Guide to Programming with Python

Yuzhen Ye (yye@indiana.edu)
School of Informatics and Computing, IUB
Objectives

- Python basics
  - How to run a python program
  - How to write a python program
    - Variables
    - Basic data types: number, string, list, and dictionary
    - Control flow:
      - Branching structure: if, if-else, if-elif-else
      - Loops: for loop and while loop
    - Write a function & a class
    - I/O (read from files and write to files)
    - Write python programs with graphical user interface (GUI)
  - Comments & modules (e.g., random module)

- Your first bioinformatics program in python
Algorithms & Computer programs

- An algorithm is a set of well-defined instructions for accomplishing a task (e.g., S’mores algorithm for making s'mores)
- When we write computer program, we are generally implementing a method (an algorithm) devised previously to solve some problem.
- A computer program is a sequence of instructions that are executed by a CPU
- Computer programs can be written in high-level (e.g., Python, Perl, C, C++, Java), or primitive programming languages
Hello World

- Python is an interpreted (scripting), high-level language (different from compiled programming language, such as C)

- “Hello World” program: By tradition, prints "Hello, world!"
  - Often used as first program
  - print “Hello world”

- Console window: Provides a text-based interface to Windows operating system

- Terminal application: Provides a text-based interface to Mac OS X and Linux operating systems
Setting up Python

- Windows
- Linux
  - Python probably already installed
  - Test: try running `python` at command prompt
- Mac OS 10.5.x
  - Leopard (10.5.x) already has Python 2.5.1 installed, but you need to install IDLE.app following instructions at http://wiki.python.org/moin/MacPython/Leopard
- Earlier Mac OS X and other systems
- If not installed, go to http://www.python.org/download/

- Remember: your computer needs a python “interpreter” to understand python codes
Introducing IDLE/vi/Emacs

- **Integrated Development Environment (IDE):** Application that helps software developers write programs
  - Like a word processor for your code
- IDE that ships with Python
- Has two “modes”: Interactive and Script (see demo)
- You need to be able to use vi or Emacs
Interactive and Script Mode

- Iterative mode: You tell Python what to do, and it will do it immediately
- Script mode: You write, edit, load, and save python programs (just like you write a document in Word processor, and any other types of text processors). But definitely you do not want to write your Python codes with Word!
Start to Talk Like a Pro

- **Statement**: Single unit in programming language that performs some action
  - `print "ACGT"`
- `print Statement` can display a **string** (actually, any **expression**)
- **Expression**: Something which has a value or that can be evaluated to a single value
  - "ACGT"
  - `7 + 2`
- **Code**: Sequence of programming statements
  - **Syntax error**: Error in the rules of usage; often a typo (versus **logic error**)
  - **Bug**: Error in programming code
1. Variables

- **Variable**: Represents a value; provides way to get at information in computer memory
- Variables allow you to store and manipulate information
- You can create variables to organize and access this information
- **Assignment statement**: Assigns a value to a variable; creates variable if necessary
- `name = "E.coli"`
  - Stores string "E.coli" in computer memory
  - Creates variable `name`, which refers to "E.coli"
Naming Variables

- Rules for legal variable names
  - Can contain only numbers, letters, and underscores
  - Can’t start with a number
  - Can’t be a keyword

- **Keyword**: Built-in word with special meaning

- **Legal Names**
  - enzyme, dna, prot, player2, max_health

- **Illegal Names**
  - ?again, 2nd_player, print
Naming Variables (continued)

- Guidelines for good variable names
  - Choose descriptive names; score instead of s
  - Be consistent; high_score or highScore
  - Follow traditions; Names that begin with underscore have special meaning
  - Keep the length in check
    personal_checking_account_balance - too long?
  - Self-documenting code: Code written so that it’s easy to understand, independent of any comments
2. Using the Right Types

- Python does not need to specify the type of a variable in advance (by contrast, C does)
  
  **Python:**
  
  ```python
  protlen = 100
  ```

  **C:**
  
  ```c
  int protlen = 10;
  ```

- Important to know which data types are available
- Equally important to know how to work with them
- If not, might end up with program that produces unintended results
- Converting values: e.g., `int("3") = 3`
2.1 Working with Strings

- Using quotes inside strings
  - Define with either single ('') or double quotes (")
    - "ribosomal RNA" or "ribosomal RNA"
  - Define with one type, use other type in string
    - "Program 'Game Over' 2.0"

- Triple-quoted strings can span multiple lines
  ""
  I am a
  triple-quoted string
  ""

- Line-continuation character \ 

- Escape sequences \n \t \

- String concatenation
  - "ACGT" + "ACGT"
  - "ACGT" * 10
Working with Biological Sequences

- Biological sequences are strings of different alphabets
  - seq1 = 'gcatgacgattacgactctgtcacgctctgcgttg'
  - seq1 = 'gcaugacguuuacgacucucugacgcg'
  - seq2 = 'STNGWEMVPA'

- Some functions you will use often
  - len(seq1)
  - 'cat' in seq1
  - count(dna, 'a')
  - replace(dna, 'a', 'A')

- Indexing/Slicing a string
  - seq1[2], seq1[-1]
  - seq1[:], seq1[:-1], seq1[1:], seq[3:6]
2.2 Working with Numbers

- **Numeric types**
  - **Integers**: Numbers without a fractional part
    - $1, 0, 27, -100$
  - **Floating-Point Numbers** (or **Floats**): Numbers with a fractional part
    - $2.376, -99.1, 1.0$

- **Addition, Subtraction and Division**
  - `print 2000 - 100 + 50` displays $1950$

- **Modulus (remainder of integer division)**
  - `print 107 % 4` displays $3$
Augmented Assignment Operators

- Common to assign a value to a variable based on its original value
- Augmented assignment operators provide condensed syntax
  - Original: `score = score + 1`
  - Augmented: `score += 1`

<table>
<thead>
<tr>
<th>Operator</th>
<th>Example</th>
<th>Is Equivalent To</th>
</tr>
</thead>
<tbody>
<tr>
<td>*=</td>
<td>x *= 5</td>
<td>x = x * 5</td>
</tr>
<tr>
<td>/=</td>
<td>x /= 5</td>
<td>x = x / 2</td>
</tr>
<tr>
<td>%=</td>
<td>x %= 5</td>
<td>x = x % 5</td>
</tr>
<tr>
<td>+=</td>
<td>x += 5</td>
<td>x = x + 5</td>
</tr>
<tr>
<td>-=</td>
<td>x -= 5</td>
<td>x = x - 5</td>
</tr>
</tbody>
</table>
2.3. Working with Lists (and Tuples)

- **List**: A mutable (changeable) sequence of **any** type

- **Creating List**
  
  ```python
  bases = ["A", "T", "C", "G"]
  Tuple: bases = ("A", "T", "C", "G")
  ```

- **Using `len()` function and `in` operator**
  
  ```python
  if abase in bases:
      print "it is a base. "
  ```

- **Indexing and slicing**
  
  ```python
  bases[1], bases[1:3]
  ```

- **Concatenating lists**
  
  ```python
  bases + bases
  ```
Deleting an Element or a Slice

```python
>>> bases = ["A", "T", "C", "G"]
>>> del bases[2]
>>> print bases

>>> del bases[:2]
>>> print bases
```
# List Methods

## Table 5.1 Selected List Methods

<table>
<thead>
<tr>
<th>Method</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td><code>append(value)</code></td>
<td>Adds <code>value</code> to end of a list.</td>
</tr>
<tr>
<td><code>sort()</code></td>
<td>Sorts the elements, smallest value first.</td>
</tr>
<tr>
<td><code>reverse()</code></td>
<td>Reverses the order of a list.</td>
</tr>
<tr>
<td><code>count(value)</code></td>
<td>Returns the number of occurrences of <code>value</code>.</td>
</tr>
<tr>
<td><code>index(value)</code></td>
<td>Returns the first position number where <code>value</code> occurs.</td>
</tr>
<tr>
<td><code>insert(i, value)</code></td>
<td>Inserts <code>value</code> at position <code>i</code>.</td>
</tr>
<tr>
<td><code>pop([i])</code></td>
<td>Returns value at position <code>i</code> and removes value from the list. Providing the</td>
</tr>
<tr>
<td></td>
<td>position number <code>i</code> is optional. Without it, the last element in the list is</td>
</tr>
<tr>
<td></td>
<td>removed and returned.</td>
</tr>
<tr>
<td><code>remove(value)</code></td>
<td>Removes the first occurrence of <code>value</code> from the list.</td>
</tr>
</tbody>
</table>
Using Nested Sequences

- **Nested Sequence**: A sequence inside another sequence
- A list can contain lists or tuples
- A tuple can contain tuples or lists

```python
prots = [['170079667', 'threonine synthase'],
         ['170079668', 'hypothetical protein']]
#gi + description
#prots[1]
#prots[1][1]
#prots[1][1] multiple indexing
```
Unpacking a Sequence

```python
>>> gi, des = ["170079667", "threonine synthase"]
>>> print gi
>>> print des
```

- **Sequence unpacking**: Automatically accessing each element of a sequence
- The list is unpacked as result of assignment statement
Variable References

- A variable refers to a place in memory where the value (or empty) is stored
  
  \[
  \text{language} = \text{“Python”}
  \]

- Variable assignment can be
  - initial (creates a new box in the computer’s memory the first time a variable name is seen)
  - shared (assign lists; default for mutable items)
    - \( a = b = [\] \) # both names will point to the same list
  - copied (numbers, strings, tuples)

```
# All variables refer to same single list
```

```
.. figure:: my-figure.png
   :width: 700

```

```
```
Avoid Shared References

gene1 = ["170079667", "170079668"]
gene2 = gene1
gene2.append("170079690")
#now how many genes does gene1 has?
gene3 = gene1[:]
gene3.append("170079698")
#now how many genes does gene1 has?

- List slicing can create a new copy of a list and avoid shared references (but NOT for nested sequences)

    a = [1, 2, [3, 4]]
b = a[:]
b[1] = "22"
b[2][0] = "33"
Using copy.deepcopy()

- **Module:** copy
  - ref: [http://docs.python.org/library/copy.html](http://docs.python.org/library/copy.html)

```python
import copy
b = copy.copy(a)  # shallow copy, => b = a[:]

b = copy.deepcopy(a)  # deep copy of an object

Example: sokodul1 = copy.deepcopy(sokodul)
```
Accessing Elements of a Nested Sequence Using for Loop

```python
prots = [["170079667", "threonine synthase"],
         ["170079668", "hypothetical protein"]]

for entry in prots:
    gi, des = entry
    print gi, "\t", des
```

**Sequence unpacking:** Automatically accessing each element of a sequence as a result of assignment statement.
3. Control the flow

```python
baddna = 'tgagaatuctaugatctcnnn'
gooddna = ""
for base in baddna:
    if base in 'atcgATCG':
        gooddna += base
    elif base == 'u':
        gooddna += 't'
    elif base == 'U':
        gooddna += 'T'
    else:
        gooddna += '*'
print "baddna: ", baddna
print "cleandna: ", gooddna
```
3.1 Branching structures

- Make choices based on conditions – to selectively execute certain portions of the code
  - Use `if` to execute code based on a condition
  - Use `if-else` to make a choice based on a condition
  - Use `if-elif-else` structures to make a choice based on a series of conditions
- Plan programs
from string import *

dna = 'tgagaattctatgaattc'

enz = 'gaattc'
print "dna", dna

site = find (dna, enz)
while site != -1:
    print "restriction site %s at position %d" % (enz, site)
    site = find (dna, enz, site + 1)
3.3 Using for Loops

- **for** loop
  - Like **while** loop, repeats a loop body
  - Unlike **while** loop, doesn’t repeat based on condition
  - Repeats loop body for each element in a sequence
  - Ends when it reaches end of the sequence
  - e.g., go through sequence of game titles and print each
3.4 Understanding conditions

- **Condition**: Expression that is **True** or **False**
- **True** and **False** are values of type **boolean**
- `password == "secret"` is condition - **True** or **False**
  - If variable `password` is equal to string "secret" condition evaluates to **True**
  - Otherwise, condition evaluates to **False**
- The password program
- Often **create conditions by comparing values** (`==, !=, >, <, >=, <=`)
Treating Values as Conditions

- Any value can be interpreted as True or False when used as condition
  - Any empty (None) or zero value is False
    - So, 0, "", and None are False
  - Any other value is True
    - So for example, -10, 2.5, "banana" are True

- if money:
  - money is treated as condition
  - True when money not 0; False when money is 0
Using Compound Conditions

- Can create more complex conditions by joining simple conditions seen so far with logical operators to create a compound condition.

**Logical operator:** An operator *(and, or, not)* that joins conditions to form a large condition.

```python
dna = ""
while not dna:
    dna = raw_input("dna: ")
```

**Compound condition:** A larger condition formed by joining simpler conditions.

```python
A or B and C
# be aware of the precedence of logical operators
# not > and > or
```
4. Working with Files!

- A typical sequence file in fasta format

>seq1
STATGPNEDKRVMLVIPGPNT
Opening and Closing a Text File

text_file = open("read_it.txt", "r")

Must open before read (or write); then you read from and/or write to the file by referring to the file object.

Always close file when done reading or writing.

Can open a file for reading, writing, or both.
# File Access Modes

## Table 7.1 Selected File Access Modes

<table>
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<tr>
<th>Mode</th>
<th>Description</th>
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</thead>
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<tr>
<td>&quot;r&quot;</td>
<td>Read from a file. If the file doesn’t exist, Python will complain with an error.</td>
</tr>
<tr>
<td>&quot;w&quot;</td>
<td>Write to a file. If the file exists, its contents are overwritten. If the file doesn’t exist, it’s created.</td>
</tr>
<tr>
<td>&quot;a&quot;</td>
<td>Append a file. If the file exists, new data is appended to it. If the file doesn’t exist, it’s created.</td>
</tr>
<tr>
<td>&quot;r+&quot;</td>
<td>Read from and write to a file. If the file doesn’t exist, Python will complain with an error.</td>
</tr>
<tr>
<td>&quot;w+&quot;</td>
<td>Write to and read from a file. If the file exists, its contents are overwritten. If the file doesn’t exist, it’s created.</td>
</tr>
<tr>
<td>&quot;a+&quot;</td>
<td>Append and read from a file. If the file exists, new data is appended to it. If the file doesn’t exist, it’s created.</td>
</tr>
</tbody>
</table>

Files can be opened for reading, writing, or both.
Reading a Line from a File

text_file = open("read_it.txt", "r")

line1 = text_file.readline()
line2 = text_file.readline()
line3 = text_file.readline()

- **readline()** file object method
  - Returns the entire line if no value passed
  - Once read all of the characters of a line (including the newline), next line becomes current line

```python
text_file.readline(number_of_characters) # a little confusing
```
Reading All Lines into a List

text_file = open("read_it.txt", "r")
lines = text_file.readlines()
#lines is a list!

- **readlines()** file object method
  - Reads text file into a list
  - Returns list of strings
  - Each line of file becomes a string element in list

Compared to: read(), which reads the entire file into a string (instead of a list of strings)
Looping Through a Text File

```python
>>> text_file = open("read_it.txt", "r")
>>> for line in text_file:
    print line
Line 1
This is line 2
That makes this line 3
```

- Can iterate over open text file, one line at a time
strip() & split()

e.g., read_it.txt:
Hunter 98
Nathan 67

#The following lines for reading names and scores:
text_file = open("read_it.txt", "r")
for line in text_file:
    line = line.strip()
    (name, score) = line.split()

str.split([sep[, maxsplit]]) -- Return a list of the words in the string, using sep as the delimiter string. If sep is not specified or None, any whitespace string is a separator '1<>2<>3'.split('<>') returns ['1', '2', '3'])

str.strip([chars]) -- Return a copy of the string with the leading and trailing characters removed '   spacious   '.strip() returns 'spacious'
Writing to Text Files

text_file = open("write_it.txt", "w")
text_file.write(">seq1\n")
text_file.write("ACGTTGAACATGGC\n")

- `write()` file object method writes new characters to file open for writing

text_file = open("write_it.txt", "w")
lines = [">seq1\n", "ACGTTGAACATGGC\n"]
text_file.writelines(lines)

- `writelines()` file object method writes list of strings to a file
5. Use and Write Functions

- Divide and conquer: divide complicated tasks into simpler and more manageable tasks.
- Avoid writing redundant program code (many programs require that a specific function is repeated many times)
- Enhance the readability of codes (a code can be broken up into manageable chunks; easy to follow the flow of the program)
- Testing and correcting errors is easy because errors are localized and corrected
- A single function written in a program can also be used in other programs also (software reuse)
User-defined Functions

def usage():
    """Display instructions."""
    print "Welcome to use ...!"

- Functions make programs easier to read, write and maintain
- **Function definition**: Code that defines what a new function does
- **Function header**: First line of a function definition
- Give function name that conveys what it does or produces
Calling a Function

usage()

- Call tells the computer to execute function usage()
- Call works just like call to built-in function
- Tells the computer to execute previously-defined function
Encapsulation

- Encapsulation: A technique of keeping independent code separate by hiding the details.
- Variables created in a function cannot be directly accessed outside the function.
- Parameters and return values allow for information exchange:
  - Functions with no arguments and no return values.
  - Functions with arguments and no return values.
  - Functions with no arguments and return values.
  - Functions with arguments and return values.
import random

def RandDNA(totbp):
    alphabets = ["A", "C", "G", "T"]
    seq = ""
    for i in range(totbp):
        seq += alphabets[random.randrange(4)]
    return seq

- Receives one value and returns another
- **Parameter:** A variable name inside the parentheses of a function header that can receive a value
- **Argument:** A value passed to a parameter
- **Sample call:** `seq = RandDNA(50)`
def AddProt(gi, des):
    print "You added a protein, gi=", gi, "des=", des
AddProt("170079667", "threonine synthase")
AddProt("hypothetical protein", "170079668")

#using default parameter value
def AddProt(gi = "170079667", des = "threonine synthase"):  
    print "You added a protein, gi=", gi, "des=", des
AddProt(gi="170079667", des="threonine synthase")
AddProt(des="hypothetical protein", gi="170079668")

**Positional arguments**
Arguments passed to the parameters in order

**Keyword argument**
Argument passed to a specific parameter using the **parameter name**

The biggest benefit of using keyword arguments is clarity.
Global versus Local Scopes

- **Scopes**: Different areas of a program that are separate from each other
- Every function has its own scope
- Functions can't directly access each other's variables
- **But can exchange information through parameters and return values**
Shadowing/Changing a Global Variable from Inside a Function

```python
def demo():
    global value1  # full access of global variable value1
    value1 = -value1
    value2 = -20  # a new variable with same name (shadow)
    print "Inside local scope:" , value1, value2, value3
    value1 = 10
    value2 = 20
    value3 = 30
    print "In the global scope:" , value1, value2, value3
    demo()  # value1 is changed; value2 and value3 not
    print "Back in the global scope", value1, value2, value3

- Shadow: To hide a global variable inside a scope by creating a new local variable of the same name
- Not a good idea to shadow a global variable
```
6. Object-Oriented Programming

- OOP allows representation of real-life objects as software objects (e.g., a dictionary as an object)
- **Object**: A single software unit that combines attributes and methods

  - **Attribute**: A "characteristic" of an object; like a variable associated with a kind of object
  - **Method**: A "behavior" of an object; like a function associated with a kind of object

- **Class**: Code that defines the attributes and methods of a kind of object (A class is a collection of variables and functions working with these variables)
Creating Classes for Objects

class Dna(object):
    def __init__(self, name, seq):
        self.name = name
        self.seq = seq
    def translate(self):
        ...

dna1 = Dna("gene1", "atcggttttgact")
dna2 = Dna("gene2", "ttcgcagcggtt")
dna2.translate()

- **Class**: Code that defines the **attributes** and **methods** of a kind of object
- **Instantiate**: To create an object (an **Instance**)
- dna.2.translate() **invokes** translate() method of Dna object dna2
Using Constructors

- **Constructor**: A special method that is automatically invoked right after a new object is created.
- Usually write one in each class.
- Usually sets up the initial attribute values of new object in constructor.
class Seq(object):
...
    def __str__(self):
        rep = "Seq object\n"
        rep += "id: " + self.id + "\n"
...
seq1 = Seq()
print seq1

__str__ is a special method that returns string representation of object
7. Handling Exceptions

>>> 1/0

Traceback (most recent call last):
  File "$pyshell#0"", line 1, in -toplevel-
    1/0
ZeroDivisionError: integer division or modulo by zero

- **Exception**: An error that occurs during the execution of a program
- Exception is **raised** and can be **caught** (or **trapped**) then **handled**
- Unhandled, halts program and error message displayed
try-except Statement

try:
    file = open("seq.txt", "r")
except IOError:
    sys.exit("open file error! ")

- try statement sections off code that could raise exception
- Instead of raising exception, except block run
- If no exception raised, except block skipped
8. Using Modules

- Module imported using filename, just like built-in modules

```python
from Bio import SeqIO
handle = open("ls_orchid.gbk")
for seq_record in SeqIO.parse(handle, "genbank") :
    print seq_record.id
```

```python
from Bio import Entrez
handle = Entrez.esearch
    (db="nucleotide",term="Cypripedioideae[Orgn]
     AND matK[Gene]"
)
record = Entrez.read(handle)
print record["Count"]
print record["IdList"]
```

Only use Biopython after you are getting quite familiar with python!!
Writing Modules

- Write module as a collection of related programming components, like functions and classes, in a single file

```python
class MySeqIO(object):
    def __init__(self, file):
        self.ReadGenbank(file)
    def ReadGenbank(self, file):
        ...
    def WriteFasta(self, outfile):
        ...

if __name__ == '__main__':
    infile = "test.gnk"
    test = MySeqIO(infile)
    outfile = "test.fasta"
    test.WriteFasta(outfile)```
9. Debugging Your Programs

- Logic errors are difficult to find
- Uses examples (from simple to complex ones) and check if your program gives correct results
- Using print statements to trace the progress (especially for those jobs that are going to take a while to finish)
Getting User Input by raw_input()

- **raw_input() function**
  - Prompts the user for text input
  - Returns what the user entered as a string

- **name = raw_input("type in the file name: ")**
  - Argument "type in your file name: "
  - Returns what user entered as a string
  - In assignment statement, name gets returned string

  num = int(raw_input("enter your seed number: "))

- You may use it for debugging purpose (to pause the program)
Sorry, there is no easy way to learn programming

- Python basics
  - Variables
  - Basic data types: number, string, list, and dictionary
  - Control flow:
    - Branching structure: if, if-else, if-elif-else
    - Loops: for loop and while loop
  - Write function & class
  - I/O (read from files and write to files)
- Learning programming takes a lot of practice! And crappy codes are ok (in the beginning), as long as they work!