Discussion Section 4

- HW2 comments/HW3 questions
- Edit graph optimization
- Useful data structures

- Comment on HW2:
 - Hard coding an initial negative weight for non-start nodes is problematic
 - Any suggestions for what else you could do?

- Comment on HW2:
 - Hard coding an initial negative weight for non-start nodes is problematic
 - Any suggestions for what else you could do?
 - Iteratively remove nodes without parents except for the start node

- Comment on HW2:
 - Hard coding an initial negative weight for non-start nodes is problematic
 - Any suggestions for what else you could do?
 - Iteratively remove nodes without parents except for the start node
 - Give each node a flag indicating if the path to it includes the start node

- Create an edit graph for 3 sequences using the BLOSUM62 score matrix
- Output in the same format as HW2
- Run your highest-weight path program on the edit graph to find the highest scoring path (local alignment)

Protein 1: M R Y I I V Y ...

Protein 2: M L V V L A N ...

Protein 3: M Y V I L V Y ...

Protein 1:MRYIVY...Protein 2:MLVLAN...Protein 3:MYVILVY...

Protein 1: M R Y I I V Y ... Protein 2: M L V V L A N ... Protein 3: M Y V I L V Y ...

Possible edges:

Protein 1: M R Y I I V Y ... Protein 2: M L V V L A N ... Protein 3: M Y V I L V Y ...

Possible edges:

MMM MM- M-M M-- - MM - M- - - M

Protein 1:MRYIVY...Protein 2:MLVVLAN...Protein 3:MYVILVY...

Possible edges:

MMM MM- M-M M-- -MM -M- -M

Protein 1:MRYIVY...Protein 2:MLVVLAN...Protein 3:MYVILVY...

Possible edges:

MMM MM- M-M M-- - MM - M- - - M

RVI RV- R-I R-- -VI -V- --I









 Suppose scores are either 1 for a match (diagonal) or 0 for a skip (horizontal or vertical)



 Suppose scores are either 1 for a match (diagonal) or 0 for a skip (horizontal or vertical)



 Suppose scores are either 1 for a match (diagonal) or 0 for a skip (horizontal or vertical)





Maximum difference between these two values?

• By definition, Y >= X – min(horizontal transition score)



- By definition, $Y \ge X min(horizontal transition score)$
- What about Y > X + max(difference in transition scores)?



- By definition, $Y \ge X min(horizontal transition score)$
- What about Y > X + max(difference in transition scores)?
 - If the best path to Y came from the vertical or diagonal edge, then that came from some vertex Z in the same column as X



- By definition, $Y \ge X min(horizontal transition score)$
- What about Y > X + max(difference in transition scores)?
 - If the best path to Y came from the vertical or diagonal edge, then that came from some vertex Z in the same column as X
 - The vertical path from Z to X differs from the path from Z to Y by either



- By definition, $Y \ge X min(horizontal transition score)$
- What about Y > X + max(difference in transition scores)?
 - If the best path to Y came from the vertical or diagonal edge, then that came from some vertex Z in the same column as X
 - The vertical path from Z to X differs from the path from Z to Y by either
 - a single horizontal



- By definition, $Y \ge X min(horizontal transition score)$
- What about Y > X + max(difference in transition scores)?
 - If the best path to Y came from the vertical or diagonal edge, then that came from some vertex Z in the same column as X
 - The vertical path from Z to X differs from the path from Z to Y by either
 - a single horizontal
 - a diagonal edge that replaced a vertical edge



 Suppose scores are either 1 for a match (diagonal) or 0 for a skip (horizontal or vertical)



 Suppose scores are either 1 for a match (diagonal) or 0 for a skip (horizontal or vertical)


















The Edit Graph for a Pair of Sequences



The Edit Graph for a Pair of Sequences



The Edit Graph for a Pair of Sequences



• Given two sequences of length N and M

- Given two sequences of length N and M
- Use t-by-t blocks

- Given two sequences of length N and M
- Use t-by-t blocks
 - Reduces the dimensions to O(N/t * M/t)

- Given two sequences of length N and M
- Use t-by-t blocks
 - Reduces the dimensions to O(N/t * M/t)
 - For every block you compute O(t) new scores

- Given two sequences of length N and M
- Use t-by-t blocks
 - Reduces the dimensions to O(N/t * M/t)
 - For every block you compute O(t) new scores
 - So new time is O(NM/t) + time to precompute blocks

- Given two sequences of length N and M
- Use t-by-t blocks
 - Reduces the dimensions to O(N/t * M/t)
 - For every block you compute O(t) new scores
 - So new time is O(NM/t) + time to precompute blocks
 - Usually you choose t = O(log N) or O(log M), which you can show will give a total time of O(NM/log N) or O(NM/log M)

- Given two sequences of length N and M
- Use t-by-t blocks
 - Reduces the dimensions to O(N/t * M/t)
 - For every block you compute O(t) new scores
 - So new time is O(NM/t) + time to precompute blocks
 - Usually you choose t = O(log N) or O(log M), which you can show will give a total time of O(NM/log N) or O(NM/log M)
 - The exact value of t depends on the total number of possible transition scores

- Arrays
 - Fast, pointer math is easy

- Arrays
 - Fast, pointer math is easy
- Linked lists
 - Inserting/deleting/reordering is easy

- Arrays
 - Fast, pointer math is easy
- Linked lists
 - Inserting/deleting/reordering is easy
- Hash tables/maps
 - Good for looking up things

- Arrays
 - Fast, pointer math is easy
- Linked lists
 - Inserting/deleting/reordering is easy
- Hash tables/maps
 - Good for looking up things
- Trees
 - Useful for sorting/searching

- Arrays
 - Fast, pointer math is easy
- Linked lists
 - Inserting/deleting/reordering is easy
- Hash tables/maps
 - Good for looking up things
- Trees
 - Useful for sorting/searching
- Heaps
 - Keeping track of extreme values

- Arrays
 - Storing a sequence, accessing the N-th position
 - Many other data structures use an underlying array

- Arrays
 - Storing a sequence, accessing the N-th position
 - Many other data structures use an underlying array
- Linked lists
 - Graph searching (breadth-first)

- Arrays
 - Storing a sequence, accessing the N-th position
 - Many other data structures use an underlying array
- Linked lists
 - Graph searching (breadth-first)
- Hash tables/maps
 - Storing sample features
 - Counting k-mer frequency

- Arrays
 - Storing a sequence, accessing the N-th position
 - Many other data structures use an underlying array
- Linked lists
 - Graph searching (breadth-first)
- Hash tables/maps
 - Storing sample features
 - Counting k-mer frequency
- Trees
 - k-dimensional trees for nearest neighbor searching (PyCogent)

- Arrays
 - Storing a sequence, accessing the N-th position
 - Many other data structures use an underlying array
- Linked lists
 - Graph searching (breadth-first)
- Hash tables/maps
 - Storing sample features
 - Counting k-mer frequency
- Trees
 - k-dimensional trees for nearest neighbor searching (PyCogent)
- Heaps
 - Constructing a minimum spanning tree (Monocle does this, not sure if it uses a heap though)

• Getting the element at a particular index is fast

Contiguous Memory



















• Easier to modify than an array

• Easier to modify than an array



• Easier to modify than an array



5748

• Easier to modify than an array


Linked Lists

• Easier to modify than an array





































 Should generate uniformly distributed hash values

- Should generate uniformly distributed hash values
 - Why?

- Should generate uniformly distributed hash values
 - Why?
- Often used in cryptography to verify data

- Should generate uniformly distributed hash values
 - Why?
- Often used in cryptography to verify data
 - Difficult to reverse engineer a hash value to a matching input

- Should generate uniformly distributed hash values
 - Why?
- Often used in cryptography to verify data
 - Difficult to reverse engineer a hash value to a matching input

size_t myhash(const string& s)

```
// Inspired by xkcd comic 153 and the Cha Cha slide
```

```
size_t hash = 0;
```

```
// This time we're gonna get funky
// (Convert the string to a number and do some strange things
to it)
// (Inspired by Jenkins one-at-a-time hash function (found on
Wikipedia))
for (size t i = 0; i < s.size(); ++i) {
   hash += s[i];
   hash += (hash << 8); // Two measure of 4 is 8 beats
    hash ^= (hash >> 5); // Funky has 5 letters
// Everybody clap your hands
// Clap clap clap clap your hands
// Clap clap clap clap your hands
// (Flip the bits)
hash = ~hash;
// Alright we gonna do the basic steps
// Slide to the left
// (The Cha Cha slide is in 4)
hash = hash << (hash % 4);
// Slide to the right
// (But it really should be in 3)
hash = hash >> (hash % 3);
// Take it back now y'all
// (Subtract - No one wants to walk back that far, so 1)
hash -= (hash >> 1);
// One hop this time
// (Bunnies hop and bunnies eat carrots. Some bunnies can hop
5 feet)
hash ^= (hash % 5);
// Right foot lets stomp
// (Add, make it dependent on the hash function for more
randomness
```

Trees

Good for searching ranges



Trees

Good for searching ranges



Good for searching ranges



Good for searching ranges



Good for searching ranges



Heaps

• Good for keeping track of extreme values



Heaps

• Good for keeping track of extreme values

What's the largest value?



Trees and Heaps

• Similar in structure, but different rules



Operation

	Access	Search	Insert	Delete
Array	O(1)	O(N)	O(1) or O(N)	O(1) or O(N)
Linked List	O(N)	O(N)	O(1) or O(N)	O(1) or O(N)
Hash Map	N/A	O(1)	O(1)*	O(1)*
Tree	O(log N)	O(log N)	O(log N)	O(log N)

Data Structure

Operation

	Access	Search	Insert	Delete
Array	O(1)	O(N)	O(1) or O(N)	O(1) or O(N)
Linked List	O(N)	O(N)	O(1) or O(N)	O(1) or O(N)
Hash Map	N/A	O(1)	O(1)*	O(1)*
Tree	O(log N)	O(log N)	O(log N)	O(log N)

* Actual worst case is O(N), but 'amortized' it's O(1)

Data Structure

Operation

	Access	Search	Insert	Delete
Array	O(1)	O(N)	O(1) or O(N)	O(1) or O(N)
Linked List	O(N)	O(N)	O(1) or O(N)	O(1) or O(N)
Hash Map	N/A	O(1)	O(1)*	O(1)*
Tree	O(log N)	O(log N)	O(log N)	O(log N)

* Actual worst case is O(N), but 'amortized' it's O(1)

Heaps are specialized for find-min/max = O(1), deletemin/max = $O(\log N)$, and insert = $O(\log N)$

Data Structure















How much time does this take?

How much time does this take?

- If sequence 1 has length N and sequence 2 has length M
 - First pass: NM time (update N nodes M times)
- If sequence 1 has length N and sequence 2 has length M
 - First pass: NM time (update N nodes M times)
 - Second pass: (NM)/2 time (half of the area)

- If sequence 1 has length N and sequence 2 has length M
 - First pass: NM time (update N nodes M times)
 - Second pass: (NM)/2 time (half of the area)
 - Third pass: (NM)/4 (quarter of the area)

- If sequence 1 has length N and sequence 2 has length M
 - First pass: NM time (update N nodes M times)
 - Second pass: (NM)/2 time (half of the area)
 - Third pass: (NM)/4 (quarter of the area)
 - And so on

- If sequence 1 has length N and sequence 2 has length M
 - First pass: NM time (update N nodes M times)
 - Second pass: (NM)/2 time (half of the area)
 - Third pass: (NM)/4 (quarter of the area)
 - And so on
 - 1 + 1/2 + 1/4 + ... = 2, so 2NM or O(NM)

- If sequence 1 has length N and sequence 2 has length M
 - First pass: NM time (update N nodes M times)
 - Second pass: (NM)/2 time (half of the area)
 - Third pass: (NM)/4 (quarter of the area)
 - And so on
 - 1 + 1/2 + 1/4 + ... = 2, so 2NM or O(NM)
 - Awesome! That's the same asymptotic time as before!

- If sequence 1 has length N and sequence 2 has length M
 - First pass: NM time (update N nodes M times)
 - Second pass: (NM)/2 time (half of the area)
 - Third pass: (NM)/4 (quarter of the area)
 - And so on
 - 1 + 1/2 + 1/4 + ... = 2, so 2NM or O(NM)
 - Awesome! That's the same asymptotic time as before!
 - But can we do better?