Practical Bioinformatics

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Resources

Router:

- SSID: BMS270
- password: deoxyribose

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Getting Python

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Course website:

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Resources on the course website:

- Syllabus
  - Papers and code (for downloading *before* class)
  - Slides and transcripts (available *after* class)
- On-line textbooks (Safari Bookshelf, Numerical Recipes, ...)
- Programs for this course (Python, Cluster3, JavaTreeView, ...)

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At the end of this class, you should have the con dence to take on the day to day tasks of \bioinformatics".

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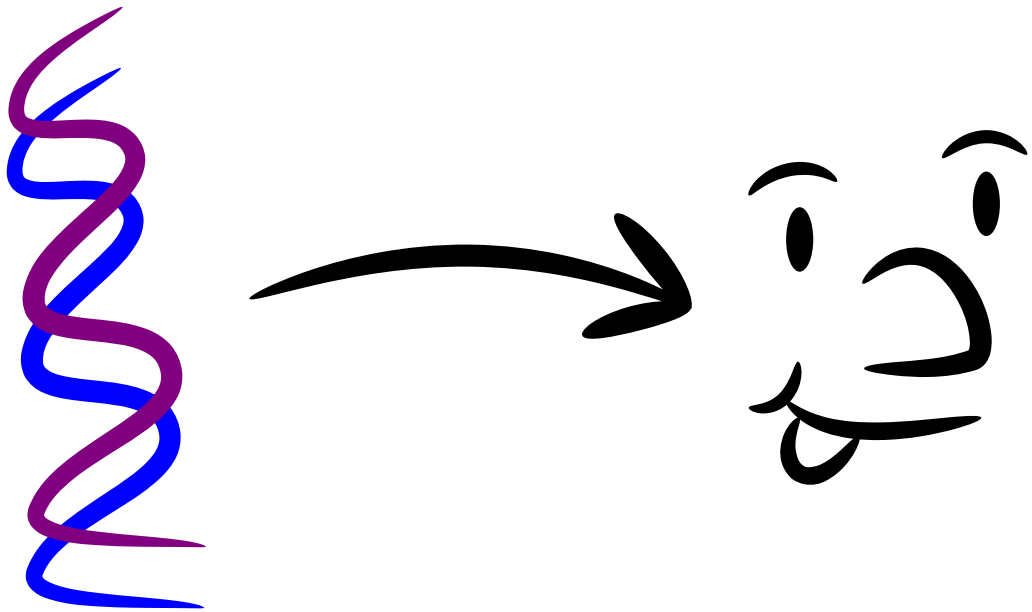
- Writing standalone scripts.
- Shepherding data between analysis tools.
- Aggregating data from multiple sources.
- Implementing new methods from the literature.

Course problems: microarray and sequence analysis



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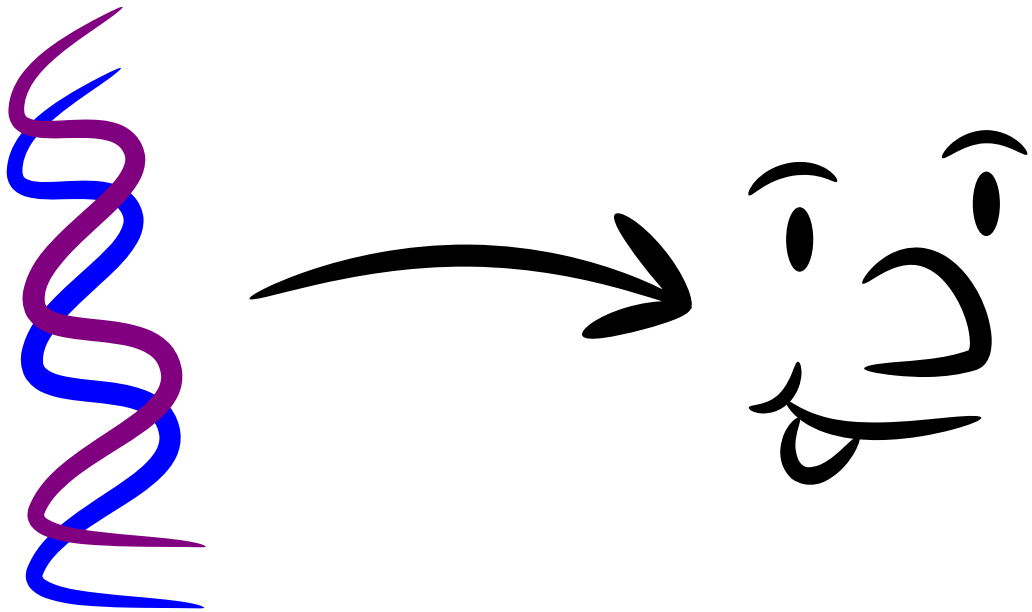
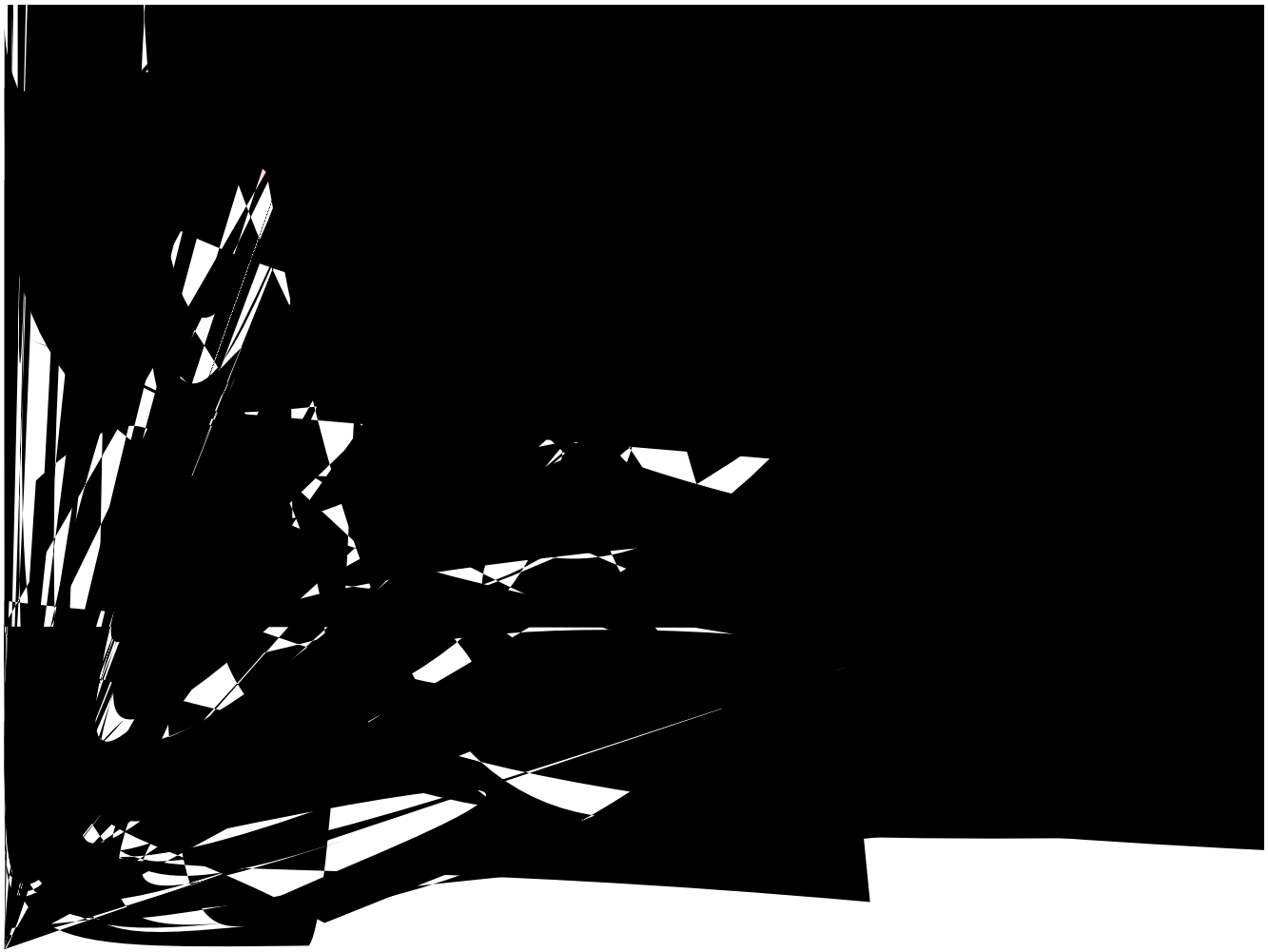


Part 2: Genotype
(Sequence analysis)

Part 1: Phenotype
(Expression pro ling)

Anatomy of a Programming Language



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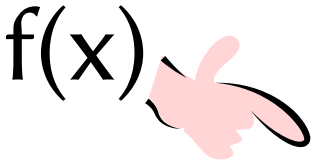

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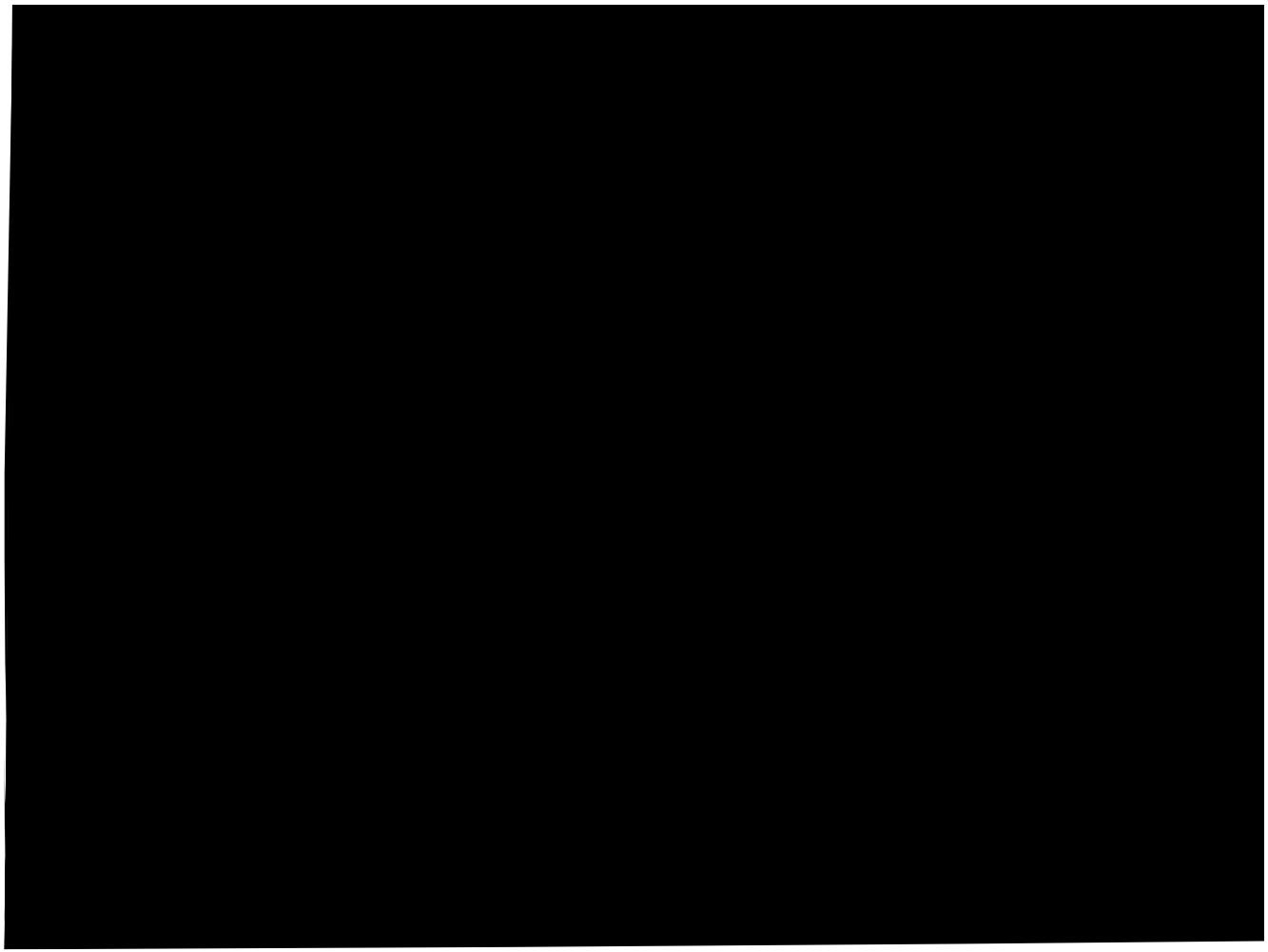
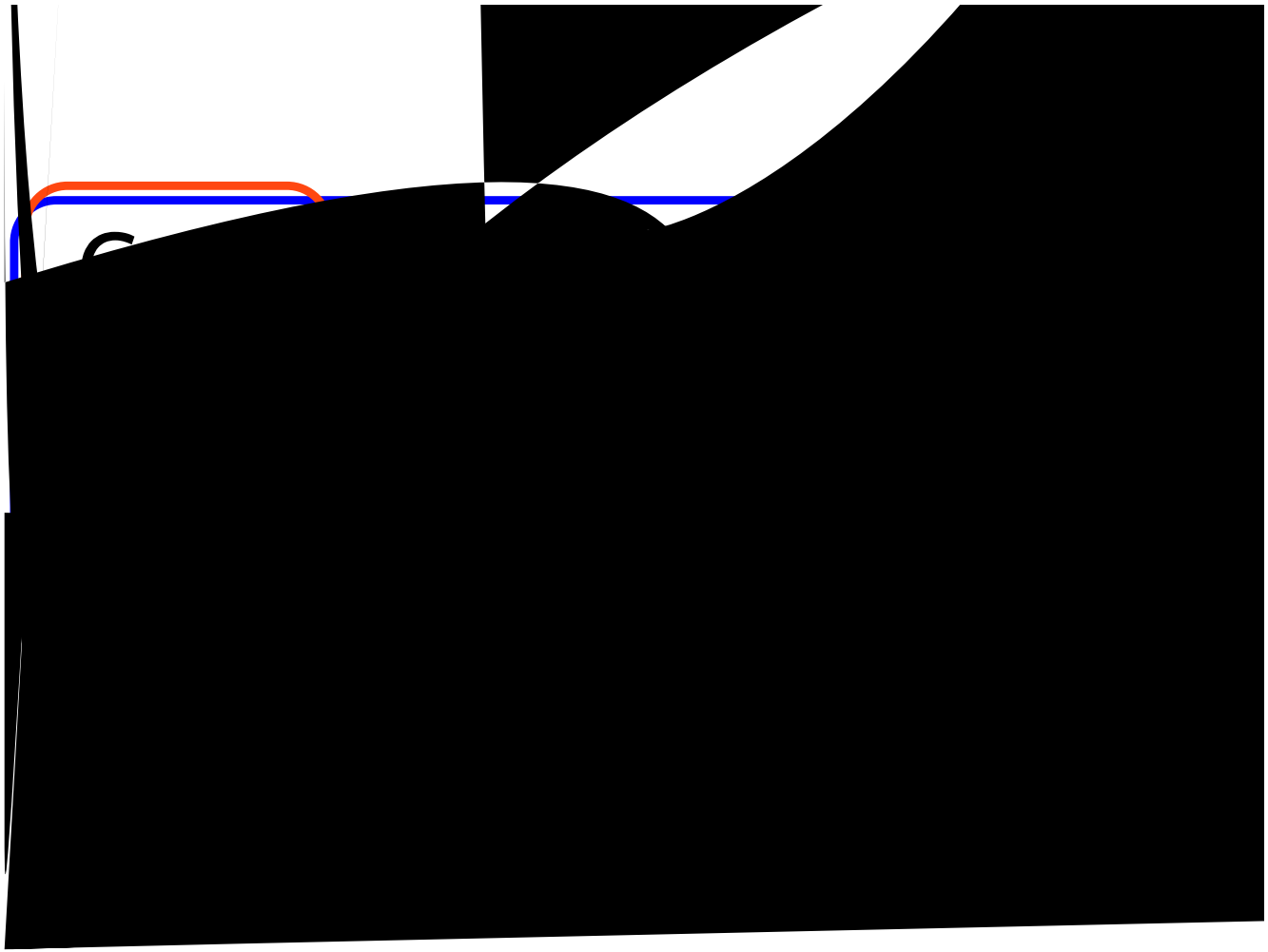


Course tool: Python



Two ways to start Python on OS X

- Using IDLE (like Windows)
  1. Open a terminal window
  2. python -m idlelib.idle
- Using command-line Python and Emacs (more stable)
  1. Open a terminal window
  2. python
  3. Open a second terminal window (or a new tab)
  4. emacs

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
```

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:

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

3. Find the original concentration assuming 10μL of oligo diluted into 990μL of solvent for the measurement.

Saving and comparing 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
```

Checking 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
```

Saving and 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
```

Saving and comparing objects

```
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[:]
```

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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Given a list of $\log_2$ expression ratios:
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1. Calculate the mean (average) $\log_2$ ratio:

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

using functions to simplify your calculation.

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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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?

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 IDLE's working directory

OS X

- Open a terminal
- cd path/to/working/directory
- python -m idlelib.idle

Windows

-

Emacs cheat sheet

C = control, M = meta

C-x C-c	Quit
C-g	Break out of current command
C-_	Undo last edit
C-x C-s	Save
C-x C-w	Save as
C-x C-f	Open/create file (in new buffer)
C-x b	Switch buffers
C-x k	Kill buffer (close file)
C-k	Kill (cut) line
C-w	Kill (cut) selection
C-y	Yank (paste)

Loading and re-loading your functions

```
# 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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- 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

1. Practice writing your own functions and importing them into Python.
2. Read Sections 4.1{4.4 of Learning Python, 3rd edition.
   - (If you are feeling ambitious, read 8.1-8.2, 12, and 13).
3. Remember to come to class tomorrow!