Practical Bioinformatics

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5/13/2019

Resources

Course website:

- http://histo.ucsf.edu/BMS270/

Resources on the course website:

- Syllabus
  - Papers and code (for downloading *before* class)
  - Slides and transcripts (available *after* class)
- On-line textbooks (Dive into Python, Numerical Recipes, ...)
- Programs for this course (VirtualBox, JavaTreeView, ...)

Homework

- E-mail Mark your python sessions (.ipynb files) after class
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- If you get stuck, try working things out on paper first.

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At the end of this class, you should have the confidence to take on the day to day tasks of “bioinformatics”.

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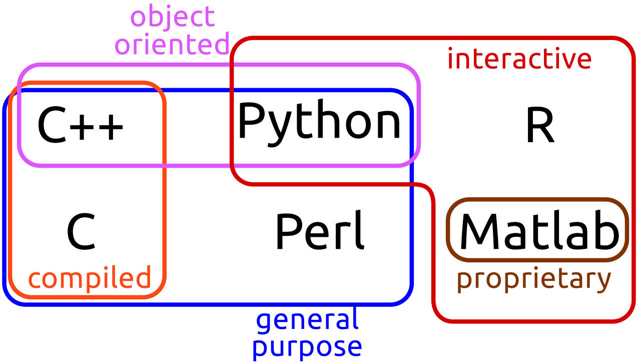
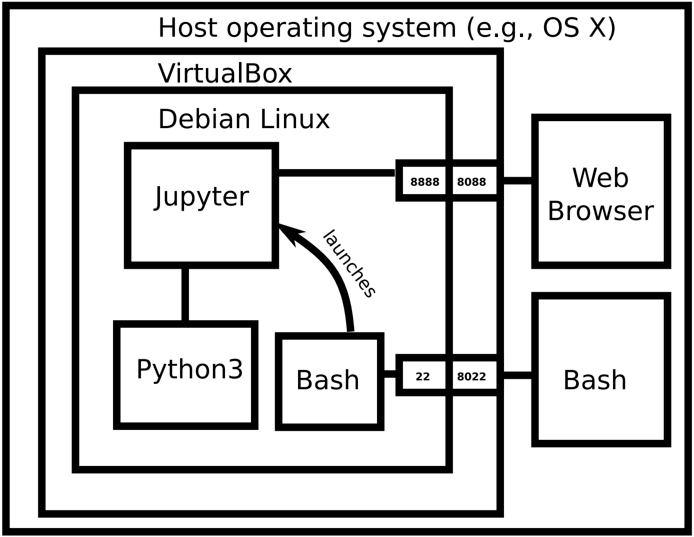
This is also good preparation for communicating with computational collaborators.

Course tool: Python



Course platform: VirtualBox



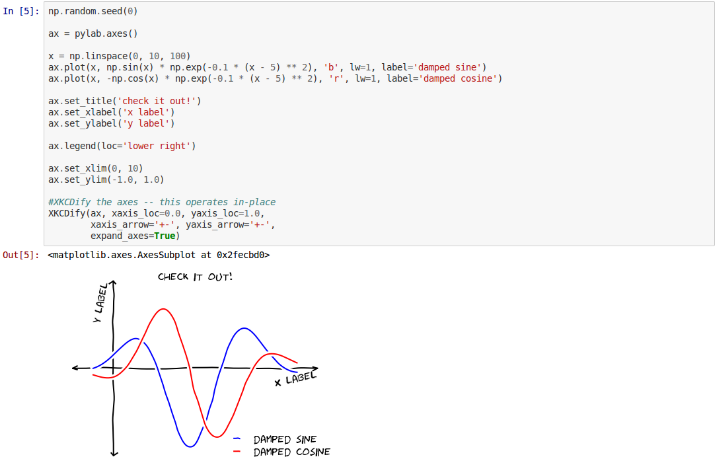
Host side bash commands

```
# Unlock your RSA private key
ssh-add ~/.ssh/VM_rsa
# Copy a file to the VM
scp -P 8022 myfile.txt explorer@localhost:
# Log into the VM
ssh -p 8022 explorer@localhost
# Get help on a command
man ssh
```

Guest side bash commands

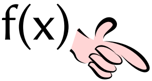
```
# Reboot the VM
su
shutdown -r now
# Shut down the VM
su
shutdown -hP now
# Start a screen session
screen
# Start Jupyter
jupyter notebook
```

Python shell: ipython (jupyter) notebook



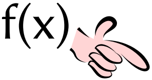
```
In [5]: np.random.seed(0)

        ax = pylab.axes()

        x = np.linspace(0, 10, 100)
        ax.plot(x, np.sin(x) * np.exp(-0.1 * (x - 5) ** 2), 'b', lw=1, label='damped sine')
        ax.plot(x, -np.cos(x) * np.exp(-0.1 * (x - 5) ** 2), 'r', lw=1, label='damped cosine')

        ax.set_title('check it out!')
        ax.set_xlabel('x label')
        ax.set_ylabel('y label')

        ax.legend(loc='lower right')

        ax.set_xlim(0, 10)
        ax.set_ylim(-1.0, 1.0)

        #XKCDify the axes -- this operates in-place
        XKCDify(ax, xaxis_loc=0.0, yaxis_loc=1.0,
                xaxis_arrow='+-', yaxis_arrow='+-',
                expand_axes=True)

Out[5]: <matplotlib.axes.AxesSubplot at 0x2fecbd0>
```

Anatomy of a Programming Language

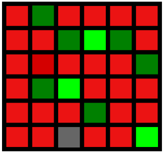


functions

Anatomy of a Programming Language



functions



data structures

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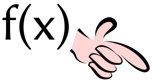
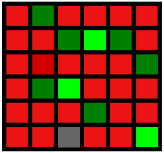


functions



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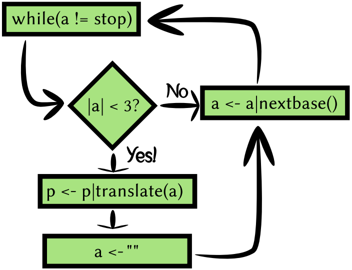


while(a != stop)

|a| < 3?

No

a <- a|nextbase()

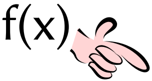
Yes!

p <- p|translate(a)

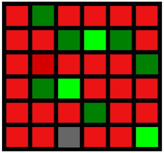
a <- ""

control statements

Anatomy of a Programming Language



functions



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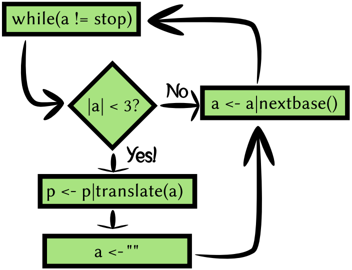

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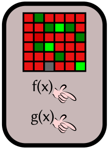

objects

Binary files are like genomic DNA

hexdump -C computers.png

```
00000000  89 50 4e 47 0d 0a 1a 0a  00 00 00 0d 49 48 44 52  |.PNG........IHDR|
00000010  00 00 03 5f 00 00 02 cc  08 06 00 00 00 1b c3 08  |..._............|
00000020  30 00 00 00 04 73 42 49  54 08 08 08 08 7c 08 64  |0....sBIT....|.d|
00000030  88 00 00 00 09 70 48 59  73 00 00 2e 23 00 00 2e  |.....pHYs...#...|
00000040  23 01 78 a5 3f 76 00 00  00 19 74 45 58 74 53 6f  |#.x.?v....tEXtSo|
00000050  66 74 77 61 72 65 00 77  77 77 2e 69 6e 6b 73 63  |ftware.www.inksc|
00000060  61 70 65 2e 6f 72 67 9b  ee 3c 1a 00 00 20 00 49  |ape.org..<... .I|
00000070  44 41 54 78 9c ec 9d 79  9c 25 57 59 fe bf cf 39  |DATx...y.%WY...9|
00000080  75 6f 2f 33 93 cc 92 c9  1e 48 42 08 01 45 92 a0  |uo/3.....HB..E..|
00000090  04 c2 26 88 08 8a 80 0a  b2 28 18 14 54 14 45 04  |..&......(..T.E.|
000000a0  7f 02 a2 2c b2 aa 2c 0a  28 22 3b ca 26 20 8b b2  |...,..,.(";.& ..|
000000b0  08 c8 26 9b 61 4d 08 6b  08 d9 c8 be cd 4c 4f 77  |..&.aM.k.....LOw|
000000c0  df 7b eb 9c f7 f7 c7 7b  aa fb e6 ce bd 3d dd 93  |.{.....{.....=..|
000000d0  59 32 a4 9e fe d4 e7 76  55 9d 53 75 ea d4 a9 aa  |Y2.....vU.Su....|
000000e0  77 7d 8e cc 8c 16 2d 5a  b4 68 d1 a2 c5 8f 27 24  |w}....-Z.h....'$|
000000f0  75 81 00 f4 cc cc 24 45  a0 03 d4 66 56 8f 94 ed  |u.....$E...fV...|
00000100  00 b1 ac ee b2 7f 42 d9  15 cb ed 2f 48 da 0a 9c  |......B..../H...|
00000110  08 1c 0d 5c 0f 5c 05 9c  6f 66 fd 03 da b0 9b 29  |...\.\..of.....)|
00000120  24 4d 03 66 66 bd b2 5e  01 15 30 30 b3 b4 86 e3  |$M.ff..^..00....|
00000130  3c 1c 78 2a f0 25 33 7b  f2 1a db b0 01 f8 58 59  |<.x*.%3{......XY|
00000140  7d a0 99 5d bf 96 fa 2d  f6 0c 92 8e 01 9e 08 dc  |}..]...-........|
00000150  01 38 0a 10 f0 7b 66 f6  8d 03 d4 9e 67 01 0f 02  |.8...{f.....g...|
00000160  de 69 66 2f 3f 10 6d d8  9f 08 07 ba 01 2d 5a b4  |.if/?.m......-Z.|
00000170  68 d1 a2 45 8b 7d 8a af  01 0b c0 ed cb fa 6f 97  |h..E.}........o.|
```

```
fp = open("computers.png")
fp.read(50)
fp.close()
```

Text files are like ORFs

hexdump -C 3_4_2010.txt

```
00000000  4d 65 65 74 20 77 2f 20  4a 6f 65 20 72 65 3a 20  |Meet w/ Joe re: |
00000010  77 69 72 65 6c 65 73 73  20 74 68 65 72 6d 6f 73  |wireless thermos|
00000020  74 61 74 73 0a 20 20 20  2d 2d 3e 20 64 6f 6e 65  |tats.   --> done|
00000030  0a 20 20 20 20 20 20 42  75 79 20 74 68 65 72 6d  |.      Buy therm|
00000040  6f 73 74 61 74 73 20 66  72 6f 6d 20 68 74 74 70  |ostats from http|
00000050  3a 2f 2f 77 77 77 2e 6f  6d 65 67 61 2e 63 6f 6d  |://www.omega.com|
00000060  0a 20 20 20 20 20 20 20  20 20 20 53 74 61 72 74  |.          Start|
00000070  20 77 69 74 68 3a 0a 20  20 20 20 20 20 20 20 20  | with:.         |
00000080  20 20 20 20 52 6f 75 74  65 72 20 55 57 54 43 52  |    Router UWTCR|
00000090  45 43 33 20 28 61 62 6f  75 74 20 24 31 32 30 29  |EC3 (about $120)|
000000a0  0a 20 20 20 20 20 20 20  20 20 20 20 20 20 20 20  |.               |
000000b0  20 43 61 6e 20 72 65 63  65 69 76 65 20 66 72 6f  | Can receive fro|
000000c0  6d 20 31 32 20 74 72 61  6e 73 6d 69 74 74 65 72  |m 12 transmitter|
000000d0  73 0a 20 20 20 20 20 20  20 20 20 20 20 20 20 20  |s.              |
000000e0  20 20 43 61 6e 20 70 75  73 68 20 63 6f 6e 66 69  |  Can push confi|
000000f0  67 75 72 61 74 69 6f 6e  20 74 6f 20 74 72 61 6e  |guration to tran|
00000100  73 6d 69 74 74 65 72 73  0a 20 20 20 20 20 20 20  |smitters.       |
00000110  20 20 20 20 20 20 20 20  20 43 6f 6d 6d 75 6e 69  |         Communi|
00000120  63 61 74 65 20 76 69 61  20 65 74 68 65 72 6e 65  |cate via etherne|
00000130  74 20 70 6f 72 74 20 61  6e 64 20 65 6d 62 65 64  |t port and embed|
00000140  64 65 64 20 77 65 62 20  73 65 72 76 65 72 0a 20  |ded web server. |
00000150  20 20 20 20 20 20 20 20  20 20 20 20 20 20 20 41  |               A|
00000160  73 73 69 67 6e 20 73 74  61 74 69 63 20 49 50 20  |ssign static IP |
00000170  61 64 64 72 65 73 73 20  61 6e 64 20 63 6f 6e 6e  |address and conn|
```

OS X *sometimes* uses CR newlines

hexdump -C macfile.txt

```
00000000  4d 65 65 74 20 77 2f 20  4a 6f 65 20 72 65 3a 20  |Meet w/ Joe re: |
00000010  77 69 72 65 6c 65 73 73  20 74 68 65 72 6d 6f 73  |wireless thermos|
00000020  74 61 74 73 0d 20 20 20  2d 2d 3e 20 64 6f 6e 65  |tats.   --> done|
00000030  0d 20 20 20 20 20 20 42  75 79 20 74 68 65 72 6d  |.      Buy therm|
00000040  6f 73 74 61 74 73 20 66  72 6f 6d 20 68 74 74 70  |ostats from http|
00000050  3a 2f 2f 77 77 77 2e 6f  6d 65 67 61 2e 63 6f 6d  |://www.omega.com|
00000060  0d 20 20 20 20 20 20 20  20 20 20 53 74 61 72 74  |.          Start|
00000070  20 77 69 74 68 3a 0d 20  20 20 20 20 20 20 20 20  | with:.         |
00000080  20 20 20 20 52 6f 75 74  65 72 20 55 57 54 43 52  |    Router UWTCR|
00000090  45 43 33 20 28 61 62 6f  75 74 20 24 31 32 30 29  |EC3 (about $120)|
000000a0  0d 20 20 20 20 20 20 20  20 20 20 20 20 20 20 20  |.               |
000000b0  20 43 61 6e 20 72 65 63  65 69 76 65 20 66 72 6f  | Can receive fro|
000000c0  6d 20 31 32 20 74 72 61  6e 73 6d 69 74 74 65 72  |m 12 transmitter|
000000d0  73 0d 20 20 20 20 20 20  20 20 20 20 20 20 20 20  |s.              |
000000e0  20 20 43 61 6e 20 70 75  73 68 20 63 6f 6e 66 69  |  Can push confi|
000000f0  67 75 72 61 74 69 6f 6e  20 74 6f 20 74 72 61 6e  |guration to tran|
00000100  73 6d 69 74 74 65 72 73  0d 20 20 20 20 20 20 20  |smitters.       |
00000110  20 20 20 20 20 20 20 20  20 43 6f 6d 6d 75 6e 69  |         Communi|
00000120  63 61 74 65 20 76 69 61  20 65 74 68 65 72 6e 65  |cate via etherne|
00000130  74 20 70 6f 72 74 20 61  6e 64 20 65 6d 62 65 64  |t port and embed|
00000140  64 65 64 20 77 65 62 20  73 65 72 76 65 72 0d 20  |ded web server. |
00000150  20 20 20 20 20 20 20 20  20 20 20 20 20 20 20 41  |               A|
00000160  73 73 69 67 6e 20 73 74  61 74 69 63 20 49 50 20  |ssign static IP |
00000170  61 64 64 72 65 73 73 20  61 6e 64 20 63 6f 6e 6e  |address and conn|
```

tr '\r' '\n' < macfile.txt > unixfile.txt

Windows uses CRLF newlines

hexdump -C dosfile.txt

```
00000000  4d 65 65 74 20 77 2f 20  4a 6f 65 20 72 65 3a 20  |Meet w/ Joe re: |
00000010  77 69 72 65 6c 65 73 73  20 74 68 65 72 6d 6f 73  |wireless thermos|
00000020  74 61 74 73 0d 0a 20 20  20 2d 2d 3e 20 64 6f 6e  |tats..   --> don|
00000030  65 0d 0a 20 20 20 20 20  20 42 75 79 20 74 68 65  |e..      Buy the|
00000040  72 6d 6f 73 74 61 74 73  20 66 72 6f 6d 20 68 74  |rmostats from ht|
00000050  74 70 3a 2f 2f 77 77 77  2e 6f 6d 65 67 61 2e 63  |tp://www.omega.c|
00000060  6f 6d 0d 0a 20 20 20 20  20 20 20 20 20 20 53 74  |om..          St|
00000070  61 72 74 20 77 69 74 68  3a 0d 0a 20 20 20 20 20  |art with:..     |
00000080  20 20 20 20 20 20 20 20  52 6f 75 74 65 72 20 55  |        Router U|
00000090  57 54 43 52 45 43 33 20  28 61 62 6f 75 74 20 24  |WTCREC3 (about $|
000000a0  31 32 30 29 0d 0a 20 20  20 20 20 20 20 20 20 20  |120)..          |
000000b0  20 20 20 20 20 20 43 61  6e 20 72 65 63 65 69 76  |      Can receiv|
000000c0  65 20 66 72 6f 6d 20 31  32 20 74 72 61 6e 73 6d  |e from 12 transm|
000000d0  69 74 74 65 72 73 0d 0a  20 20 20 20 20 20 20 20  |itters..        |
000000e0  20 20 20 20 20 20 20 20  43 61 6e 20 70 75 73 68  |        Can push|
000000f0  20 63 6f 6e 66 69 67 75  72 61 74 69 6f 6e 20 74  | configuration t|
00000100  6f 20 74 72 61 6e 73 6d  69 74 74 65 72 73 0d 0a  |o transmitters..|
00000110  20 20 20 20 20 20 20 20  20 20 20 20 20 20 20 20  |                |
00000120  43 6f 6d 6d 75 6e 69 63  61 74 65 20 76 69 61 20  |Communicate via |
00000130  65 74 68 65 72 6e 65 74  20 70 6f 72 74 20 61 6e  |ethernet port an|
00000140  64 20 65 6d 62 65 64 64  65 64 20 77 65 62 20 73  |d embedded web s|
00000150  65 72 76 65 72 0d 0a 20  20 20 20 20 20 20 20 20  |erver..         |
00000160  20 20 20 20 20 20 20 41  73 73 69 67 6e 20 73 74  |       Assign st|
00000170  61 74 69 63 20 49 50 20  61 64 64 72 65 73 73 20  |atic IP address |
```

Talking to Python: Nouns

```
# This is a comment
# This is an int (integer)
42
# This is a float (rational number)
4.2
# These are all strings (sequences of characters)
'ATGC'

"Mendel's Laws"

""">CAA36839.1 Calmodulin
MADQLTEEQIAEFKEAFSLFDKDGDGTITTKELGTVMRSLGQNPTEAEL
QDMINEVDADDLPGNGTIDFPEFLTMMARKMKDTDSEEEIREAFRVFDK
DGNGYISAAELRHVMTNLGEKLTDEEVDEMIREADIDGDGQVNYEEFVQ
MMTAK"""
```

Python as a Calculator

```
# Addition
1+1
# Subtraction
2-3
# Multiplication
3*5
# Division
5/3
# Exponentiation
2**3
# Order of operations
2*3-(3+4)**2
```

Remembering objects

```
# Use a single = for assignment:
TLC = "GATACA"
YFG = "CTATGT"
MFG = "CTATGT"

# A name can occur on both sides of an assignment:
codon_position = 1857
codon_position = codon_position + 3

# Short-hand for common updates:
codon += 3
weight -= 10
expression *= 2
CFU /= 10.0
```

Displaying values with print

```
# Use print to show the value of an object
message = "Hello, world"
print(message)
# Or several objects:
print(1,2,3,4)
# Older versions of Python use a
# different print syntax
print "Hello, world"
```

Collections of objects

```
# A list is a mutable sequence of objects
mylist = [1, 3.1415926535, "GATACA", 4, 5]
# Indexing
mylist[0] == 1
mylist[-1] == 5
# Assigning by index
mylist[0] = "ATG"
# Slicing
mylist[1:3] == [3.1415926535, "GATACA"]
mylist[:2] == [1, 3.1415926535]
mylist[3:] == [4,5]
# Assigning a second name to a list
also_mylist = mylist
# Assigning to a copy of a list
my_other_list = mylist[:]
```

Repeating yourself: iteration

```
# A for loop iterates through a list one element
# at a time:
for i in [1,2,3,4,5]:
    print(i, i**2)

# A while loop iterates for as long as a condition
# is true:
population = 1
while(population < 1e5):
    print(population)
    population *= 2
```

Verb that noun!

return_value = function(parameter, ...)
“Python, do *function* to *parameter*”

```
# Built-in functions
#  Generate a list from 0 to n-1
a = range(5)
#  Sum over an iterable object
sum(a)
#  Find the length of an object
len(a)
```

Verb that noun!

return_value = function(parameter, ...)
"Python, do *function* to *parameter*"

```
# Importing functions from modules
import numpy
numpy.sqrt(9)

import matplotlib.pyplot as plt
fig = plt.figure()
plt.plot([1,2,3,4,5],
         [0,1,0,1,0])

from IPython.core.display import display
display(fig)
```

New verbs

```python
def function(parameter1, parameter2):
    """Do this!"""
    # Code to do this
    return return_value
```

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- Saving interactive sessions is a good way to document our computer "experiments".
- Likewise, we can use modules and scripts to document our computer "protocols".
- Most of these statements are applicable to any programming language (Perl, R, Bash, Java, C/C++, FORTRAN, ...)

Homework: Exploring Files

1. Try reading the first few bytes of different files on your computer. Can you distinguish binary files from text files?
2. Create a simple data table in your favorite spreadsheet program and save it in a text format (*e.g.*, save as CSV or tab-delimited text from Excel[1]). Practice reading the data from Python.

[1] Note for Mac users: Excel will offer you Macintosh and DOS/Windows text formats. Choose *DOS/Windows*