Quiz Section Week 5
April 26, 2018

Review
Topics (not guaranteed to be comprehensive!)

• Alignments
  • Reasons to align sequences
  • Needleman-Wunsch algorithm
  • Smith-Waterman algorithm
  • Effects of parameter variation (including gap penalties)
  • Testing for statistical significance of an alignment

• Phylogenetic trees
  • Rooted and unrooted topologies
  • Defining the best tree with UPGMA and Neighbor Joining
  • Concept of parsimony
  • Fitch algorithm: quantifying how parsimonious a tree is, assigning internal states
  • Finding the most parsimonious tree: Hill climbing w/ Nearest-Neighbor interchanges
  • Bootstrapping to quantify confidence in tree partitions

• Clustering
  • Defining a clustering problem
  • Hierarchical clustering
    • Impact of using single/complete/average linkage
  • K-means: Objective and algorithm

• Networks
  • Reasons to make and analyze networks
  • Basic network definitions
  • Dijkstra’s Algorithm
  • Network motifs and their uses
Topics (not guaranteed to be comprehensive!)

- Programming
  - Variables and types
  - String methods
  - List methods
  - Conditionals
  - Loops
  - Functions
Phylogenetic trees

UPGMA/Neighbor Joining
• Define the best tree: based on distance between leaves
• Find the best tree using: polynomial time algorithm to construct the best tree from a distance matrix

Parsimony approach
• Define the best tree: Minimum # of mutations required to traverse tree
• Find the best tree: by enumerating all trees (exhaustive search), or by heuristic approach like Nearest-Neighbor Interchange Hill-Climbing
Tree topologies

Are these the same tree?
Tree topologies

Are these the same tree?

How about these?
Counting tree topologies

For N leaves

# of unrooted topologies = 3*5*7*…*(2N-5)
# of branches = 2N-3

E.g. an unrooted tree with 6 nodes

How many different topologies?
Counting tree topologies

For N leaves

# of unrooted topologies = 3*5*7*...*(2N-5)
# of branches = 2N-3

E.g. an unrooted tree with 6 nodes

How many different topologies?
3*5*7 = 105
Counting tree topologies

For N leaves

# of unrooted topologies = 3*5*7*...*(2N-5)
# of branches = 2N-3

E.g. an unrooted tree with 6 nodes

How many different topologies?
3*5*7 = 105

How many branches?
Counting tree topologies

For N leaves

# of unrooted topologies = 3*5*7*...*(2N-5)
# of branches = 2N-3

E.g. an unrooted tree with 6 nodes

How many different topologies?
3*5*7 = \textbf{105}

How many branches?
2N-3 = \textbf{9}
Counting tree topologies

For N leaves

# of unrooted topologies = $3 \times 5 \times 7 \times \ldots \times (2N-5)$
# of branches = $2N-3$

E.g. an unrooted tree with 6 nodes

How many different topologies? $3 \times 5 \times 7 = 105$
How many branches? $2N-3 = 9$
The root could be placed on any branch

E.g. an unrooted tree with 6 nodes

How many different topologies?
3*5*7 = 105

How many branches?
2N-3 = 9
The root could be placed on any branch

E.g. an unrooted tree with 6 nodes

How many different topologies?
3*5*7 = 105

How many branches?
2N-3 = 9

Total options = 105*9
= 945
Nearest Neighbor Interchange trees

For each internal branch generate two variant trees that swap the relationships of the four outside branches.
Nearest Neighbor Interchange trees

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Nearest Neighbor Interchange trees

For each internal branch generate two variant trees that swap the relationships of the four outside branches.
NN Practice: Draw both interchanges from swapping this branch
NN Practice: Draw both interchanges from swapping this branch.
Fitch algorithm practice
Fitch algorithm practice: bottom-up
Fitch algorithm practice: top-down
Hierarchical clustering with complete linkage example

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Dijkstra’s Algorithm
Another data type: Dictionaries

• a data structure that consists of an unordered set of \textit{key}: \textit{value} pairs
  • think of as \textit{word}: \textit{definition} pairs!

Q: How could we encode the entire genetic code?
Dictionaries: How could we encode the entire genetic code?

```python
>>> genetic_code = {"ATG": "Start", "TGA": "Stop", "TAG": "Stop"}
>>> genetic_code["TAA"] = "Stop"
>>> genetic_code.get("TGA")
 'Stop'
>>> genetic_code["TGA"]
 'Stop'
>>> genetic_code.get("sss") #nothing or 'None' if not defined
>>> genetic_code["sss"]
KeyError: 'ttt'
```
Creating a dictionary

# create an empty dictionary
myDict = {}

# create a dictionary with three entries
myDict = {"Curly":4123, "Larry":2057, "Moe":1122}

# add another entry
myDict["Shemp"] = 2232

# change Moe's phone number
myDict["Moe"] = 4040

# delete Moe from dictionary
del myDict["Moe"]
Rules for dictionaries

• The first item is a **key**.

• Each key can appear only once in a dict.

• A key must be an **immutable** object: number, string, or tuple.

• Lists cannot be keys (they are mutable).

• The key is the item you'll use to do look-ups.

• Each **key** is paired with a **value**.
Some useful dictionary methods

```python
>>> genetic_code.items()
[('TAA', 'Stop'), ('TGA', 'Stop'), ('TAG', 'Stop'), ('ATG', 'Start')]

>>> genetic_code.keys()
['TAA', 'TGA', 'TAG', 'ATG']

>>> genetic_code.values()
['Stop', 'Stop', 'Stop', 'Start']
```
Another use of dictionaries: store counts of named elements

Example: Calculate # of each nucleotide in a sequence

```python
sequence = "GACCCT"
nuc_counts = {'A': 0, 'C': 0, 'T':0, 'G': 0}
for nuc in sequence:
    #Add to the count for the given nucleotide
```
Another common use of dictionaries: store counts of named elements

Calculate # of each nucleotide in a sequence

```python
sequence = "GACCCCT"
nuc_counts = {'A': 0, 'C': 0, 'T': 0, 'G': 0}
for nuc in sequence:
    nuc_counts[nuc] = nuc_counts[nuc] + 1
```
Traversing a dictionary by key

```python
# birthdays is a dictionary with names as keys
# and birth dates as values

for person in birthdays.keys():
    print "Send", person, "a card on", birthdays[person]
```
dictionary basics

D = {'dna': 'T', 'rna': 'U'}  # dictionary literal assignment
D = {}  # make an empty dictionary
D.keys()  # get the keys as a list
D.values()  # get the values as a list
D['dna']  # get a value based on key
D['dna'] = 'T'  # set a key:value pair
del D['dna']  # delete a key:value pair
'dna' in D  # True if key 'dna' is found in D, else False

The keys must be immutable objects (e.g. string, int, tuple).

The values can be anything (including a list or another dictionary).

The order of elements in the list returned by D.keys() or D.values() is arbitrary (effectively random).

Each key can be stored only once in the dictionary, so if you set the value for a key for a second time it OVERWRITES the old value!