Practical Bioinformatics

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4/24/2017

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 (Canopy, Cluster3, JavaTreeView, ...)

Homework

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- If you get stuck, try working things out on paper first.

Goals

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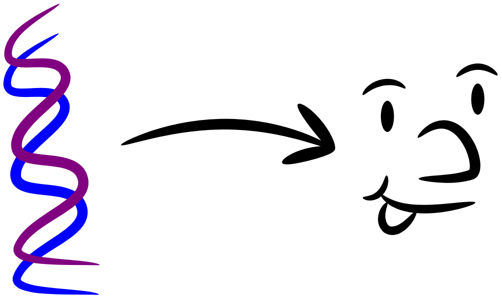
This is also good preparation for communicating with computational collaborators.

Course problems: expression and sequence analysis



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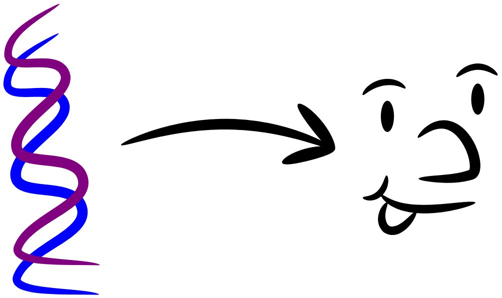
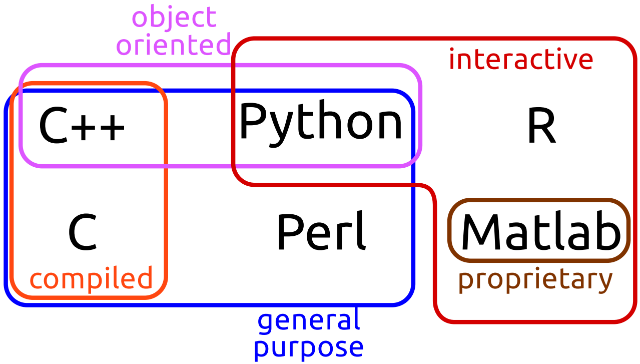


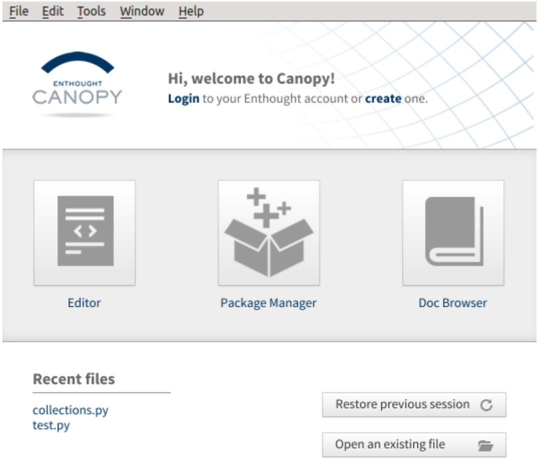
Part 2: Genotype
(Sequence analysis)

Part 1: Phenotype
(Expression profiling)

Course tool: Python



Python distribution: Enthought Canopy



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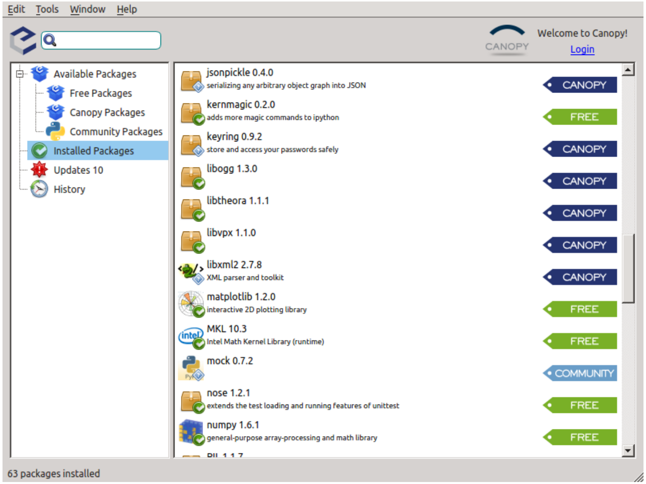


jsonpickle 0.4.0
serializing any arbitrary object graph into JSON
CANOPY

kernmagic 0.2.0
adds more magic commands to ipython
FREE

keyring 0.9.2
store and access your passwords safely
CANOPY

libogg 1.3.0
CANOPY

libtheora 1.1.1
CANOPY

libvpx 1.1.0
CANOPY

libxml2 2.7.8
XML parser and toolkit
CANOPY

matplotlib 1.2.0
interactive 2D plotting library
FREE

MKL 10.3
Intel Math Kernel Library (runtime)
FREE

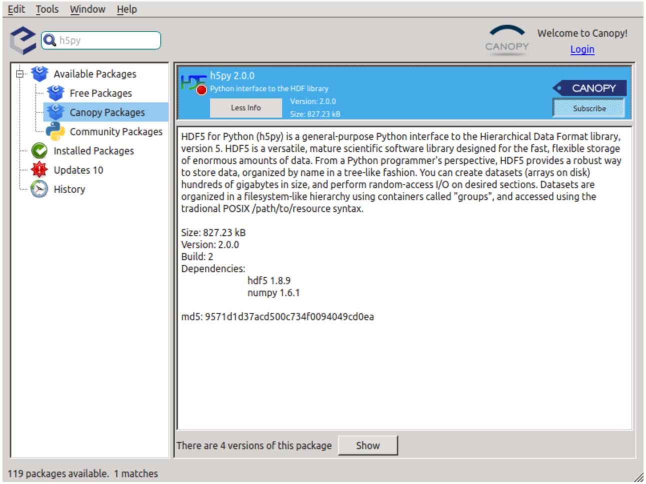
mock 0.7.2
COMMUNITY

nose 1.2.1
extends the test loading and running features of unittest
FREE

numpy 1.6.1
general-purpose array-processing and math library
FREE

63 packages installed

Python distribution: Enthought Canopy



HDF5 for Python (h5py) is a general-purpose Python interface to the Hierarchical Data Format library, version 5. HDF5 is a versatile, mature scientific software library designed for the fast, flexible storage of enormous amounts of data. From a Python programmer's perspective, HDF5 provides a robust way to store data, organized by name in a tree-like fashion. You can create datasets (arrays on disk) hundreds of gigabytes in size, and perform random-access I/O on desired sections. Datasets are organized in a filesystem-like hierarchy using containers called "groups", and accessed using the tradional POSIX /path/to/resource syntax.

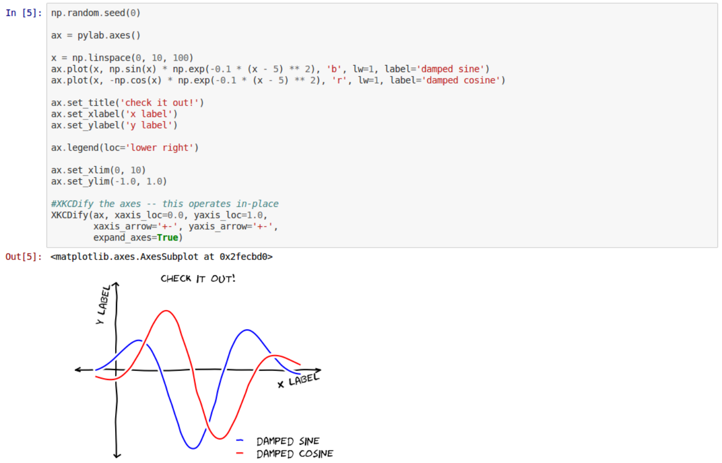
Size: 827.23 kB
Version: 2.0.0
Build: 2
Dependencies:
hdf5 1.8.9
numpy 1.6.1

md5: 9571d1d37acd500c734f0094049cd0ea

There are 4 versions of this package

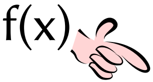
119 packages available. 1 matches

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

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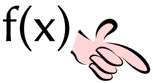

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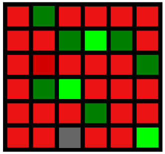

data structures

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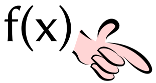

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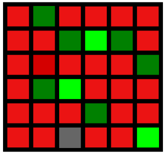

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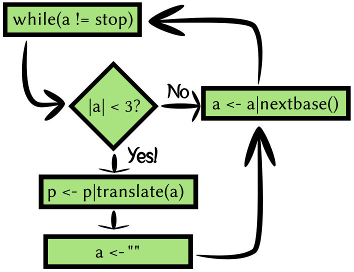
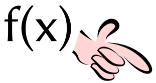
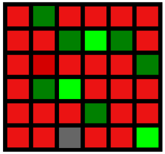


control statements

Anatomy of a Programming Language



functions



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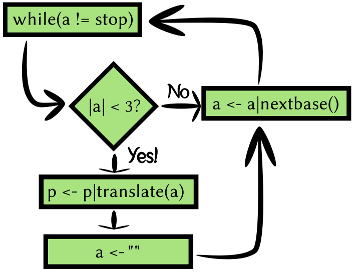

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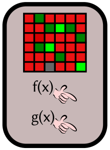

objects

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 (gotcha: be sure to use floats)
5/3.0
# 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
```

Python as a Calculator

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

$$C = \frac{.02A_{260}}{330L} \tag{1}$$

2. 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:

$$T_m = 81.5 + \frac{41n_{GC} - 100n_{MM} - 675}{L} \tag{2}$$

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)
# Older versions of Python use a
# different print syntax
print "Hello, world"
```

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
```

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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```
# 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

```
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: Make your own Fun

Write functions for these calculations, and test them on random data:

1. Mean:

$$\bar{x} = \frac{\sum_i^N x_i}{N}$$

2. Standard deviation:

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

3. Correlation coefficient (Pearson's r):

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