Today's Lecture

- Algorithm generalities / complexity
- Directed graphs, WDAGs

Genomes are big but computers are fast!

- Typical laptop clock speed: ~ 1 Ghz
  - Potentially billions of CPU instructions / sec
- Important practical consideration in dealing with genome-scale data sets: compared to CPU operations,
  - *non-cache memory accesses* are very slow (100s of cycles)
  - *disk accesses* are even slower (1000s of cycles)
  - for both, random (non-sequential) accesses are much slower than sequential accesses

Algorithms – Some General Remarks

- The most widely used algorithms are the oldest
  - e.g. sorting lists, traversing trees, dynamic programming.

The challenge in CMB is usually *not* finding *new* algorithms, but rather

  - finding ***biologically appropriate applications*** of old ones.

- Often prefer
  - suboptimal but easy-to-program algorithm over more optimal one
  - or space-efficient algorithm over time-efficient one.
- *Probabilities* are important in
  - interpreting results
  - guiding search

The most powerful analyses generally involve probabilistic models, rather than deterministic ones.

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.

Algorithmic Complexity (cont'd)

- 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 = $O(N^3)$.

Algorithmic Complexity (cont’d)

- 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.

Algorithmic Complexity (cont'd)

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

Algorithmic Complexity (cont'd)

- 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.

Algorithmic Complexity (cont'd)

- 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

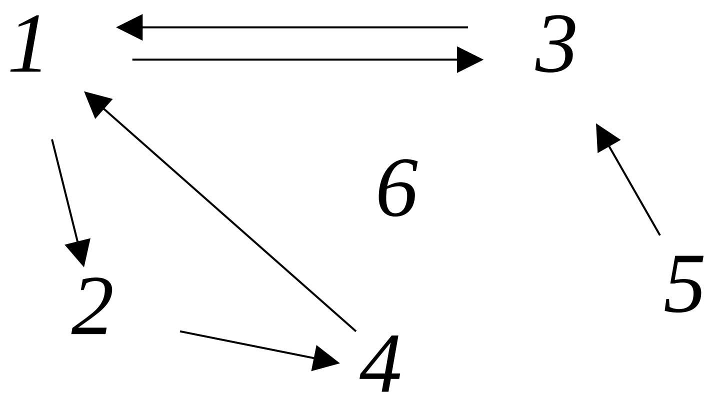
- we need *some* solution anyway, for data sets occurring in practice
- average *biologically relevant* case may be quite manageable

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.

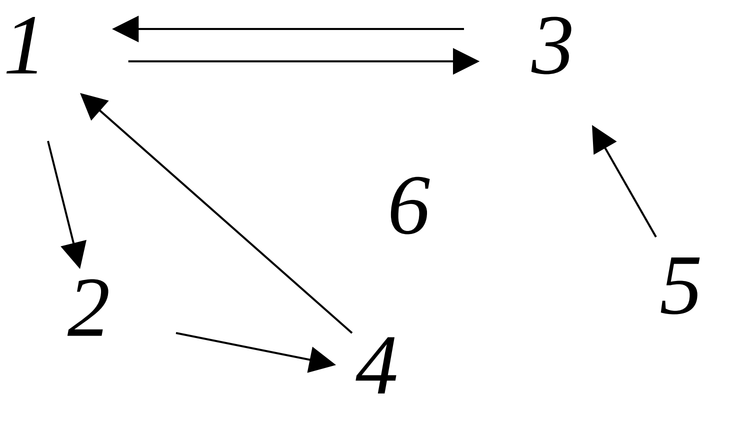
Example:

- $V = \{1,2,3,4,5,6\}$,
- $E = \{(1,2), (1,3), (2,4), (4,1), (5,3), (3,1)\}$
- 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.



Paths and Cycles (cont'd)

- 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;

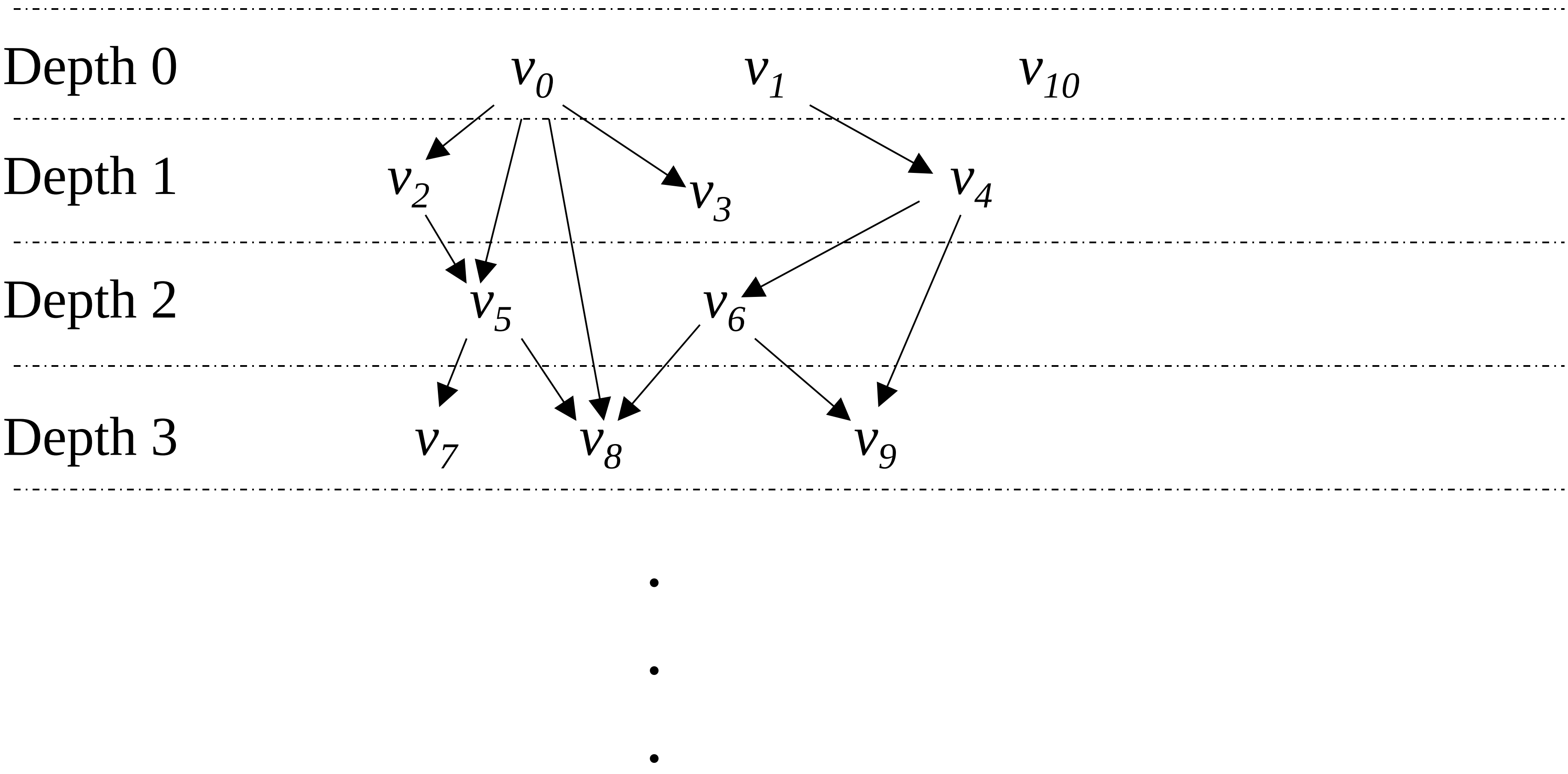
  by above, the depth is well-defined and $\leq |V| - 1$.
- *Every descendant w of a node v has higher depth than v*: If
  - $(u, \ldots, v)$ is path of length n = depth(v) ending at v, and
  - $(v, \ldots, w)$ is path from v to w,

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

Structure of DAGs (cont'd)

- *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*.

Structure of DAGs (cont'd)

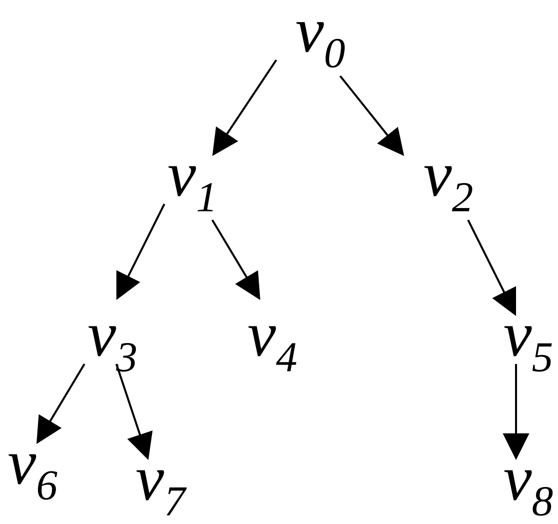


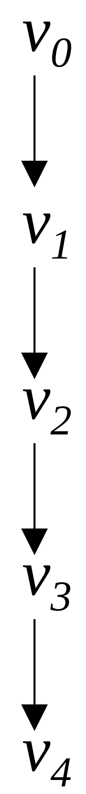
Important special cases:

- 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 ∃ at most one node of each depth

binary tree

linked list





Remarks on Depth Structure

- For *dynamic programming* algorithm
  - we need an order $v_1, v_2, ..., v_n$ 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