Genome Sciences 373 Genome Informatics

Quiz Section #2

April 5, 2016

Today

- Local alignment review
- Debugging strategies
- Python: data types review, input/output, if/else, for loops

Reminder: Office hours Mondays 4:30-5:30, Foege S-040

Additional background question: stats and probability background?

- Can you define a p-value right now?
- Can you define null and alternative hypotheses right now?
- Are you familiar with the multiple hypothesis testing problem?

Local alignment DP

Substitution matrix:

	A	C	G	T
A	10	-5	0	-5
C	-5	10	-5	0
G	0	-5	10	-5
T	-5	0	-5	10

- Align sequence x and y.
- F is the DP matrix; s is the substitution matrix; d is the linear gap penalty.

$$F(0,0) = 0$$

Score of a match (or mismatch)

$$F(i,j) = \max \begin{cases} F(i-1, j-1) + s(x_i, y_j) \\ F(i-1, j) + d \\ F(i, j-1) + d \\ 0 \end{cases}$$

Adding a gap to one of the sequences

(corresponds to start of alignment)

Local alignment example

Substitution matrix:

	A	C	G	T
A	10	-5	0	-5
C	-5	10	-5	0
G	0	-5	10	-5
T	-5	0	-5	10

$$F(0,0) = 0$$

$$F(i,j) = \max \begin{cases} F(i-1, j-1) + s(x_i, y_j) \\ F(i-1, j) + d \\ F(i, j-1) + d \\ 0 \end{cases}$$

(corresponds to start of alignment)

		G	A	G	T	A
	0	?				
A						
G						
T						
T						
A						

Linear gap penalty d = -4

Local alignment example

Substitution matrix:

	A	C	G	T
A	10	-5	0	-5
C	-5	10	-5	0
G	0	-5	10	-5
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(corresponds to start of alignment)

		G	A	G	T	A
	0	0	0	0	0	0
A	0	?				
G	0					
T	0					
T	0					
A	0					

Linear gap penalty d = -4

Local alignment example

Substitution matrix:

	A	C	G	T
A	10	-5	0	-5
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(corresponds to start of alignment)

		G	A	G	T	A
	0	0	0	0	0	0
A	0	0				
G	0	?				
T	0					
T	0					
A	0					

Linear gap penalty d = -4

Local alignment example

Substitution matrix:

	A	C	G	T
A	10	-5	0	-5
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$$F(0,0) = 0$$

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(corresponds to start of alignment)

		G	A	G	T	A
	0	0	0	0	0	0
A	0	0				
G	0	10				
T	0	6				
T	0	2				
A	0	?				

Linear gap penalty d = -4

Local alignment example

Substitution matrix:

	A	C	G	T
A	10	-5	0	-5
C	-5	10	-5	0
G	0	-5	10	-5
T	-5	0	-5	10

$$F(0,0) = 0$$

$$F(i,j) = \max \begin{cases} F(i-1, j-1) + s(x_i, y_j) \\ F(i-1, j) + d \\ F(i, j-1) + d \\ 0 \end{cases}$$

(corresponds to start of alignment)

		G	A	G	T	A
	0	0	0	0	0	0
A	0	0	10	6	2	10
G	0	10	6	20	16	12
T	0	6	6	16	30	26
T	0	2	2	12		
A	0	0	12	8	22	36

Maximum score

Local alignment example

Substitution matrix:

	A	C	G	T
A	10	-5	0	-5
C	-5	10	-5	0
G	0	-5	10	-5
T	-5	0	-5	10

GAGT-A
AGTTA

		G	A	G	T	A
	0	0	0	0	0	0
A	0	0	10	6	2	10
G	0	10	6	20	16	12
T	0	6	6	16	30	26
T	0	2	2	12	26	25
A	0	0	12	8	22	36

When local and global alignments differ

We want to align two sequences:

AGTTA

AGAGTATTA

Optimal Local Alignment: -4

AGAG–TATTA
AGTTA

Optimal global alignment

4 gaps: -16

AGAGTATTA
AG–––––TTA

Suboptimal global alignment with 6 gaps: -24

AGAG–TATTA
- -AGTTA- - -

So many deletions/insertions might be implausible

Reminder: the alignment parameters are a model of mutational processes

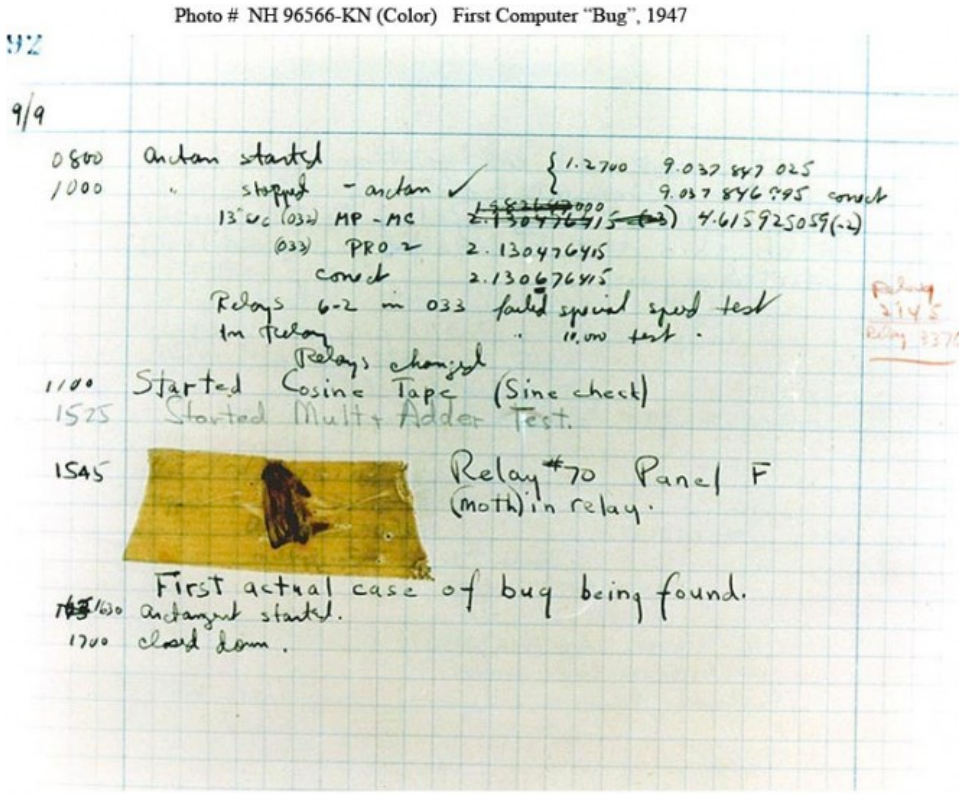
Substitution matrix:

	A	C	G	T
A	10	-5	0	-5
C	-5	10	-5	0
G	0	-5	10	-5
T	-5	0	-5	10

AGAG–TATTA
AGTTA

- What kinds of mutations?
- How do we know whether to trust the mutations described by an alignment?

Debugging your code



Big picture tips to keep in mind

- Start small! Work in pieces!
- Regular print statements to check your progress
- Read error messages…
- Use toy examples to check your work
- Be patient!
- When the above fails, Google/Stack Overflow *may* be helpful...

Python error types

- ParseError = Syntax errors - look for formatting problems
- TypeError, ValueError = check your data types
- NameError = check your variable names
- IndexError = check your list indices

Debugging workflows

- The classic: text editor + terminal
- Run chunks in a Jupyter notebook
- IDEs: PyCharm, Spyder

Here's a broken program

- Copy and paste it, save as startCodon.py
  - What's it doing?

```
x = 'atggataccagg'
print "x is", x

start_codon = 'atg'
if start_codon = x[0:3]:
    print 'Yes!'
else:
    print 'No!'
```

Here's a broken program

```
x = 'atggataccagg'
print "x is", x

start_codon = 'atg'
if start_codon == x[0:3]:
    print 'Yes!'
else:
    print 'No!'
```

There's another problem!

```
x = 'atggataccagg'
print x
print "first 3 characters in x are",
x[0:3]

start_codon = 'atg '
print "start_codon is ", start_codon

if start_codon = x[0:3]:
    print 'Yes!'
else:
    print 'No!'
```

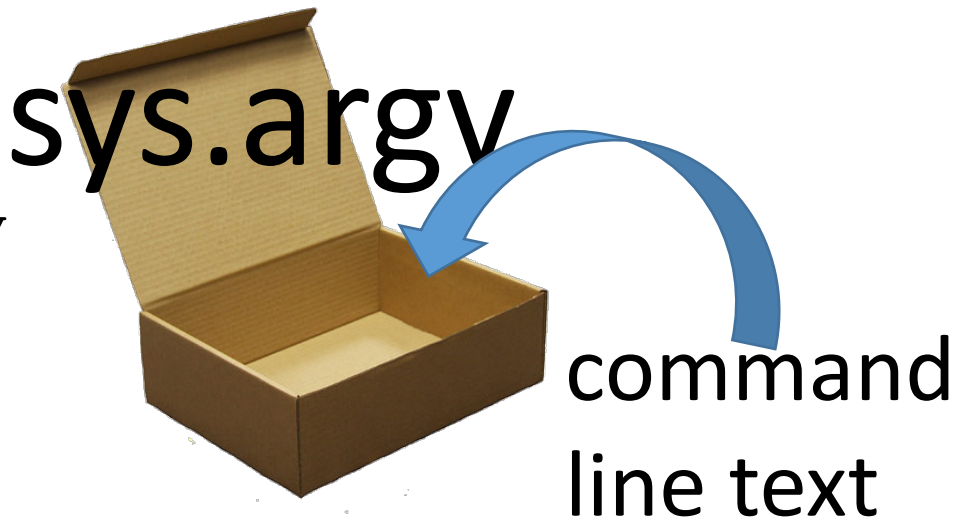
There's another problem!

```
x = 'atggataccagg'
print x
print "first 3 characters in x are",
x[0:3]

start_codon = 'atg'
print "start_codon is ", start_codon

if start_codon == x[0:3]:
    print 'Yes!'
else:
    print 'No!'
```

Let’s learn more Python!

Taking input from the terminal command line

```
# This is inputs.py
import sys
print sys.argv
print sys.argv[1]
```



python inputs.py apple banana

```
['inputs.py','apple', 'banana']
'apple'
```

sys.argv only contains strings, so to get numbers, you need to **change the variable's type**

python inputs.py 1.1 2

```
import sys
print sys.argv
print sys.argv[1]
print type(sys.argv[1])
print float(sys.argv[1])
print int(sys.argv[2])
print int(sys.argv[1])
```

sys.argv only contains strings, so to get numbers, you need to **change the variable's type**

python inputs.py 1.1 2

```
import sys
print sys.argv
print sys.argv[1]
print type(sys.argv[1])
print float(sys.argv[1])
print int(sys.argv[2])
print int(float(sys.argv[1]))
```

One more example

python minus.py 3.3 1.1

```
import sys
print sys.argv
print sys.argv[1] – sys.argv[2]
```

```
['minus.py','3.3', '1.1']
TypeError: unsupported operand
type(s) for -: 'str' and 'str'
```

One more example

python minus.py 3.3 1.1

```
import sys
print sys.argv
print float(sys.argv[1])-
float(sys.argv[2])
```

```
['minus.py','3.3', '1.1']
2.2
```

Review: If/else statements

```
x = 4

if x == 5:
    print 'x is 5!'
elif x == 6:
    print 'x is 6!'
else:
    print 'x is neither 5 nor
6!'
```

Review: If/else statements

Note: Indents are important!!

```
x = 5
y = 7

if x == 5:
    print 'x is 5!'
    if y == 7:
        print 'x is 5 and y is 7!'
    else:
        print 'x is 5 and y is not 7!'
else:
    print 'x is not 5!'
```

Review: If/else statements

Note: Indents are important!!

```
x = 5
y = 7

if x == 5:
    print 'x is 5!'
    if y == 7:
        print 'x is 5 and y is 7!'
    else:
        print 'x is 5 and y is not 7!'
else:
    print 'x is not 5!'
```

A block

A block inside a block (nested)

Example

```
x = [ 1, 3, 2]
```

From a list x containing 3 numbers, print the number with the smallest value

```
smallest_value = x[0]
```

```
print smallest_value
```

Example

```
x = [ 1, 3, 2]
```

From a list x containing 3 numbers, print the number with the smallest value

```
smallest_value = x[0]
if x[1] < smallest_value:
    smallest_value = x[1]
if x[2] < smallest_value:
    smallest_value = x[2]
print smallest_value
```