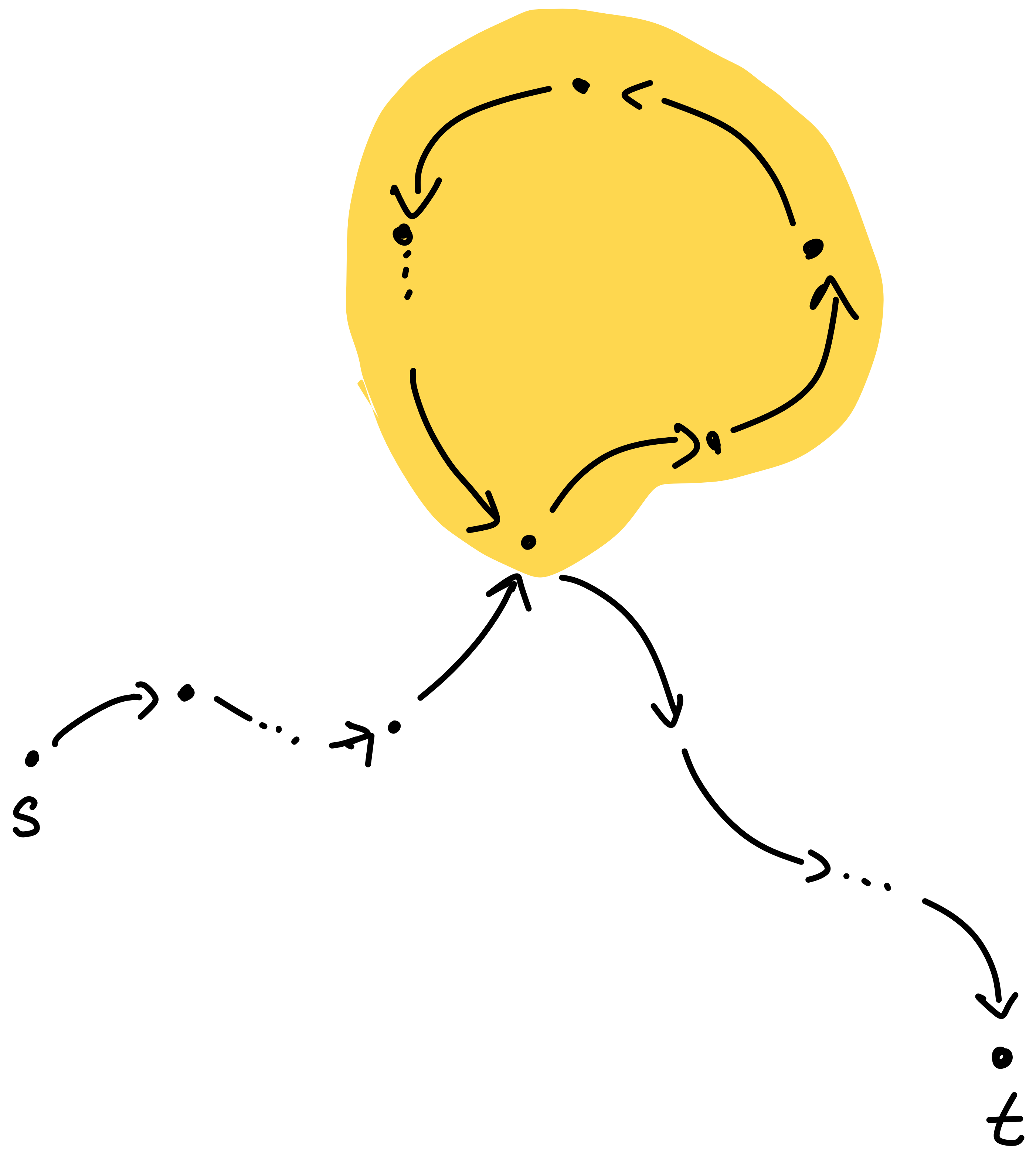
- If a graph has negative weights, let $w_{\min} = \min_{e \in E} w(e)$
- What if we adjusted every edge weight to $w'(e) = w(e) - w_{\min} \geq 0$?
- Can we just run standard Dijkstra's on the adjusted graph?
- **No**. Path weights adjust variably.
  - $w'(p) = w(p) - w_{\min} \cdot |\text{\# of edges in } p|$

Negative weight shortest path

- **Input:** Directed graph $G = (V, E)$ and weights $w : E \to \mathbb{R}$ and a vertex t
- **Output:** For all vertices s, the weight of the shortest path $d(s, t)$
- Note, we are considering shortest paths with respect to the endpoint t
- Its easy enough to convert it to an algorithm for shortest paths with respect to the source

Negative weight shortest path

- **Input:** Directed graph $G = (V, E)$ and weights $w : E \to \mathbb{R}$ and a vertex t
- **Output:** For all vertices s, the weight of the shortest path $d(s, t)$
- **Observation:** If a path $s \rightsquigarrow t$ contains a negative weight cycle, then a shortest path doesn't exist.
- **Observation:** If G has no negative cycles then the shortest path $s \rightsquigarrow t$ is of length $\leq n - 1$.
- **Proof:** A path of length $\geq n$ exists, it has a repeated vertex (i.e. a cycle). That cycle has weight ≥ 0, so removing it only decreases weight. Repeat till path is of length $\leq n - 1$.



Dynamic programming algorithm

- **Definition.** For $i \in \{0,\ldots,n-1\}, s \in V$, let $d(i,s)$ be the length of the *shortest path* $s \rightsquigarrow t$ consisting of *at most* i edges
    - Case 1: The shortest path uses $\leq i-1$ edges. Then

      $$d(i,s) = d(i-1,s)$$

    - Case 2: The shortest path uses exactly i edges. Let u be the first the first vertex on the path. Then

      $$d(i,s) = w(s,u) + d(i-1,u)$$

Dynamic programming algorithm

- **Definition.** For $i \in \{0, \ldots, n-1\}$, $s \in V$, let $d(i, s)$ be the length of the *shortest path* $s \rightsquigarrow t$ consisting of *at most* i edges
- **DP recursive definition**:

$$d(i,s) = \begin{cases} 0 & \text{if } i = 0 \text{ and } s = t \\ \infty & \text{if } i = 0 \text{ and } s \neq t \\ \min\left\{ d(i-1,s),\ \min\limits_{u:s\to u} w(s,u) + d(i-1,u) \right\} & \text{otherwise} \end{cases}$$

Dynamic programming implementation

(Assuming no negative cycles)

- **Table generation:**
  - Generate table d of size $(n-1) \times n$ and table next of size n
  - Set $d(0,s) \leftarrow \infty$ for $s \neq t$ and $d(0,t) \leftarrow 0$
  - For $i \leftarrow 1$ to n and edge $(s \rightarrow u) \in E$
    - If $w(s,u) + d(i-1,u) < d(i-1,s)$,
      - Set $d(i,s) \leftarrow w(s,u) + d(i-1,u)$ and $\mathrm{next}(s) \leftarrow u$
      - Else, set $d(i,s) \leftarrow d(i-1,s)$.
- **Path recovery:** Follow $\mathrm{next}(\,\cdot\,)$ from s until it reaches t.

Space saving techniques

- The end result is a DAG mapping paths from every vertex s to the sink t
- The entries of $\mathrm{next}(\cdot)$ list the edges in the path
- $d(i, s)$ only depends on entries $d(i-1,\cdot)$. Rows $i-2,\ldots,1$ can be discarded.

Better DP implementation

(Assuming no negative cycles)

- **Table generation:**
  - Generate table d of size n and table next of size n
  - Set $d(s) \leftarrow \infty$ for $s \neq t$ and $d(t) \leftarrow 0$
  - For $i \leftarrow 1$ to n and edge $(s \rightarrow u) \in E$
    - If $w(s,u) + d(u) < d(s)$,
      - Set $d(s) \leftarrow w(s,u) + d(u)$ and $\mathrm{next}(s) \leftarrow u$
- **Path recovery:** Follow $\mathrm{next}(\,\cdot\,)$ from s until it reaches t.

Even more trimming (in practice)

- If $d(u)$ doesn't decrease in round i, then we don't need to consider any edges $s \to u$ in round $i+1$ as the best paths through u have already been considered
- Keep a list Q of vertices updated in the previous round and only update edge $s \to u$ if u was in Q

Even better DP implementation

(Assuming no negative cycles)

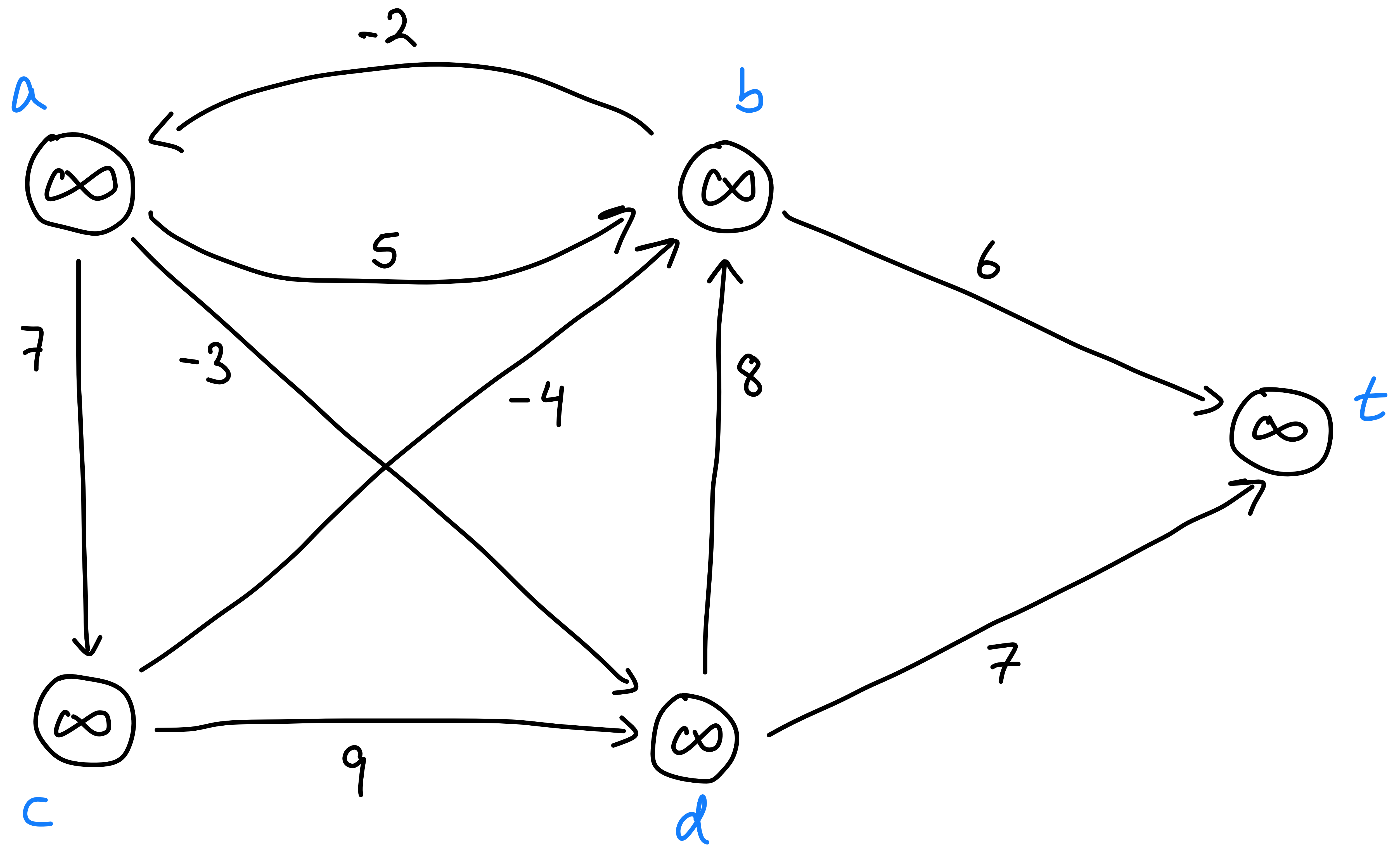
- Compute the reverse adjacency list: For every $u \in V$, $\text{pre}(u) = \{s : s \to u\}$.
- Generate tables d, next of size n with $d(s) \leftarrow \infty \ \forall \ s \neq t$ and $d(t) \leftarrow 0$
- Initialize counter $i \leftarrow 0$ and generate a queue $Q \leftarrow \{t, \perp\}$.
- While $i < n$
  - Pop u off the queue Q.
  - If $u = \perp$, increment $i \leftarrow i + 1$ and push $\perp$ to Q.
  - Else, for each $s \in \text{pre}(u)$,
    - If $w(s,u)+d(u) < d(s)$, set $d(s) \leftarrow w(s,u)+d(u)$ and $\text{next}(s) \leftarrow u$
    - Push s into queue Q.

everytime $\perp$ is seen in queue,
we've done one iteration of BF.
We need to do $n-1$.

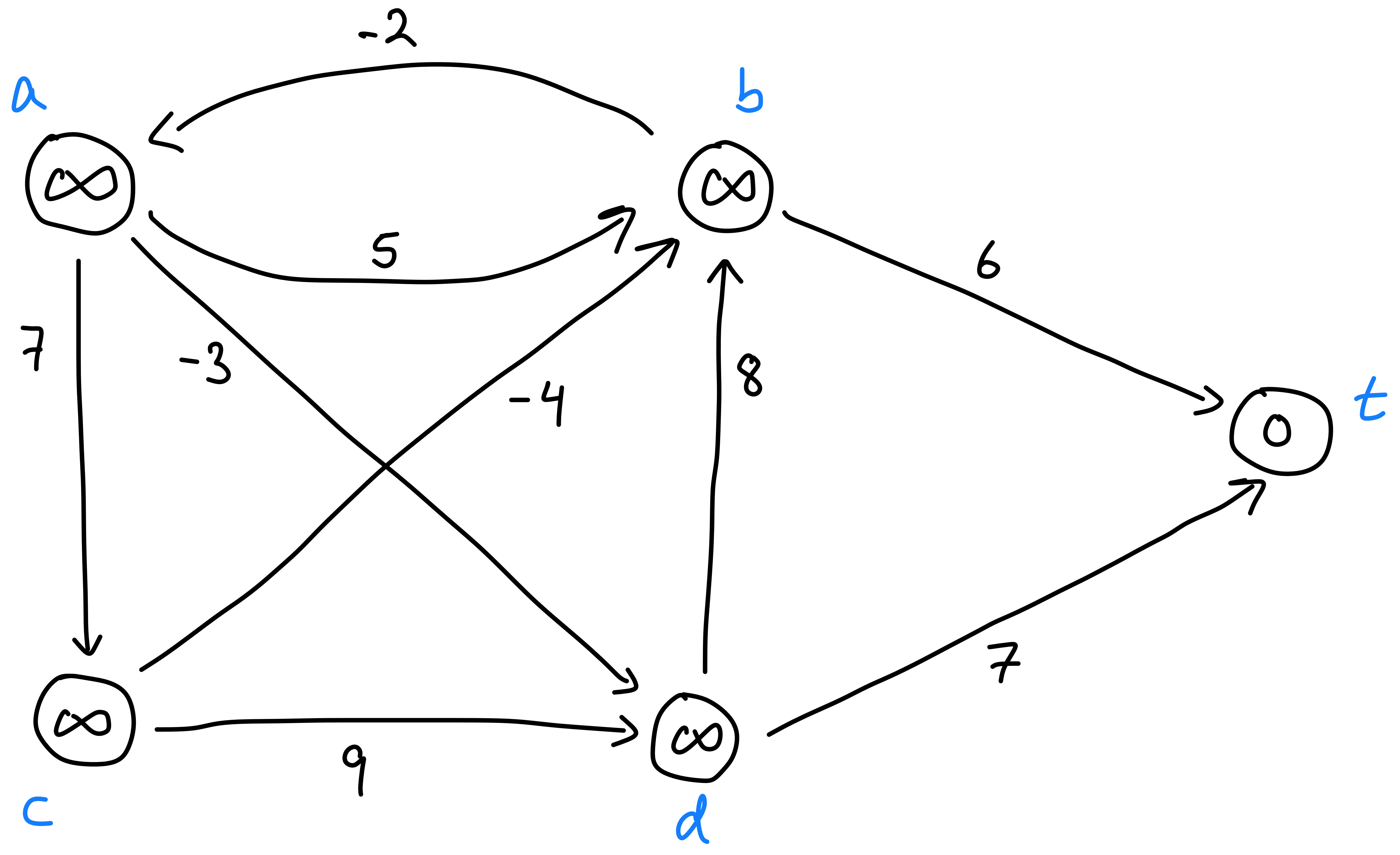
Bellman-Ford properties

- **Theorem**: Throughout the algorithm, $d(s)$ is the length of some path and that path has weight less than the lightest path of $\leq i$ edges after i rounds of updates
- **Impact:** Space decreases to $O(n+m)$ but runtime is still $O(nm)$ in the worst case. In practice, the runtime is much faster!
- **New:** [S.Rao, '25] Bellman-Ford in time $O(n^{2/3}m)$, first major upgrade in half a century

Bellman-Ford example



Bellman-Ford example

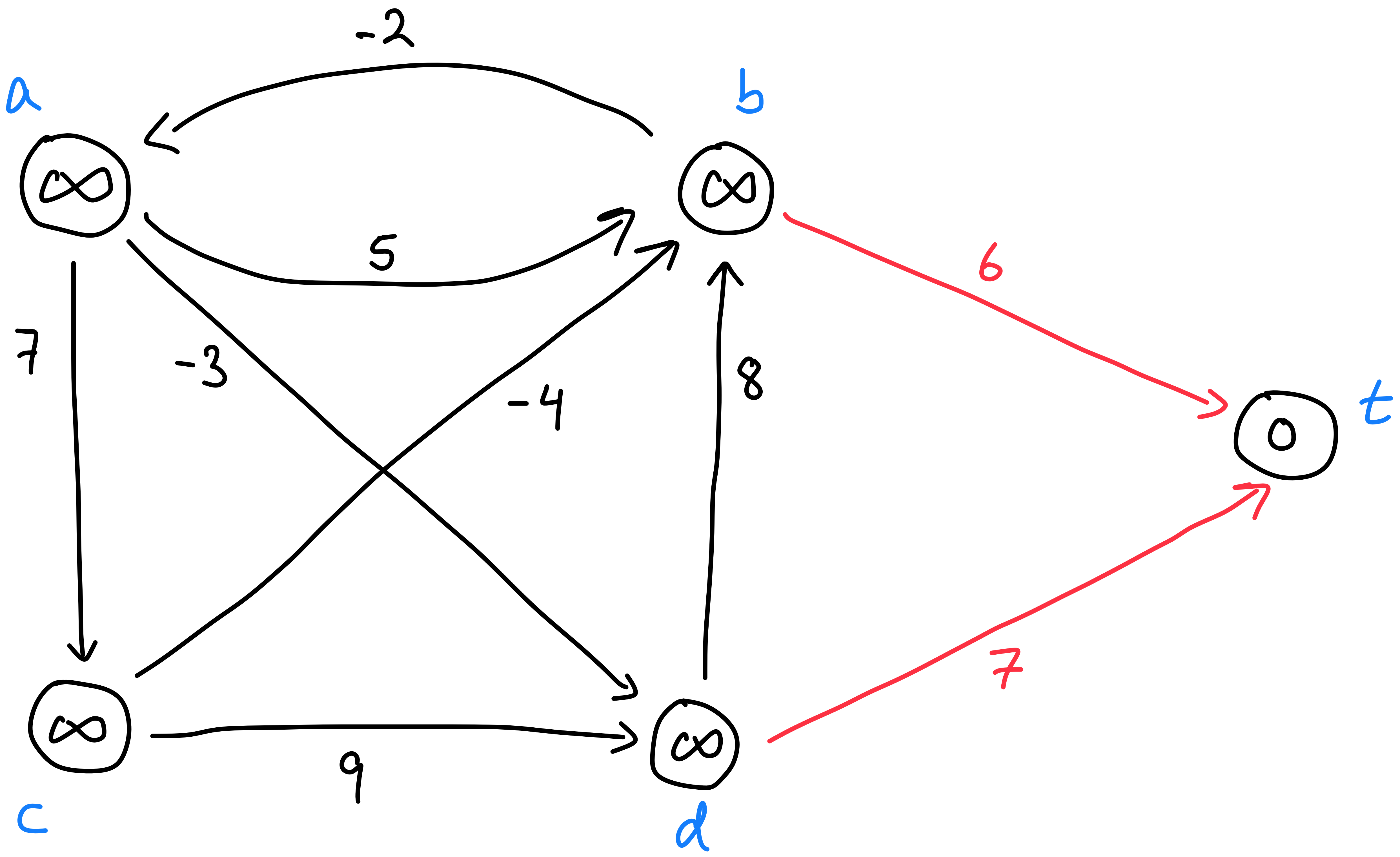


Queue

t

⊥

Bellman-Ford example



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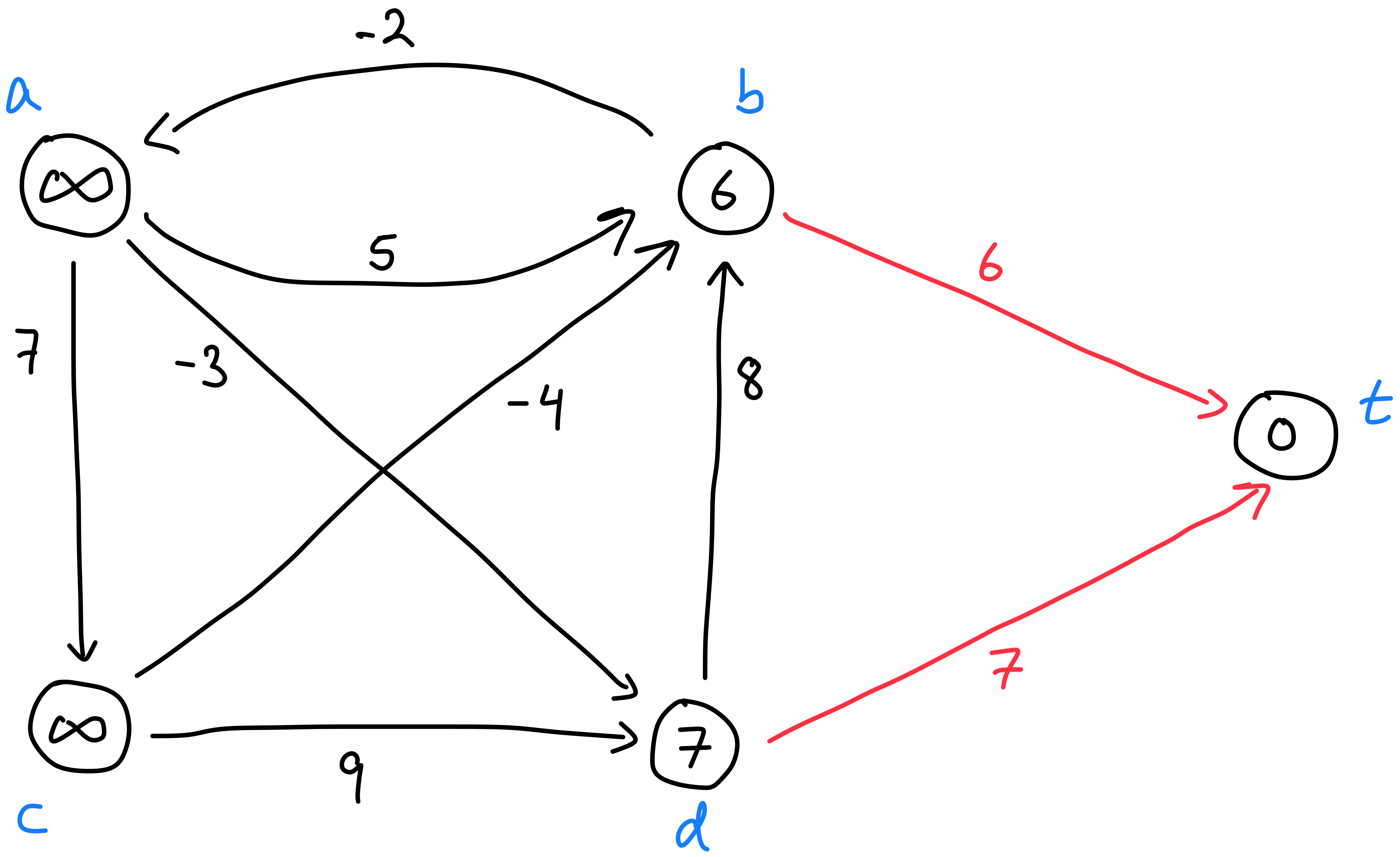


Queue

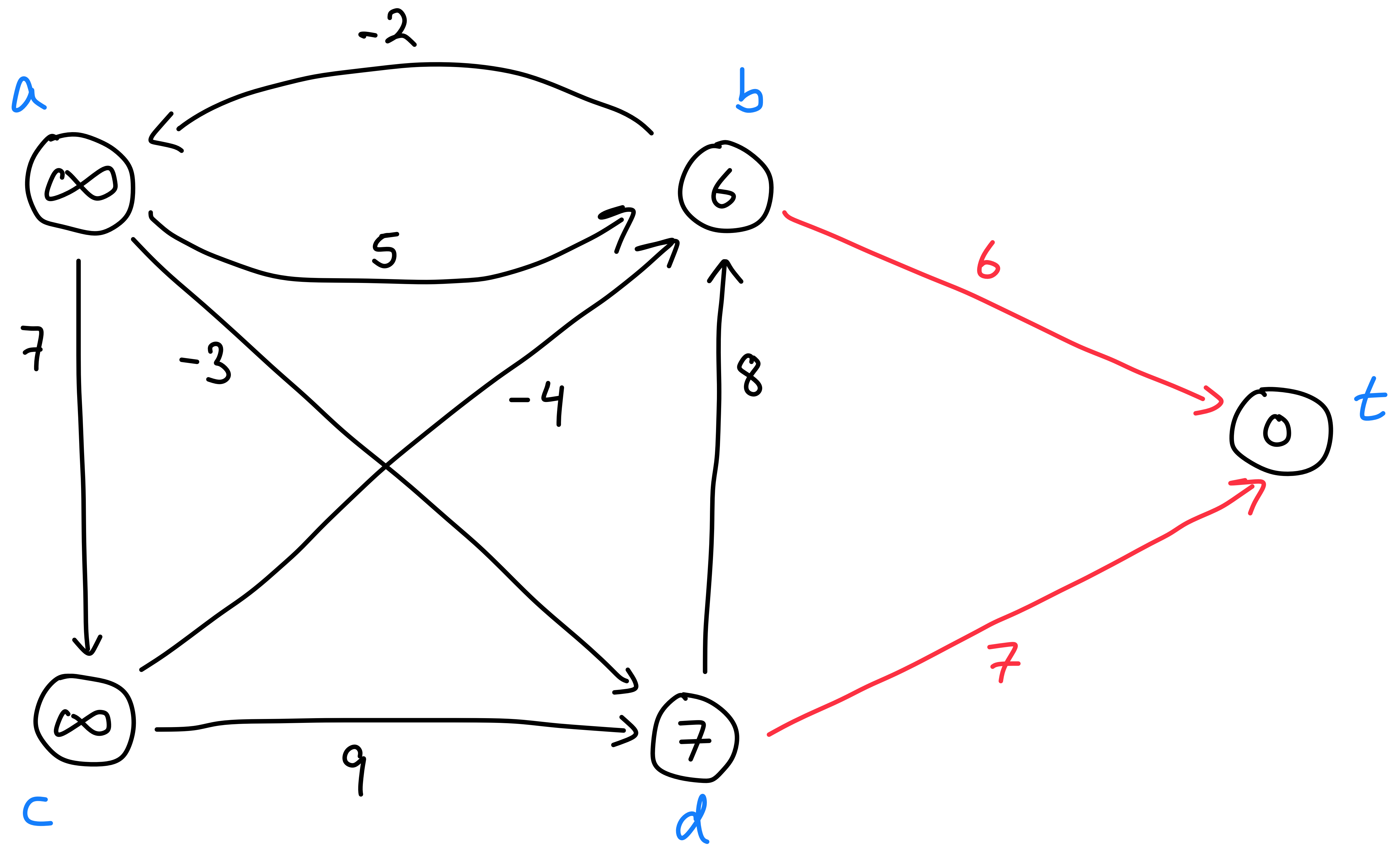
~~t~~

$\perp$

b

d

Bellman-Ford example



Queue

~~t~~
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b
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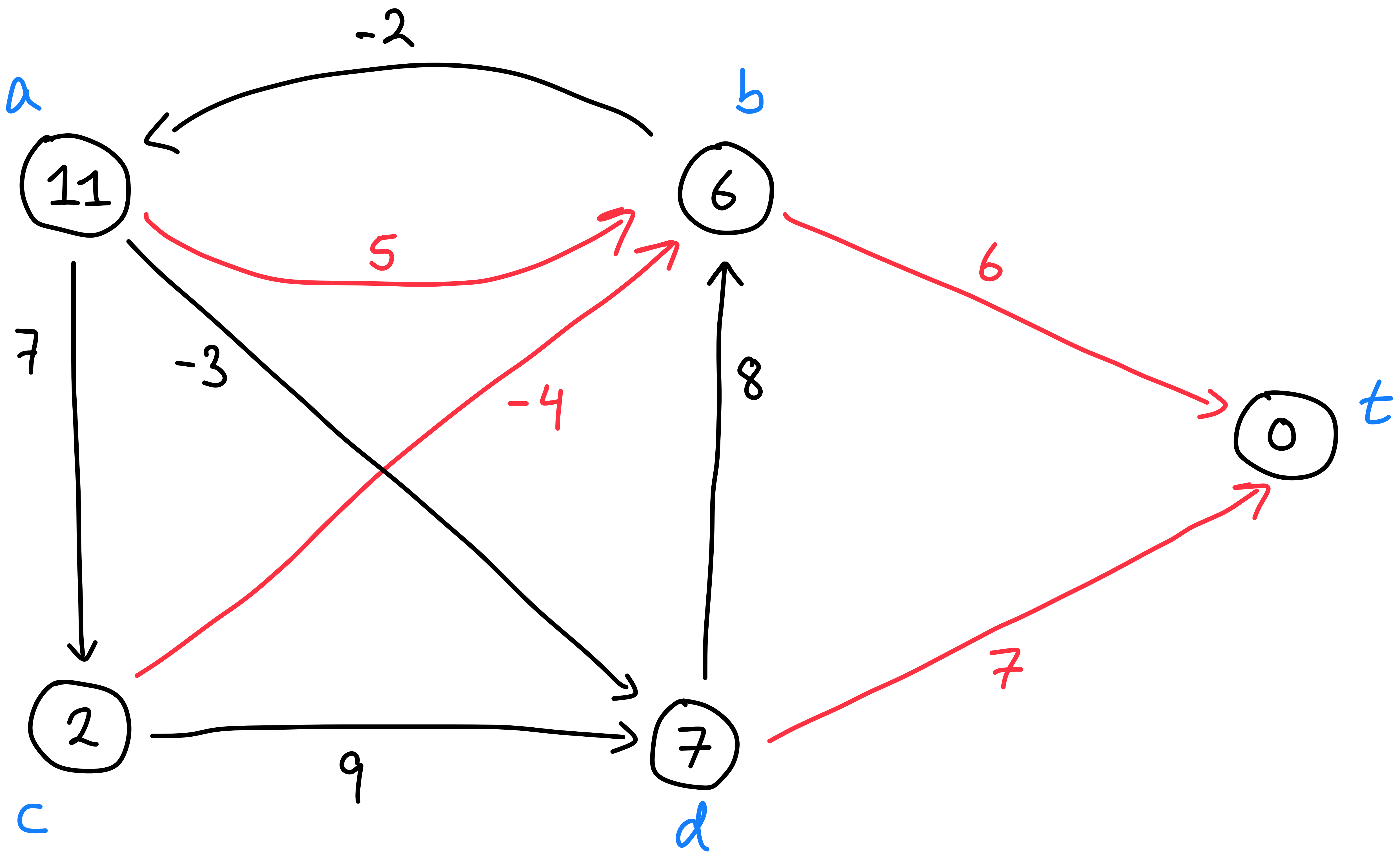
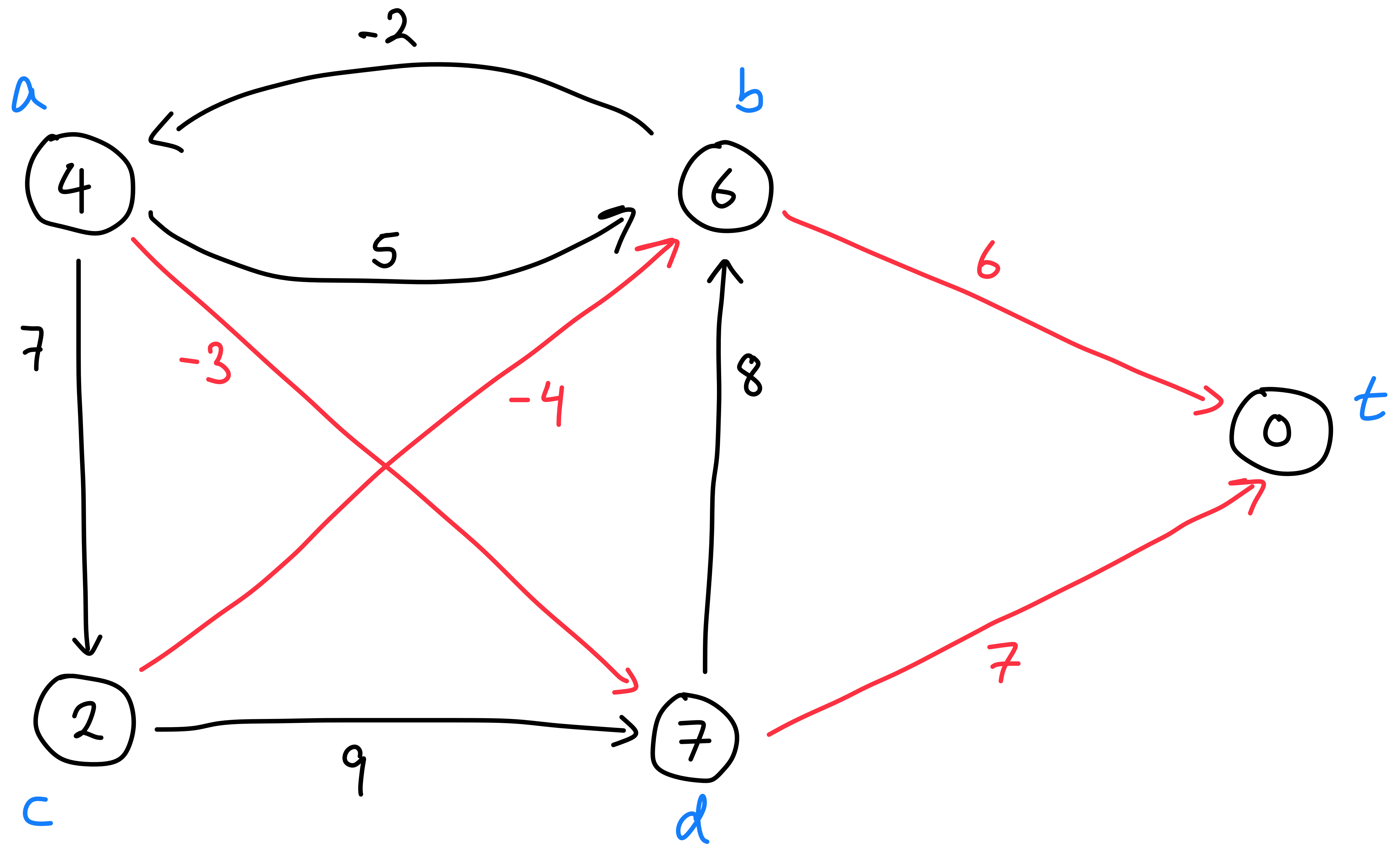
Bellman-Ford example



Queue

~~t~~
~~⊥~~
~~b~~
d
⊥
a
c

Bellman-Ford example



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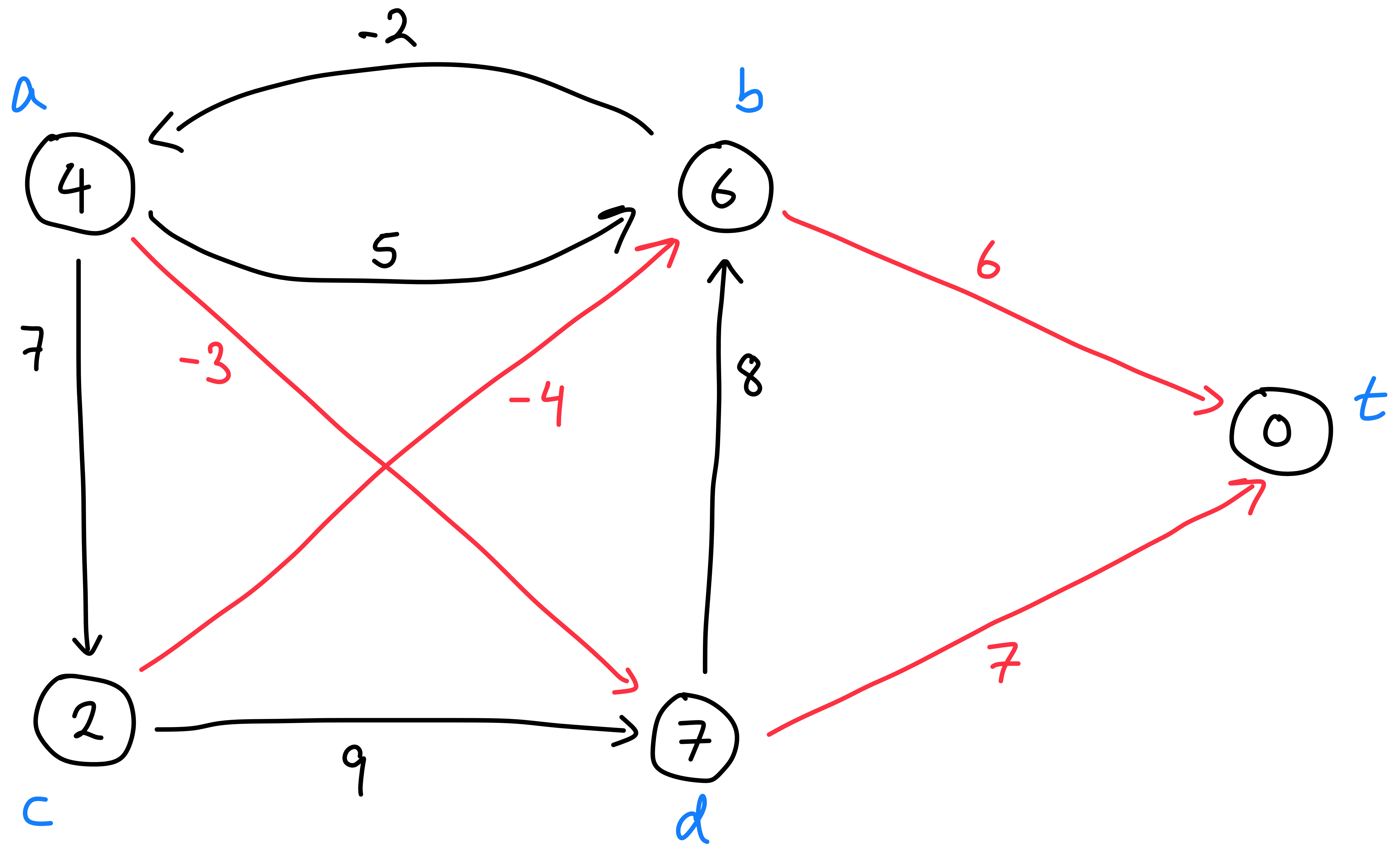
c

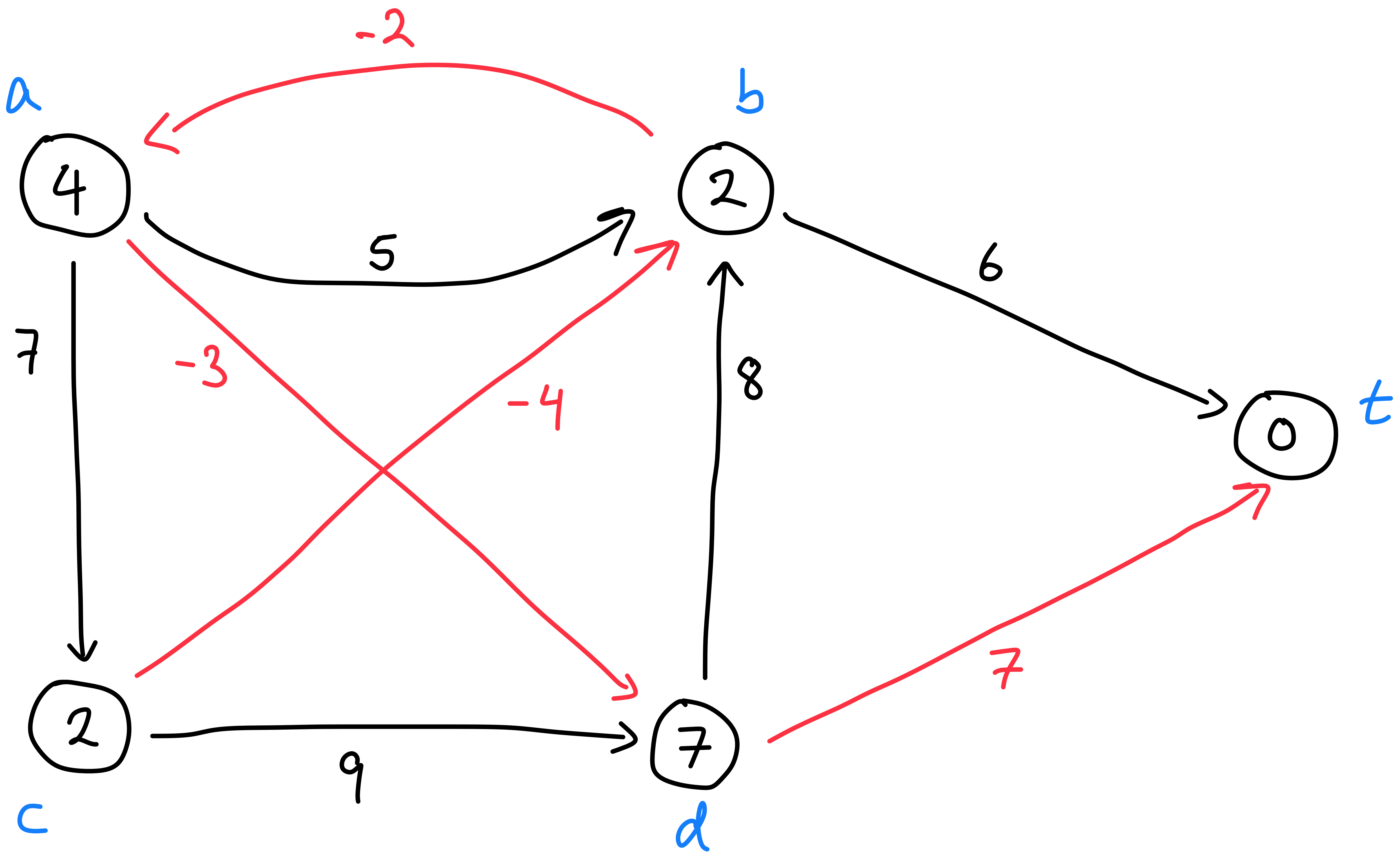
Bellman-Ford example



Queue

~~t~~
~~⊥~~
~~b~~
~~d~~
~~⊥~~
a
c
⊥

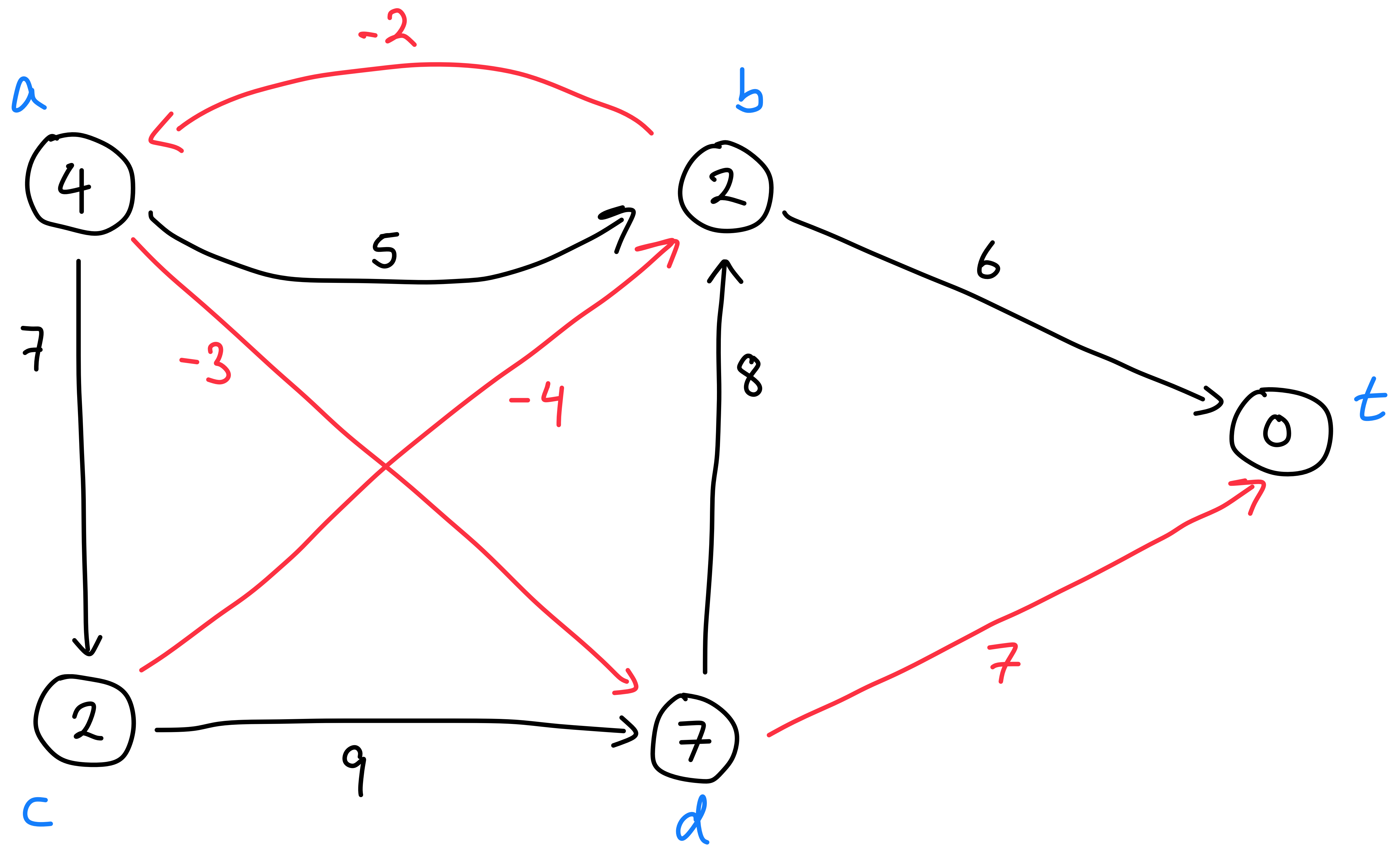
Bellman-Ford example

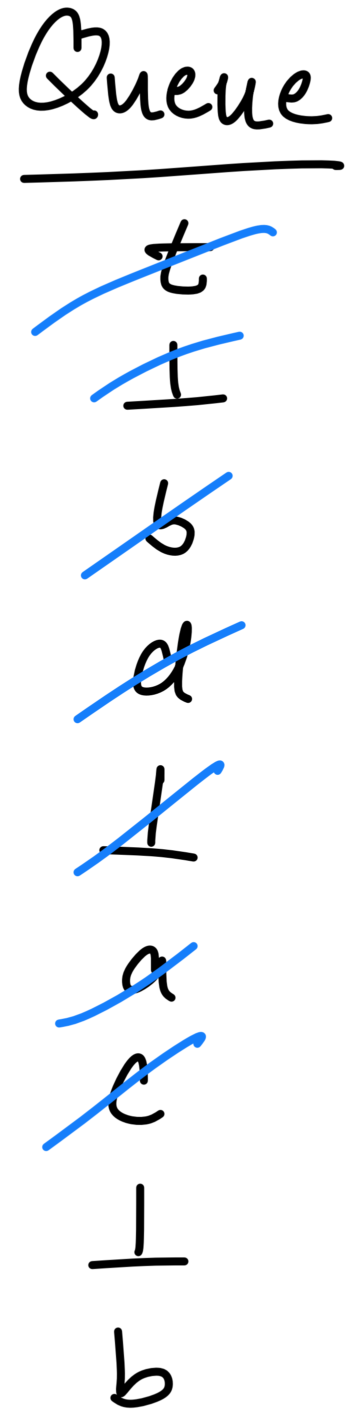


Queue

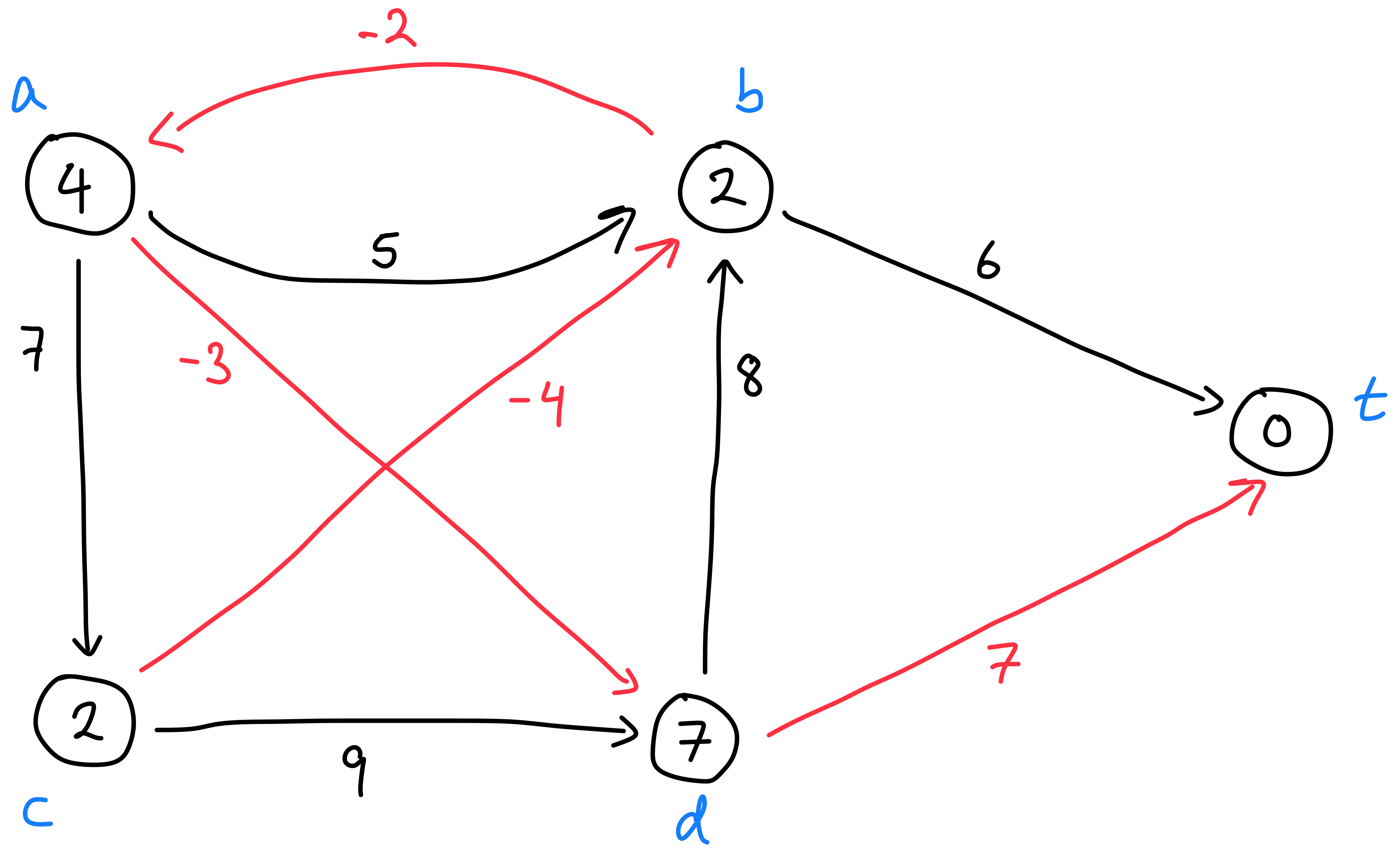
~~t~~
~~⊥~~
~~b~~
~~d~~
~~⊥~~
~~a~~
c
⊥
b

Bellman-Ford example





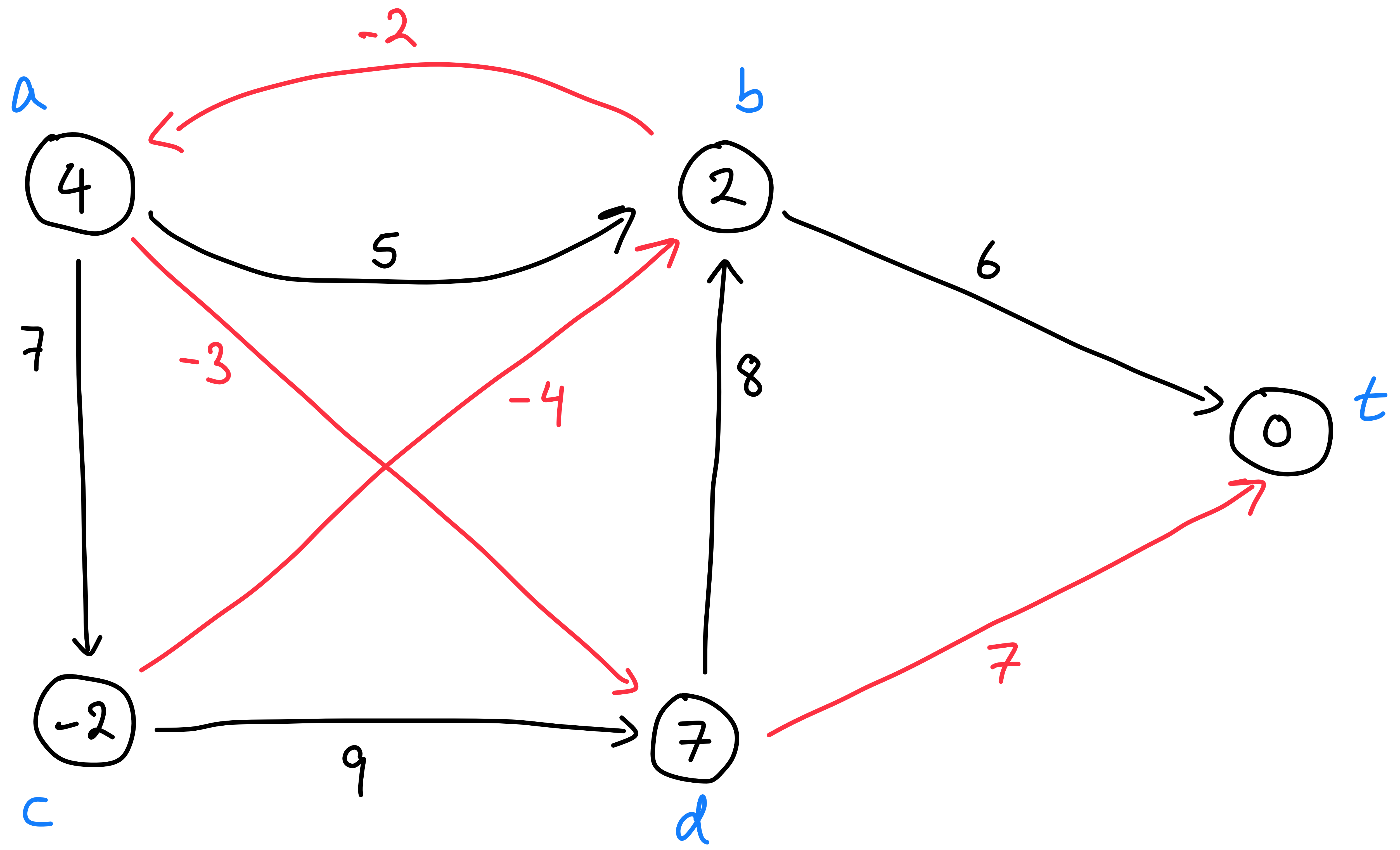
Bellman-Ford example

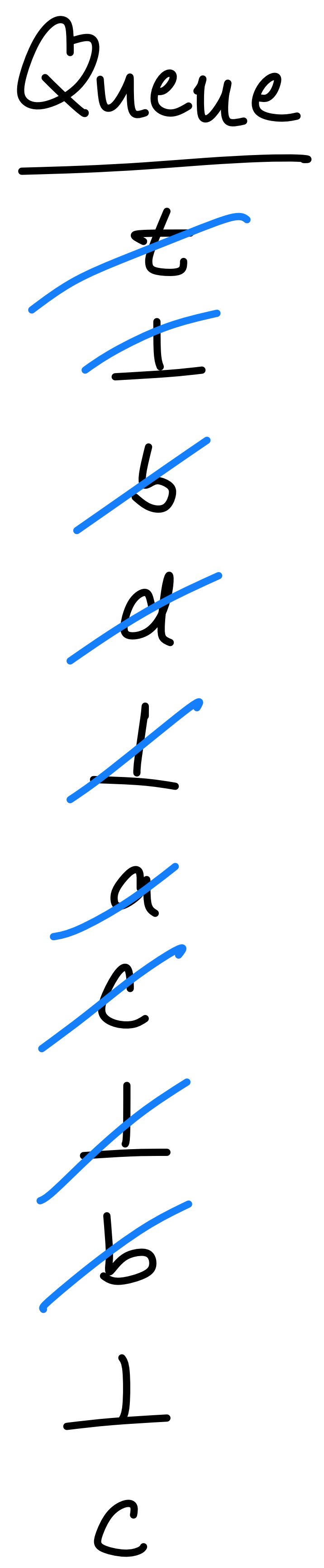


Queue

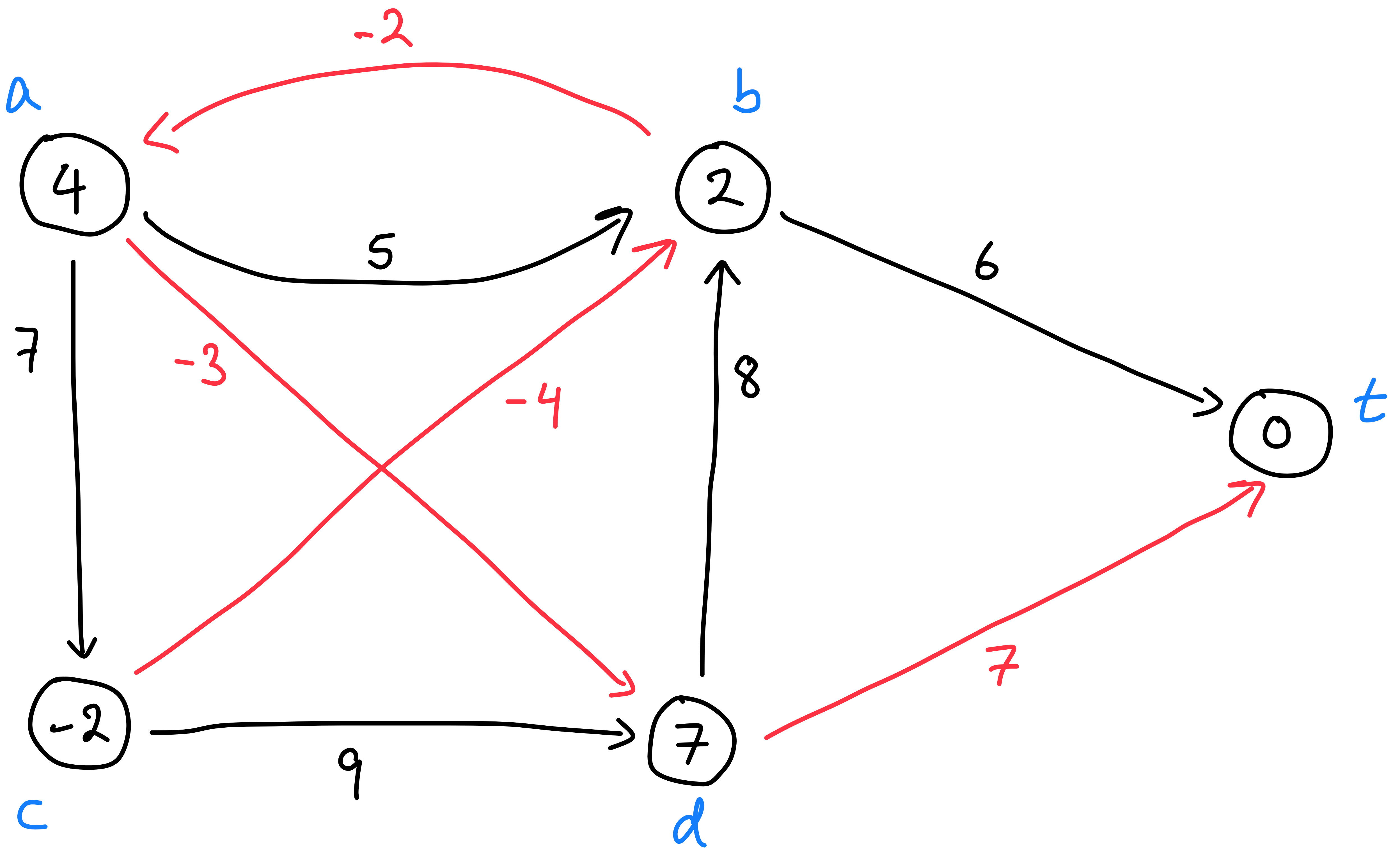
~~t~~
~~⊥~~
~~b~~
~~d~~
~~⊥~~
~~a~~
~~c~~
~~⊥~~
b
⊥

Bellman-Ford example





Bellman-Ford example



Queue

~~t~~
~~⊥~~ 1
~~b~~
~~d~~
~~⊥~~ 2
~~a~~
~~c~~
~~⊥~~ 3
~~b~~
~~⊥~~ 4
c
⊥

n-1 iterations.

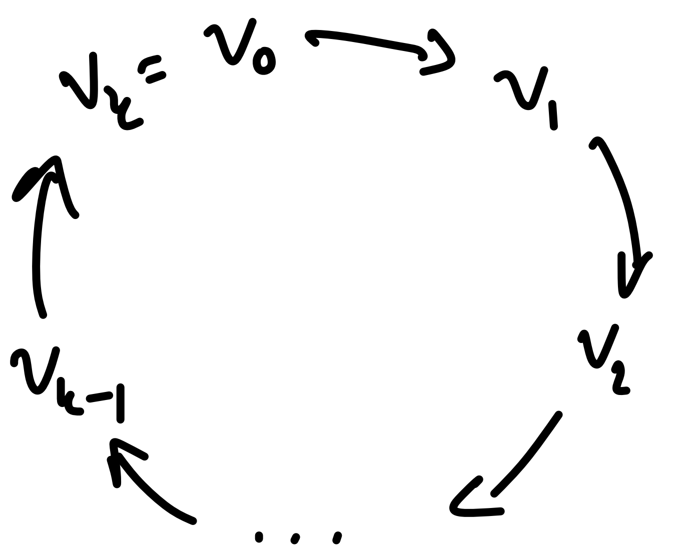
Alg concludes.

Detecting negative cycles

- **Lemma:** If every vertex s can reach t, and G has a negative cycle, then there is some edge $u \to v$ so that $d(n-1,u) > d(n-1,v) + w(u,v)$. If G has no negative cycles, then output of Bellman-Ford is correct on final iteration.

- **Proof:** By contradiction.

Let G have a negative cycle.



$$\sum_{i=0}^{k-1} w(v_i, v_{i+1}) < 0. \quad (1)$$

Assume (for $\perp$) that $\forall$ edges $u \to v$, $d(n-1,u) \le d(n-1,v) + w(u,v)$.

Adding up these equations for the cycle,

$$\underbrace{\sum_{i=0}^{k-1} d(n-1, v_i)} \le \underbrace{\sum_{i=0}^{k-1} d(n-1, v_{i+1})} + \sum_{i=0}^{k-1} w(v_i, v_{i+1})$$

same term

$$\Longrightarrow \quad 0 \le \sum_{i=0}^{k-1} w(v_i, v_{i+1}) \quad (2)$$

(1) and (2) are inconsistent, proving the contradiction.

Detecting negative cycles

- **Lemma:** If every vertex s can reach t, and G has a negative cycle, then there is some edge $u \to v$ so that $d(n-1,u) > d(n-1,v) + w(u,v)$. If G has no negative cycles, then output of Bellman-Ford is correct on final iteration.

- **Proof:** The previous slide proves the first part of the statement.

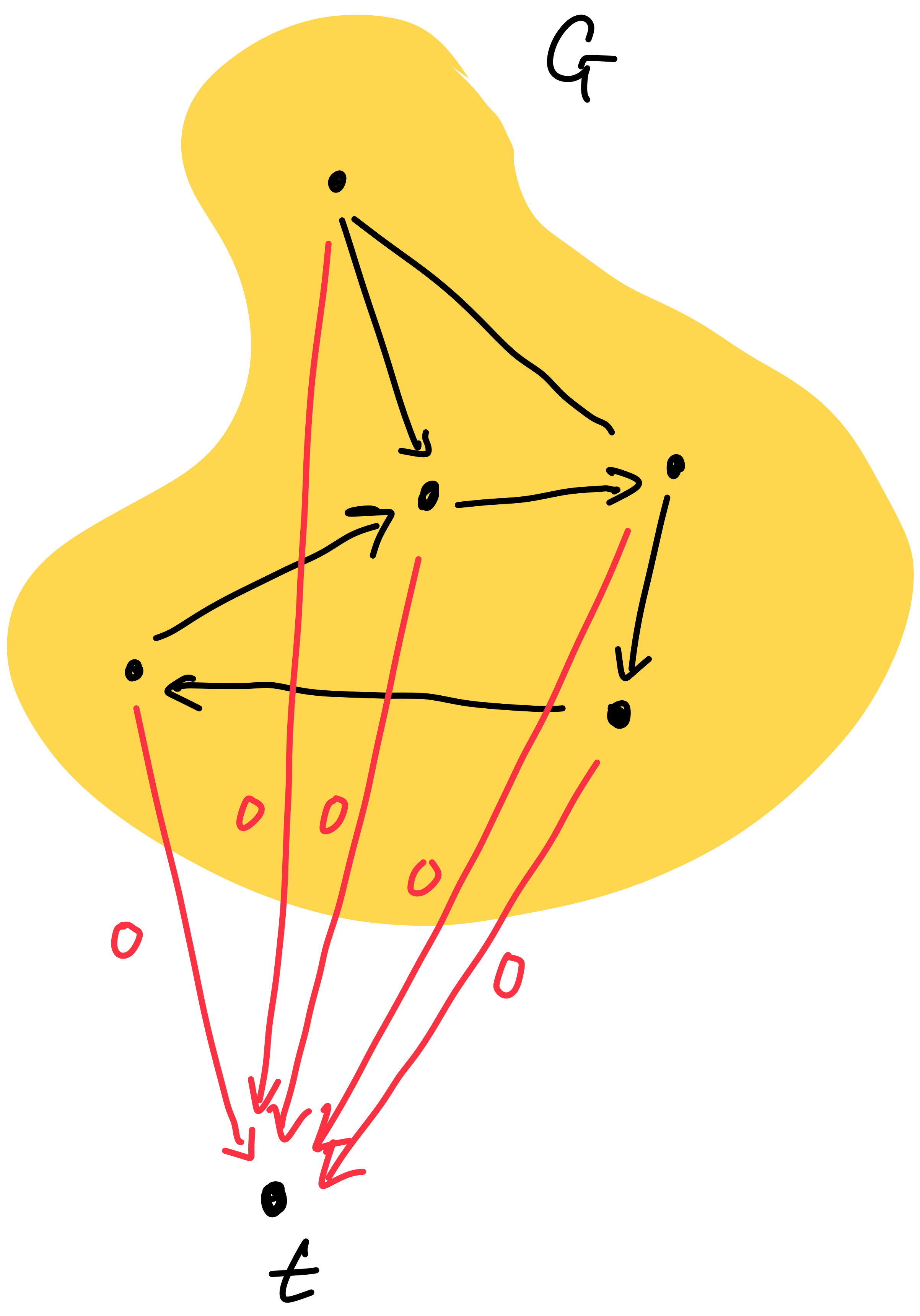
  - If there are no negative cycles, the shortest path $s \rightsquigarrow t$ consists of unique vertices and has length $\leq n-1$.

  - We previously proved that $d(i,s)$ was optimal length of path $s \rightsquigarrow t$ of length $\leq i$.

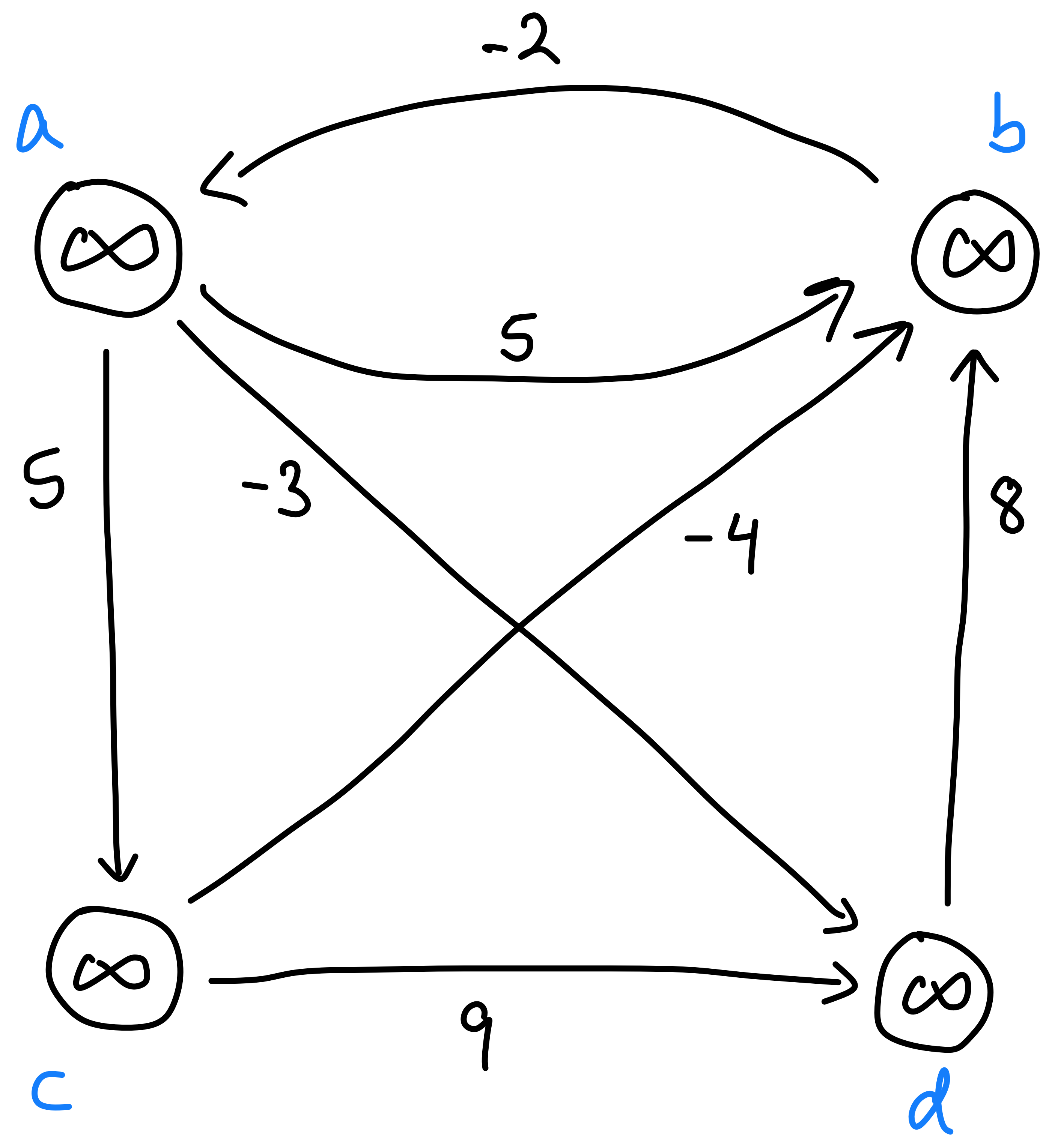
  - Together, concludes proof.

Negative cycle detection

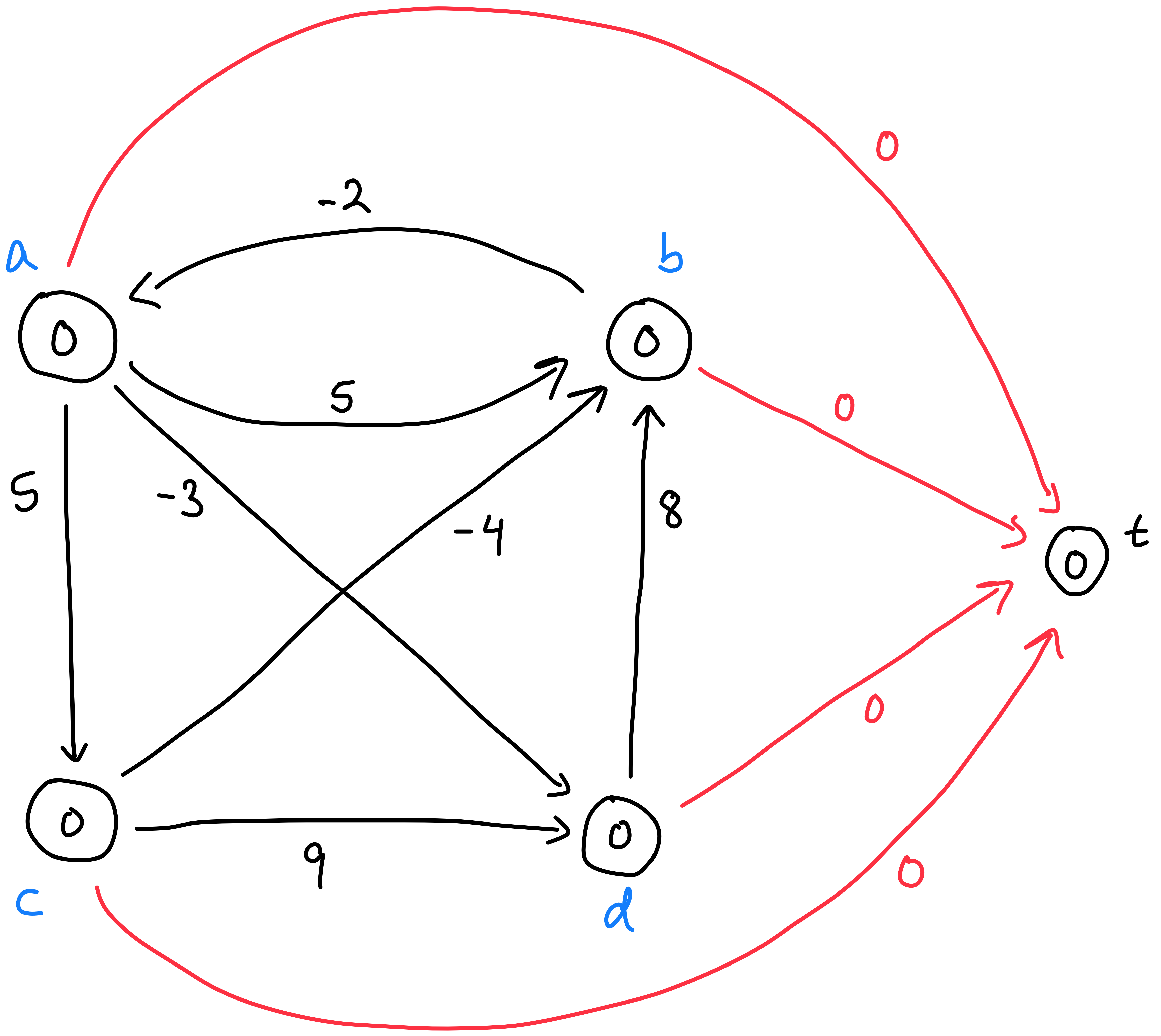
- **Negative cycle detection algorithm:**
  - Run Bellman-Ford assuming there are no negative cycles
  - For each edge $u \to v$, verify that $d(u) \leq d(v) + w(u, v)$. Else, report “negative cycle detected”.
- This will only detective negative cycles amongst vertices that have paths to t. Might not be the entire graph for bad choice of t.
- Solution: Add a new “sink” t to the graph and add edge $v \to t$ of weight 0 for all vertices. Run detection algorithm w.r.t this sink.



Bellman-Ford with negative cycles example



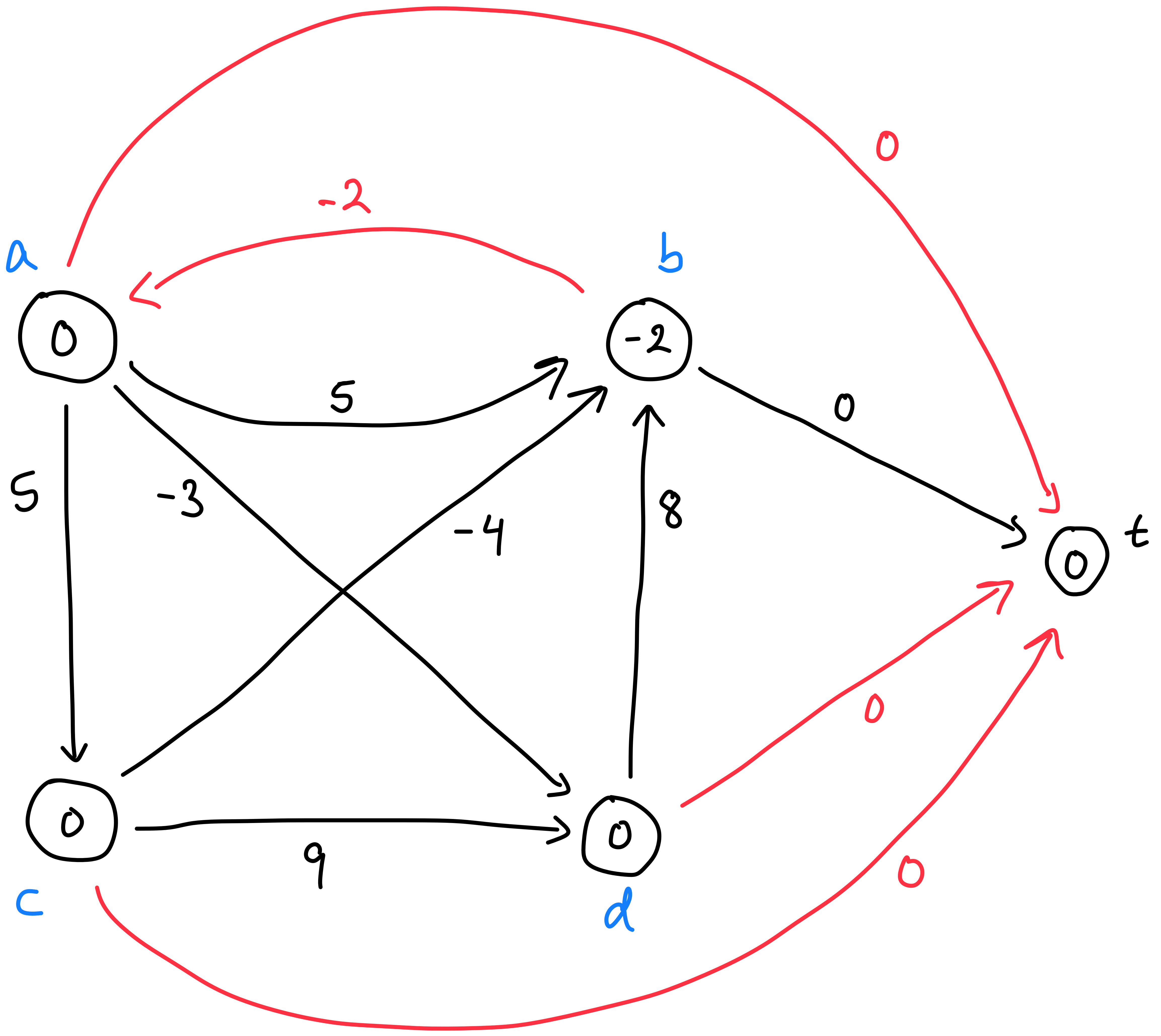
Bellman-Ford with negative cycles example

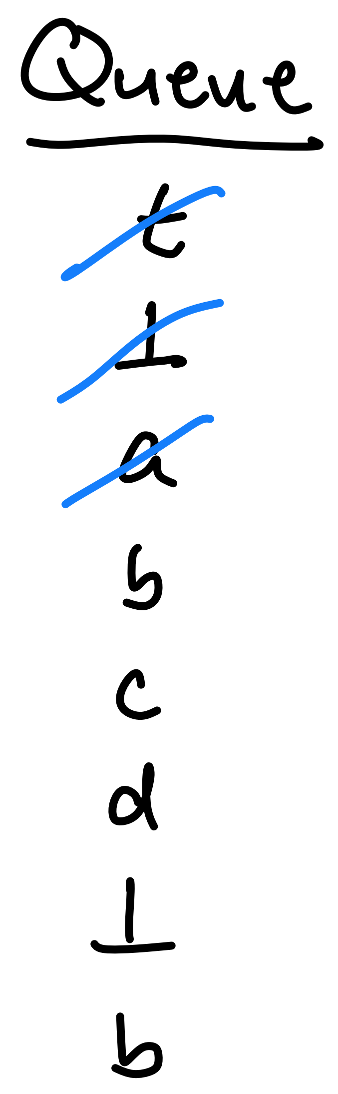


Queue

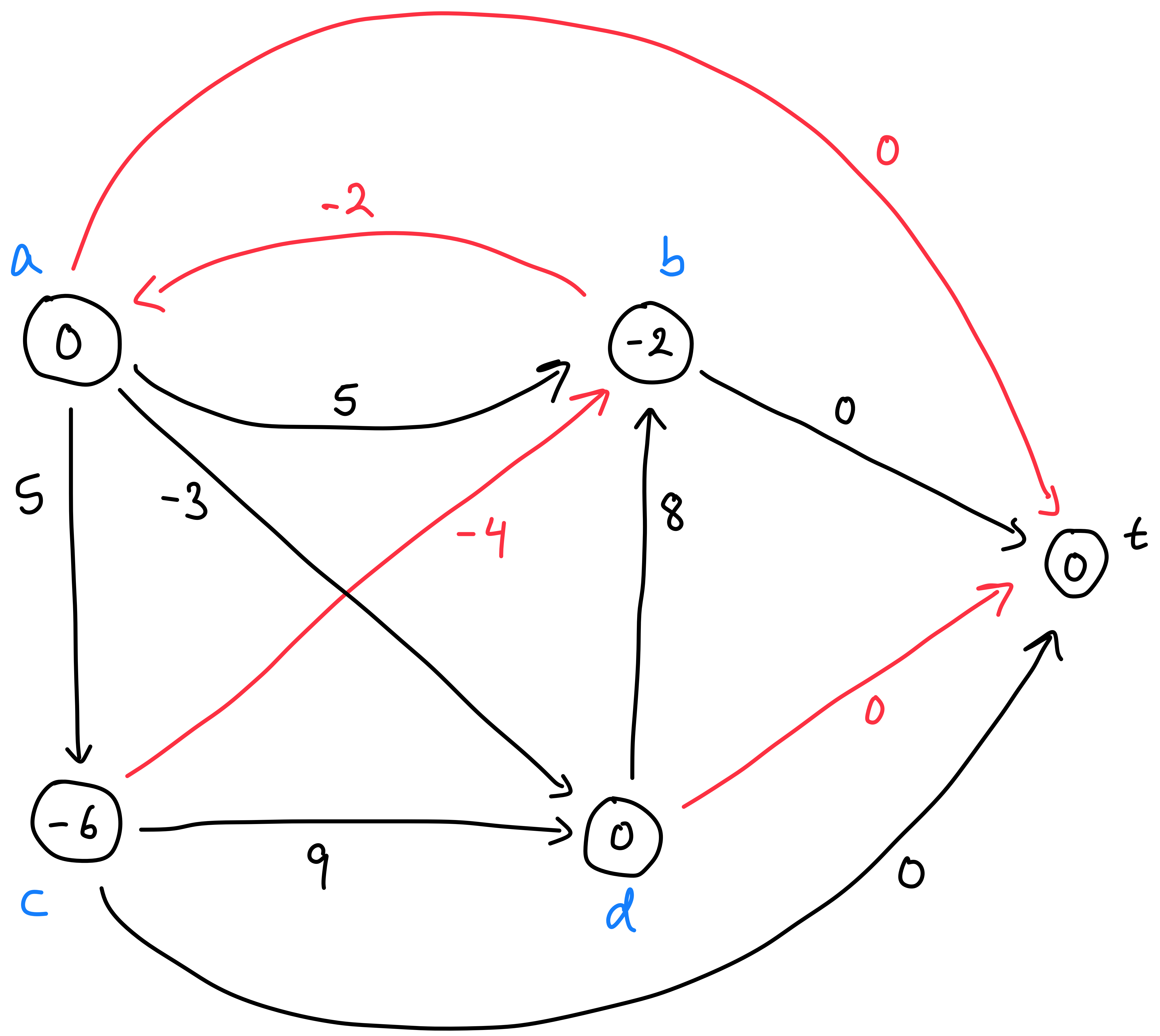
~~t~~
~~⊥~~
a
b
c
d
⊥

Bellman-Ford with negative cycles example





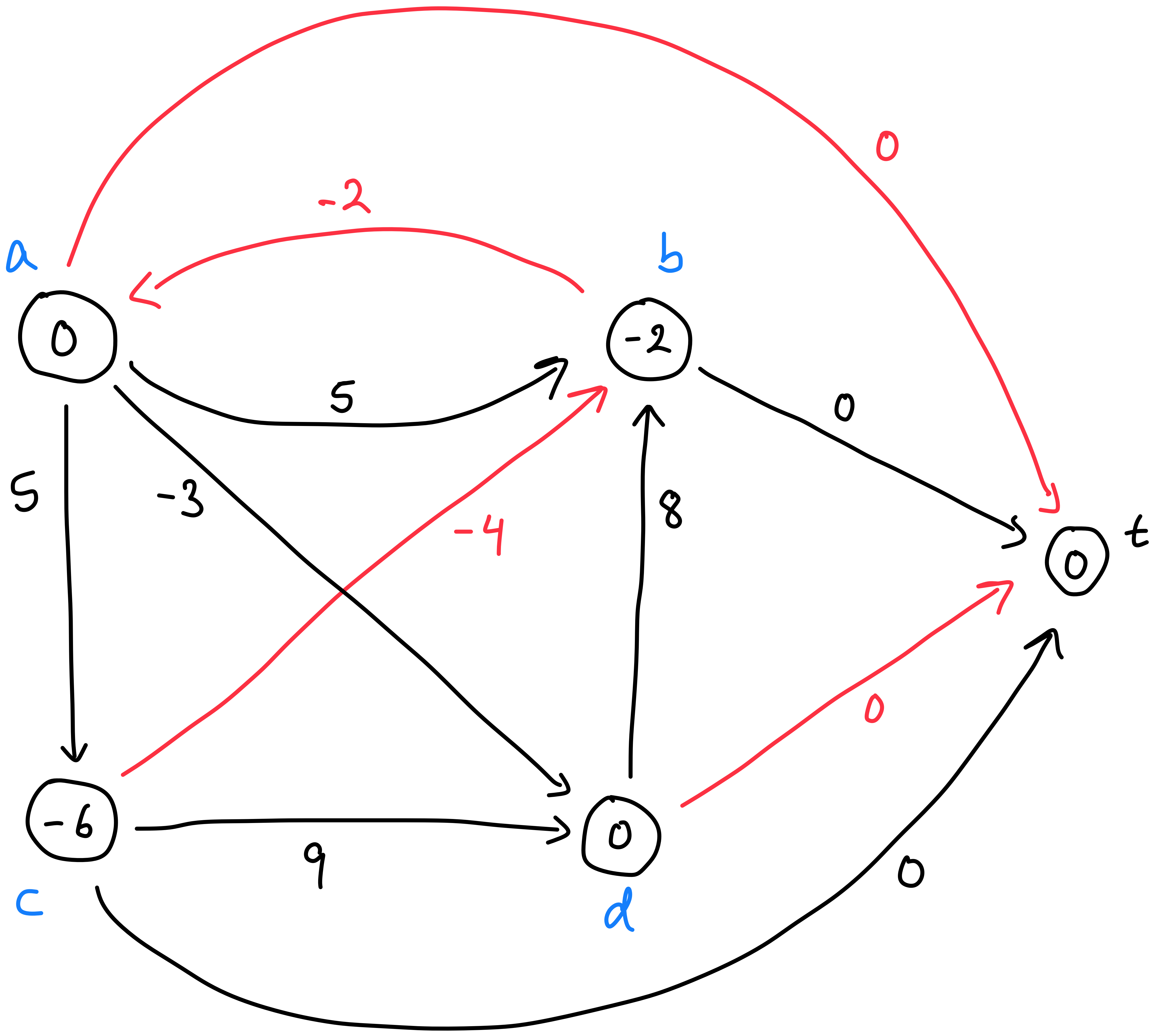
Bellman-Ford with negative cycles example



Queue

~~t~~
~~⊥~~
~~a~~
~~b~~
c
d
⊥
b
c

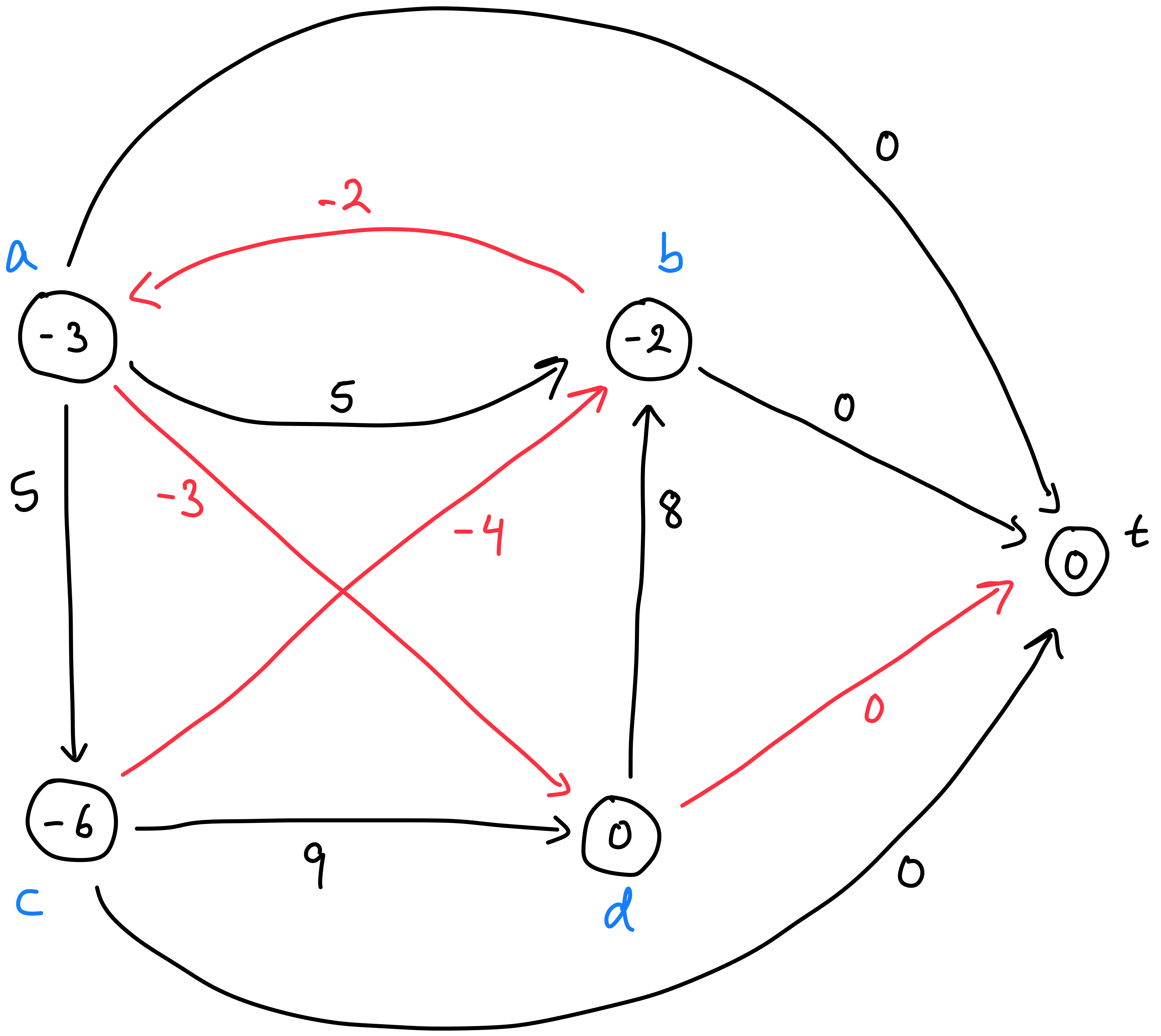
Bellman-Ford with negative cycles example

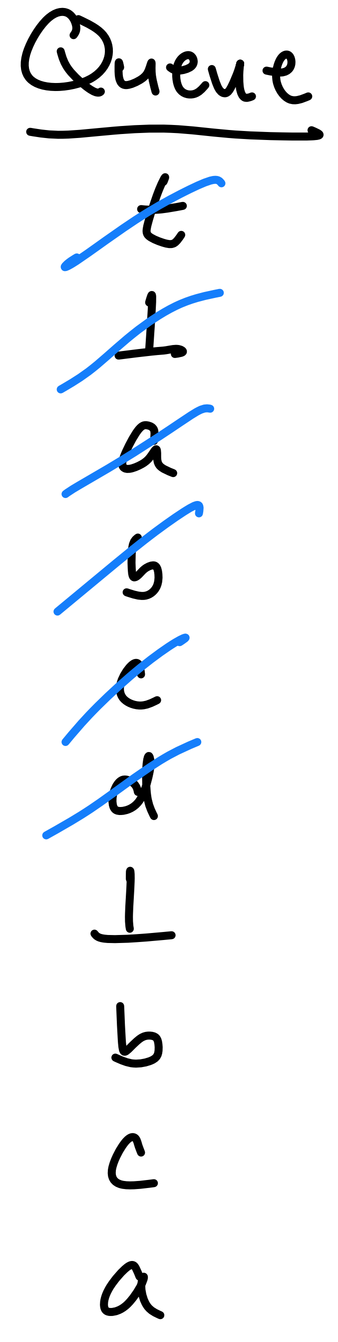


Queue

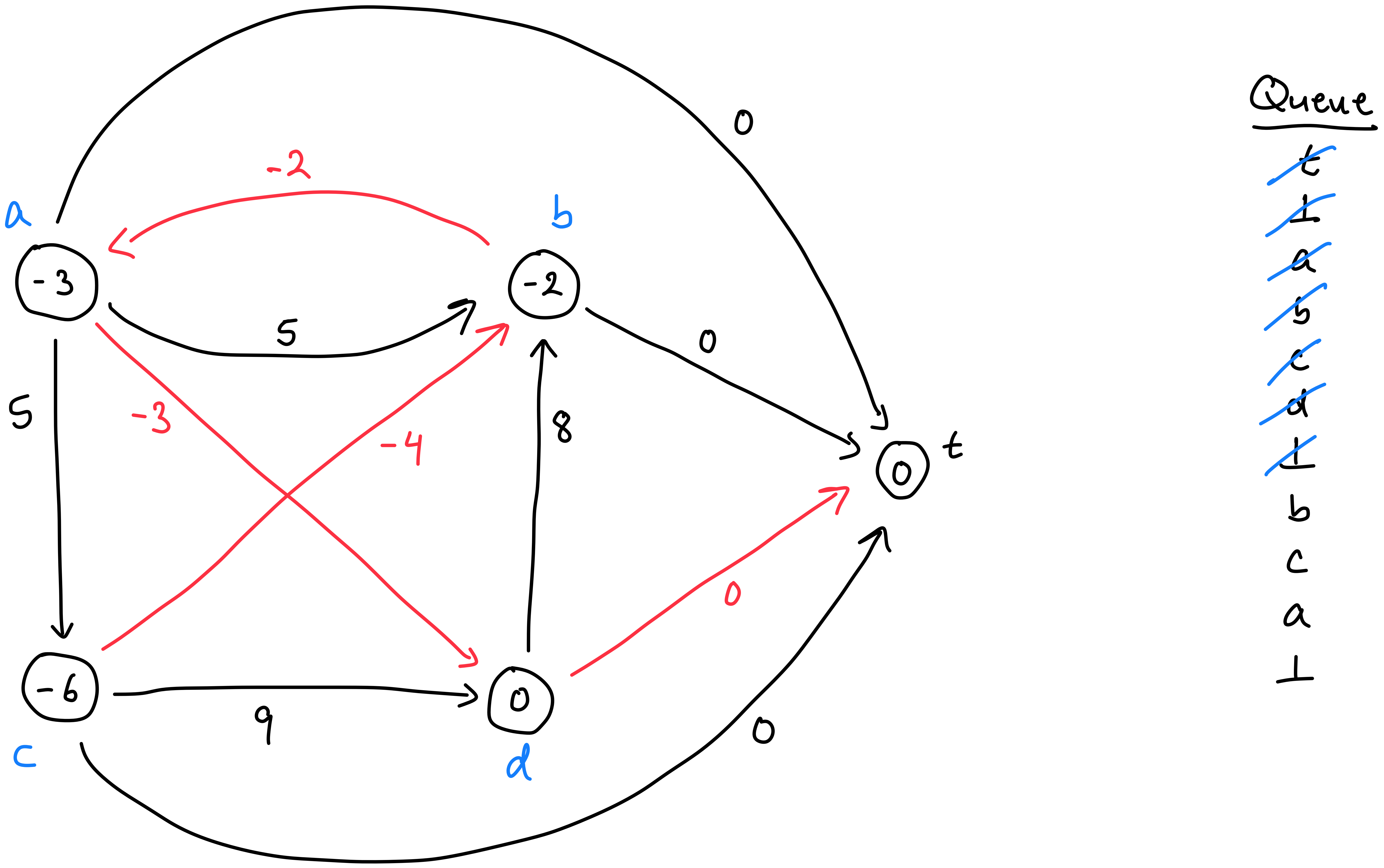
~~t~~
~~⊥~~
~~a~~
~~b~~
~~c~~
d
⊥
b
c

Bellman-Ford with negative cycles example

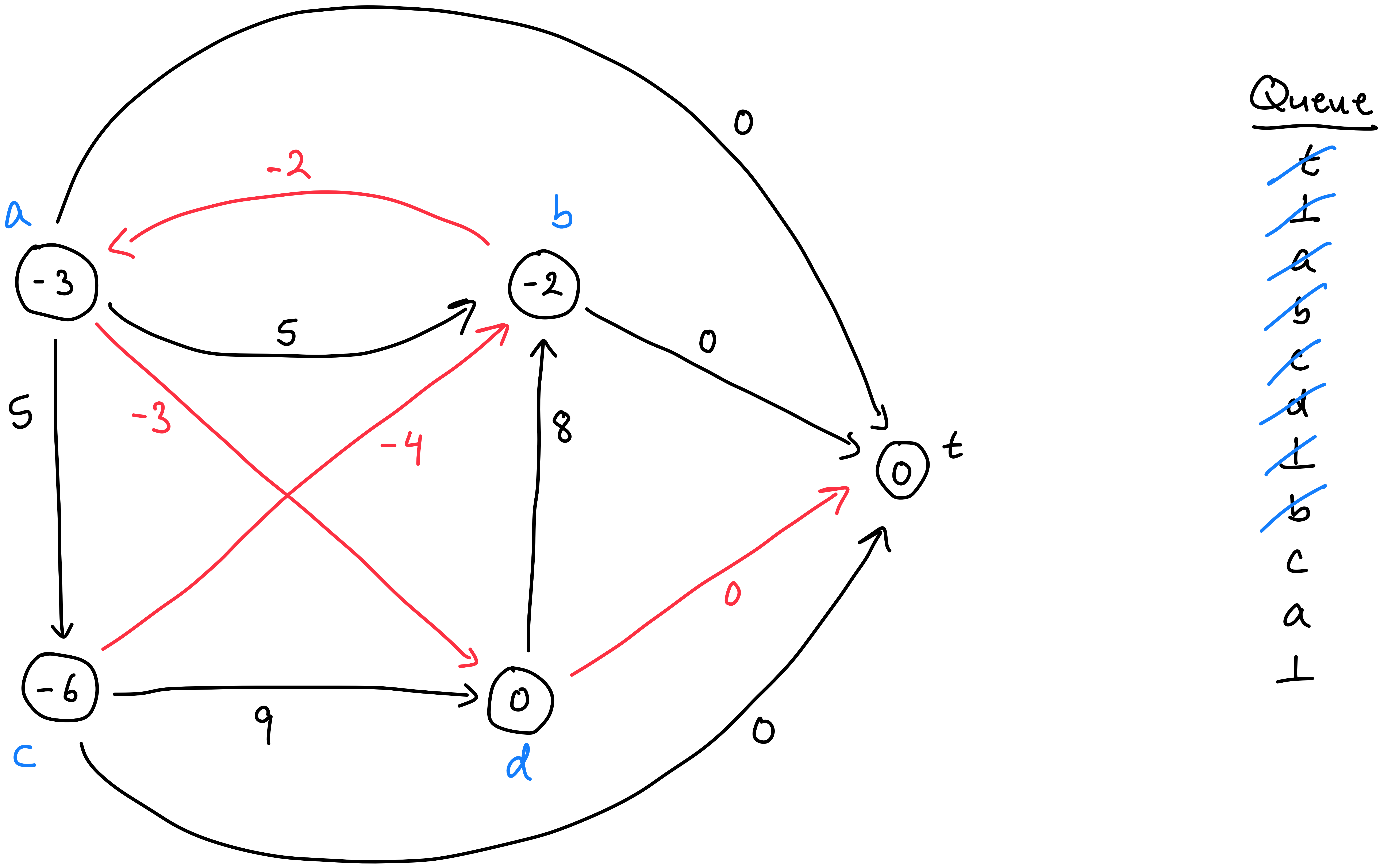




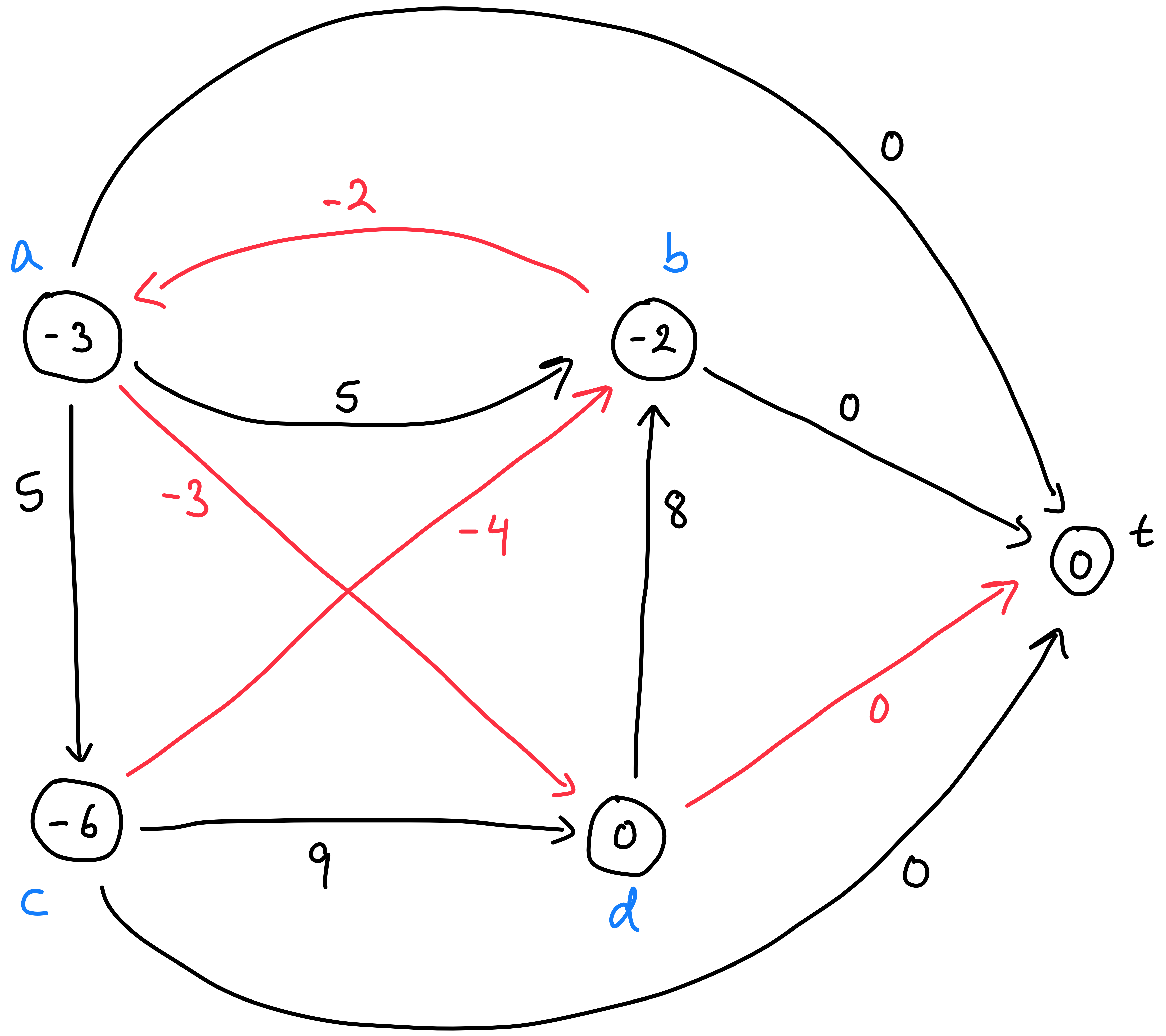
Bellman-Ford with negative cycles example



Bellman-Ford with negative cycles example



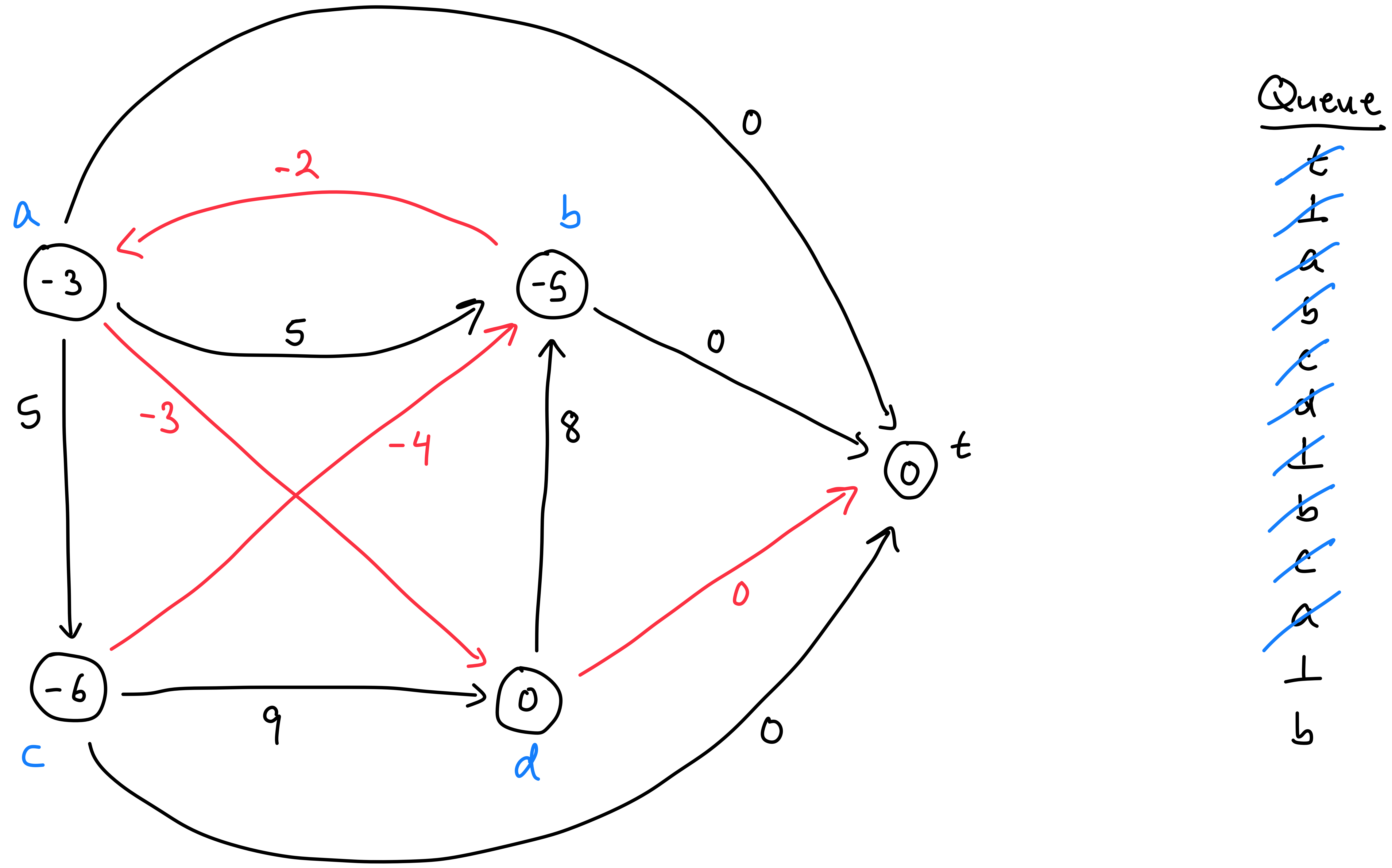
Bellman-Ford with negative cycles example



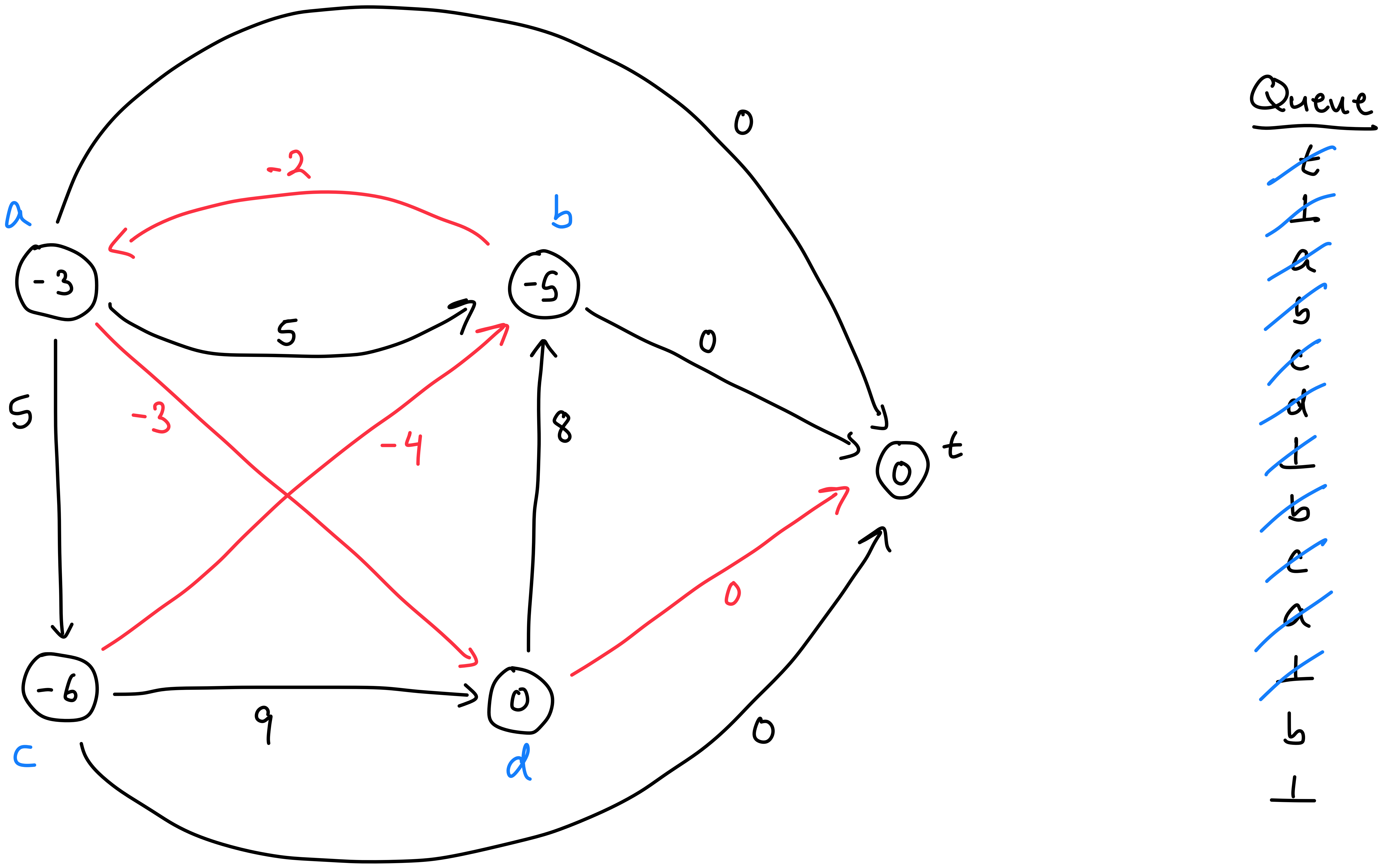
Queue

~~t~~
~~⊥~~
~~a~~
~~b~~
~~c~~
~~d~~
~~⊥~~
~~b~~
~~c~~
a
⊥

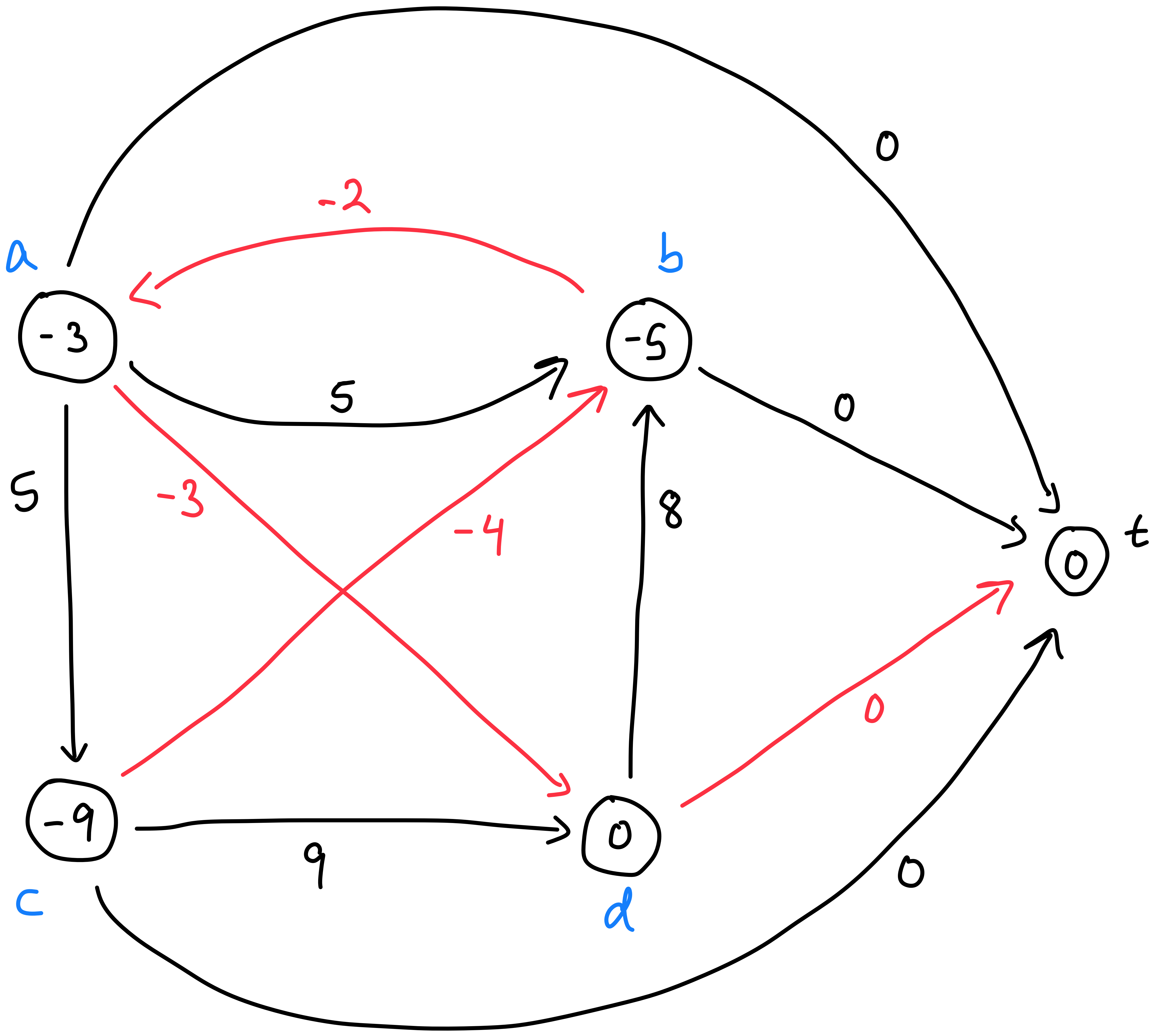
Bellman-Ford with negative cycles example



Bellman-Ford with negative cycles example



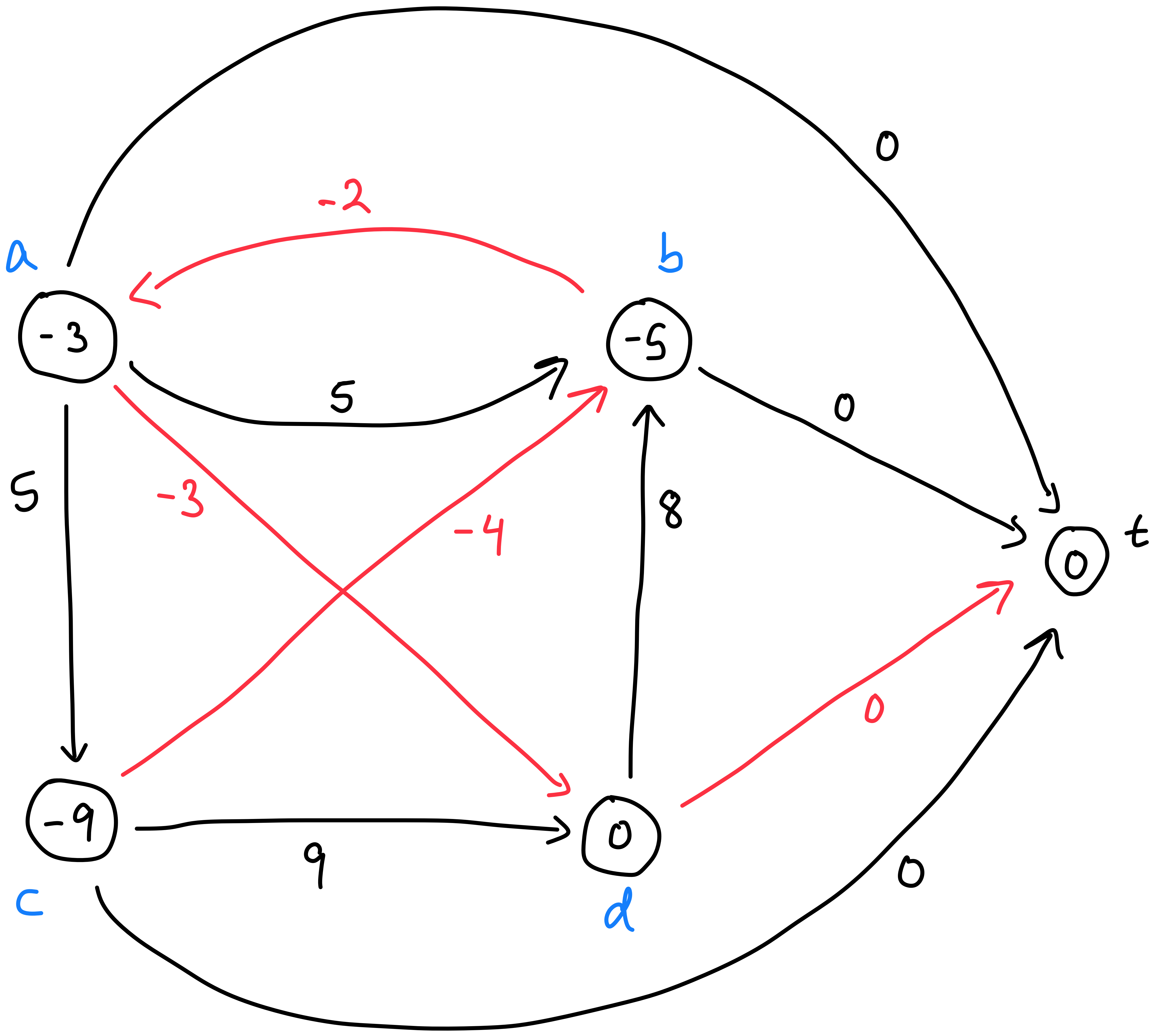
Bellman-Ford with negative cycles example



Queue

~~t~~
~~⊥~~
~~a~~
~~b~~
~~c~~
~~d~~
~~⊥~~
~~b~~
~~c~~
~~a~~
~~⊥~~
~~b~~
⊥
c

Bellman-Ford with negative cycles example



Queue

~~t~~
~~⊥~~ 1
~~a~~
~~b~~
~~c~~
~~d~~
~~⊥~~ 2
~~b~~
~~c~~
~~a~~
~~⊥~~ 3
~~b~~
~~⊥~~ 4
c

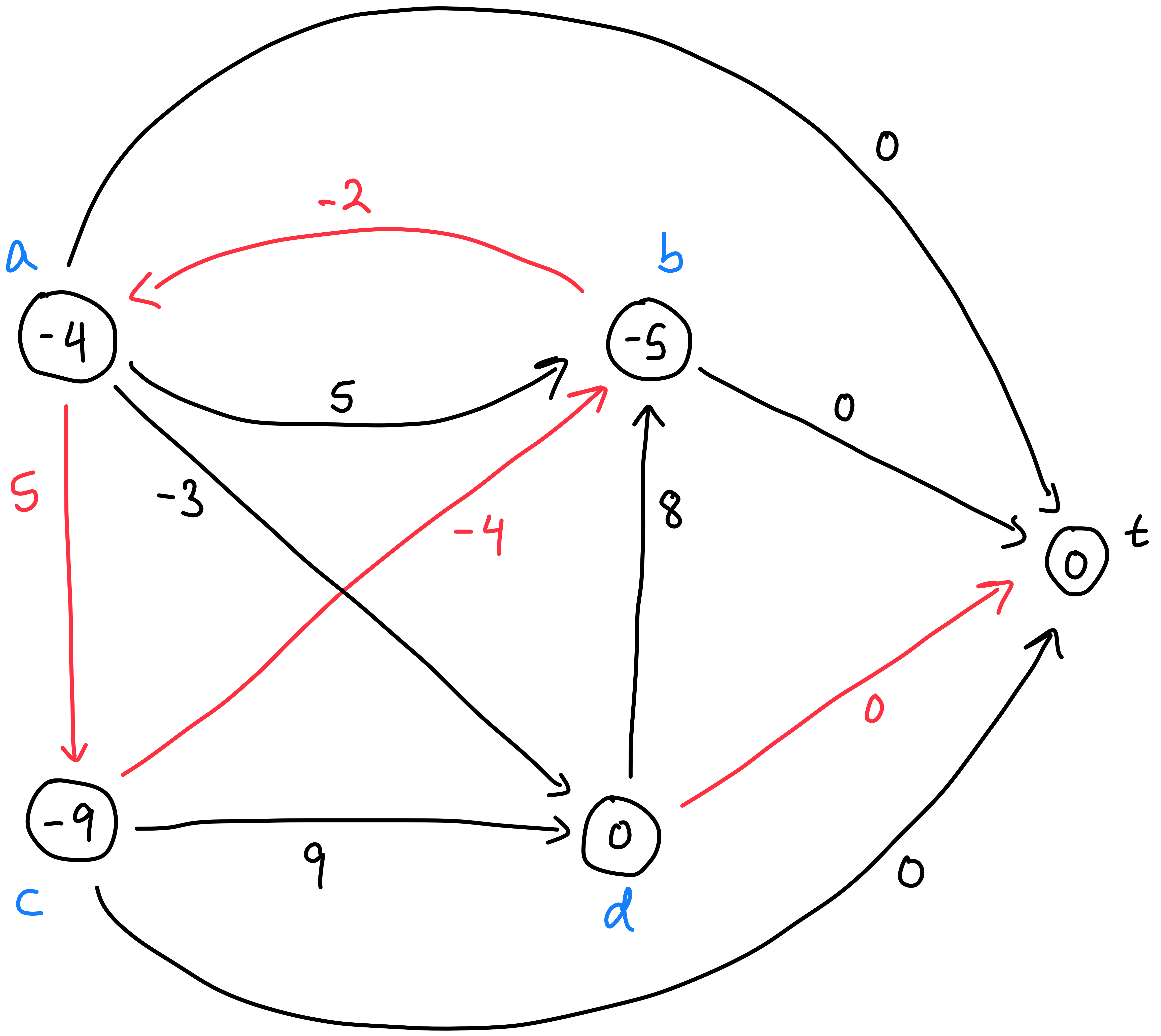
4 iterations completed.

Now checking edges, we notice that

$$\underbrace{d(a)}_{-3} > \underbrace{d(c)}_{-9} + \underbrace{w(a,c)}_{5}$$

So a negative cycle exists (a → c → b).

Bellman-Ford with negative cycles example



Queue

~~t~~
~~⊥~~ ①
~~a~~
~~b~~
~~c~~
~~d~~
~~⊥~~ ②
~~b~~
~~c~~
~~a~~
~~⊥~~ ③
~~b~~
~~⊥~~ ④
~~c~~
⊥
a

Observe what would happen if we updated once more.

Shortest paths with negative weights on a DAG

- No cycles by definition
- Under topological sort, edges only go from low to high numbered vertices
- One pass through the vertices in reverse topological order suffices
- **Runtime**: $O(n + m)$