Practical Bioinformatics

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5/20/2013

Resources

Getting \Scienti c" Python

- https://www.enthought.com/products/canopy/academic/

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Resources on the course website:

- Syllabus
  - Papers and code (for downloading *before* class)
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Resources on the course website:

- Syllabus
  - Papers and code (for downloading *before* class)
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- On-line textbooks (Dive into Python, Numerical Recipes, ...)
- Programs for this course (Canopy, Cluster3, JavaTreeView, ...)

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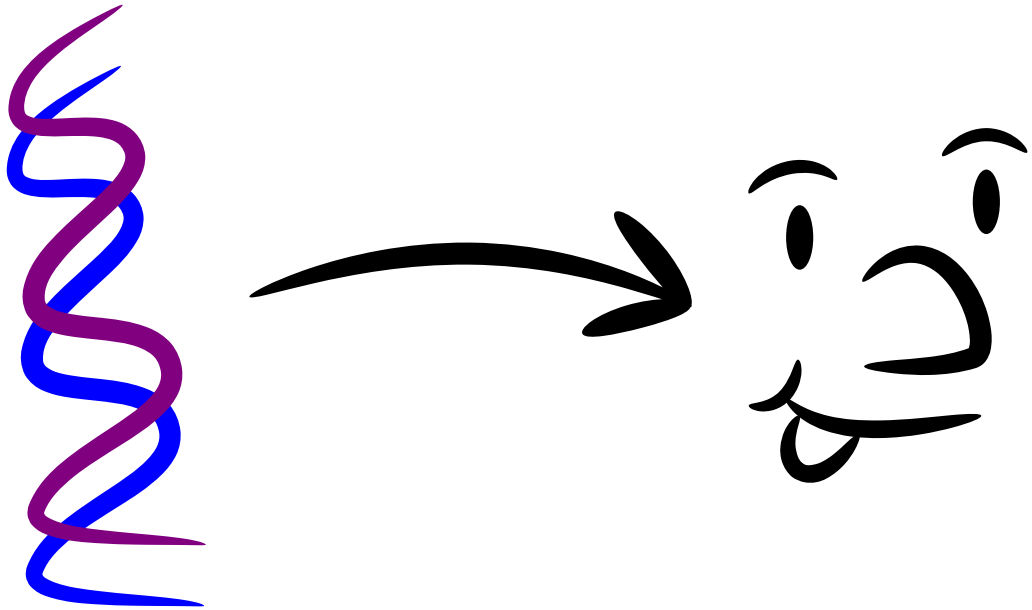
- Writing standalone scripts.
- Shepherding data between analysis tools.
- Aggregating data from multiple sources.
- Implementing new methods from the literature.

Course problems: expression and sequence analysis



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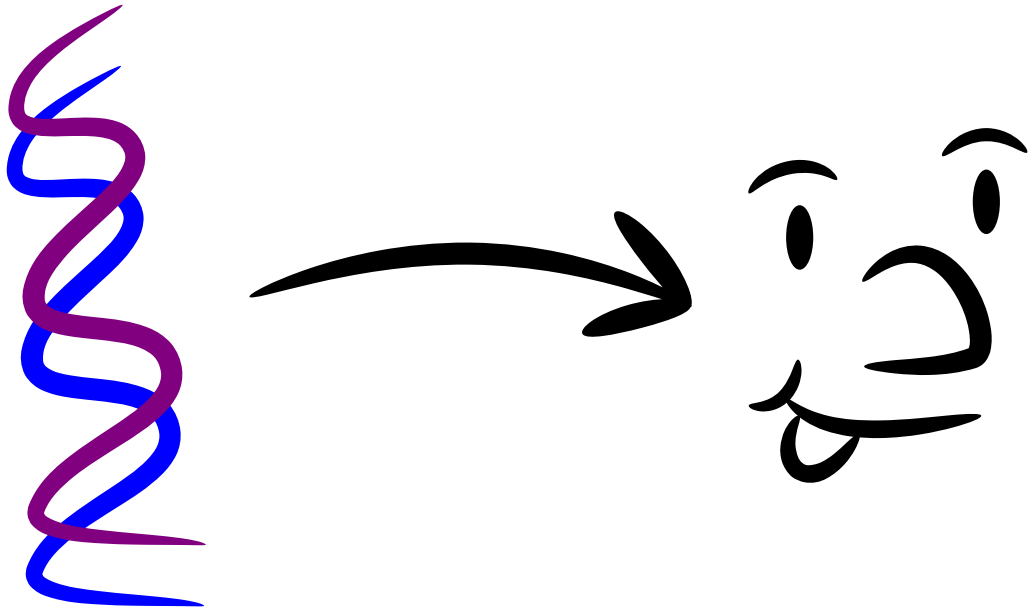
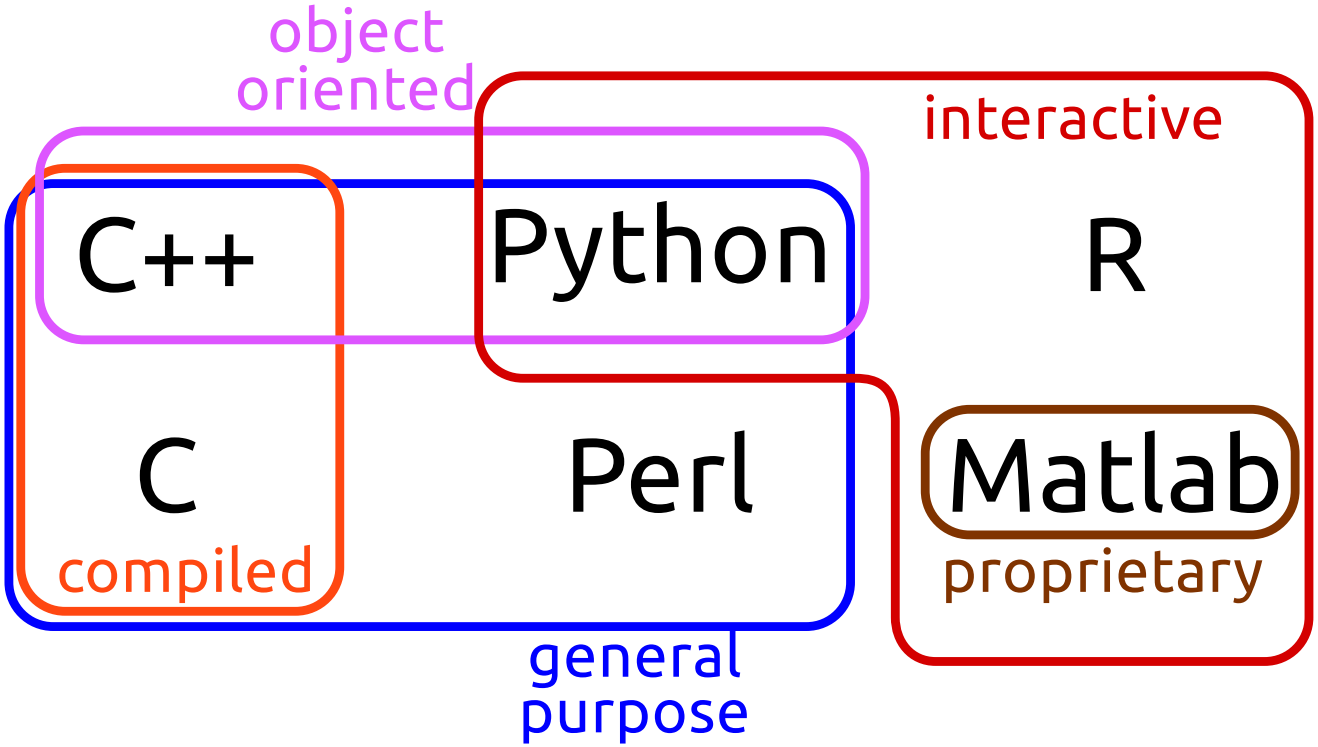


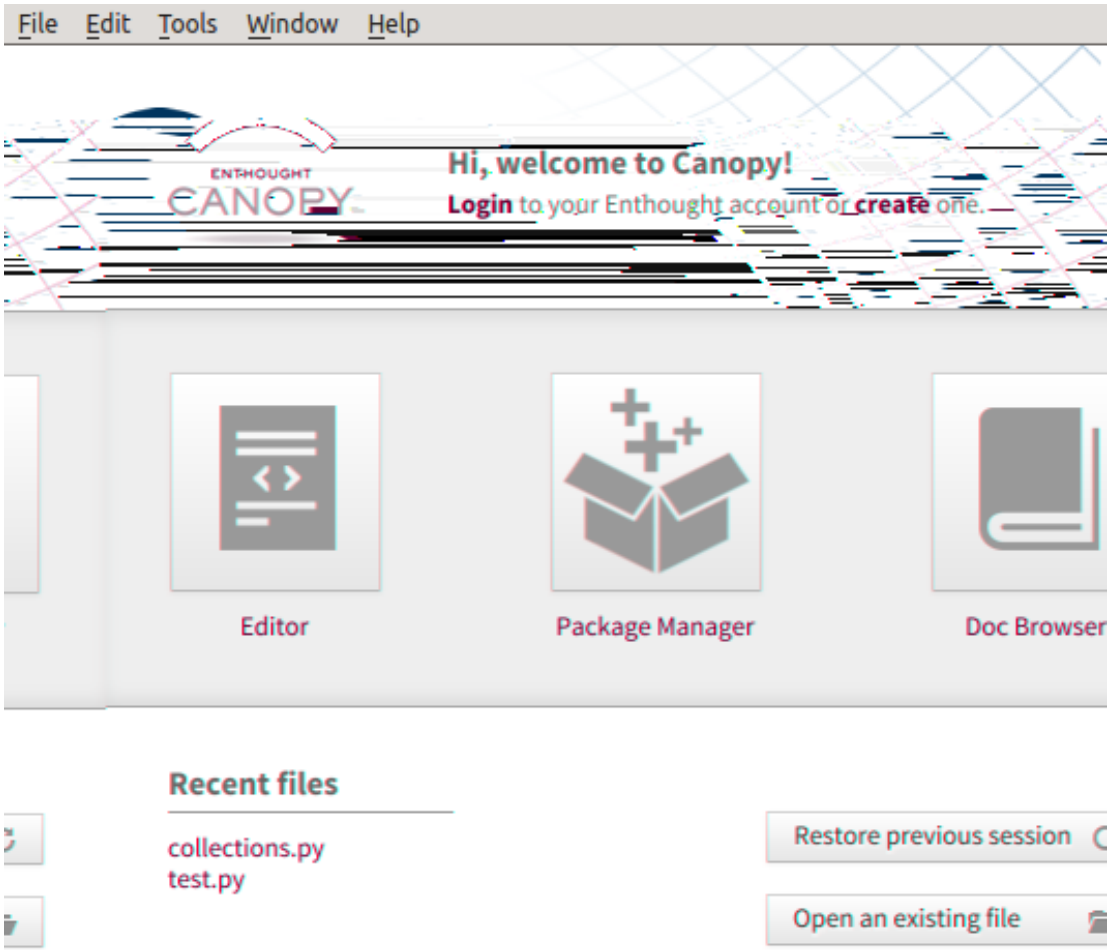
Part 2: Genotype
(Sequence analysis)

Part 1: Phenotype
(Expression pro ling)

Course tool: Python



Python distribution: Enthought Canopy



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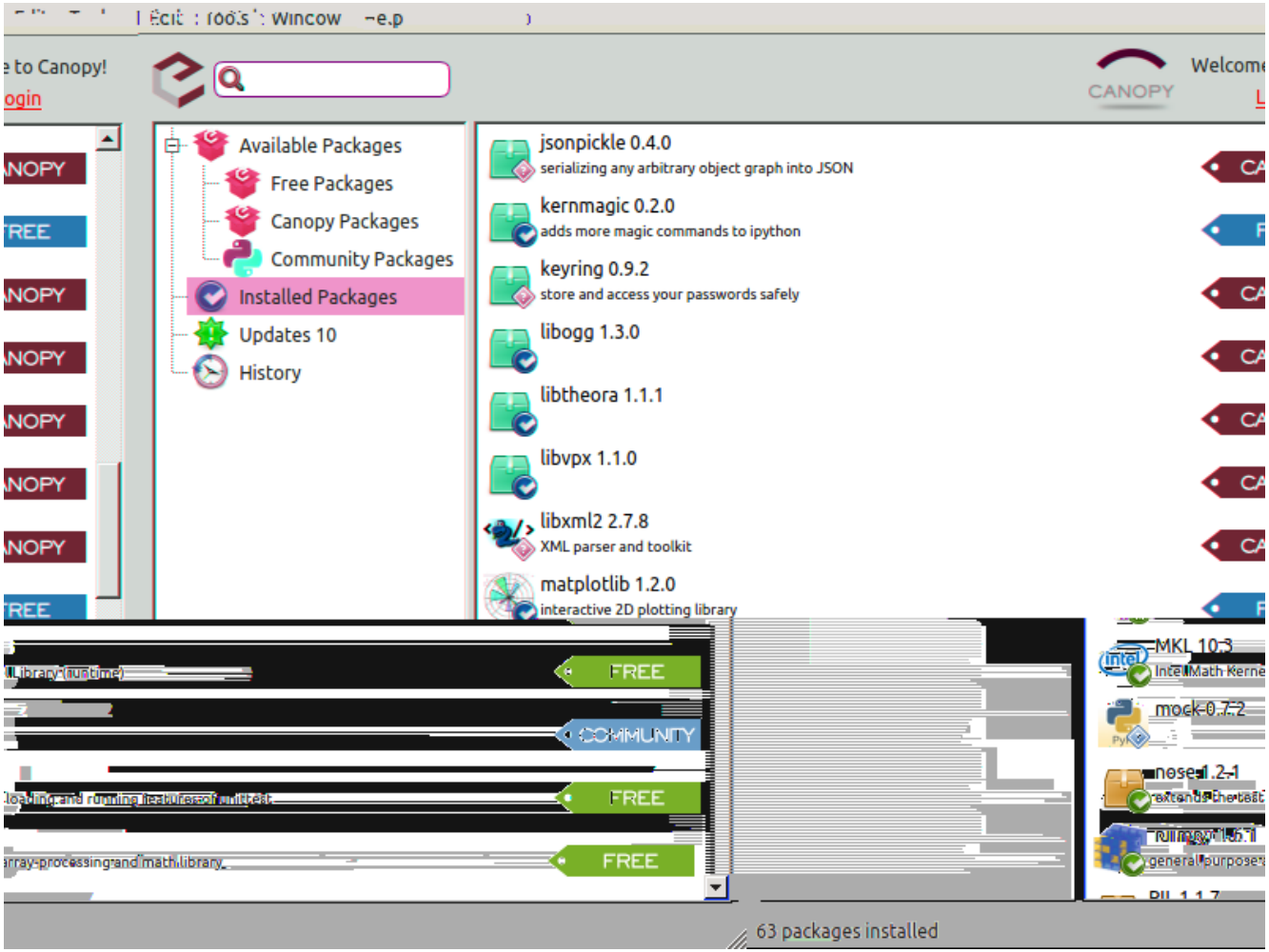

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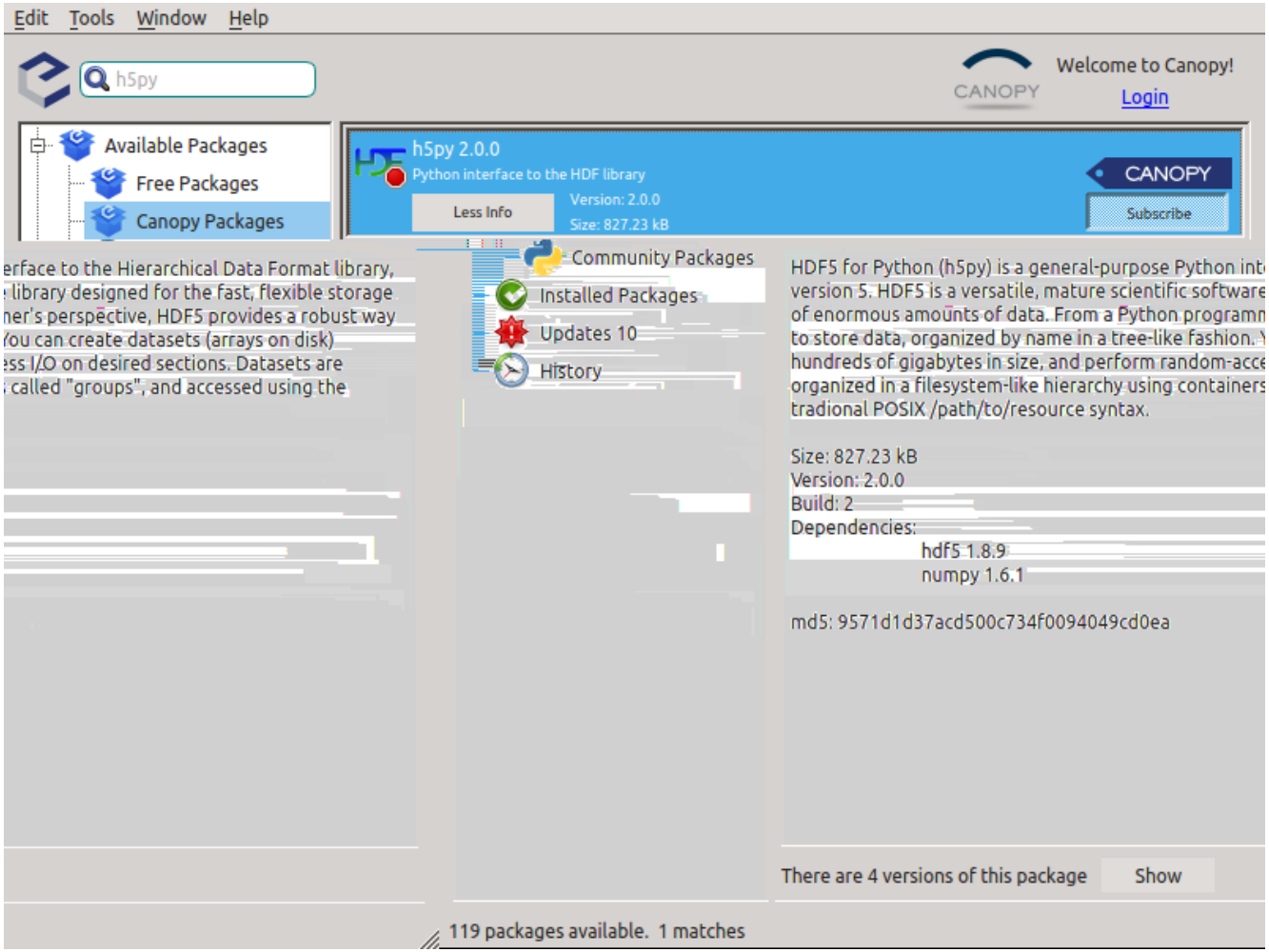
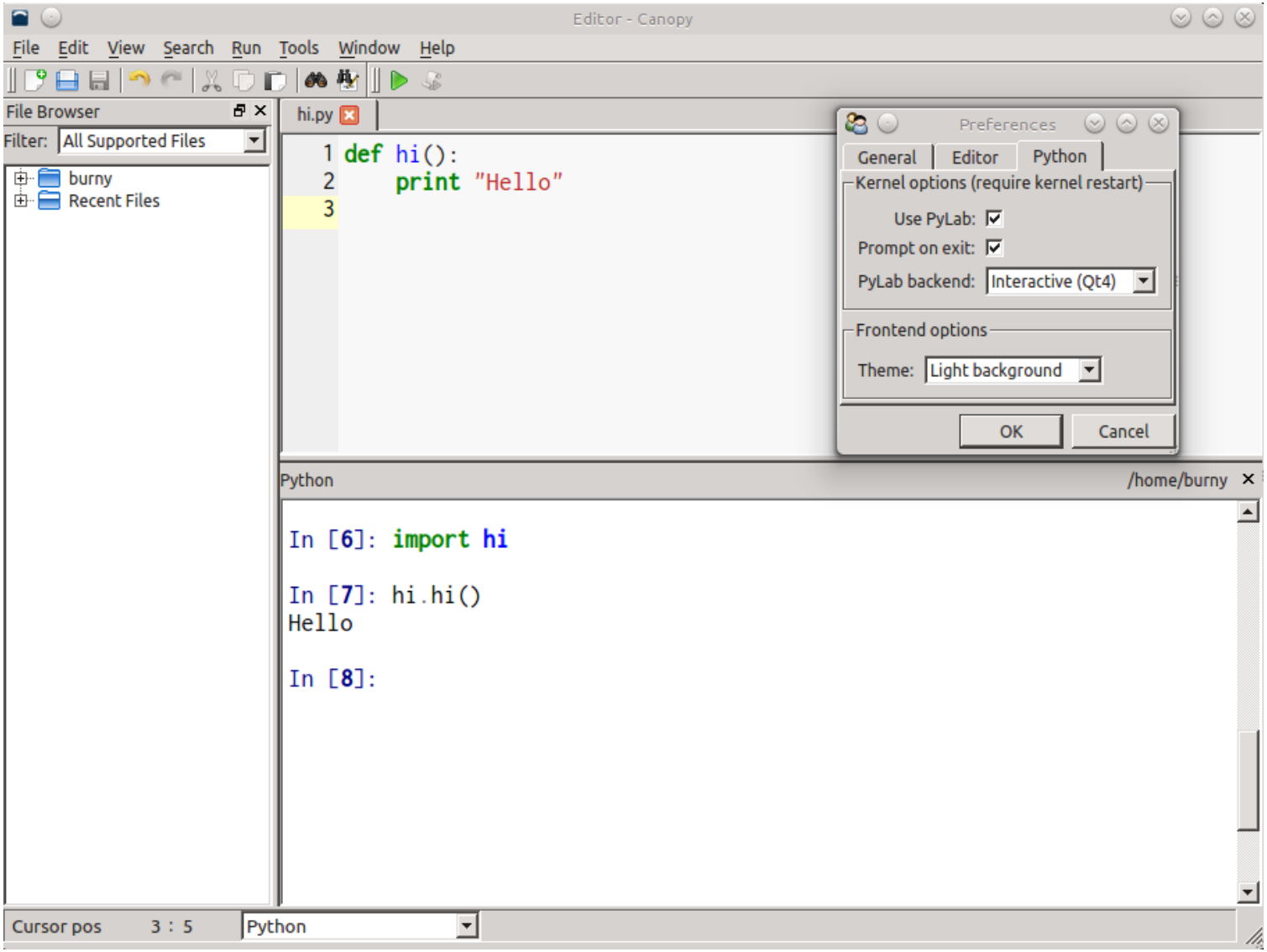
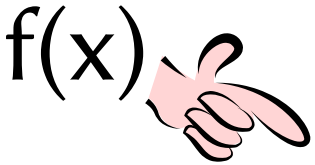


Python shell: IPython (qtconsole)

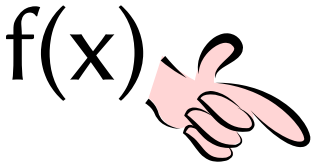


Anatomy of a Programming Language



functions

Anatomy of a Programming Language



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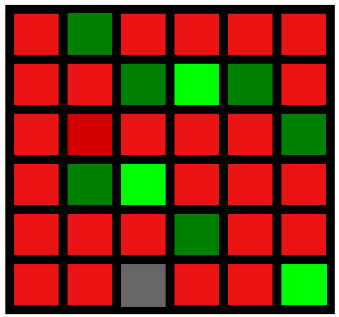

data structures

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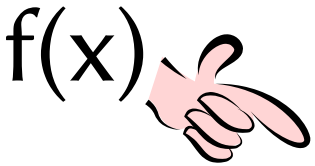
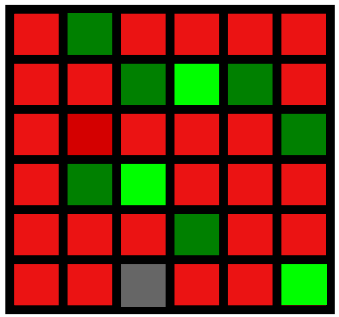


functions



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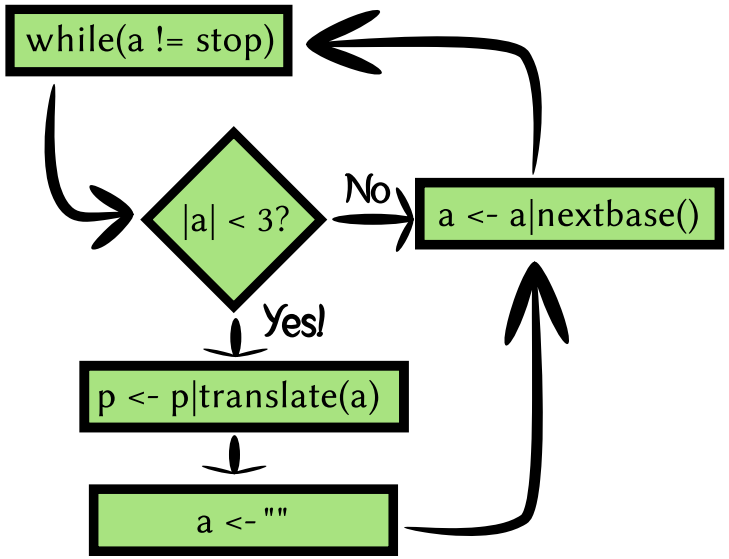

control statements

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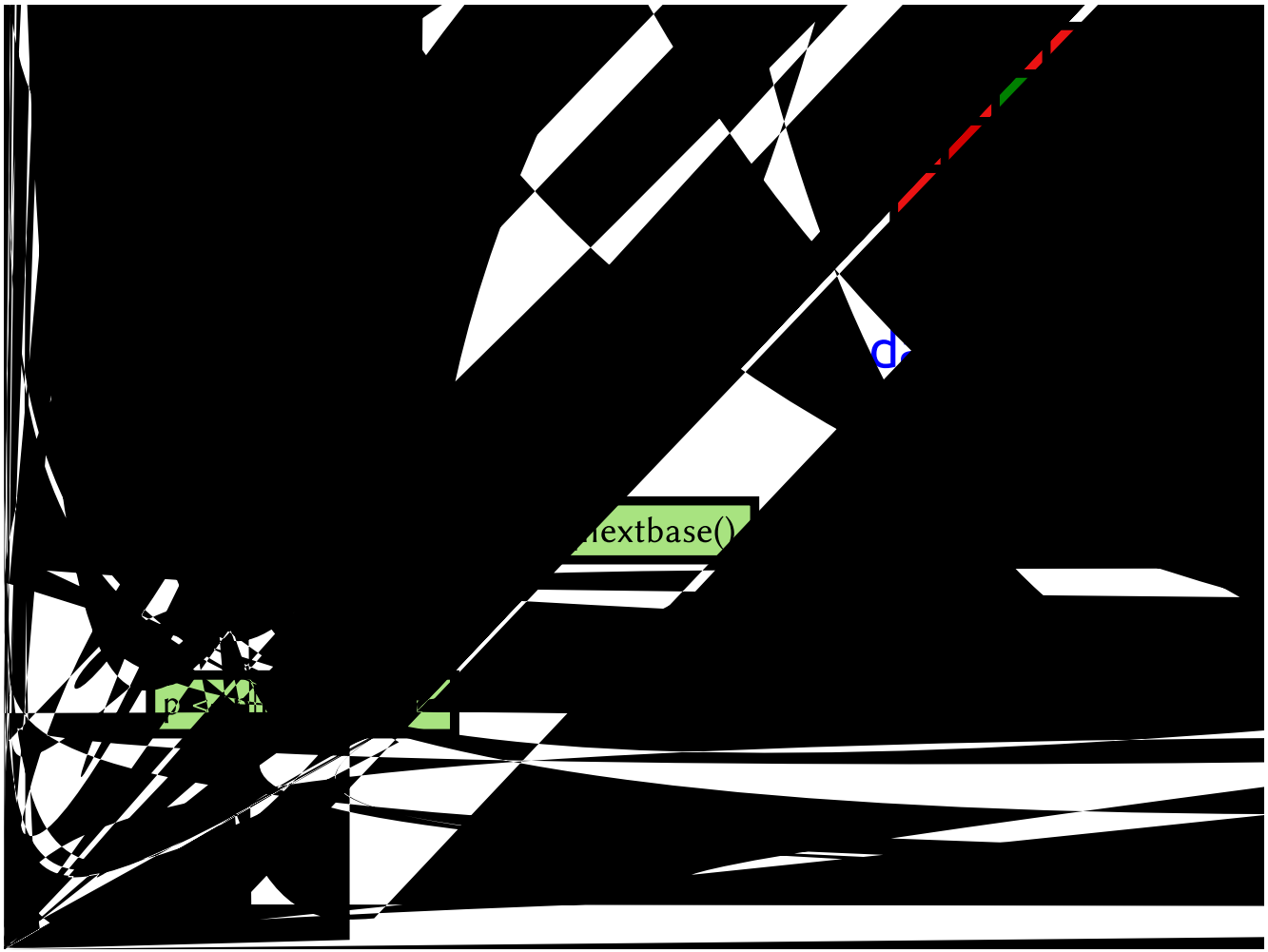

Talking to Python: Nouns

```
# 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
"""
```

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
```

Python as a Calculator

```
# Addition
1+1
# Subtraction
2-3
# Multiplication
3*5
# Division (gotcha: be sure to use floats)
5/3.0
# Exponentiation
2**3
# Order of operations
2*3-(3+4)**2
```

Python as a Calculator

1. Calculate the T_m of a QuickChange mutagenesis primer with length 25bp ($L = 25$), 13 GC bases ($n_{GC} = 13$), and 2 mismatches to the template ($n_{MM} = 2$) using the formula from Stratagene:

$$T_m = 81.5 + \frac{41n_{GC} - 100n_{MM} - 675}{L} \quad (1)$$

2. Calculate the molarity of a 70mer oligonucleotide with $A_{260} = .03$ using the formula from Maniatis:

$$C = \frac{.02A_{260}}{330L} \quad (2)$$

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
```

Comparing objects

```
# Use double == for comparison:
YFG == MFG

# Other comparison operators:
#   Not equal:
TLC != MFG
#   Less than:
3 < 5
#   Greater than, or equal to:
7 >= 6
```

Making decisions

```
if(YFG == MFG):
    print "Synonyms!"

if(protein_length < 60):
    print "Probably too short to fold."
elif(protein_length > 10000):
    print "What is this, titin?"
else:
    print "Okay, this looks reasonable."
```

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
```

Summary statistics

Given a list of $\log_2$ expression ratios:
$x = [1.8, 2.0, 1.7, 1.9, 2.3, 1.6, 2.2, 1.8, 1.9, 4.0, 1.7]$

1. Print the corresponding expression ratio values
2. Calculate the mean (average) $\log_2$ ratio:

$$x = \frac{\sum_{i=1}^{N} x_i}{N}$$

3. Calculate the mean expression ratio
4. In what situations do either of these mean values capture useful information about our measurements?

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)
```

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$x = [1.8, 2.0, 1.7, 1.;\ \ :7, :\ ;\ \ :7,\ \ :0,1$

Fun with logarithms

In log space, multiplication and division become addition and subtraction:

$$\begin{aligned} \log(xy) &= \log(x) + \log(y) \\ \log(x/y) &= \log(x) - \log(y) \end{aligned}$$

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Therefore, exponentiation becomes multiplication:

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Also, we can change of the base of a logarithm like so:

$$\log_A(x) = \log(x)/\log(A)$$

Verb that noun!

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```
# Importing functions from modules
import math
math.sqrt(9)
math.log(8)/math.log(2)

from math import log
log(16)/log(2)
```

Summary statistics

Given a list of expression ratios:
$r = [4.00, 4.59, 3.73, 4.29, 5.66, 3.48, 5.28, 4.00, 4.29, 18.38, 3.73]$

1. Write a for loop to convert the list to $\log_2$ ratios
2. How can you do this conversion without destroying the original list?
3. How can you invert the transform (covert the new list back to the original list)?

Short-hand for converting lists

```
from math import log
log2 = log(2)
logratios = [log(i)/log2 for i in ratios]
```

New verbs

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

Setting Canopy's working/import directory

OS X

- Open a terminal
- cd path/to/working/directory
- env PYTHONPATH="$PYTHONPATH:$PWD" canopy

Windows (or OS X)

- Start canopy
- %cd path/to/working/directory
- import sys, os
- sys.path.append(os.getcwd())

Loading and re-loading your functions

```
# For now, we will keep code and data in a
# single directory
%cd /home/state_your_name/BMS270
%logstart -o /home/state_your_name/BMS270/day3.log

# Use import the first time you load a module
#   (And keep using import until it loads
#    successfully)
import my_module

my_module.my_function(42)

# Once a module has been loaded, use reload to
#   force python to read your new code
reload(my_module)
```

Make your own Fun

Write functions for these calculations:

1. Mean:

$$x = \frac{\sum_i^N x_i}{N} \tag{3}$$

2. Standard deviation:

$$\sigma_x = \sqrt{\frac{\sum_i^N (x_i - x)^2}{N - 1}} \tag{4}$$

3. Correlation coe cient (Pearson's r):

$$r(x, y) = \frac{\sum_i (x_i - x)(y_i - y)}{\sqrt{\sum_i (x_i - x)^2} \sqrt{\sum_i (y_i - y)^2}} \tag{5}$$

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- 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

1. Practice writing your own functions and importing them into Python.
2. E-mail Mark your python sessions after class
3. E-mail Mark any homework code/results before tomorrow's class