# Lecture 6

- Algorithmic complexity
- Directed graphs, DAGs
- DAG structure
- Dynamic programming to find highest weight paths in WDAGs

# Algorithmic Complexity

- Basic questions about an algorithm:
  - how long does it take to run?
  - how much space (RAM or disk space) does it require?
- Would like precise function $f(N)$, e.g.

$$f(N) = .05\,N^3 + 50.7\,N^2 + 6.03\,N$$

for

  - running time in secs, or
  - space in kbytes,

as function of the size $N$ of input data set.

- But
  - tedious to derive &
  - depends on (often uninteresting – though important!) hardware & software implementation details.

- Instead, more customary to give "the" *asymptotic complexity*, i.e. expression $g(N)$ such that

$$C_1 g(N) < f(N) < C_2 g(N)$$

for some constants $C_1$ and $C_2$, and $N$ large enough.

- This is written $O(g(N))$, where notation $O()$ means "up to an unspecified multiplicative constant".
  – e.g. for the $f(N)$ above, the dominating term for large $N$ is .05 $N^3$, so
    - can take $g(N) = N^3$
    - asymptotic complexity = $O(N^3)$.

- Can be misleading, since
  - for small $N$ a different term may dominate
    - (e.g. 2[d] term in above example much more important for $N <$ 1000)
  - size of constant may be quite important
    - (big difference between .05 and 5,000,000!)
    - e.g. BLAST and Smith-Waterman both $O(N^2)$, but size of constant enormously different
- *but* very useful as rough guide to performance.

- Cache misses (non-cache memory accesses) and disk accesses often dominate running time, yet are ‘invisible’ to complexity analysis (because affect constant factor only)

- Another limitation to complexity analysis:
  - time or space requirement may depend on specific characteristics of input data.
- Usually give “worst case” complexity
  - applies to the worst data set of a given size,

*but*

  - in biological situations the *average biologically occurring case* is
    - more relevant
    - often much easier than worst case (which may never arise in practice), or even “average case” in some idealized sense.

- Proof that a problem is *NP-hard*
  - (has complexity very likely greater than any polynomial function of *N* and therefore effectively unsolvable for large *N*)

can be useful in guiding search for more efficient algorithms

*but* can also be misleading, since

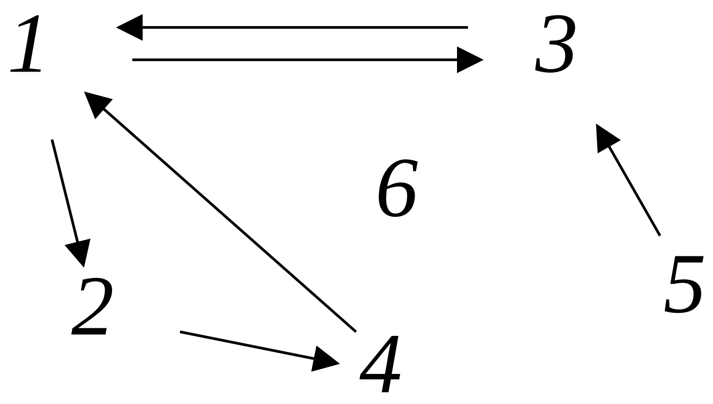
- we need *some* solution anyway, for data sets occurring in practice
- average *biologically relevant* case may be quite manageable

# Directed Graphs

- A *directed graph* is a pair ($V$, $E$) where
  - $V$ is a finite set of *vertices*, or *nodes*.
  - $E$ is a set of ordered pairs (called *edges*) of vertices in $V$.
- An edge ($v_i$, $v_j$) is said to *leave* $v_i$ and to *enter* $v_j$.
  - ($v_i$ and $v_j$ are vertices)
- *in-degree* of a vertex = # edges entering it;
- *out-degree* = # edges leaving it.

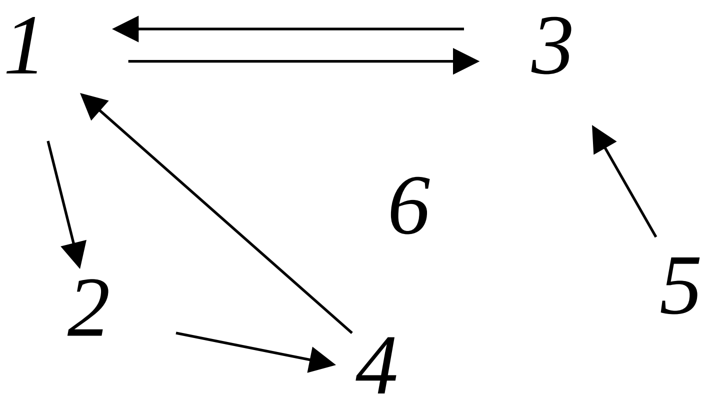
# Example:

- $V = \{1,2,3,4,5,6\}$,
- $E = \{(1,2), (1,3), (2,4), (4,1), (5,3), (3,1)\}$
- Vertex *3* has in-degree 2 and out-degree 1.



# Paths and Cycles

- A *path* of *length k* in *G from u* to *u'* (vertices) is
  - a sequence *P* of vertices $(v_0, v_1, \ldots, v_k)$ such that
    - $v_0 = u$,
    - $v_k = u'$, and
    - $(v_{i-1}, v_i)$ is an edge for $i = 1,2, \ldots, k$.
- A path can have length 0.
- We write $|P| = k$.
- A *cycle* is a path of length ≥ 1 from a vertex to itself.
- In example at right,
  - (*1*,*2*,*4*) is a path,
  - (*1*,*3*,*5*) is not, and
  - (*1*,*2*,*4*,*1*) and (*1*,*3*,*1*) are cycles.



- Can join
  - any path ($u$, ... , $v$) from $u$ to $v$, to
  - any path ($v$, ... , $w$) from $v$ to $w$

to get a path ($u$, ... , $v$, ... , $w$) from $u$ to $w$.

# DAGs

- A *directed acyclic graph* (DAG) is a directed graph with no cycles.
- In a DAG, for distinct nodes $v_i$ and $v_j$, we say
  - $v_i$ is a *parent* of $v_j$, and $v_j$ is a *child* of $v_i$, if
    - there is an edge $(v_i, v_j)$
  - $v_i$ is an *ancestor* of $v_j$, and $v_j$ is a *descendant* of $v_i$, if
    - there is a path from $v_i$ to $v_j$
- In a DAG the length of a path cannot exceed $|V| - 1$,
  - (where $|V|$ = total # vertices in graph)

  because
  - in a path of length $\geq |V|$,
    - at least one vertex $v$ would have to appear twice in the path;
  - but then there would be a path from $v$ to $v$, i.e. a cycle.

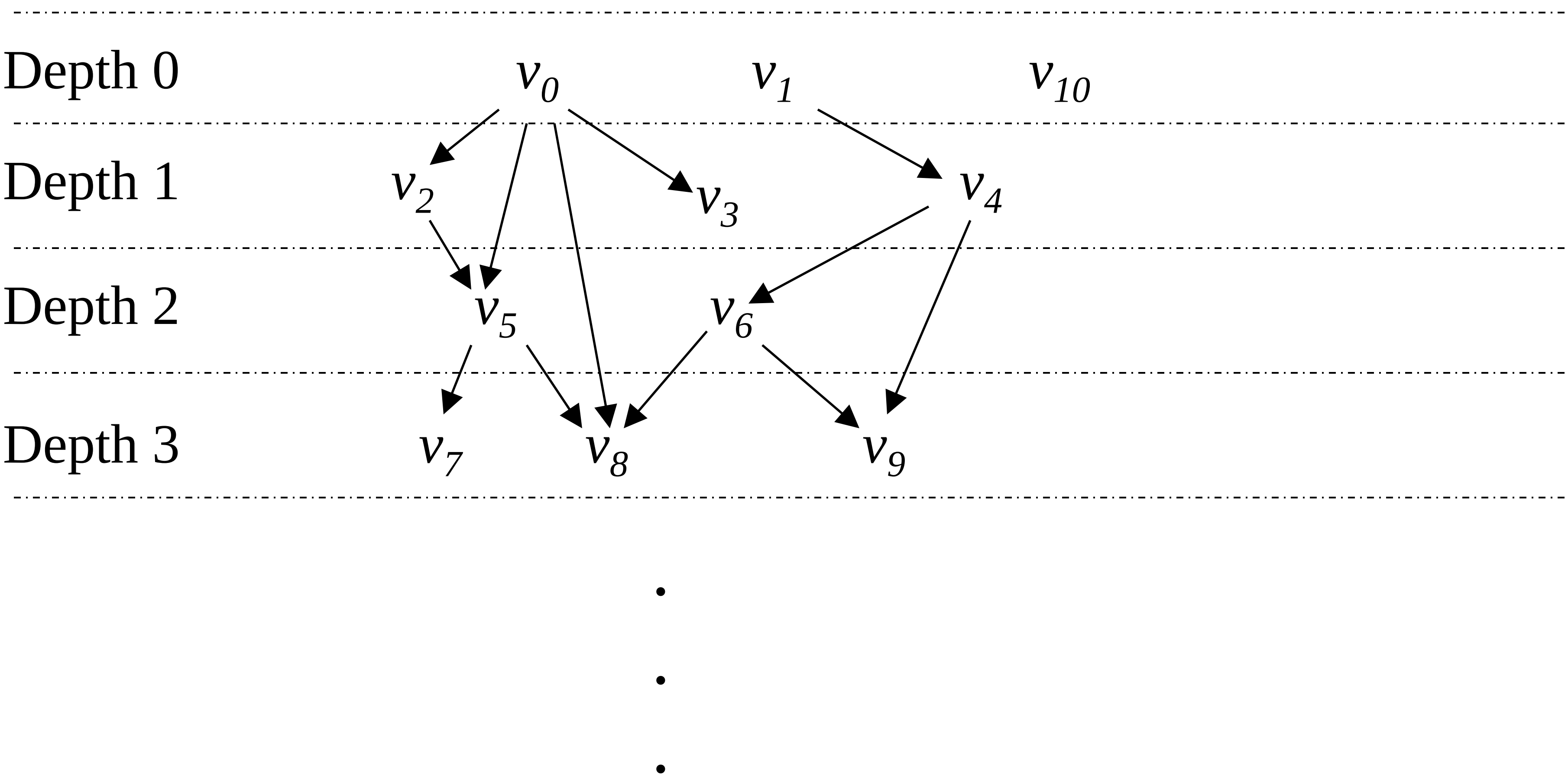
# Structure of DAGs

- Define the *depth* of a node $v$ in $V$ as:
  - the length of the longest path ending at $v$;

  by above, the depth is well-defined and $\leq |V| - 1$.
- *Every descendant $w$ of a node $v$ has higher depth than $v$*: If
  - $(u, \ldots, v)$ is path of length $n = \text{depth}(v)$ ending at $v$, and
  - $(v, \ldots, w)$ is path from $v$ to $w$,

  then $(u, \ldots, v, \ldots, w)$ is a path of length $> n$ ending at $w$, so $\text{depth}(w) > n$.

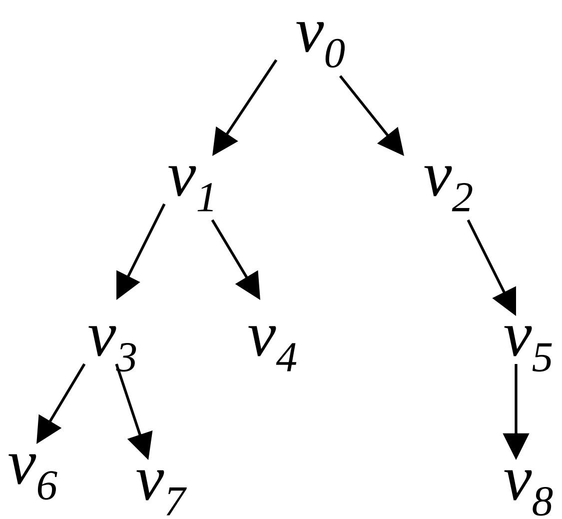
- *Every node v of positive depth has a parent of depth exactly one less*:
  - Let ($u$, ... , $v'$, $v$) be path of length $n$ = depth($v$) ending at $v$.
  - Then $v'$ is a parent of $v$.
  - Since ($u$, ... , $v'$) has length $n - 1$, depth($v'$) $\geq n - 1$.
  - Since also depth($v'$) $< n$ (because $v$ is a descendant of $v'$), depth($v'$) is exactly $n - 1$.
- *The nodes on any path are of increasing depth*.


Depth 0
Depth 1
Depth 2
Depth 3
$v_0$
$v_1$
$v_{10}$
$v_2$
$v_3$
$v_4$
$v_5$
$v_6$
$v_7$
$v_8$
$v_9$

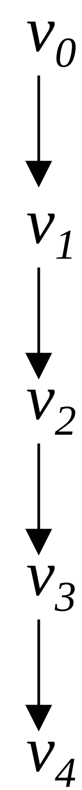
# Important special cases:

- A (*rooted*) *tree* is a DAG which
  - has unique depth 0 node (the *root*), *and*
  - every other node has in-degree 1
    - (i.e. has a unique parent, of depth one less than that of the node).
- A *binary tree* is a tree in which
  - every node has out-degree at most 2.
- A *linked list* is a tree in which
  - every node has out-degree at most 1
  - or equivalently, a DAG in which $\exists$ at most one node of each depth

binary tree




linked list



# Remarks on Depth Structure

- For *dynamic programming* algorithm
  - we need an order $v_1, v_2, \ldots, v_n$ for the vertices
    - (not a path!)

    in which parents appear before children.
  - From the above, *depth order*
    - (in which depth 0 nodes are listed first, then depth 1 nodes, etc.)

    is such an order.
  - In general there are many other such orders.
- We haven't given constructive procedure for finding the depths of all vertices.
  - For an arbitrary DAG, can be done in $O(|V| + |E|)$ time;
  - we omit algorithm, since for DAGs related to sequence analysis, the depth structure is obvious.

# Weighted Directed Graphs

- A *weighted directed graph* is
  - a directed graph ($V$, $E$) together with
  - a function $w$ from $E$ to the real numbers,
    - i.e. with a numerical *weight* $w(e)$ (which may be positive, negative, or 0) associated to each edge $e$.

A weighted DAG is called a WDAG.

- The (*sum*) *weight of a path* is defined to be the sum of the weights on the edges of the path.
- Similarly, the *product weight of a path* is the product of the edge weights
  - usually only consider this when all weights are non-negative.
- weight of a path P is written $w(P)$
- For a path of length 0 (i.e. consisting of a single vertex):
  - the sum weight is 0
  - the product weight is 1

# Highest Weight Paths on WDAGs

- *Problem*: find a path with the highest possible weight.
- *Solution*:
  - "Brute force" approach
    - i.e. simply enumerating all possible paths and comparing their weights

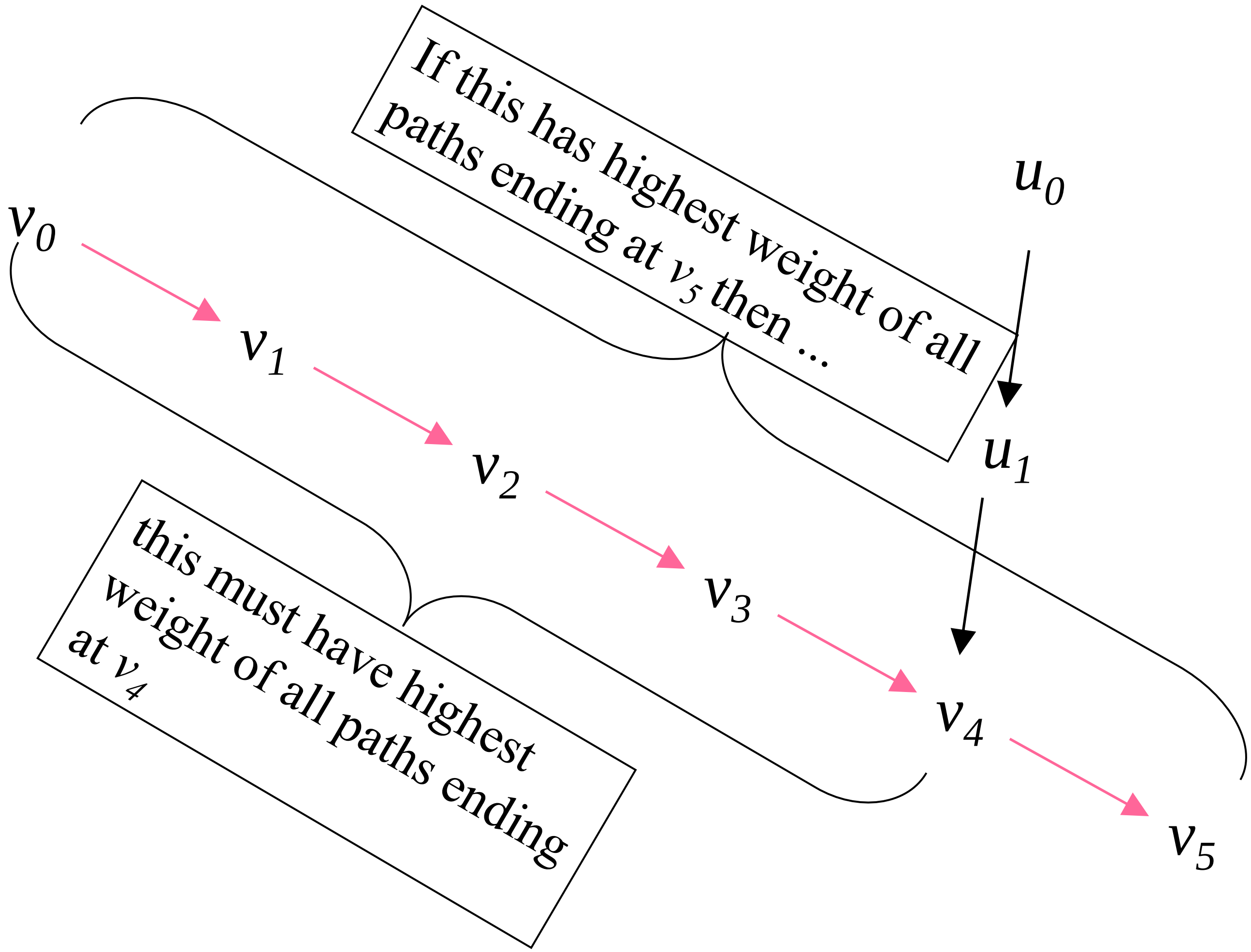
    is usually impractical (too many paths!)
  - Instead, use the method of *dynamic programming* ('The Fundamental Algorithm of Computational Biology').

- Let $P_n = (v_0, v_1, \ldots, v_n)$ be a path of highest weight.
- Then for each $k < n$, the sub-path $P_k = (v_0, v_1, \ldots, v_k)$ must have highest weight of all paths ending at $v_k$, because
  - *if* $Q = (u_0, u_1, \ldots, v_k)$ were another path ending at $v_k$ and having higher weight than $P_k$,
  - *then* the path $(Q, v_{k+1}, \ldots, v_n)$ would have weight

$$w((Q, v_{k+1}, \ldots, v_n)) = w(Q) + w((v_k, \ldots, v_n))$$
$$> w(P_k) + w((v_k, \ldots, v_n)) = w(P_n),$$

contradicting assumption that $P_n$ has highest weight.

# Subpaths of a highest-weight path can't be improved:



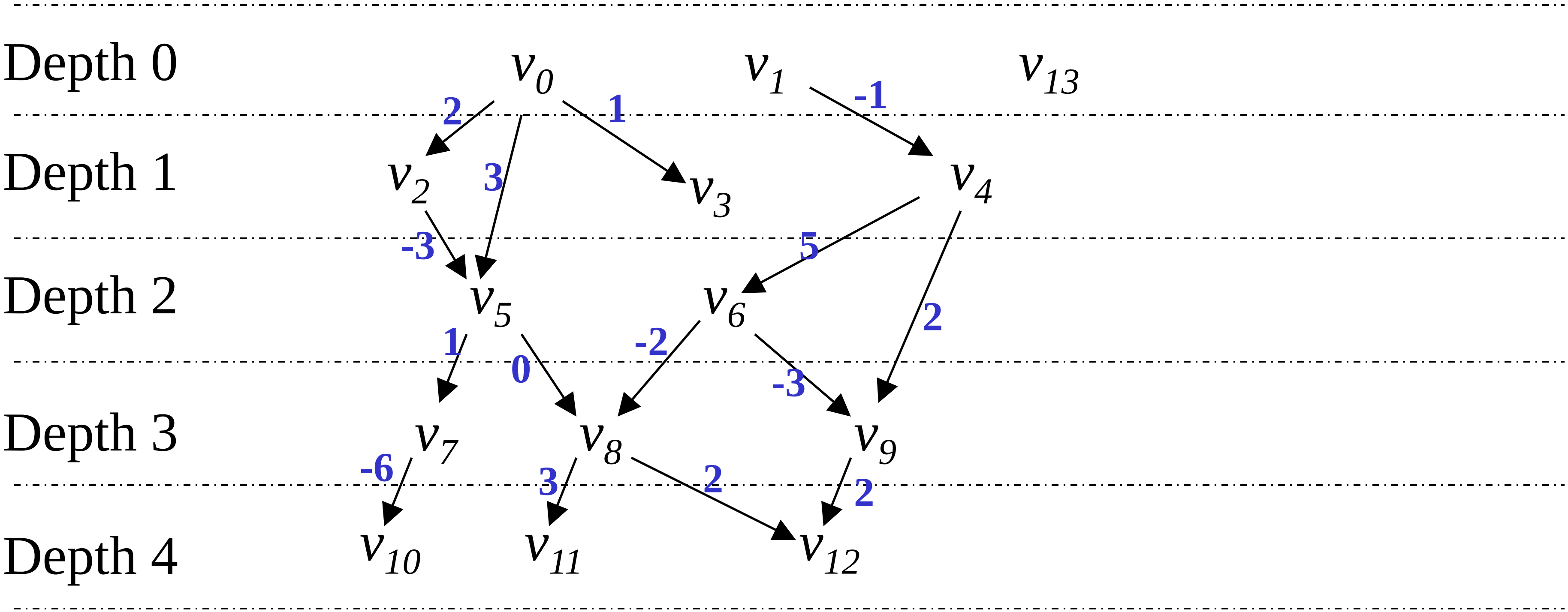
- So generalize the problem as follows:
- find, for *each* vertex $v$, the highest weight of all paths ending at $v$ – call this $w(v)$
- Can find $w(v)$ in single pass through $V$, as follows:
  - process the $v$ in depth order (*or any order in which parents precede children*)
  - if $v$ has no parents, $w(v) = 0$ (the only path ending at $v$ is $(v)$).
  - for any other $v$, except for the path $(v)$ (which has weight 0), any path ending at $v$ is of form $(v_0, v_1, \ldots, v_k, u, v)$. Then
  - $u$ is a parent of $v$, so $w(u)$ has already been computed, and

    $$w((v_0, v_1, \ldots, v_k, u, v)) \leq w(u) + w((u,v))$$

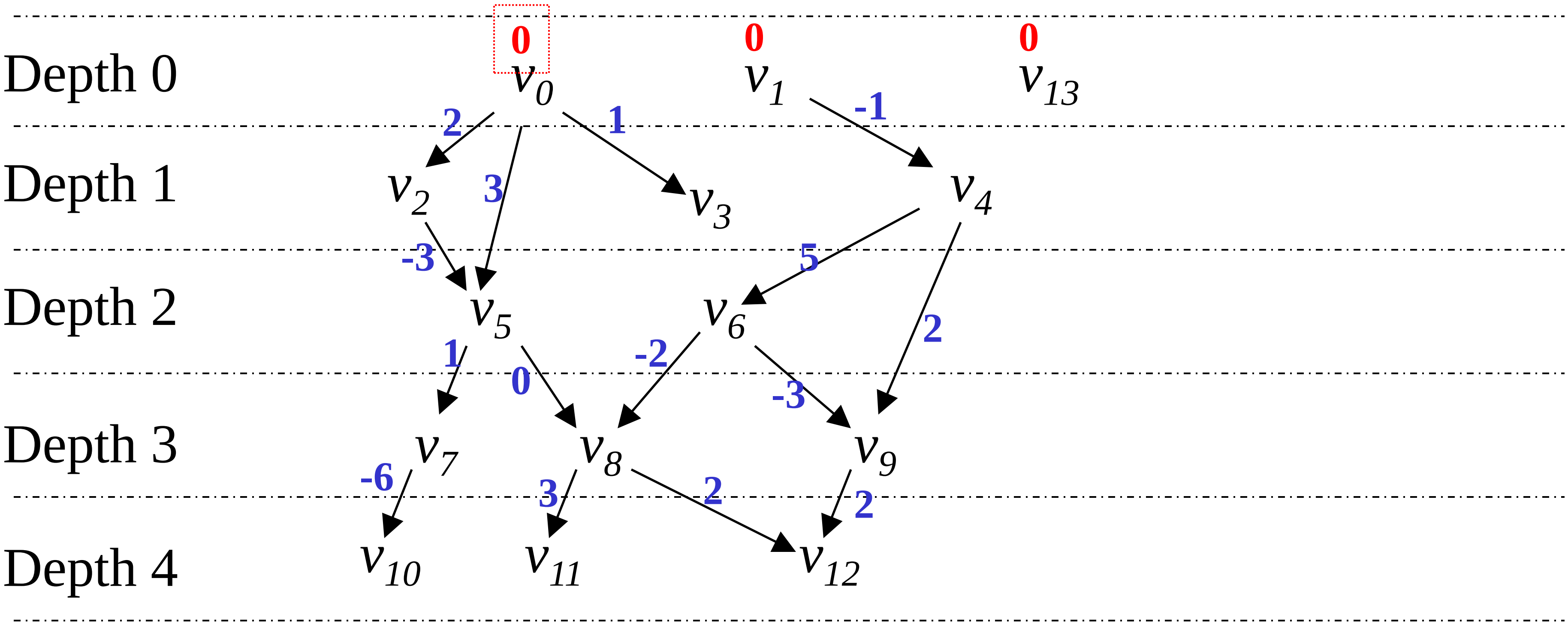
    with equality for an appropriate choice of $v_i$.
  - Therefore we may compute $w(v)$ as

$$w(v) = \max(0, \max_{u \in parents(v)} (w(u) + w((u,v))))$$

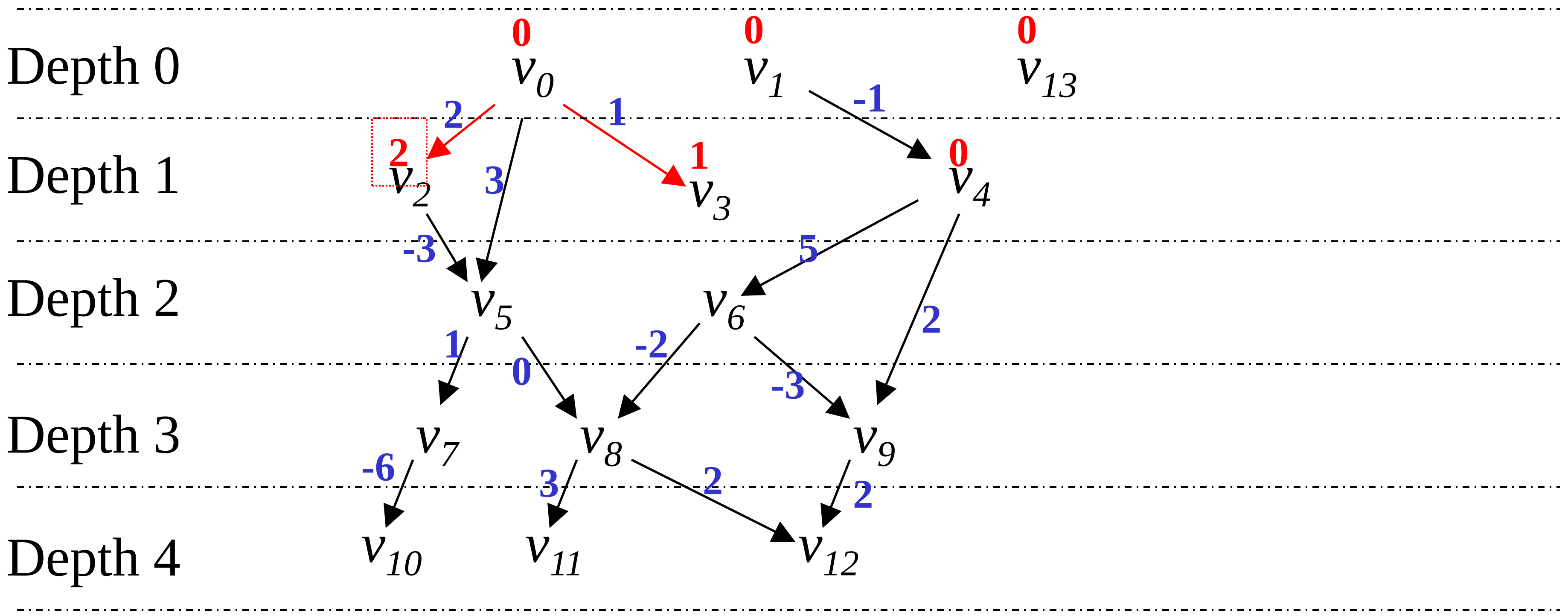
# Example


Depth 0
Depth 1
Depth 2
Depth 3
Depth 4
$v_0$
$v_1$
$v_{13}$
$v_2$
$v_3$
$v_4$
$v_5$
$v_6$
$v_7$
$v_8$
$v_9$
$v_{10}$
$v_{11}$
$v_{12}$
2
1
-1
3
-3
5
2
1
0
-2
-3
-6
3
2
2

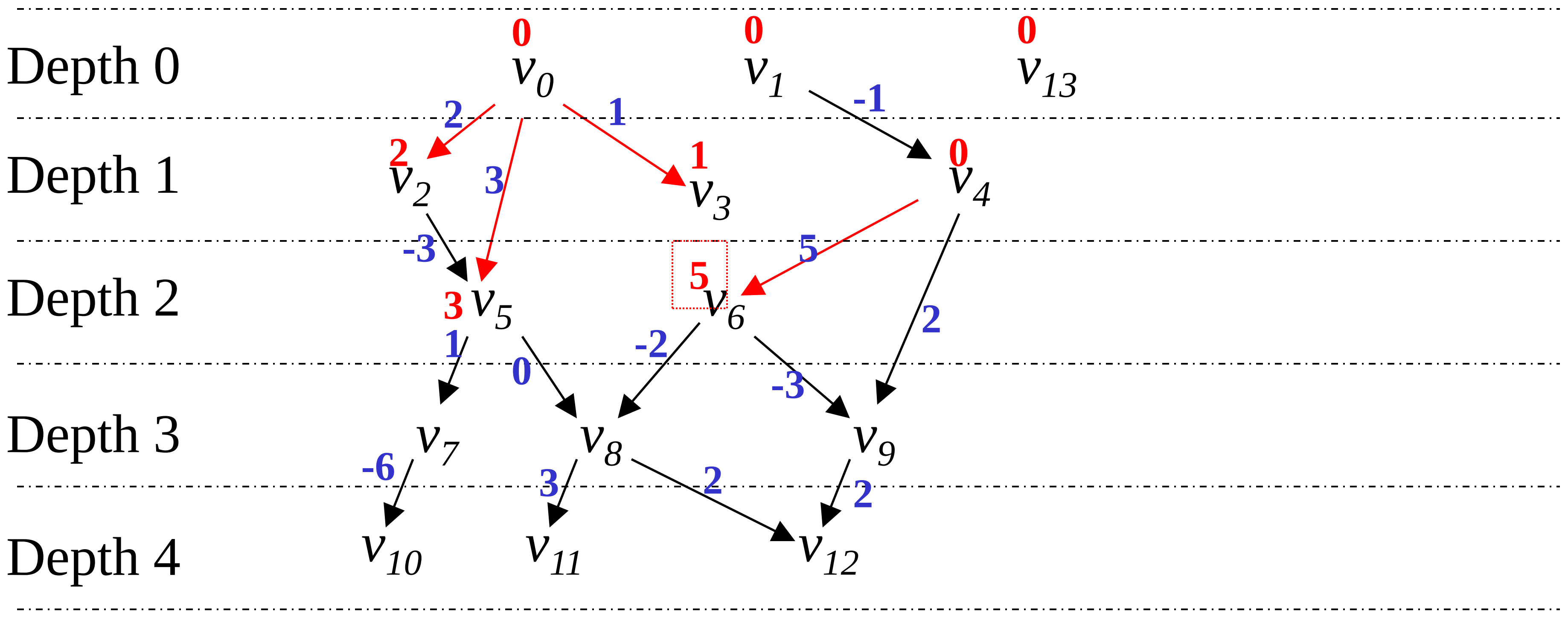
# $w(v)$ – depth 0 nodes



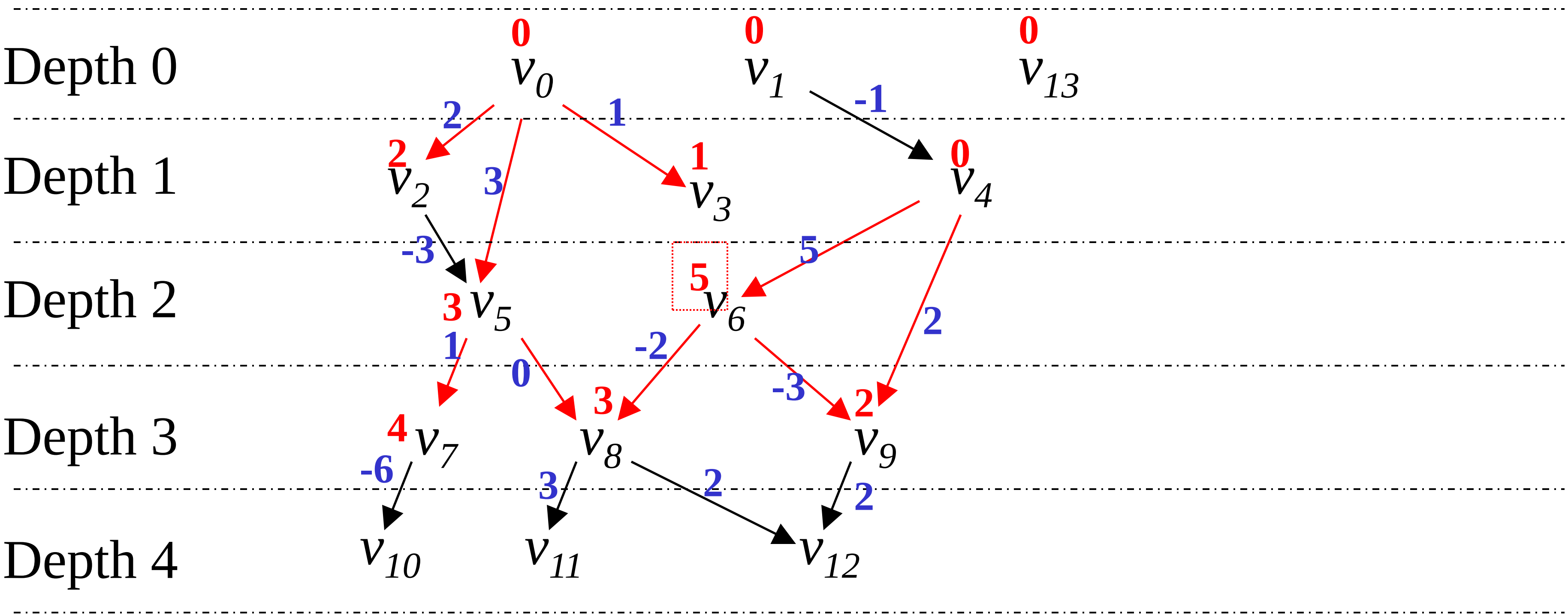
# $w(v)$ – depth 1 nodes



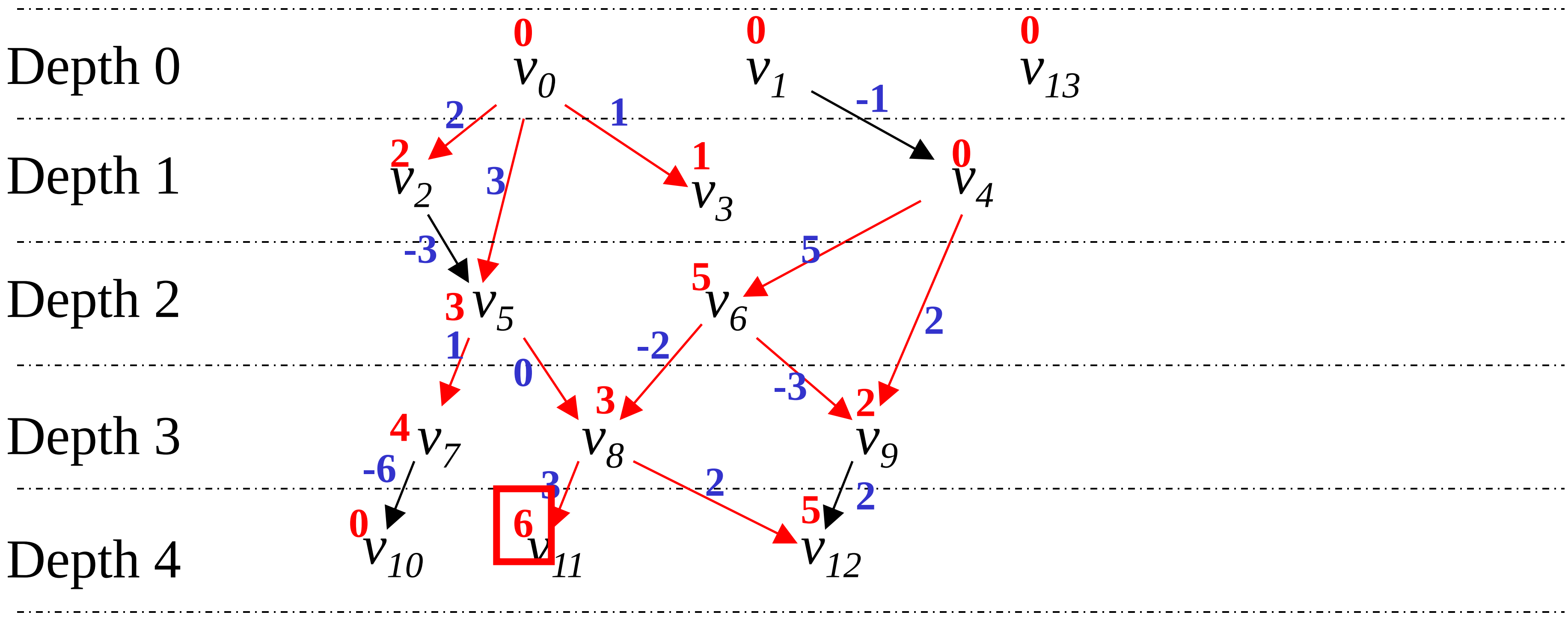
# $w(v)$ – depth 2 nodes



# $w(v)$ – depth 3 nodes



# $w(v)$ – depth 4 nodes



- To reconstruct best path, need "traceback" pointer to immediate predecessor of *v* in best path:

$$T(v) = \begin{cases} v & w(v) = 0 \\ \underset{u \in \text{parents}(v)}{\arg\max} \; (w(u) \; + \; w((u,v)) & w(v) \neq 0 \end{cases}$$

  - in preceding graph, $T(v)$ is the *parent* on *red edge* coming into *v*
    - if more than one such edge, pick one at random;
    - if no such edge, $T(v) = v$
- Sometimes useful to record *beginning* of best path:

$$B(v) = \begin{cases} v & w(v) = 0 \\ B(T(v)) & w(v) \neq 0 \end{cases}$$

- Then highest weight of any path in graph is

$$\max_{v \in V} (w(v))$$

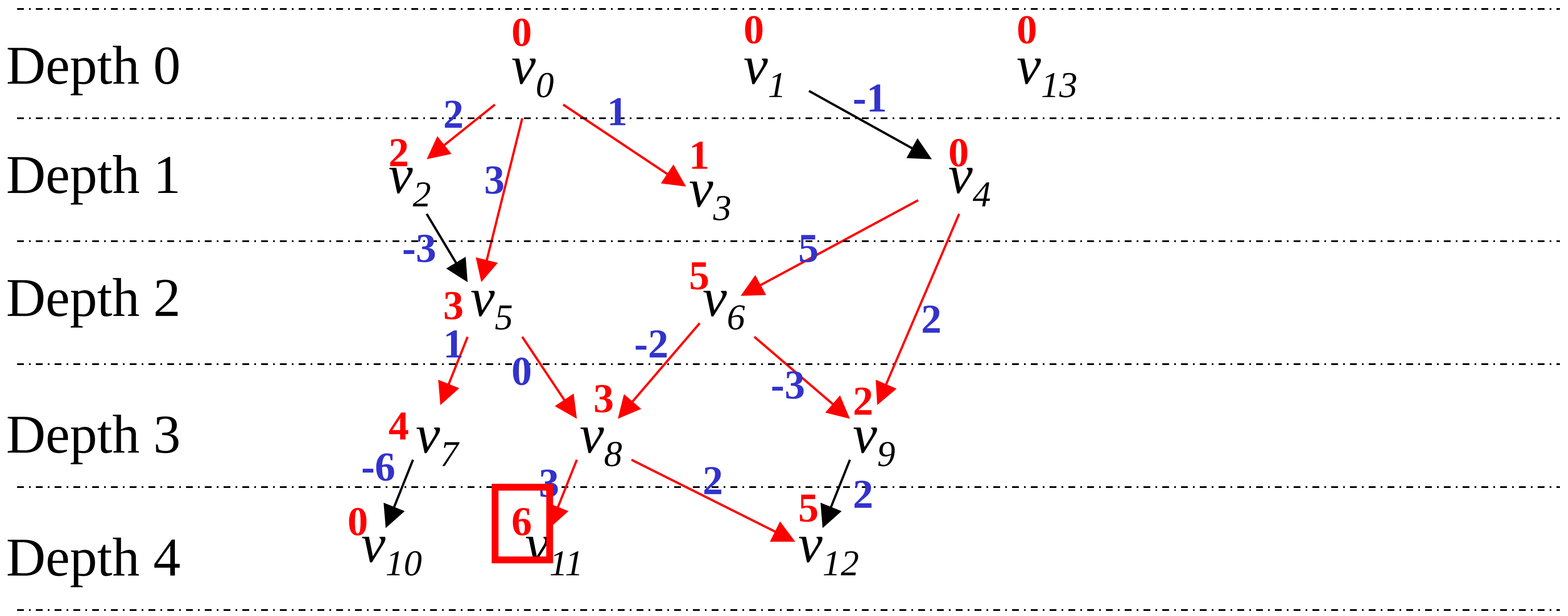
  - updated as each node is visited
    - indicated by in preceding graph –

  and so doesn't require additional pass through vertices

- if $u = \text{argmax}_{v \in V} (w(v))$, can reconstruct highest weight path by tracing back from $u$, using $T$:
  - path ends at $u$;
  - immediate predecessor of $u$ is $T(u)$;
  - predecessor of $T(u)$ is $T(T(u))$; etc.
  - stop when $T(v) = v$.

- In preceding example, highest weight is *6* and $u = v_{11}$

# Dynamic programming on WDAGs



# Complexity of Dynamic Programming

- Time to find a best path is $O(|E|+|V|)$:
  - in initial pass, visit each node, and each edge into that node: $O(|E|+|V|)$
  - in traceback, visit subset of nodes, and unique edge from each node: $O(|V|)$

(Complexity to find *all* highest weight paths can be higher)

For very large graphs, even $O(|E|+|V|)$ may be unacceptable!

- Space requirements:
  - If only want *weight* of best path, and beginning and end, then
    - don't need $T(v)$, and
    - only need retain $w(v)$ and $B(v)$ until have processed all children of $v$ (or when best path found so far ends at $v$).

    Space depends on graph structure, but usually $\ll O(|V|)$.
  - If want path itself, must store $T(v)\ \forall\ v$
    - space = $O(|V|)$
    - $\exists$ algorithms (for some graphs) to reduce this, but may take more time.

# Implementing Dynamic Programming in a Computer Program

- Storing entire graph has space complexity = $O(|V|+|E|)$
- If graph has regular structure, can often "create" and process vertices and edges on the fly, without storing in memory
  - cf. edit graph (to be defined later) for aligning sequences

# Same dynamic programming approach can be used to find:

1. Highest product weight path (if weights are $\geq 0$)
2. Highest weight path that
   - *starts* in particular subset $V'$ of vertices,
     - don't consider paths that start outside $V'$ :

       i.e. when computing $w(v)$, don't consider trivial path unless $v \in V'$
   - and/or *ends* in particular subset $V''$
     - only scan for the maximum $w(v)$ over $V''$
3. Sum of product weights of all paths ending at particular vertex
   - *sum* over all edges coming into $v$, instead of *maximizing*
   - this useful for probability calculations

- Will use the above variants later!