Essential Computing for Bioinformatics

Lecture 4

High-level Programming with Python

Controlling the flow of your program

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Reference: How to Think Like a Computer Scientist: Learning with Python

Essential Computing for Bioinformatics

- The following material is the result of a curriculum development effort to provide a set of courses to support bioinformatics efforts involving students from the biological sciences, computer science, and mathematics departments. They have been developed as a part of the NIH funded project “Assisting Bioinformatics Efforts at Minority Schools” (2T36 GM008789). The people involved with the curriculum development effort include:

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- Dr. Satish Bhalla, Johnson C. Smith University.

- Most recent versions of these presentations can be found at http://marc.psc.edu/

Outline

- Basics of Functions
- Decision statements
- Recursion
- Iteration statements

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Built-in Functions

```
>>> import math
>>> decibel = math.log10 (17.0)
>>> angle = 1.5
>>> height = math.sin(angle)
>>> degrees = 45
>>> angle = degrees * 2 * math.pi / 360.0
>>> math.sin(angle)
0.707106781187
```

To convert from degrees to radians, divide by 360 and multiply by 2*pi

Can you avoid having to write the formula to convert degrees to radians every time?

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Defining Your Own Functions

```
def <NAME> ( <LIST OF PARAMETERS> ):
        <STATEMENTS>
```

```
import math
def radians(degrees):
    result = degrees * 2 * math.pi / 360.0
    return(result)
```

```
>>> def radians(degrees):
...     result=degrees * 2 * math.pi / 360.0
...     return(result)
...

>>> radians(45)
0.7853981633974483
>>> radians(180)
3.141592653589793
```

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Monolithic Code

```
From string import *

cds = “atgagtgaacgtctgagcattaccccgctggggccgtatatc”

gc = float(count(cds, 'g') + count(cds, 'c'))/ len(cds)

print gc
```

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```
def gcCount(sequence):
        gc = float(count(sequence, 'g') + count(sequence, 'c'))/ len(sequence)
        print gc
```

```
>>> gcCount(“actgaccgggat”)
```

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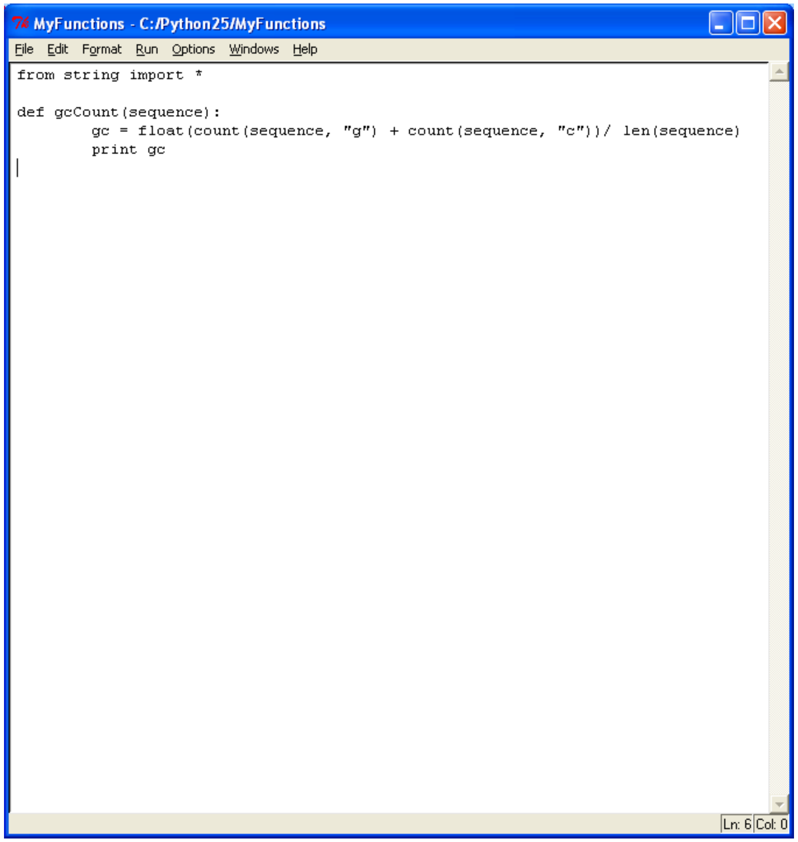
Step 2: Add function to script file



```
from string import *

def gcCount(sequence):
        gc = float(count(sequence, "g") + count(sequence, "c"))/ len(sequence)
        print gc
```

- *Save script in a file*
- *Re-load when you want to use the functions*
- *No need to retype your functions*
- *Keep a single group of related functions and declarations in each file*

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- Powerful mechanism for creating building blocks
- Code reuse
- Modularity
- Abstraction (i.e. hide (or forget) irrelevant detail)

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Function Design Guidelines

- Should have a single well defined 'contract'
  - E.g. Return the gc-value of a sequence
- Contract should be easy to understand and remember
- Should be as general as possible
- Should be as efficient as possible
- Should not mix calculations with I/O

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Applying the Guidelines

```
def gcCount(sequence):
        gc = float(count(sequence, 'g') + count(sequence, 'c'))/ len(sequence)
        print gc
```

What can be improved?

```
def gcCount(sequence):
        gc = float(count(sequence, 'g' + count(sequence, 'c'))/ len(sequence)
        return gc
```

Why is this better?

- More reusable function
- Can call it to get the *gcCount* and then decide what to do with the value
- May not have to *print* the value
- Function has ONE well-defined objective or CONTRACT

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Decision statements

Indentation has meaning in Python

```
if <$be_1$> :
    <$block_1$>
elif <$be_2$>:
    <$block_2$>
…
…
else:
    <$block_{n+1}$>
```

- *Each <$be_{i>}$ is a BOOLEAN expressions*
- *Each <$block_i$>is a sequence of statements*
- *Level of indentation determines what's inside each block*

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Compute the complement of a DNA base

```
def complementBase(base):
    if (base == ’a'):
        return ’t'
    elif (base == ’t'):
        return ’a'
    elif (base == ’c'):
        return ’g'
    elif (base == ’g'):
        return ’c'
```

How can we improve this function?

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Boolean Expressions

- Expressions that yield True of False values
- Ways to yield a Boolean value
  - Boolean constants: True and False
  - Comparison operators (>, <, ==, >=, <=)
  - Logical Operators (and, or, not)
  - Boolean functions
  - 0 (means False)
  - Empty string '' (means False)

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Some Useful Boolean Laws

- Lets assume that b,a are Boolean values:
  - (b and True) = b
  - (b or True) = True
  - (b and False) = False
  - (b or False) = b
  - not (a and b) = (not a) or (not b)
  - not (a or b) = (not a) and (not b)

} De Morgan's Laws

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A strange Boolean function

```
def test(x):
    if x:
        return True
    else:
        return False
```

What can you use this function for?

What types of values can it accept?

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Recursive Functions

A classic!

```
def fact(n):
    if (n==0):
        return 1
    else:
        return n * fact(n - 1)
```

```
>>> fact(5)
120
>>> fact(10)
3628800
>>> fact(100)
93326215443944152681699238856266700490715968264381621468592963895217599993
22991560894146397615651828625369792082722375825118521091686400000000000000
0000000000L
>>>
```

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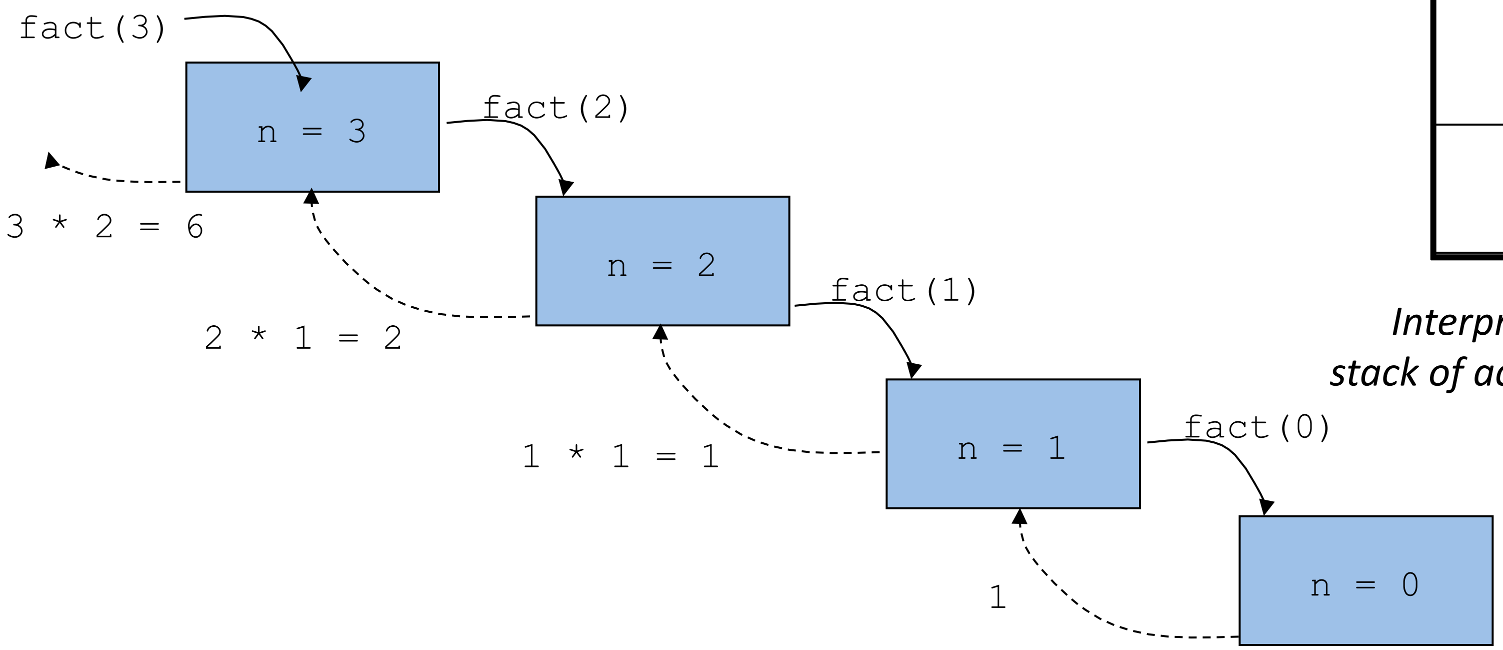
Recursion Basics

```
def fact(n):
    if (n==0):
        return 1
    else:
        return n * fact(n - 1)
```



fact(3)

n = 3

fact(2)

3 * 2 = 6

n = 2

fact(1)

2 * 1 = 2

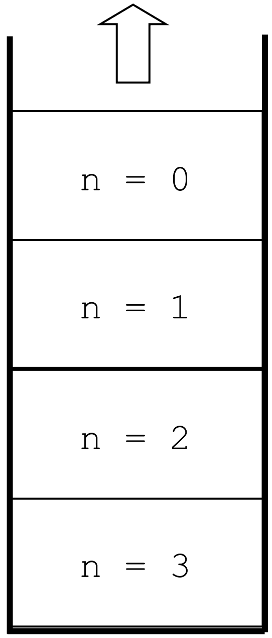
n = 1

fact(0)

1 * 1 = 1

n = 0

1



n = 0

n = 1

n = 2

n = 3

Interpreter keeps a
stack of activation records

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Beware of Infinite Recursions!

```
def fact(n):
    if (n==0):
        return 1
    else:
        return n * fact(n - 1)
```

What if you call fact 5.5? Explain

When using recursion always think about how will it stop or converge

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Write recursive Python functions to satisfy the following specifications:

- Compute the reverse of a sequence
- Compute the molecular mass of a sequence
- Compute the reverse complement of a sequence
- Determine if two sequences are complement of each other
- Compute the number of stop codons in a sequence
- Determine if a sequence has a subsequence of length greater than n surrounded by stop codons
- Return the starting position of the subsequence identified in exercise 6

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Reversing a sequence recursively

```
def reverse(sequence):

    'Returns the reverse string of the argument sequence'

    if (len(sequence)>1):

        return reverse(sequence[1:])+sequence[0]

    else:

        return sequence
```

Runtime Complexity - 'Big O' Notation

```
def fact(n):
    if (n==0):
        return 1
    else:
        return n * fact(n - 1)
```

- *How 'fast' is this function?*
- *Can we come up with a more efficient version?*
- *How can we measure 'efficiency'*
- *Can we compare algorithms independently from a specific implementation, software or hardware?*

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Big Idea

Measure the number of *steps* taken by the algorithm as an asymptotic function of the *size* of its input

- What is a step?
- How can we measure the size of an input?
- Answer in both cases: YOU CAN DEFINE THESE!

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- A 'step' is a function call to fact
- The size of an input value n is n itself

```
def fact(n):
    if (n==0):
        return 1
    else:
        return n * fact(n - 1)
```

Step 1: Count the number of steps for input n

$$T(0) = 0$$

$$T(n) = T(n-1) + 1 = (T(n-2) + 1) + 1 = \ldots = T(n-n) + n = T(0) + n = 0 + n = n$$

Step 2: Find the asymptotic function

$$T(n) = O(n)$$

A.K.A Linear Function

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Iteration

SYNTAX → *while <be>:*
<block>

SEMANTICS → *Repeat the execution of <block> as long as expression <be> remains true*

SYNTAX = FORMAT
SEMANTICS = MEANING

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Iterative Factorial

```
def iterFact(n):
    result = 1
    while(n>0):
        result = result * n
        n = n - 1
    return result
```

Work out the runtime complexity:

whiteboard

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Formatted Output using % operator

<format> % <values>

```
>>> '%s is %d years old' % ('John', 12)
'John is 12 years old'
>>>
```

- <format> is a string
- <values> is a list of values n parenthesis (a.k.a. a tuple)
- % produces a string replacing each %x with a correding value from the tuple

For more details visit: http://docs.python.org/lib/typesseq-strings.html

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The For Loop: Another Iteration Statement

SYNTAX

```
for <var> in <sequence>:
    <block>
```

SEMANTICS

Repeat the execution of the <block> binding variable <var> to each element of the sequence

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```
def iterFact2(n):
    result = 1
    for i in xrange(1,n+1):
        result = result * i
    return result
```

xrange(start,end,step) generates a sequence of values :

- start = first value
- end = value right after last one
- step = increment

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Revisiting code from Lecture 1

```
seq="ACTGTCGTAT"
print seq
Acount= seq.count('A')
Ccount= seq.count('C')
Gcount= seq.count('G')
Tcount= seq.count('T')
Total = float(len(seq))
APct = int((Acount/Total) * 100)
print 'A percent = %d ' % APct
CPct = int((Ccount/Total) * 100)
print 'C percent = %d ' % CPct
GPct = int((Gcount/Total) * 100)
print 'G percent = %d ' % GPct
TPct = int((Tcount/Total) * 100)
print 'T percent = %d ' % TPct
```

Can we reduce the amount of repetitive code?

Approach: Use For Loop

```
bases = ['A', 'C', 'T', 'G']
sequence = "ACTGTCGTAT"
for base in bases:
    nextPercent = 100 * sequence.count(base)/float(len(sequence))
    print 'Percent %s: %d' % (base, nextPercent)
```

How many functions would you refactor this code into?

Write iterative Python functions to satisfy the following specifications:

1. Compute the reverse of a sequence
2. Compute the molecular mass of a sequence
3. Compute the reverse complement of a sequence
4. Determine if two sequences are complement of each other
5. Compute the number of stop codons in a sequence
6. Determine if a sequence has a subsequence of length greater than n surrounded by stop codons
7. Return the starting position of the subsequence identified in exercise 6

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Finding Patterns Within Sequences

```
from string import *
def searchPattern(dna, pattern):
        'print all start positions of a pattern string inside a target string’
        site = find (dna, pattern)
        while site != -1:
                print ’pattern %s found at position %d' % (pattern, site)
                site = find (dna, pattern, site + 1)
```

```
>>> searchPattern("acgctaggct","gc")

pattern gc at position 2

pattern gc at position 7

>>>
```

Example from: *Pasteur Institute Bioinformatics Using Python*

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- Extend searchPattern to handle unknown residues