Practical Computing for Biologists

Release 1.0

Cliburn Chan

June 01, 2012

CONTENTS

CHAPTER

ONE

UPDATES

24 April 2012 Personal web space on the Duke servers is not turned on by default for DUMC perosnnel. However, if you make a request for AFS space to help@oit.duke.edu, it will be available to you within 24 hours.

9 April 2012 The PCfB textbook is now available for collection for course participants at Room 120, Surgical Oncology Research Facility. Please read or at least scan the book before the workshop starts. There are also pre-workshop *Assignments* that you will need to do. We will shortly be contacting course participants for data sets/repetitive tasks that could serve as relevant demonstrations or examples of regular expression manipulation, programming or use of relational databases.

3 April 2012 The course is now fully subscribed, and new registrants will be placed on a wait list. Please continue to register if you are interested - if there is sufficient demand, we will plan for a second workshop. Thanks so much for your enthusiasm and support!

CHAPTER

TWO

INTRODUCTION

The CFAR Biostatistics and Computational Biology Core is conducting a *free* four-day workshop for Duke researchers to learn how to use the computer more effectively for scientific work. It is designed for people who *need to work with large and complex data sets and suspect that there is a better and faster way to get their work done*. The course will use the textbook *Practical Computing for Biologists (PCfB)* by Steven Haddock and Casey Dunn, and *CFAR is generously giving each participant a free copy of the book*. The main intent of the course is to teach researchers how to use the Unix shell, the Python programming language, databases and image manipulation tools to execute common scientific chores. An OS X system is preferred since Macs provide a Unix command line natively. Windows users can also participate by setting up Linux in an emulator (this is perfectly safe and instructions are given in the *PCfB* textbook).

The course is designed for people trained in biology, and *no previous Unix or programming experience is necessary*. The course will be limited to 12 participants and will be held at the Surgical Oncology Research Facility (SORF) Beard Conference Room from 29 May 2012 to 1 June 2012. Please email cliburn.chan@duke.edu if you have any enquiries or wish to register for the course. Acceptance will be on a first-come first-serve basis, but CFAR investigators and their trainees will be given priority.

We will contact course participants before the workshop starts to collect your copy of *Practical Computing for Biologists*. To make it relevant for your needs, participants will also be asked to suggest computational tasks that you would like to automate or simplify, as well as to contribute data sets that are tedious to preprocess and filter manually. We will try to work these examples into the demonstrations or class assignments if at all possible. Updates and course materials will be posted at http://www.duke.edu/~ccc14/pcfb/.

CHAPTER

THREE

COURSE DESCRIPTION

29 May 2012 (Tuesday)

AM: Software installation and working with text editors. We will install the TextWrangler editor (jEdit for Linux users), the Enthought Python distribution (Academic license), ImageMagick, ImageJ, MySQL Community Server and MySQL Workbench. Participants are expected to install the software ahead of the workshop following instructions in *PCfB*, but help and troubleshooting will be provided in the morning session if necessary. Many operations on large file sets, especially for text data, are performed much more efficiently from the command line than from a graphical interface. We will learn how to open a Terminal, and perform text processing, access material from the web, and write simple shell scripts to automate common tasks.

Installation and introduction

Basic Unix commands

PM: We will learn to use the TextWranger/jEdit editor to understand the basics of regular expressions, and how to reformat text using regular expressions. TextWrangler/jEdit will also be used to develop programs from Day 2. We will also learn to transfer and synchronize files with remote computers from the command line, or run programs on remote computers using the command line (ssh)). We will conclude by showing how to construct a simple homepage using Sphinx and upload it to the Duke server.

Using a text editor and regular expressions

Remote computing and web page generation

30 May 2012 (Wednesday)

AM: Day 2 introduces you to the Python programming language, a modern dynamic language that is (relatively) easy to learn. The morning session will introduce you to the powerful IPython interpreter, where you will test out code snippets with instant feedback, and learn about the Python documentation and help system. We wil then move on to Python scripting, including decisions and loops, reading from and writing to files, and writing your own functions.

Python Basics I

Python Basics II

PM: The afternoon will introduce you to the most useful Python modules in the standard library, followed by an introduction to the NumPy module for numerical work, and Matplotlib for graphics.

Python Modules

NumPy and Matplotlib

31 May 2012 (Thursday)

AM: You will learn more about Numpy and Matplotlib, together with how to use the Biopython module for sequenc and array analysis, as well as how to access the NCBI databases programmatically.

Biopython I

Biopython II

PM: The afternoon starts with an introduction to relational databases and how to query them using SQL, then concludes with some intermediate examples of using Python for data analysis and statistical simulation.

Data management and relational databasesI

Data analysis with Python

01 June 2012 (Friday)

AM: On the final day, we will have a tutorial for how to create scientific diagrams using the vector illustration program Inkscape. The course will conclude with working through developing a moderately complex Python program to parse, summarize and display data from a cytokine assay experiment.

Vector graphics with Inkscape

Capstone example

CHAPTER

FOUR

INSTRUCTOR: CLIBURN CHAN, BIOSTATISTICS AND BIOINFORMATICS.

Cliburn is a computational biologist whose main research interest is in data analysis and modeling of immune responses. He teaches the Introduction to the Practice of Biostatistics I & II courses for the Duke Masters in Biostatistics program, and has been programming in Python for over a decade. Other instructors will be Jacob Frelinger, a PhD student in the Computational Biology and Bioinformatics (CBB) program and Adam Richards, a postdoctoral fellow in the department of Biostatistics and Bioinformatics.

4.1 Data Samples

4.1.1 Basic Unix commands

1. `hamlet`

4.1.2 Using a text editor and regular expressions

1. `TextWrangler tutorial`
2. `Lorem ipsum`
3. `Email`
4. `Find and replace`
5. `Ch3observations`

4.1.3 Remote computing and web page generation

No data samples.

4.1.4 Python Basics I

No data samples.

4.1.5 Python Basics II

1. `sequence1`
2. `hamlet`

4.1.6 Python Modules

1. `CSV sample data`
2. `CSV exercise solution`

4.1.7 NumPy and Matplotlib

1. `cell cycle microarray`

4.1.8 Biopython I

1. `orchid FASTA file`

4.1.9 Biopython II

4.1.10 Data management and relational database

`SQLite example database` `Code to generate the database`

4.1.11 Data analysis with Python

1. `Ch3observations`

4.1.12 Vector graphics with Inkscape

1. `tux image`

4.1.13 Capstone Example

1. `Cytokine assay (Excel)`
2. `Cytokine assay (TDL)`

4.2 Assignments

4.2.1 Pre-workshop

#1 Software installation

Once you have collected your copy of the PCfB book from SORF, install the following software. If you will be using a Windows system, please follow the instructions starting on page 458 under **Installing VirtualBox** till the end of Appendix 1.

For Mac users, install **TextWrangler** (Page 12) and **MySQL** (Page 260). We also recommend installing the Enthought Python Distribution by requesting a free academic copy from http://www.enthought.com/products/edudownload.php (this will email you a download link). It will also be useful to learn how to compile and install software from *source* by following the instructions given in Chapter 21. If you find the instructions extremely confusing, an alternative is to use a package management system such as *MacPorts*. MacPorts and how to use it to install software are described on Page 415.

At the end of this assgnment, you should have installed the following software:

1. TextWranger (jEdit for Windows/Ubuntu)
2. MySQL
3. Enthought Python Distribution
4. ImageMagick (compiling from source or using a package management system such as MacPorts)

#2 Creating your Duke home page

Requesting for AFS space All DUMC personnel with a NetID are eligible for AFS space (5GB) for hosting personal web pages. However it is not available by default. Please email help@oit.duke.edu to request for AFS space if necessary to complete this assignment. It should be available to you within 24 hours of the request.

1. Create a filed called index.html in your text editor (TextWranger or jEdit) and type or copy the following text:

```
<html>
   <head>
      <title>My home page for PCfB</title>
   </head>
   <body>
     Congratulations, you have successfully created your home page!
   </body>
</html>
```

2. Use your NetID and password to log into WebFiles. You'll be connected to your home directory.
3. Click the *Shared Spaces* tab.
4. Under *Your Personal Web Space*, click *Create public_html*
5. Under *Your Personal Web Space*, click *Upload to public_html* and upload the *index.html* file you downloaded to your desktop in Step 1.
6. To view your Web site, visit http://www.duke.edu/~NetID. (Replace NetID with your NetID but kep the ~)

4.3 References

The website for the textbook Practical Computing for Biologists.

4.3.1 The course website as a PDF

```
Workshop tutorials
```

4.3.2 NCBI eSearch

- ESearch parameters

4.3.3 Unix

- Unix Cheat Sheet

4.3.4 Regular expressions

- Regular Expression Cheat Sheet

4.3.5 Python

Online tutorials

Learn Python the Hard Way: If you have found the learning curve for our exercises to be too steep, try the 52 exercises at this site, which provide a much more gentle ramp. The author shares our philosophy that the only way to effectively learn programming is by working on programming exercises. Don't be put off by the title - the exercises are not as "hard" as the ones in the workshop - by "the hard way" the author just means learning by *doing* instead of learning by *reading*.

Think Python - How to Think Like a Computer Scientist: Once you are comfortable with the basic syntax of Python (e.g. from the book above), this book introduces you gently to the conceptual ideas you willl need to program effectively..

PyPi - A repository of software for the Python programming language

- pypi

Useful packages for scientific computing

- Python
- Numpy
- Scipy
- Matplotlib
- Sphinx

4.3.6 Relational Databases

- SQLite
- SQLite tutorial

4.3.7 Inkscape Tutorials

- How to draw flow charts in Inkscape

4.3.8 Software used

- TextWrangler
- EPD Academic Version
- MySQL
- ImageMagick
- ImageJ

1. Spellman P T, Sherlock, G, Zhang, M Q, Iyer, V R, Anders, K, Eisen, M B, Brown, P O, Botstein, D, Futcher, B. Comprehensive identification of cell cycle-regulated genes of the yeast Saccharomyces cerevisiae by microarray hybridization. *Molecular biology of the cell*, Vol. 9 (12): 3273-97, 1998. PubMed.
2. Duda, R O, Hart, P E & Stork, D G, *Pattern Classification*, John Wiley & Sons, Inc., 2001.
3. Cock, P J A and Antao, Tiago and Chang, J T and Chapman, B A and Cox, C J and Dalke, A and Friedberg, I and Hamelryck, T and Kauff, F and Wilczynski, B and de Hoon, M J L, Biopython: freely available Python tools for computational molecular biology and bioinformatics, *Bioinformatics*, Jun, 2009, 25, 11, 1422-3. PubMed.

4.3.9 Archival material

```
Snapshot of web content for workshop on June 1, 201
```

4.4 Participants

4.4.1 Registered

1. Will Williams <will.williams@duke.edu>
2. Jessica Peel <jessica.peel@duke.edu>
3. John Yi <john.yi@dm.duke.edu>
4. Alex Price <alexander.price@duke.edu>
5. Christopher J. Pierick <pieri008@umn.edu>
6. Sandeep Dave <ssd9@duke.edu>
7. Janet Staats <janet.staats@duke.edu>
8. Joe Saelens <jsaelens71@gmail.com>
9. Anna Maria Masci <annamaria.masci@duke.edu>

10. Herman Staats <herman.staats@duke.edu>
11. Adam Whisnant <adam.whisnant@duke.edu>
12. Pinghuang Liu <ping.liu@duke.edu>

4.4.2 Wait list

1. Luigi Racioppi <luigi.racioppi@duke.edu> (non-CFAR)
2. Kelly Seaton <kelly.seaton@duke.edu>
3. Derrick Pulliam <derrick.pulliam@duke.edu>
4. Guido Ferrari <gflmp@duke.edu>

4.5 Installation and introduction

4.5.1 Introduction to PCfB

This workshop is intended to provide an introduction to the most useful tools for computation in biology. This includes a basic command of the Unix shell, using text editors, regular expressions, scripting in the Python programming language, data management/using a relational database, and creating vector graphics for scientific communication. As there is a lot of new material to cover, we have created extensive documentation for each topic that will be accessible at this website for your reference. Please let us know if any of the documentation is unclear or has errors - we want this to be a useful resource for the future, and will fix documentation issues during the workshop itself as far as possible.

These are the specific topics that we will cover over the next few days

1. *Basic Unix commands*
2. *Using a text editor and regular expressions*
3. *Remote computing and web page generation*
4. *Python Basics I*
5. *Python Basics II*
6. *Python Modules*
7. *NumPy and Matplotlib*
8. *Biopython I*
9. *Biopython II*
10. *Data management and relational databases*
11. *Data analysis with Python*
12. *Vector graphics with Inkscape*

4.5.2 Software installation

But before we start, we just need to check that everyone has installed the required tools:

> # An operating system based on Unix (Mac or Linux) # A text editor that understands regular expressions # The Enthought Python distribution # A relational database system # Inkscape for vector graphics # A web account on the Duke server with public_html access

If any of you have had trouble installing software, we will spend some time helping you to troubleshoot.

4.5.3 Feedback

Preparing for and running such a workshop takes a lot of time and effort. We are therefore very interested in any feedback that you can provide that will help us improve. During the workshop, if you have any suggestions for improvement, please let us know on the spot. Since this is a small class, we want the sessions to be highly informal and welcome questions and interruptions.

We will probably run this course again in the future if you found it useful. It is also possible that we will run other similar workshops, depending on interest. As a simple survey, what computational topics would you be interested in?

1. Practical programming for biologists - An intermediate course on the use of Python for scientific computation.
2. Practical statistics for biologists - An introduction to basic statistics in Python and R.
3. Practical data management for biologists - An introduction to creating and using relational database systems to manage laboratory data.
4. Practical data visualization for biologists - An introduction to statistical and scientific graphics for exploratory data analysis and scientific communication.
5. Modeling and simulations in biology - How to construct and simulate computational models of biological phenomena.
6. Others (please specify)

4.5.4 Pre-test

1. Do you know how to open a Unix shell/console/terminal on your computer?
2. How do you create a directory `foo` that has a subdirectory `bar` that has a subdirectory `baz` with a single command?
3. How do you write a regular expression to find sequences that lie between specific restriction enzyme motifs?
4. What is the difference between `ssh` and `scp`?
5. How do you write a function in Python to plot a histogram of some data?
6. How do you use BioPython to get information from the NCBI databases?
7. What does this mean `select f.name, b.value from foo f, bar b where f.foo_id = b.foo_id;`?
8. How can you estimate the 95% confidence intervals for a statistic without using any formulas?
9. Can you illustrate a conceptual biological model using a vector graphics program?
10. Can you write a program to summarize data from a typical laboratory spreadsheet?

Record your score from 0 to 10. We are curious to see if there is any improvement in your score by the end of the workshop!

4.6 Basic Unix Commands

4.6.1 Working with the file system

Overview:

- cd - change directories
- pwd - print working directory
- mkdir - make directory
- rmdir - remove directory
- ls - list directory
- cp - copy files
- mv - move files
- rm - remove files

Changing and Making Directories

pwd is a command that prints the current directory. Depending on how your shell is configured, your current directory or part of it is displayed in your prompt (the prompt is the bit in your shell that looks like this `iMac:pcfb cliburn$`). Typically your shell starts you in your home directory, where you would have permissions to write and create files. To change directories you would use *cd*, the *c*hange *d*irectory command.

```
[jacob@moku ~]$ pwd
/home/jacob
[jacob@moku ~]$ cd /tmp
[jacob@moku /tmp]$ pwd
/tmp
[jacob@moku /tmp]$ cd
[jacob@moku ~]$ pwd
/home/jacob
```

You can use *cd* without specifying a directory - this returns you to your home directory. You can also use ~ as an alias for your home directory too. Creating directories uses the *mkdir* command. If you don't specify a full path (a path starting with a /) it tries to create one in the current directory.

```
[jacob@moku ~]$ pwd
/home/jacob
[jacob@moku ~]$ mkdir foo
[jacob@moku ~]$ cd foo
[jacob@moku ~/foo]$ pwd
/home/jacob/foo
[jacob@moku ~/foo]$ mkdir /tmp/bar
[jacob@moku ~/foo]$ cd /tmp/bar
[jacob@moku /tmp/bar]$ pwd
/tmp/bar
```

If you need to make a deep hierarchy of directories all at once, you can use the *-p* argument to *mkdir* to create all the necessary preceding directories.

```
[jacob@moku ~]$ pwd
/home/jacob
[jacob@moku ~]$ cd foo
foo: No such file or directory.
[jacob@moku ~]$ mkdir -p foo/bar
[jacob@moku ~]$ cd foo
[jacob@moku ~/foo]$ cd bar
[jacob@moku ~/foo/bar]$ pwd
/home/jacob/foo/bar
```

The *rmdir* command removes directories. Directories must be empty to be removed. Just like *mkdir*, if a full path is not specified it tries to remove the directory from the current directory. Similar to *mkdir*, the *-p* argument tries to remove all the preceding directories

```
[jacob@moku /tmp/bar]$ cd
[jacob@moku ~]$ rmdir /tmp/bar
[jacob@moku ~]$ rmdir -p foo/bar
[jacob@moku ~]$ mkdir bar
[jacob@moku ~]$ touch bar/foo
[jacob@moku ~]$ rmdir bar
rmdir: bar: Directory not empty
```

touch is a command that creates an empty file. We will find out about it when we look at working with files

Examining directories

Now that we understand directories, we'd want to look at what files the directories contain. *ls* will list the files in a directory.

```
[jacob@moku ~]$ ls
A.txt   B.txt   C.txt   bar
[jacob@moku ~]$ ls bar
foo
```

Just like *mkdir*, *ls* has several useful command line options. *ls -l* will list out all the extra properties of the directory listed (file permissions, owner, last time modified). *ls -a* will list hidden files (those files whose name begin with a .). *ls -F* will append directories names */* and (along with other symbols after other special file types).

```
[jacob@moku ~]$ ls -l
total 5
-rw-r--r--  1 jacob  jacob  32 May 25 08:48 A.txt
-rw-r--r--  1 jacob  jacob  32 May 25 08:49 B.txt
-rw-r--r--  1 jacob  jacob  64 May 25 08:53 C.txt
drwxr-xr-x  2 jacob  jacob   3 May 23 15:54 bar
[jacob@moku ~]$ ls -a
.       .cshrc      .mail_aliases   .rhosts     A.txt       bar
..      .login      .mailrc     .shrc       B.txt
.bash_history   .login_conf .profile    .ssh        C.txt
[jacob@moku ~]$ ls -laF
total 20
drwxr-xr-x  4 jacob  jacob    16 May 27 12:11 ./
drwxr-xr-x  4 root   wheel     5 May 23 15:12 ../
-rw-------  1 jacob  jacob   459 May 25 09:32 .bash_history
-rw-r--r--  1 jacob  jacob  1014 May 23 15:12 .cshrc
-rw-r--r--  1 jacob  jacob   257 May 23 15:12 .login
-rw-r--r--  1 jacob  jacob   167 May 23 15:12 .login_conf
-rw-------  1 jacob  jacob   379 May 23 15:12 .mail_aliases
-rw-r--r--  1 jacob  jacob   339 May 23 15:12 .mailrc
-rw-r--r--  1 jacob  jacob   753 May 23 15:12 .profile
-rw-------  1 jacob  jacob   284 May 23 15:12 .rhosts
-rw-r--r--  1 jacob  jacob   978 May 23 15:12 .shrc
drwx------  2 jacob  jacob     3 May 23 16:15 .ssh/
-rw-r--r--  1 jacob  jacob    32 May 25 08:48 A.txt
-rw-r--r--  1 jacob  jacob    32 May 25 08:49 B.txt
-rw-r--r--  1 jacob  jacob    64 May 25 08:53 C.txt
drwxr-xr-x  2 jacob  jacob     3 May 23 15:54 bar/
```

Working with files

Coping files uses the *cp* command, copying from the first argument (*source*) to the last (*destination*):

```
[jacob@moku ~]$ cp A.txt bar/A.txt
```

if the destination is a directory it copes the file into the directory.

```
[jacob@moku ~]$ cp A.txt bar/
[jacob@moku ~]$ ls bar
A.txt   foo
```

You can also copy multiple files at once. *cp* will copy all the files listed on the command line into the directory specified in the last argument.

```
[jacob@moku ~]$ cp A.txt B.txt C.txt bar/
[jacob@moku ~]$ ls bar
A.txt   B.txt   C.txt   foo
```

Globbing will allow us to use many files at once rather than typing them all out explicitly. Globbing is a form of wildcards.

Glob	Effect
*	any number of any character
?	any single character
[abc]	one of a, b, or c

```
[jacob@moku ~]$ cp *.txt bar/
[jacob@moku ~]$ ls bar
A.txt   B.txt   C.txt   foo
```

or

```
[jacob@moku ~]$ cp ?.txt bar/
[jacob@moku ~]$ ls bar
A.txt   B.txt   C.txt   foo
```

or even

```
[jacob@moku ~]$ cp [ABC].txt bar/
[jacob@moku ~]$ ls bar
A.txt   B.txt   C.txt   foo
```

with the *-r* command line argument you can recursively copy whole directories

```
[jacob@moku ~]$ cp -r bar foo
[jacob@moku ~]$ ls foo
A.txt   B.txt   C.txt   foo
```

Similar to the copy command is the move command *mv*.

```
[jacob@moku ~]$ mv A.txt foo
[jacob@moku ~]$ mv [BC].txt foo
[jacob@moku ~]$ mv foo/*.txt bar/
[jacob@moku ~]$ mv foo baz
```

To remove files, use the *rm* command. A word of caution, there is no trash can or waste basket. Removed files are **gone**. It is very easy to accidentally shoot your self in the foot when blindly removing files.

```
[jacob@moku ~]$ rm bar/A.txt
[jacob@moku ~]$ rm bar/[BC].txt
```

```
[jacob@moku ~]$ ls bar
foo
[jacob@moku ~]$ rm -rf bar/
```

the *-r* command line flag removes files recursively, while *-f* attempts to ignore permissions on the file. The combination of *-r* and *-f* flags can be useful to remove whole directory tree. **BE VERY CAREFUL** using *-r* and *-f* flags.

4.6.2 Working with file contents

- cat - concatenate command
  - pipes and redirects - Why con**cat**enate prints to the screen
  - globbing - Working with wildcards
- less - a more sensible way to look at the contents of file
- grep - searching for patterns in files
  - basics of regular expressions

Examining files

The *cat* command will display files on the screen

```
[jacob@moku ~]$ cat A.txt
This is file A.
It has 2 lines.
[jacob@moku ~]$ cat B.txt
This is file B.
It has
3 lines.
```

cat will also concatenate files to print to the screen.

```
[jacob@moku ~]$ cat A.txt B.txt
This is file A.
It has 2 lines.
This is file B.
It has
3 lines.
```

Using redirects allows us to save the concatenated file.

```
[jacob@moku ~]$ cat A.txt B.txt > C.txt
[jacob@moku ~]$ cat C.txt
This is file A.
It has 2 lines.
This is file B.
It has
3 lines.
```

> is a redirect to create a new file (and delete the old file if it exists). >> is the append redirect, while | (pipe) allow you to send the output of one command as input to a new command.

```
[jacob@moku ~]$ cat [AB].txt
This is file A.
It has 2 lines.
This is file B.
```

```
It has
3 lines.
```

While *cat* is useful for displaying small files, longer files would page off the screen quickly. To display longer files, a page aware program will be used, *less*.

```
[jacob@moku ~]$ less <file name>
```

Common useful less keys

key	effect
G	Go to the last line
1G	Go to the first line
#G	Go to line number #
/foo	Search forward for foo
?foo	Search Backward for foo
q	Quit less

Quitting (or how to escape when you are lost)

You may at some point find you self lost, and your prompt doing interesting things you don't expect. Here are some keys to try and get your prompt back in the state you expect.

- q
- Esc
- ctrl-d (sends an end of file saying there is no more input)
- typing Quit
- typing exit
- ctrl-c (sends a break, telling the program to abruptly halt)

Regexp, *grep*, and searching in files

The *grep* command allows you to tap into the powerful regular expression language to search the contests of file for complex patterns.

```
[jacob@moku ~]$ grep 'poor Yorick' hamlet.txt
  Ham. Let me see. [Takes the skull.] Alas, poor Yorick! I knew him,
```

The first argument passed to grep is the pattern to search for, in the above example *poor Yorick*.

Regular expressions provide the ability to search beyond known text, using wildcards to build complex patterns.

key	Meaning
.	any single character
+	one or more of the preceding character
*	zero or more of the preceding character
^	matches the beginning of the line
$	matches the end of the line
[abc]	matches a singular character of a, b, or c

so to find all the lines beginning with the word *HAMLET* and end withs *DEMARK*

```
[jacob@moku ~]$ grep '^HAMLET.*DENMARK$' hamlet.txt
HAMLET, PRINCE OF DENMARK
```

Ever wonder how many lines in hamlet contain eight l's in them?

```
[jacob@moku ~]$ grep 'l.*l.*l.*l.*l.*l.*l.*l' hamlet.txt
    Till then sit still, my soul. Foul deeds will rise,
    all welcome. We'll e'en to't like French falconers, fly at
    married already- all but one- shall live; the rest shall keep as
  Clown. I like thy wit well, in good faith. The gallows does well.
```

4.6.3 Man Pages

Unix documentation is typically stored in man pages acces by the *man* command. Try typing *man cat* into the console to see the manual page for the *cat* command. Note, man pages are notoriously terse, technical, and often confusing to new users, so while learning it may be better to ask google instead, but if all you want is to know optional command arguments the man page is the first place to look.

4.6.4 Exercise

Make a directory in your home folder named *spam* containing subfolders *eggs*, *bacon*, *foo* and *bar* and then remove *spam/foo* and *spam/bar*

4.7 Using a text editor and regular expressions

4.7.1 What is a text editor?

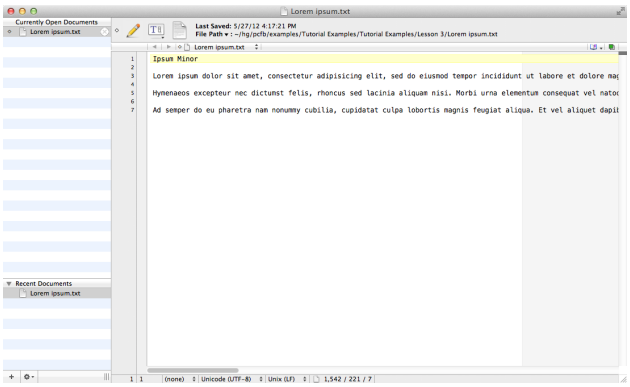
Unlike a word processor, a text editor only handles plain text (i.e. no graphics or fancy formating). However, in return, text editors provide powerful tools for manipulating text, including the ability to use regular expressions, highlight differences between two or more files, and search and replace functionality on steroids. Since most data is available in or can be exported to plain text, and computer programs are written in plian text, a text editor is one of the most basic and useful applcations for anyone dealing with massive amounts of data. Text is universal - unlike binary formats (try to open a WordPerfect 4.2 document), text documents are editable on any platform, and will still be readable in 30 years time.

4.7.2 First look

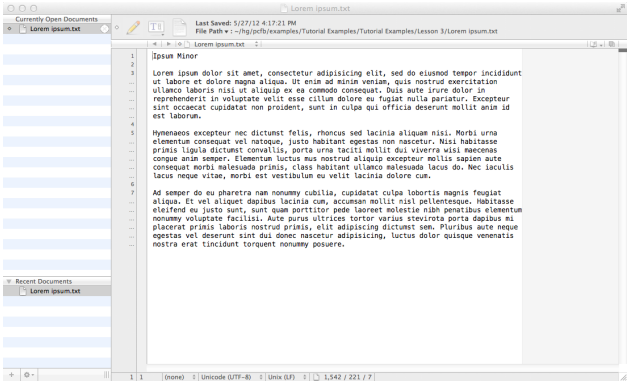
This session will asume that you are using the TextWrangler editor on a Mac. The functionality of most text editors is very similar, and you should be able to follow along if you are using a different editor. We will take the lazy option of familiarizing you to TextWrangler by using the official tutorial. Open TextWrangler and take a few minutes to familiarize yourself with its anatomy - look at the menus, toolbars, icons etc. Most of this should be pretty familiar to you from other programs. Open the file Lorem ipsum.txt in the Tutorial Examples/Lesson 3 folder. Now read the description of the toolbar on Page 10 of the tutorial.

4.7.3 Mini-exercise

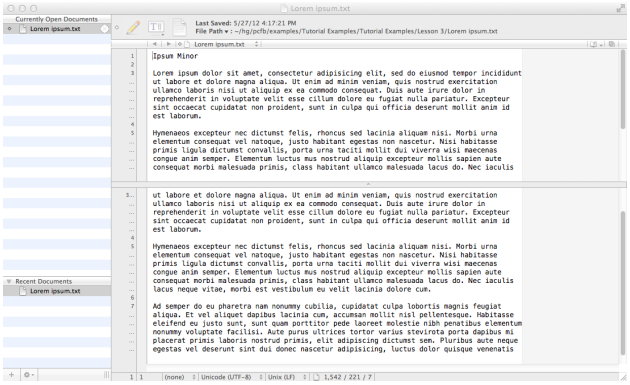
When you first open the Lorem ipsum.txt file, it looks like



Use the TextWrangler toolbar Text Options to get here



Then use the splitbar to split into two windows



Now drag the splitbar all the way to the top to get back a single window.

4.7.4 Finding and replacing

You can read all about TextWrangler in the tutorial at your leisure at home, but most things such as cut, copy and paste and undo/redo work as expected. Since we have a lot to cover, we'll just skip ahead to lesson 7. Open the file Find and Replace Sample.txt in the Lesson 7 folder and work through the exercise on page 39.

Next, open the Email Table.txt file in the Lesson 7 folder and work through the exercise on page 42 to learn how to do search and replace on *invisible* characters.

4.7.5 Regular expressions

We now come to the main part of this session, which is how to use *regular expressions* (or regex) for text manipulation described in pages 44 to 51 of the TextWrangler tutorial. You have already come across regular expressions in the Unix session - now you will see how to use them to manipulate text files.

We'll continue with the cats and dogs file just to get comfortable with the basic elements of regular expressions. Open the Find dialog and check the `Grep` and `Wrap around` boxes. The Grep option tells TextWrangler that we are using regular expressions, and wrap around that we want to do search and replace on the whole document regardless of where our cursor/insertion point is. If at any point you get confused over the next few paragraphs, look at the examples from page 47-49 for concrete illustrations of how to use regular expressions.

On page 45, there is a table of *Wildcards*. Put a period `.` in the Find box and click Next to see what matches. Keep clicking Next - you will see that the `.` matches every character as advertised. Next try `\s` in the Find box and click Next. What does it match? Repeat for all the Wildcards to get a good intuition of what each wildcard matches.

Now do the same with the *Class* patterns. Feel free to edit the text to include new words or numbers if you are curious as to how they will be matched. Also experiment with creating your own class search patterns - for example, what would a class to match DNA nucleotide symbols look like?

Now try the *Repetition* patterns `*`, `*?`, `+`, `+?` and `?`. There is another repetition pattern `{n, m}` that means match at least `n` but not more than `m` of the previous character or pattern. If `n` is left out, we have `{,m}` which means match no more than `m` characters or patterns. If `m` is left out, we have `{n,}` which means match at least `n` occurrences. What is the difference between `*` and `*?` or `+` and `+?`? When would you use the greedy and non-greedy versions?

Now figure out what the `^` and `$` positional assertions and the alternation patterns mean. You can use parenthesis to enclose alternations if you need to also match stuff before and/or after the alternation.

4.7.6 Mini-exercise

1. Construct a regular expression to find two or more consecutive vowels in the cats and dogs file.
2. Use a regular expression pattern to delete all punctuation from the example.
3. Use a positional assertion with the alternation pattern to find all cat, cats, dog or dogs that occur at the end a sentence. You should find that the ends of sentences 1, 3, 5, 9 and 11 match.

4.7.7 Subpatterns and replace patterns

Regular expressions really begin to show their power when we use *subpatterns* and *replace patterns*. This can be a little tricky to wrap your head around when encountered for the first time, so we start with some simple contrived examples to give you some practice.

Subpatterns are simply any regular expression enclosed by parenthesis. For example, `(.)` is a subpattern that matches any character, just like `.` by itself. However, we can refer to *captured* subpatterns to refer to whatever is in the parenthesis. For example, what does the regex `(.)\1` find? See if you can guess, then use TextWrangler to check if you were correct.

We can also use the captured subpatterns in the replace pattern. Here again, `\1` refers to the first regex in parenthesis, *2'* to the second one etc, and `&` to refer to the full regular expression matched (not just an individual subpattern). As an example, what does putting `(.)\1([aeiou]+)` in the Find box and `&\2\1&` do? Test it out in TextWrangler to find out what word is changed and what it is changed to.

4.7.8 Exercise

Open the file `Ch3observations.txt` in the examples folder. It looks like this

```
13 January, 1752 at 13:53 -1.414 5.781 Found in tide pools
17 March, 1961 at 03:46 14 3.6 Thirty specimens observed
1 Oct., 2002 at 18:22 36.51 -3.4221 Genome sequenced to confirm
20 July, 1863 at 12:02 1.74 133 Article in Harper's
```

Write a regular expression to convert it into this:

```
1752 Jan.  13 13 53 -1.414 5.781
1961 Mar.  17 03 46 14 3.6
2002 Oct.  1 18 22 36.51 -3.4221
1863 Jul.  20 12 02 1.74 133
```

Hint: Construct a regular expression to match one single line. Look at the patterns that you must capture from the original to perform the conversion. Construct the appropriate subpatterns to do so. Now construct the regular patterns between the subpatterns to match the unwanted separating characters. When you have a regular expression that matches a single line, check by clicking Next - the highlighted match should jump from one complete line to the other. Now use the references `\1`, `\2` etc, re-ordering if necessary, and adding in filler such as extra punctuation or tabs to construct the desired replacement string. Save the regular expression by clicking the little `g` button on the Find dialog box and clicking `Save ...`. Now hit Replace and see if it does what you expect. If it works, hit replace a few more times or click Replace All. If it doesn't work, Undo and try again.

If you are totally lost and about to pull all your hair out, the construction of the solution is described in detail on pages 38-40 of the PCfB textbook. However, you should not peek at the answer without trying for at least 15 minutes.

4.8 Remote computing and web page generation

Sometimes it is useful to be able to synchronize files or execute programs on a remote computer, or to transfer files from one computer to another. This can be easily done from the command line very easily using the `ssh`, `scp` and `rsync` commands.

The `ssh` (secure shell) command allows you to securely connect to a remote computer for which you have access. For example, you can access your account on the Duke system:

```
eris:pcfb cliburn$ ssh ccc14@login.oit.duke.edu
ccc14@login.oit.duke.edu's password:
Last login: Sat May 26 10:14:19 2012 from 152.3.189.147
###############################################################################
#                                                                             #
#           *****   ATTENTION    *****   ATTENTION   *****                    #
#                                                                             #
# This is a Duke University computer system.  This computer system,           #
# including all related equipment, networks and network devices               #
# (includes internet access) are provided only for authorized Duke            #
# University use. Duke University computer systems may be monitored for       #
# all lawful purposes, including to ensure that their use is authorized,      #
# for management of the system, to facilitate protection against              #
# unauthorized access, and to verify security procedures, survivability,      #
# and operational security. During monitoring, information may be             #
# examined, recorded , copied , and used for authorized purposes. All         #
# information, including personal information, placed on or sent over         #
# this system may be monitored. use of this Duke University computer          #
# system, authorized or unauthorized, constitutes consent to                  #
# monitoring. Unauthorized use of this Duke University computer system        #
# may subject you to criminal prosecution. Evidence of unauthorized use       #
```

```
# collected during monitoring may be used for administrative, criminal,  #
# or other adverse action. Use of this system constitutes consent to     #
# monitoring for all lawful purposes.                                    #
##########################################################################

Self provisioned systems are now available for remote usage through OIT's Virtual Computing Lab servi
Mon May 28 00:44:43 EDT 2012
[ccc14@login5 ~]$ ls
AFSDocs  public_html  Sites
[ccc14@login5 ~]$
```

If you know the IP address of a Linux or Mac computer that you have login rights to, you can usually connect to it via ssh. For example, this is how we typically access departmental servers or computing workstations from home. If you work with the Duke Beowulf cluster, you will also use ssh to connect and run your programs remotely.

If you can `ssh` to a computer, you can also copy files to or from the remote computer using `scp` (secure copy). Here is an example:

```
[ccc14@login5 ~]$ cat > remote.txt
This is my remote file on lgoin.oit.duke.edu
[ccc14@login5 ~]$ exit
logout
Connection to login.oit.duke.edu closed.
eris:pcfb cliburn$ scp ccc14@login.oit.duke.edu:~/remote.txt .
ccc14@login.oit.duke.edu's password:
remote.txt                                    100%   45     0.0KB/s   00:00
eris:pcfb cliburn$ cat remote.txt
This is my remote file on lgoin.oit.duke.edu
```

If you wish to synchronize entire directory trees between computers, it is more efficient to use `rsync` which performs data compression, only tranfers files that are differnet, and allows resuming of interrupted transfers. For example, `rsync` is a simple way to back up your files to another computer.

```
eris:tmp cliburn$ rsync -avz foo ccc14@login.oit.duke.edu:~/
ccc14@login.oit.duke.edu's password:
building file list ... done
foo/
foo/foo.txt
foo/bar/
foo/bar/bar.txt
foo/bar/baz/
foo/bar/baz/baz.txt

sent 376 bytes  received 104 bytes  73.85 bytes/sec
total size is 75  speedup is 0.16
```

The flags `-avz` are short for `--archive`, `--verbose` and `--compress`. The `--archive` flag preserves symbolic links and is perfect for remote backups. As usual, you can look at `man rsync` if you want to know the details of how `rsync` works.

4.8.1 Web page construction with sphinx

Sphinx (http://sphinx.pocoo.org/) is a Python tool to create documentation, but it is also great for creating highly structured webpages with minimal effort. The entire workshop website was created with Sphinx.

We start by asking Sphinx to generate the initial directory for us with the `sphinx-quickstart` command. The program will ask some configuration questions - you can just accept the defaults or give any sensible answer for now - the options can all be changed later if necessary.

```
eris:tmp cliburn$ sphinx-quickstart homepage
Welcome to the Sphinx 1.1.2 quickstart utility.

Please enter values for the following settings (just press Enter to
accept a default value, if one is given in brackets).

Selected root path: homepage

You have two options for placing the build directory for Sphinx output.
Either, you use a directory "_build" within the root path, or you separate
"source" and "build" directories within the root path.
> Separate source and build directories (y/N) [n]:

Inside the root directory, two more directories will be created; "_templates"
for custom HTML templates and "_static" for custom stylesheets and other static
files. You can enter another prefix (such as ".") to replace the underscore.
> Name prefix for templates and static dir [_]:

The project name will occur in several places in the built documentation.
> Project name: Demo home page
> Author name(s): Cliburn Chan

Sphinx has the notion of a "version" and a "release" for the
software. Each version can have multiple releases. For example, for
Python the version is something like 2.5 or 3.0, while the release is
something like 2.5.1 or 3.0a1.  If you don't need this dual structure,
just set both to the same value.
> Project version: 0.0
> Project release [0.0]:

The file name suffix for source files. Commonly, this is either ".txt"
or ".rst".  Only files with this suffix are considered documents.
> Source file suffix [.rst]:

One document is special in that it is considered the top node of the
"contents tree", that is, it is the root of the hierarchical structure
of the documents. Normally, this is "index", but if your "index"
document is a custom template, you can also set this to another filename.
> Name of your master document (without suffix) [index]:

Sphinx can also add configuration for epub output:
> Do you want to use the epub builder (y/N) [n]:

Please indicate if you want to use one of the following Sphinx extensions:
> autodoc: automatically insert docstrings from modules (y/N) [n]:
> doctest: automatically test code snippets in doctest blocks (y/N) [n]:
> intersphinx: link between Sphinx documentation of different projects (y/N) [n]:
> todo: write "todo" entries that can be shown or hidden on build (y/N) [n]:
> coverage: checks for documentation coverage (y/N) [n]:
> pngmath: include math, rendered as PNG images (y/N) [n]:
> mathjax: include math, rendered in the browser by MathJax (y/N) [n]:
> ifconfig: conditional inclusion of content based on config values (y/N) [n]:
> viewcode: include links to the source code of documented Python objects (y/N) [n]:

A Makefile and a Windows command file can be generated for you so that you
only have to run e.g. 'make html' instead of invoking sphinx-build
directly.
> Create Makefile? (Y/n) [y]:
```

```
> Create Windows command file? (Y/n) [y]:

Creating file homepage/conf.py.
Creating file homepage/index.rst.
Creating file homepage/Makefile.
Creating file homepage/make.bat.

Finished: An initial directory structure has been created.

You should now populate your master file homepage/index.rst and create other documentation
source files. Use the Makefile to build the docs, like so:
   make builder
where "builder" is one of the supported builders, e.g. html, latex or linkcheck.
```

The next thing to do is to `cd homepage` to enter the directory that was just created for us and edit the `conf.py` file to setup a configuraiton that we like. The only change to be made for now is to change the `html_theme` from `defautl` to `agogo` to match our workshop website theme. The themes that come with Sphinx can be viewed at http://sphinx.pocoo.org/theming.html.

The first page to edit is the `index.rst` file. The `rst` extension is for ReStructuredText, a simple plain text markup language that is much easier to work with than HTML. Look at the primer on ReStructuredText at http://sphinx.pocoo.org/rest.html to see examples of how to use it. Open the index.rst file in your text editor:

```
.. Demo home page documentation master file, created by
   sphinx-quickstart on Mon May 28 01:12:56 2012.
   You can adapt this file completely to your liking, but it should at least
   contain the root `toctree` directive.

Welcome to Demo home page's documentation!
==========================================

Contents:

.. toctree::
   :maxdepth: 2



Indices and tables
==================

* :ref:`genindex`
* :ref:`modindex`
* :ref:`search`
```

Since this is to be a home page rather than documentation page, we can simplify the structure. Edit the file so that the last part looks like this:

```
Contents:

.. toctree::
   :maxdepth: 2
   :hidden:

   Home <self>
   research
   publications
```

We want to keep the table of contents *hidden*, and have set up a simple structure where the home page (index.html)

links to a research.html and a publications.html file. Just as the index.html file will be generated by thiis index.rst file, the other two files are also generated by a research.rst and publications.rst file that we write using ReStructuredText. The full contents of the 3 rst files are included verbatim for reference:

4.8.2 index.rst

```
Cliburn's very boring home page
=======================================

Stuff I do
------------------

Tongue ribeye pig, tenderloin turducken salami frankfurter strip
steak. T-bone turducken meatball flank, beef ribs brisket corned
beef tail. Ball tip tongue flank beef ribs, biltong tri-tip salami
chicken sausage leberkas chuck tail. Kielbasa shankle pork chop
sirloin, leberkas bresaola tail. Ham hamburger venison sausage
biltong, pork loin brisket pig sirloin pastrami short loin shank
chicken. Pig andouille leberkas beef short loin ribeye turkey ham
hock. Cow ham kielbasa, capicola short ribs brisket shoulder
pancetta t-bone pork belly tri-tip pork loin tenderloin.

Ground round pork belly pastrami pork chop, drumstick corned beef
t-bone tail bresaola filet mignon meatloaf. Boudin spare ribs ham
hock short loin. Prosciutto ham hock sausage, biltong leberkas
turkey hamburger pork meatball bresaola pork belly. Shankle tri-tip
frankfurter ribeye leberkas ham hock, tongue beef ribs speck venison
pork chop andouille chuck. Rump pastrami bresaola, strip steak short
loin andouille pork chop beef boudin capicola bacon shank prosciutto
beef ribs swine. Meatloaf leberkas pancetta beef.

More stuff I do
--------------------

Enim do boudin officia labore tail. Pork exercitation short ribs
deserunt laboris, tenderloin drumstick in dolor tongue sunt ex. Ham
hock t-bone exercitation pork loin non mollit. Jowl boudin magna
adipisicing in dolore. Brisket quis shoulder nostrud tempor
ea. Aliquip officia consequat deserunt, dolore nostrud est tri-tip
ut pancetta speck shank excepteur. Sausage cillum ground round velit
rump, dolore laboris.

Commodo consectetur ut, officia proident eu cillum jowl aute flank
sausage ut beef ribs. Deserunt occaecat pariatur elit. Pork chop ut
tempor, enim aliqua laborum cillum eiusmod t-bone occaecat aute
laboris labore. Ham hock turkey beef nostrud excepteur
dolor. Consectetur meatball chicken deserunt exercitation, corned
beef beef in short ribs ut ea velit beef ribs. Enim andouille in,
dolore ut meatball ea ut tail proident short ribs leberkas ground
round filet mignon.

Andouille sirloin chicken tempor aute, cow salami commodo dolore
leberkas culpa in ea esse. Id ground round tongue velit. Ex elit
minim sirloin fatback laboris. Irure andouille shankle cupidatat,
nostrud bresaola id shank do jowl. Swine sirloin pork loin,
prosciutto bresaola rump cillum in exercitation capicola.
```

```
Contents:

.. toctree::
   :maxdepth: 2
   :hidden:

   Home <self>
   research
   publications
```

4.8.3 research.rst

```
Cliburn's boring research page
==============================================

Current research interests
--------------------------------------

 1. Bacon
 2. Pork rind
 3. Trotters

.. image:: bacon.jpg
  :width: 60%

Past research interests
---------------------------------------

 1. LOL cats

.. image:: Lolcat.JPG
```

4.8.4 publications.rst

```
Not really Cliburn's publications
================================

First 5 hits on Pubmed search for "Sphinx"
------------------------------------------

  1. Quadrature RF Coil for In Vivo Brain MRI of a Macaque Monkey in
  a Stereotaxic Head Frame.  Roopnariane CA, Ryu YC, Tofighi MR,
  Miller PA, Oh S, Wang J, Park BS, Ansel L, Lieu CA, Subramanian T,
  Yang QX, Collins CM.  Concepts Magn Reson Part B Magn Reson
  Eng. 2012 Feb;41B(1):22-27. Epub 2012 Feb 18.  PMID: 22611340
  [PubMed]

  2. The place of general practitioners in cancer care in
  Champagne-Ardenne.  Tardieu E, Thiry-Bour C, Devaux C, Ciocan D,
  de Carvalho V, Grand M, Rousselot-Marche E, Jovenin N.  Bull
  Cancer. 2012 May 1;99(5):557-562.  PMID: 22522646 [PubMed - as
  supplied by publisher]
```

```
3. Spontaneous Endometriosis in a Mandrill (Mandrillus sphinx).
Nakamura S, Ochiai K, Ochi A, Ito M, Kamiya T, Yamamoto H.  J Comp
Pathol. 2012 Apr 18. [Epub ahead of print] PMID: 22520805
[PubMed - as supplied by publisher]

4. [Reality of healthcare access for migrant children in Mayotte].
Baillot J, Luminet B, Drouot N, Corty JF.  Bull Soc Pathol
Exot. 2012 May;105(2):123-9. Epub 2012 Mar 1. French.  PMID:
22383116 [PubMed - in process]

5. Craniodental features in male Mandrillus may signal size and
fitness: an allometric approach.  Klopp EB.  Am J Phys
Anthropol. 2012 Apr;147(4):593-603. doi: 10.1002/ajpa.22017. Epub
2012 Feb 10.  PMID: 22328467 [PubMed - indexed for MEDLINE]
```

4.8.5 HTML Generation

With these files written, we now ask Sphinx to generate the HTML

```
eris:homepage cliburn$ make html
sphinx-build -b html -d _build/doctrees   . _build/html
Making output directory...
Running Sphinx v1.1.2
loading pickled environment... not yet created
building [html]: targets for 3 source files that are out of date
updating environment: 3 added, 0 changed, 0 removed
reading sources... [100%] research

Not really Cliburn's publications
================================
looking for now-outdated files... none found
pickling environment... done
checking consistency... done
preparing documents... done
writing output... [100%] research
writing additional files... genindex search
copying images... [100%] bacon.jpg
copying static files... done
dumping search index... done
dumping object inventory... done
build succeeded, 1 warning.

Build finished. The HTML pages are in _build/html.
```

And now the directory looks like this:

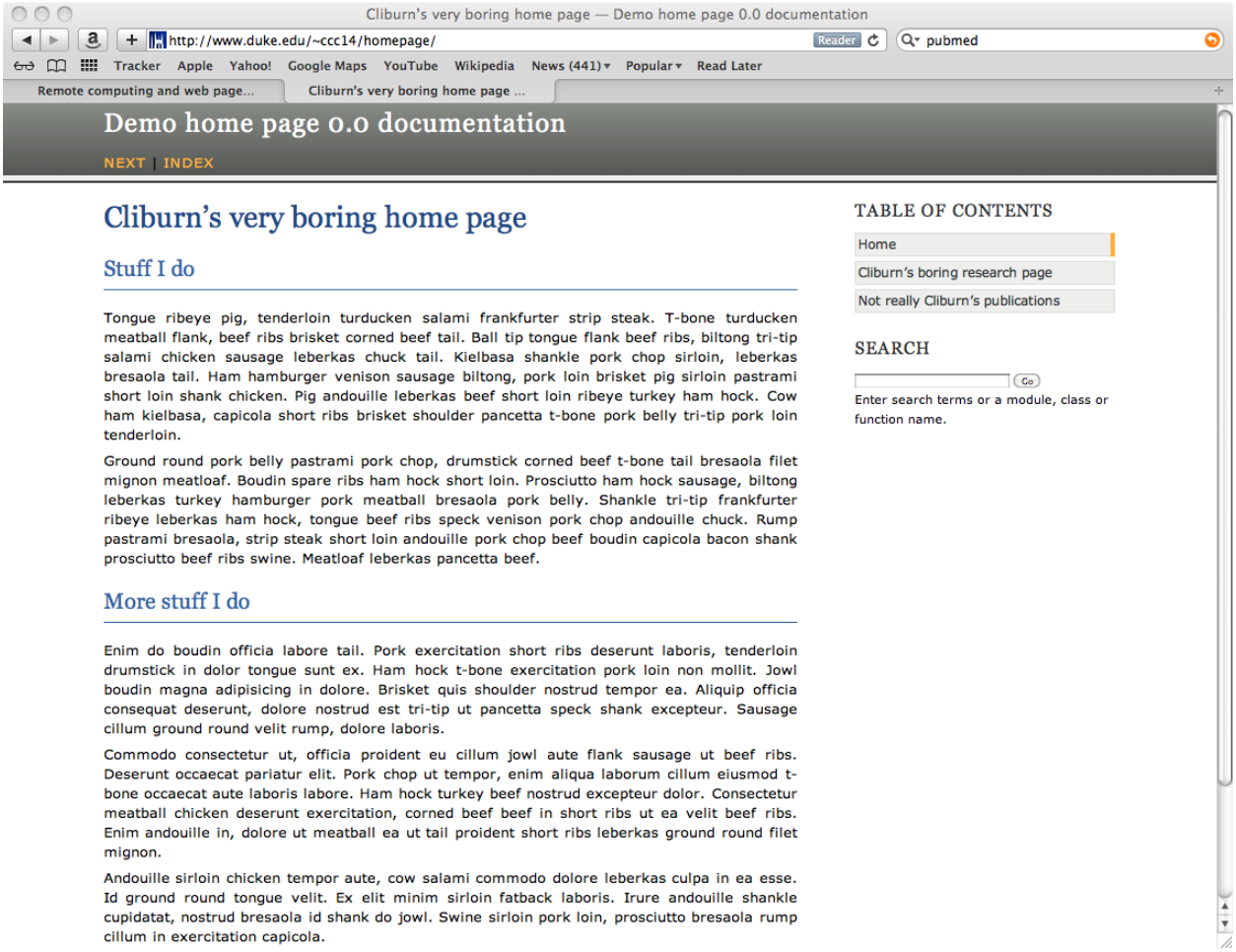
```
eris:homepage cliburn$ ls
Lolcat.JPG              _templates              make.bat
Makefile                bacon.jpg               publications.rst
_build                  conf.py                 research.rst
_static                 index.rst
```

4.8.6 Copy generated HTML to public_html on Duke server

Now all we need to do is to `rsync` the `_build/html` folder to the Duke server:

```
eris:homepage cliburn$ rsync -avz _build/html/ ccc14@login.oit.duke.edu:~/public_html/homepage
ccc14@login.oit.duke.edu's password:
building file list ... done
created directory /afs/acpub/users/c/c/ccc14/public_html/homepage
./
.buildinfo
genindex.html
index.html
objects.inv
publications.html
research.html
search.html
searchindex.js
_images/
_images/Lolcat.JPG
_images/bacon.jpg
_sources/
_sources/index.txt
_sources/publications.txt
_sources/research.txt
_static/
_static/agogo.css
_static/ajax-loader.gif
_static/basic.css
_static/bgfooter.png
_static/bgtop.png
_static/comment-bright.png
_static/comment-close.png
_static/comment.png
_static/doctools.js
_static/down-pressed.png
_static/down.png
_static/file.png
_static/jquery.js
_static/minus.png
_static/plus.png
_static/pygments.css
_static/searchtools.js
_static/underscore.js
_static/up-pressed.png
_static/up.png
_static/websupport.js

sent 164472 bytes  received 792 bytes  22035.20 bytes/sec
total size is 286369  speedup is 1.73
```

Now, if we navigate to http://www.duke.edu/~ccc14/homepage/, we will see the homepage and the links on the sidebar to publications and research work as well.



4.9 Python Basics I

4.9.1 Why program?

Biology is increasingly data-rich. And the amount of data is growing exponentially, as I am sure you are all only too well aware. Wouldn't it be really nice if you had some unpaid slaves that would help you sort through your data, check for problems, find the most interesting bits, and generate pretty pictures for you to include in your next manuscript? Well, you are in luck, for the computer is a slave factory, and the slaves are called programs. And today, I have some slaves to give away ...

4.9.2 What can my slave do?

In this workshop, we will focus on 3 types of jobs for our slaves that are essential whenever there is a lot of data:

1. Data munging
2. Data analysis
3. Data visualization

Data munging means taking that error-riddled, color-coded, highly redundant Excel spreadsheet that biologists love to create, and cleaning, parsing and proofing it so that it is suitable for analysis. There is a related skill of how to

create persistent data stores that allow you to slice and dice well-structured data that will be briefly touched upon in the session on :doc:`Data management and relational databasesI</database>`, but will require another full workshop to cover in any depth.

Data analysis is largely about how to do statistics. We will show very simple examples of analysis in :doc:`Data analysis with Python</analysis>`, but the proper cultivation of the statistical way of thinking probably requires not just another workshop, but returning to graduate school.

Finally, there are two main reasons for data visualization - the first is for exploratory data analysis, since the human brain is highly optimized to detect patterns in pictures; and the second is for communicating results, since every biologist I've ever met is only ever interested in the figures in a paper and never the raw data. Making pictures from data for exploratory analysis and communication are covered in `NumPy and Matplotlib</numerics>` and the creation of schematics to illustrate concepts in :doc:`Vector graphics with Inkscape</inkscape>`.

But first - in order to tell your slave how to do these jobs, you need to think like a programmer.

4.9.3 Thinking like a programmer

Computers are stupid. And very literal. So to be able to program, we need to tell the computer what to do in very simple language without any ambiguity. Almost all programs we will deal with involve only 5 basic operations:

```
1. Get input data
2. Store data in variables
3. Do some calculation or check logic
4. Repeat
5. Generate some output
```

For now, we simply define a *variable* as a name we give to data so that we can retrieve it later. The other terms should be familiar to everyone.

For example, here is a simple example that checks if a word is a palindrome:

```
# get input and store in variable word
word = raw_input("Enter a word: ")
# check if word is the same when reversed
if word == word[::-1]:
    print "%s is a palindrome!" % word
else:
    print "%s is a regular old word" % word
```

Here is another program that makes use of these 5 concepts:

```
"""Count the number of vowels in a name."""

# input data and store in variable name
name = raw_input("What's your name? ")
# store count of vowels in variable num_vowels
num_vowels = 0
# repeat updating of vowel count
for vowel in 'aeiou':
    # simple calculation (count occurences of vowel in string)
    num_vowels += name.count(vowel)
# output result
print "Hello %s, there are %d vowels in your name." % (name, num_vowels)
```

Since the 5 operations are about all that a computer can do, even big complex projects must boil down to smaller tasks that mix and match these operations. Essentially, if you know these 5 operations, you know how to program. The rest are details.

4.9.4 Introducing Python

We will learn to program in a language called *Python*, named after the British comedy skit *Monty Python*. Python is possibly the simplest programming language to learn and has an amazing range of libraries for just about any biomedical data processing need, making it an ideal first language for biologists to learn. When you are comfortable with Python, a very useful second language to learn is *R*, another open source language specialized for statistical analysis.

Python is an interpreted language, meaning that instructions are executed as soon as you complete a programming statement. To see the Python interpreter in action, we will use the **IPython** interpreter, which you can start by opening a Terminal window and typing `ipython`, after which you will see this welcome message:

```
eris:pcfb cliburn$ ipython
Enthought Python Distribution -- http://www.enthought.com

Python 2.6.6 |EPD 6.3-2 (32-bit)| (r266:84292, Sep 23 2010, 11:52:53)
Type "copyright", "credits" or "license" for more information.

IPython 0.10.1 -- An enhanced Interactive Python.
?         -> Introduction and overview of IPython's features.
%quickref -> Quick reference.
help      -> Python's own help system.
object?   -> Details about 'object'. ?object also works, ?? prints more.
```

There is also a vanilla `python` interpreter, but `ipython` provides so many nice features such as Unix shell integration, tab completion, history etc that I hardly ever use the `python` interpreter. Try typing `?` in `ipython` to see what it offers. To exit the information screen, type `q` to quit. There are several ways to get more information about a Python language feature - for example, what does the python `range` function do? Type `help(range)` or `help range` or `range?` or `?range`.

4.9.5 Python as a calculator

To get comfortable with `ipython`, let's just use it as a calculator:

```
In [1]: 1+2*3**2
 Out[1]: 19

In [2]: 3/2
 Out[2]: 1

In [3]: 3/2.0
 Out[3]: 1.5

In [4]: 13 % 4
 Out[4]: 1

In [5]: import math

In [6]: math.pi
 Out[6]: 3.141592653589793

In [7]: math.e
 Out[7]: 2.718281828459045

In [8]: math.pi/4
 Out[8]: 0.7853981633974483
```

```
In [9]: math.sin(math.pi/4)
 Out[9]: 0.7071067811865475

In [10]: math.asin(math.sin(math.pi/4))
Out[10]: 0.7853981633974482

In [11]: math.sqrt(16)
Out[11]: 4.0

In [12]: 16**0.5
Out[12]: 4.0
```

Note the gotcha in the [2] calculation - when both numerator and denominator are integers, the division operator returns an integer, which might not be what you want. Make either numerator or denominator a float (a number with a decimal point) as in [3] to get the usual answer.

4.9.6 Types

As we have already seen in the previous example, there is a difference between `2` and `2.0`. In particular, they differ in *type* - `2` is an integer, while `2.0` is a float. Types are necessary so that Python can distinguish between different *kinds* of things that may have different behaviors. Here are the most commonly used basic types in Python:

1. `Integers` are natural numbers, `..., -3, -2, -1, 0, 1, 2, 3 ...`
2. `Floats` are "decimal" numbers e.g. `0.01, 1e-6, math.pi` etc
3. `Bools` are the values `True` and `False`
4. `Strings` are anything within single quotes, double quotes, or "triple" quotes such as `'hello'`, `"hello"`, `"'hello"'` and `"""hello"""`.

While the first 3 types are atomic, *strings* are actually sequences of characters, and we can retrieve characters at specific postions by *indexing* and *slicing*. An example of how we can slice and dice sequences is useful here:

```
In [1]: s = "My first string"

In [2]: s[0]
 Out[2]: 'M'

In [3]: s[1]
 Out[3]: 'y'

In [4]: s[-1]
 Out[4]: 'g'

In [5]: s[0:2]
 Out[5]: 'My'

In [6]: s[3:8]
 Out[6]: 'first'

In [7]: s[3:8:2]
 Out[7]: 'frt'

In [8]: s[::-1]
 Out[8]: 'gnirts tsrif yM'
```

Note that in Python, we count from *zero*, not one. Note also that a negative index means count backwards from the *end* of the sequence.

Another type of sequence that is ubiquitous in Python programs is the `list`, consisting of a sequence of other types delimited by square brackets `[` and `]`. Unlike strings which only contain characters, list elements can be anything, including other lists. Another difference between strings and lists is that the elements in a list can be changed by assigning new values to them. In geek-speak, lists are *mutable* and strings are *immutable*. You may also see `tuples` which are items separated by commas, and typically delimited by `(` and `)`. For the most part, we can just consider tuples to be immutable lists. A neat trick we can do with tuples is *unpacking*, perhaps easier demonstrated than explained:

In the first example above, we *unpacked* the length 3 list into the variables `a`,‘‘ b‘‘, `c` in a single statement. In the second example, we swapped the contents of `a` and `b`.

Time for more experimentation in `ipython`:

```
In [1]: alist = [1,2,3.14,'foo','bar',['a','b',True]]

In [2]: alist[5]
 Out[2]: ['a', 'b', True]

In [3]: alist[5][2]
 Out[3]: True

In [4]: alist[1] = 99

In [5]: alist
 Out[5]: [1, 99, 3.14, 'foo', 'bar', ['a', 'b', True]]

In [6]: atuple = (1,2,3.14,'foo','bar',['a','b',True])

In [7]: atuple[5]
 Out[7]: ['a', 'b', True]

In [8]: atuple[5][2]
 Out[8]: True

In [9]: atuple[1] = 99
---------------------------------------------------------------------------
TypeError                                 Traceback (most recent call last)
/Volumes/HD3/hg/pcfb/<ipython-input-9-5a8168f444b1> in <module>()
----> 1 atuple[1] = 99

TypeError: 'tuple' object does not support item assignment

In [10]: astring = "hi there"

In [11]: astring[2] = 'x'
---------------------------------------------------------------------------
TypeError                                 Traceback (most recent call last)
/Volumes/HD3/hg/pcfb/<ipython-input-11-71b2376dea24> in <module>()
----> 1 astring[2] = 'x'

TypeError: 'str' object does not support item assignment
```

Here the difference between *mutable* and *immutable* is clearly shown. We can grow lists in several ways - using an `insert`, and `append` and list `concatenation`. We can remove items from a list by using `pop`, `del` or assigning a slice to the empty list.

```
In [1]: blist = []

In [2]: blist.append(1)
```

```
In [3]: blist.append(99)

In [4]: blist = blist + [3,4,5]

In [5]: blist
 Out[5]: [1, 99, 3, 4, 5]

In [6]: blist[2:2] = ['a','b','c']

In [7]: blist
 Out[7]: [1, 99, 'a', 'b', 'c', 3, 4, 5]

In [8]: blist[2:4] = []

In [9]: blist
 Out[9]: [1, 99, 'c', 3, 4, 5]

In [10]: blist.pop()
Out[10]: 5

In [11]: blist
Out[11]: [1, 99, 'c', 3, 4]

In [12]: del blist[3]

In [13]: blist
Out[13]: [1, 99, 'c', 4]
```

The final basic type we will look at is the `dictionary`. A dictionary consists of `(key, value)` pairs, where the key is an immutable type (e.g. a number, a string, a tuple) and the value is anything. We retrieve the value in a dictionary by using the associated key. Dictionaries are delimited by `{` and `}`. For example, we can make a dictionary of email addresses:

```
In [1]: emails = {}

In [2]: emails['cliburn'] = 'cliburn.chan@duke.edu'

In [3]: emails['jacob'] = 'jacob.frelinger@duke.edu'

In [4]: emails['cliburn']
 Out[4]: 'cliburn.chan@duke.edu'

In [5]: emails.keys()
 Out[5]: ['jacob', 'cliburn']

In [6]: emails.values()
 Out[6]: ['jacob.frelinger@duke.edu', 'cliburn.chan@duke.edu']

In [7]: emails
 Out[7]: {'cliburn': 'cliburn.chan@duke.edu', 'jacob': 'jacob.frelinger@duke.edu'}
```

We can also think of dictionaries as fancy lists that are not restricted to consecutive integers for indexing. Note that we create dictionaries with curly braces `{}` but assign element to and retrieve elements from dictionaries with square brackets `[key]`. If the key is not found in the dictionary, Python will raise a KeyError exception and abort. To avoid that, we can either check for the key before retrieval, tell Python to ignore KeyErrors in a `try-except` statement, or return a default value using the `get` method instead of `[]` to access the dictionary. Here are more examples of dictionary creation and usage:

```
In [1]: zip(['a','b','c','d'], [1,2,3,4])
 Out[1]: [('a', 1), ('b', 2), ('c', 3), ('d', 4)]

In [2]: adict = dict(zip(['a','b','c','d'], [1,2,3,4]))

In [3]: adict
 Out[3]: {'a': 1, 'b': 2, 'c': 3, 'd': 4}

In [4]: adict['b']
 Out[4]: 2

In [5]: adict.get('e', 0)
 Out[5]: 0

In [6]: adict
 Out[6]: {'a': 1, 'b': 2, 'c': 3, 'd': 4}

In [7]: adict.setdefault('e', 0)
 Out[7]: 0

In [8]: adict
 Out[8]: {'a': 1, 'b': 2, 'c': 3, 'd': 4, 'e': 0}
```

Dictionaries can also be constructed from a list of (key, value) pairs (or 2-tuples). The `zip` function takes the first element from list 1 and the first element from list 2 to make a tuple, then does the same for the second element etc until one or both lists are exhausted. It is used here to construct a list of pair from two matching lists of keys and values. The `get` method returns the default (second) argument when the key given by its first argument is not found in the dictionary. The `setdefault` method does the same thing, but additionally inserts the new key / default value into the dictionary if not found. If we want to ingore missing keys but just retrieve values for valid keys, we can wrap the dictionary access in a `try-except` statement:

```
In [1]: adict
 Out[1]: {'a': 1, 'b': 2, 'c': 3, 'd': 4, 'e': 0}

In [2]: for ch in "ajfljldjajfeljad":
   ...:     try:
   ...:         print adict[ch]
   ...:     except KeyError:
   ...:         pass
   ...:
   ...:
1
4
1
0
1
4
```

The `pass` keyword means "do nothing". Without the `try-except` statement, the program would crash with a `KeyError` the first time ``ch was not found in the dictionary keys `a, b, c, d, e`.

You might have noticed that we sometimes used a funny notation with a *dot* `.` between names, for example `list.append(1)`. This is because Python is an *object-oriented language*, and these basic types are also *classes*. We won't discuss classes here except to note that we use the dot notation to access values (attributes) and functions (methods) associated with the class. In `ipython`, hit the `tab` key after the dot to see what types are available.

```
In [1]: blist
 Out[1]: [1, 99, 'c', 4]
```

```
In [2]: [b for b in dir(blist) if not b.startswith('_')]
 Out[2]:
['append',
 'count',
 'extend',
 'index',
 'insert',
 'pop',
 'remove',
 'reverse',
 'sort']
```

The code ‘‘ [b for b in dir(blist) if not b.startswith(‘_’)] ‘‘ is a `list comprehension` to show all the normal methods of the list class, filtering out methods that look like __xxx__. The methods with __ prefixes and suffixes are “special” internal methods that we won’t use in this workshop. You can use help to find out what `extend`, `index` etc do. The `count`, `reverse` and `sort` methods are quite simple:

```
In [1]: numlist = [3,1,4,1,5,1,6,9]

In [2]: numlist.sort()

In [3]: numlist
 Out[3]: [1, 1, 1, 3, 4, 5, 6, 9]

In [4]: numlist.reverse()

In [5]: numlist
 Out[5]: [9, 6, 5, 4, 3, 1, 1, 1]
```

Strings have an even longer list of methods:

```
In [1]: quote = "My philosophy, like color television, is all there in black and white"

In [2]: [m for m in dir(quote) if not m.startswith('_')]
 Out[2]:
['capitalize',
 'center',
 'count',
 'decode',
 'encode',
 'endswith',
 'expandtabs',
 'find',
 'format',
 'index',
 'isalnum',
 'isalpha',
 'isdigit',
 'islower',
 'isspace',
 'istitle',
 'isupper',
 'join',
 'ljust',
 'lower',
 'lstrip',
 'partition',
 'replace',
```

```
 'rfind',
 'rindex',
 'rjust',
 'rpartition',
 'rsplit',
 'rstrip',
 'split',
 'splitlines',
 'startswith',
 'strip',
 'swapcase',
 'title',
 'translate',
 'upper',
 'zfill']

In [3]: quote.lower()
 Out[3]: 'my philosophy, like color television, is all there in black and white'

In [4]: quote.upper()
 Out[4]: 'MY PHILOSOPHY, LIKE COLOR TELEVISION, IS ALL THERE IN BLACK AND WHITE'

In [5]: quote.split()
 Out[5]:
['My',
 'philosophy,',
 'like',
 'color',
 'television,',
 'is',
 'all',
 'there',
 'in',
 'black',
 'and',
 'white']

In [6]: quote = ''.join(quote)

In [7]: quote.split(',')
 Out[7]: ['My philosophy', ' like color television', ' is all there in black and white']
```

4.9.7 Operators

We have already seen some operations, such as `+` and `*` for addition and multiplication. In addition to the numeric operators, there are also Boolean operators `and`, `or` and `not`, comparison operators `<`, `<=`, `>`, `>=`, `==`, `!=`, `is` and `is not`, and some other operators we will not discuss here (e.g. bitwise operators). Most of these operators are quite self-evident, and if not, experimentation in the interpreter will clarify what they do:

```
In [1]: True and False
 Out[1]: False

In [2]: True or False
 Out[2]: True

In [3]: not True
 Out[3]: False
```

```
In [4]: 3 == 3
 Out[4]: True

In [5]: 3 == 4
 Out[5]: False

In [6]: 3 != 4
 Out[6]: True

In [7]: 3 > 4
 Out[7]: False

In [8]: 4 > 3
 Out[8]: True

In [9]: None is None
 Out[9]: True

In [10]: 0 is None
Out[10]: False

In [11]: 0 is not None
Out[11]: True
```

4.9.8 Control flow and loops

We now begin to get to the heart of programming - asking the computer to do mind-numbingly boring work many, many times. The way to perform repetitions is by *looping*, but before we go there, we will first learn about how to control the program flow with the `if-else` family of statements. Luckily, the `if-else` statement family does exactly what you'd expect it to do:

```
In [1]: if 'math' > 'football':
   ...:     print 'Nerds rule'
   ...: else:
   ...:     print 'Jocks rule'
   ...:
Nerds rule
```

The structure of the `if-else` statement has the form:

```
if (condition is true):
  do A
else:
  do B
```

Here are some more examples of the `if-else` family:

```
In [1]: grade = None

In [2]: score = 86

In [3]: if (score > 93):
   ...:     grade = 'A'
   ...: elif (score > 85):
   ...:     grade = 'B'
   ...: elif (score > 70):
   ...:     grade = 'C'
```

```
   ...: else:
   ...:       grade = 'D'
   ...:

In [4]: grade
 Out[4]: 'B'
```

As you can see, the `if` statement can be used by itself without an `else` part with the understanding that if the condition is not true, then nothing is done. If you need to make decisions based on many conditions, the `if-[elif]-else` form is useful, where the final optional `else` statement will be executed if none of the others above it are true. Note that the last example depends on the *ordering* of the conditions, and works because the `if-elif-else` statement works from top to bottom. See if you can figure out why the code below doesn't work as intended:

```
In [1]: score = 86

In [2]: grade = None

In [3]: if (score > 70):
   ...:       grade = 'C'
   ...: elif (score > 85):
   ...:       grade = 'B'
   ...: elif (score > 93):
   ...:       grade = 'A'
   ...:

In [4]: grade
 Out[4]: 'C'
```

OK, back to looping. There are two main ways to loop in Python using the `for` and `while` statements. The `for` statement goes through a sequence of items one at a time, typically performing some work on that item as it *iterates* over it. The examples below should make clear what a for loop does:

```
In [1]: range(10, 15)
 Out[1]: [10, 11, 12, 13, 14]

In [2]: for number in range(10, 15):
   ...:       print number
   ...:
10
11
12
13
14

In [3]: for char in 'abcde':
   ...:       print char
   ...:
a
b
c
d
e

In [4]: for name in ['adam', 'eve']:
   ...:       print name
   ...:
adam
eve
```

Remember that strings, lists, tuples and dictionaries are all sequences, and hence *iterable*. So we can use the for loop on any of these. It is getting rather tedious to use the word sequence, so from now on, I will use lists, or strings or dictionaries, but you should remember that the looping constructs work on all of them. Another Python idiom that is sometimes useful in looping is the use of `enumerate` to keep track of position (or index) while looping over a list. Here is how it is used:

```
In [1]: for i, name in enumerate(['cliburn', 'jacob', 'adam']):
   ...:     print i, name
   ...:
0 cliburn
1 jacob
2 adam
```

A common use of the for loop is to create a new list from an old one. For example, here is how you can create a list of all the squares from 10 to 15.

```
In [1]: squares = []

In [2]: for i in range(10, 16):
   ...:     squares.append(i**2)
   ...:

In [3]: squares
 Out[3]: [100, 121, 144, 169, 196, 225]
```

Notice that to get the numbers `[10,11,12,13,14,15]`, we call `range(10, 16)` since Python indexing includes the start but excludes the end.

We can now combine `if` checks with loops to *filter* lists that we are constructing, only adding items to our list if they meet certain conditions. Suppose we wanted to only collect the squares of the *odd* numbers and discard the *even* one in the previous example:

```
In [1]: oddsquares = []

In [2]: for i in range(10, 16):
   ...:     if i%2==1:
   ...:         oddsquares.append(i**2)
   ...:

In [3]: oddsquares
 Out[3]: [121, 169, 225]
```

This process of looping over a sequence and collecting the items in a list, filtering by some condition if necessary, is so common that Python has a short cut way of doing it known as *list comprehension*. Here is the nicer list comprehension version of the above two examples:

```
In [1]: squares = [i**2 for i in range(10, 16)]

In [2]: squares
 Out[2]: [100, 121, 144, 169, 196, 225]

In [3]: oddsquares = [i**2 for i in range(10, 16) if i%2==1]

In [4]: oddsquares
 Out[4]: [121, 169, 225]
```

We can *nest* loops within each other - for example, to generate labels for a 96-well plate, we can do this list comprehension:

```
In [1]: wells = ['%s%02d' % (r, c) for r in 'ABCDEF' for c in range(1, 13)]

In [2]: wells[:15]
 Out[2]:
['A01',
 'A02',
 'A03',
 'A04',
 'A05',
 'A06',
 'A07',
 'A08',
 'A09',
 'A10',
 'A11',
 'A12',
 'B01',
 'B02',
 'B03']
```

It might be clearer to understand what is happening using the longer version of creating an empty list, then using nested for loops:

```
In [1]: wells = []

In [2]: for r in 'ABCDEF':
   ...:     for c in range(1,13):
   ...:         wells.append('%s%02d' % (r, c))
   ...:

In [3]: wells[:15]
 Out[3]:
['A01',
 'A02',
 'A03',
 'A04',
 'A05',
 'A06',
 'A07',
 'A08',
 'A09',
 'A10',
 'A11',
 'A12',
 'B01',
 'B02',
 'B03']
```

Don't worry about the funny '%02d' and '%s' bits in the code. We will explain *string interpolation* in the next session. Congratulations! You have learnt the basic building blocks of a python program. Once you complete the exercise below, we will finish off our Python crash course with I/O and creating your own functions.

4.9.9 Storing and re-using programs

Using `ipython` is great for learning because of the instant feedback, but at some point you will want to save your code to use for another day. To do so, we use our text editor to write code in a file that ends with the extension '.py'. Open up a new page in TextWrangler, enter the following code:

```
print "I am an expert programmer"
```

then save it as "expert.py". Now open a new terminal, and run the program like so:

```
eris:~ cliburn$ python expert.py
I am an expert programmer
```

You can also run Python programs from within `ipython` with the `run` keyword:

```
In [1]: run expert.py
ERROR: File `expert.py` not found.
```

For the above two programs to run, you need to be in the same directory as `expert.py`. Later, Jacob will show you how to run programs in arbitrary locations.

4.9.10 Exercise

It is claimed by an interviewer that the majority of computer science graduates cannot write a correct solution to this problem (http://imranontech.com/2007/01/24/using-fizzbuzz-to-find-developers-who-grok-coding/). Are you better than the average computer science graduate?

```
Write a program that prints the numbers from 1 to 100.  But for multiples
of three print "Fizz" instead of the number and for the multiples of five
print "Buzz".  For numbers which are multiples of both three and five print
"FizzBuzz".
```

You should save your program in a text editor and execute it as shown above. You can experiment within ipython, and copy and paste working code from ipython into the text editor. The instruction `history -n startline:stopline` shows you code in your history without the line numbers that is convient for cutting and pasting. Do it in stages - first, how do you print the numbers from 1 to 100? Next, how do you find multiples of 3? How do you change what is printed if the number is a multiple of 3? And so on ...

4.10 Python Basics II

We left out the `while` looping construct yesterday. It is used like this:

```
initialize condition
while (condition is True):
  do stuff
```

Typically, the *condition* is updated within the body of the while statement such that it eventually becomes false. A simple example follows:

```
In [1]: i = 0

In [2]: while (i < 5):
   ...:       i = i+1
   ...:       print i
   ...:
1
2
3
4
5
```

4.10.1 Review and warm-up exercises

1. Open a terminal. What directory are you in? List the files in your current directory. Make the following new directories - 'folder1/folder2/folder3'. Navidgate to folder2 and create a file "catted.txt" using cat with the words "I made this!." Delete folder1, folder2 and folder3.

    1. Open your text editor. Load the file sequence1.txt. Find the sequences that would be cut by the EcoRI restriction enzyme that recognizes sequneces flanked on both sides by GAATTC.

    2. Create a list of cubes for all the positive inteters less than 10 (i.e. [1,8,27,...,729]) using a) a for loop and b) a list comprehension.

    3. Find all the characters that are used exactly once in the sentence 'A person who never made a mistake never tried anything new'. Ignore case, so 'A' and 'a' would be counted as 2 occurrences of 'a'.

    4. Find the second largest number in this list [9, 61, 2, 79, 58, 87, 68, 83, 61, 13]

    5. Make a dictionary from these two lists, using the author as the key and the quote as the value:

```
authors = ["Albert Einstein", "Richard Feynman", "Charles
Darwin"]
```

```
quotes = ["Any man who can drive safely while kissing a
pretty girl is simply not giving the kiss the attention it
deserves", "There is a computer disease that anybody who works
with computers knows about.  It's a very serious disease and
it interferes completely with the work.  The trouble with
computers is that you 'play' with them!", "I have tried lately
to read Shakespeare, and found it so intolerably dull that it
nauseated me"]
```

    1. Write a program that generates this list [0,1,2,3,4,5,5,4,3,2,1,0]. Your program should only contain a single integer.

    2. Write a program that uses `while` and `raw_input` and simply repeats the question "who wins?" until you type the words "you win". Here is a session with the program in the terminal:

    eris:examples cliburn$ python winner.py who wins? me who wins? cliburn who wins? someone else who wins? you win

4.10.2 String Interpolation

We start this session by learning how to construct nicely formatted strings with *holes* where we want to insert variables. The most convenient way to do this in python is by *string interpolation*. String interpolation uses codes starting with the `%` symbol as placeholders for inserting variables within the string. The codes that are most useful are:

1. `%s` for strings
2. `%d` for integers
3. `%f` for floats

So for example, we can have this string:

```
In [1]: "%s took %d courses last year and had a %f GPA" % ('Tome', 4, 3.2)
Out[1]: 'Tome took 4 courses last year and had a 3.200000 GPA'
```

Note that the variables to be inserted into the string are given as a tuple following the `%` separator. However, the default formatting leaves something to be desired. For numbers, we can specify the minimum width, as well as the number of decimal places when the number is a float.

```
In [1]: '%4d' % 123
Out[1]: ' 123'

In [2]: '%4d' % 12345
Out[2]: '12345'

In [3]: '%5f' % 3.14
Out[3]: '3.140000'

In [4]: '%5.2f' % 3.14
Out[4]: ' 3.14'
```

Sometimes it is also convenient to *pad* strings or change alignment so rows line up nicely using the flags `0` (left pad with zeros), ‘ ‘ (left pad with space), – (left align) and + (add sign character).

```
In [1]: '%05d' % 23
Out[1]: '00023'

In [2]: '% 5d' % 23
Out[2]: '   23'

In [3]: '%-5d' % 23
Out[3]: '23   '

In [4]: '%+5d' % 23
Out[4]: '  +23'
```

Simple tables are often created using loops and string interpolation. For example, here is the code to print out the layout of a 96 well plate:

```
In [1]: for r in 'ABCDEF': print ' '.join(['%s%02d' % (r, c) for c in range(1, 13)])
   ...:
A01 A02 A03 A04 A05 A06 A07 A08 A09 A10 A11 A12
B01 B02 B03 B04 B05 B06 B07 B08 B09 B10 B11 B12
C01 C02 C03 C04 C05 C06 C07 C08 C09 C10 C11 C12
D01 D02 D03 D04 D05 D06 D07 D08 D09 D10 D11 D12
E01 E02 E03 E04 E05 E06 E07 E08 E09 E10 E11 E12
F01 F02 F03 F04 F05 F06 F07 F08 F09 F10 F11 F12
```

The `join` method of a string *joins* together all the strings in a list, separated by the original string. In this case the original string is a space `' '`, so all the strings in the list comprehension will be joined with spaces separating them before being printed. Take your time to deconstruct this short example - it pulls together many concepts - looping, list comprehension, string interpolation and the use of the string method `join`.

4.10.3 Mini-exercise

1. Write a program that produces these 2 lines of output from range(1,11):

   0001 0002 0003 0004 0005 6.00 7.00 8.00 9.00 10.00

2. Write a program that starts with range(1, 6) and ends up with this string ‘1-one-thousand-2-one-thousand-3-one-thousand-4-one-thousand-5’, using a list comprehension, the `str()` function and a string join.

4.10.4 Reading from and writing to files

We open files using the built-in `open` function. We need to tell the function if the file is to be used for *reading*, *writing* or *appending* with the `r`, `w` and `a` flags. When a file is opened for reading (the default), its contents cannot be altered. When a file is open for writing, if there is an existing file with the same name, its contents are **deleted** and you can write new content to the file. Opening for appending does not delete pre-existing file contents, but allows addition of new content appended to the existing contents. If you work with files from different operating systems, an additional useful flag is `U` for universal that handles differences between how Unix, Macs and Windows systems deal with line endings. All the following do the same thing - open the file `sequnce1.txt` in the `examples` directory for reading. The last version is the most robust, and will work regardless of whether `sequnce1.txt` was created on a Unix, Mac or Windows system, while the others only work if the file was created on the same platform as you are currently using.

```
In [1]: fin = open('examples/sequence1.txt')

In [2]: fin = open('examples/sequence1.txt', 'r')

In [3]: fin = open('examples/sequence1.txt', 'rU')
```

Opening files for writing or appending is similar, but replace the `r` in the argument with `w` or `a`. Remember if you open the file `sequence1.txt` with the `w` flag, the current contents are gone forever.

OK. Now we will open a file for writing, write some lines, close it, open again for appending more lines, close it, and finally open again for reading.

```
In [1]: graffiti = '\n'.join(['Roses are red', 'Violets are blue', 'The dog is pregnant', 'Thanks to

In [2]: fo = open('graffiti.txt', 'w')

In [3]: fo.write(graffiti)

In [4]: fo.close()
```

Here, we write some lines of doggerel in a list, join them as separate lines with the newline separator `\n`, then write it to a file called `directory.txt` that has been opened for writing. Sometimes, you will see another newer idiom for opening files:

```
In [1]: with open('graffiti.txt', 'w') as fo:
   ...:     fo.write(graffiti)
   ...:
```

The difference is that when using the `with` statement, you don't need to remember to `close` the file handler. The operating system limits the numbers of file handlers that are available, and exceeding the number may lead to a system crash. Closing the file frees up the resource, but it is easy to forget to do so in more complicated programs, hence the availability of the `with` statement. Either way is fine. You can see what's in the file by using `less graffiti.txt` either in `ipython` or on the command line.

Let's add another line for the author of the poem:

```
In [1]: fo = open('graffiti.txt', 'a')

In [2]: fo.write('\n' + 'by anonymous college toilet poet')

In [3]: fo.close()
```

Note that we add a newline `\n` before the attribution string so that it appears on a separate line.

4.10.5 Mini-exercise

1. Find the AT/GC ratio in `sequence1.txt`.
2. Find all palindromes of length = 9 in `sequence1.txt` and save them to a file called `palindromes.txt`.
3. Now, re-open `palindromes.txt` and *append* all palindromes of length 8 to the file.

4.10.6 Reading files with read() and readlines()

We can also store the contents of the file read in by using the `read` and `readlines` methods for further processing later. The difference is that `read` returns the content as a single string, while `readlines` returns it as a list of lines.

```
In [1]: poem = open('graffiti.txt', 'rU').read()

In [2]: poem
Out[2]: 'Roses are red\nViolets are blue\nThe dog is pregnant\nThanks to you\nby anonymous college to

In [3]: poem = open('graffiti.txt', 'rU').readlines()

In [4]: poem
Out[4]:
['Roses are red\n',
 'Violets are blue\n',
 'The dog is pregnant\n',
 'Thanks to you\n',
 'by anonymous college toilet poet']
```

We can now process the string in poem1 or the list in poem2 as necessary.

4.10.7 Exercise

1. Convert the contents of the file 'graffit.txt' to all uppercase letters. That is, calling `cat` or `less` on graffit.txt should look like this before and after your program is run:

BEFORE

```
eris:pcfb cliburn$ cat graffiti.txt
Roses are red
Violets are blue
The dog is pregnant
Thanks to you
by anonymous college toilet poet
```

AFTER

```
eris:pcfb cliburn$ cat graffit.txt
ROSES ARE RED
VIOLETS ARE BLUE
THE DOG IS PREGNANT
THANKS TO YOU
BY ANONYMOUS COLLEGE TOILET POET
eris:pcfb cliburn$
```

2. Count the number of times each word appears in hamlet.txt found in the examples folder. For, we define a word to be any string of characters that is separated by white space (space, tab, newline). We also ignore

```
case - so 'ABC' is the same word as 'abc'.  For extra credit, strip all
punctuation before doing the word count.
```

1. Open the file 'hamlet.txt' and assign its contents to a variable as a single string
2. Convert the string to lower case
3. Remove all punctuation characters from the string (punctuation characters are '!"#$%&'()*+,-./:;<=>?@[\]^_'{|}~', which you can also find in the `string` module)
4. Split the string into a list of words, where a word is defined to be any sequence of characters separated by white space
5. Create an empty dictionary to store word counts
6. Loop over the list of words and increment the dictionary count for that word by 1
7. Print the number of occurrences of 'hamlet' in 'Hamlet'
8. Close the file if necessary

4.10.8 Writing your own functions

We are finally in the home stretch for the Python programming module. Learning to write your own functions will greatly increase the complexity of the programs that you can write. A function is a black box - it takes some input, does something with it, and spits out some output. Functions hide details away, allowing you to solve problems at a higher level without getting bogged down. For example, consider the built-in sum function:

```
In [1]: numbers = [1,6,23,8,1,2,90]

In [2]: sum(numbers)
Out[2]: 131
```

The use of the built-in `sum` function hides the details of having to initialize the sum to zero and looping over each number while adding that number to the sum variable. While Python comes with many useful built-in functions, sooner or later, you will need to write your own functions. As you will see, writing your own functions is really simple. Let's write our version of the `sum` function and a `product` function that when given a sequence of numbers, returns the product rather than the sum of numbers. We will store save the functions in `examples/functions.py`.

```
def sum(xs):
    """Given a sequence of numbers, return the sum."""
    s = 0
    for x in xs:
        s += x
    return s

def prod(xs):
    """Given a sequence of numbers, return the product."""
    s = 1
    for x in xs:
        s *= x
    return s
```

A typical function looks like this:

```
def function_name(function_arguments):
   """Optional string describing the function."""
   statements ...
   return result
```

4.10.9 Mini-exercise

1. Write a function that returns the *cumulative* sum of numbers in a list. For example, if the function is given the list [1,2,3,4,5], it should return the list [1, 3, 6, 10, 15].
2. Write a function `fib` that generates the first *n* Fibonacci numbers. The Fibonacci numbers are the sequence [1,1,2,3,5,8,13,...], where each successive number is the sum of the two preceding numbers. Here are some results that your function should give:

```
In [1]: fib(1)
Out[1]: [1]

In [2]: fib(2)
Out[2]: [1, 1]

In [3]: fib(3)
Out[3]: [1, 1, 2]

In [4]: fib(4)
Out[4]: [1, 1, 2, 3]

In [5]: fib(10)
Out[5]: [1, 1, 2, 3, 5, 8, 13, 21, 34, 55]
```

4.10.10 Importing a function from a file (module)

Now we can use the `prod` function in `ipython` or other programs just like a built-in function once we *import* the functions module we have just written. If we are not in the same directory as `functions.py`, we also need to tell the Python interpreter where to find it by adding its location to the search path `sys.path` (which is just a list of directories that Python looks for modules). The way to *call* a function is to give the function name followed by parenthesis with values for the number of arguments expected:

```
In [1]: import functions

In [2]: xs = [1,2,3,4]

In [3]: s, p = functions.sum(xs), functions.prod(xs)
```

If calling `functions.prod` is too verbose for you, you can modify the import statement like so:

Just be aware that this will make any existing function with the name `prod` inaccessible. So for instance, if we used `from functions import sum`, we would no longer have access to the built in `sum` function. Whereas if we used `import functions`, we can choose which function to use - `sum` will use the built-in function, while `functions.sum` will use our function. We recommend using the full name all the time to avoid such *name clashes*, using a shorter alias for the imported module with the `as` keyword if you are really lazy.

```
In [1]: import functions as f

In [2]: f.prod(xs)
Out[2]: 24
```

4.10.11 Functions are first class objects

In Python, functions can be treated like any other object - we can assign them to variables, use them as values in dictionaries, use them as arguments to other functions etc.

```
In [1]: foo = functions.sum

In [2]: foo([1,2,3])
Out[2]: 6

In [3]: func_dict = {'plus' : functions.sum, 'times' : functions.prod}

In [4]: xs = [1,2,3,4]

In [5]: func_dict['plus'](xs)
Out[5]: 10

In [6]: func_dict['times'](xs)
Out[6]: 24
```

There is another way to write short "throwaway" functions for one-time use that is much terser using *lamba* or anonymous functions:

```
In [1]: f = lambda x: x*x

In [2]: f(3)
Out[2]: 9
```

This use of lambda is typically seen in the context of the built-in higher order functions (functions that take functions as arguments) `map` and `filter`.

```
In [1]: filter(lambda x: x % 2==0, range(10))
Out[1]: [0, 2, 4, 6, 8]

In [2]: map(lambda x: x**2, range(5))
Out[2]: [0, 1, 4, 9, 16]
```

In general, Python programmers prefer to use defined rather than anonymous functions, and the use of list comprehensions rather than `map` and `filter` as they are more explicit and easier to understand, but you may come across `lambda`, `map` and `filter` in books or on the web.

4.10.12 Mini-Exercise

1. Replace the filter and map functionality in the above example using list comprehension.
2. Rewrite f = lambda x: x**2 as a regular function also called f using `def`.

4.10.13 Function arguments

We can define functions with more than one argument, as well as give default values to the arguments. In turn, when *calling* a function, we can supply the arguments either by position or by name. Arguments with default values do not need to be supplied when calling a function, but if provided, will overwrite the default values.

```
In [1]: def f(a, b, c=3, d=100):
   ...:     print a, b, c, d
   ...:

In [2]: f(1,2)
1 2 3 100

In [3]: f(1,2,3,4)
```

```
1 2 3 4

In [4]: f(d=1, c=2, b=3, a=4)
4 3 2 1
```

Warning: When you assign a list or a dictionary as a default value for an argument, the list is created at the same time the function is declared, and *persists* over subsequent function calls if not overwritten. That is probably not what you intended - if you do not want the default list to persist, you have set the default to None in the argument, then set it to the empty list in the function after checking that it has not been assigned. An example should make this clear:

```
# we set b to have a default of an empty list
In [1]: def f(a, b=[]):
   ...:       b.append(a)
   ...:       print a, b
   ...:

# but the behavior is rather counter-intuitive
In [2]: f(2)
2 [2]

In [3]: f(3)
3 [2, 3]

# if we over-write the default argument, everything is OK
In [4]: f(3, [1,2])
3 [1, 2, 3]

# this is the way to get the non-persistent behavior
In [5]: def f(a, b=None):
   ...:       if b is None:
   ...:           b = []
   ...:       b.append(a)
   ...:       print a, b
   ...:

In [6]: f(2)
2 [2]

In [7]: f(3)
3 [3]
```

4.10.14 Exercise

1. Write a function that finds palindromic sequences of length k from a string, and use it to find all palindromic sequences of length 9 in sequence1.txt in the examples folder. The function should take 2 arguments, the string and k, the palindrome length
2. Write a program that plays the children's guessing game with you. Running the program and playing with it looks like this:

```
eris:examples cliburn$ python guessing.py
I'm thinking of a number between 1 and 100. Guess what it is!
Guess a number: 50
Too small
Guess a number: 75
Too large
Guess a number: 63
```

```
Too large
Guess a number: 56
Too small
Guess a number: 60
Too large
Guess a number: 58
You've guessed it! The number is 58
```

The first 5 lines of the program look like this:

```
import random

number = random.randint(1, 101)
guess = None
print "I'm thinking of a number between 1 and 100. Guess what it is!"
while guess != number:
  YOUR CODE HERE
```

4.11 Python Modules

Python comes with many libraries covering a large variety of functions. During this section we will look at some of them.

Recall that libraries are accessed using the *import* statement. You can see what object a library contains by using *dir(<module>)* in ipython, and looking at *<module>.<object>.__doc__* string

```
In [1]: import math

In [2]: print math.exp.__doc__
exp(x)

Return e raised to the power of x.
```

4.11.1 os module

The os module provide a platform independent way to work with the operating system, make or remove files and directories.

```
In [1]: import os

In [2]: print os.getcwd()
/home/jacob

In [3]: os.chdir('/home/jacob/baz')

In [4]: os.getcwd()
Out[4]: '/home/jacob/baz'

In [5]: os.remove('foo')

In [6]: os.chdir('/home/jacob')

In [7]: os.rmdir('baz')
```

4.11.2 csv module

The *csv* module provides readers and writers for comma separated value data.

```
In [1]: import csv

In [2]: f = open('monty_python.csv', 'w')

In [3]: cfw = csv.writer(f, dialect='excel')

In [4]: cfw.writerow(['spam','spam','eggs','spam'])

In [5]: cfw.writerow(['spam','spam','spam and eggs', 'spam'])

In [6]: cfw.writerow(['toast'])

In [7]: f.close()

In [8]: cfr = csv.reader(open('monty_python.csv', 'rU'), dialect='excel')

In [9]: for row in cfr:
   ...:     print ', '.join(row)
   ...:
spam, spam, eggs, spam
spam, spam, spam and eggs, spam
toast
```

If you'd prefer a different separator than commas the delimiter optional argument can be used

```
In [1]: import csv

In [2]: f = open('tabbs.csv', 'rU')

In [3]: csvfile = csv.reader(f, delimiter='\t')

In [4]: for row in csvfile:
   ...:     print row
   ...:
['1', '2', '3']
['2', '3', '4']
['4', '5', '6']
```

often you'll want to skip the first row in a csv file, and a simple way to do that is

```
import csv

f = open('test_scores.csv', 'rU')
csvfile = csv.reader(f)

header = False

for row in csvfile:
   if not header:
      header = True
   else:
      print row
f.close()
```

csv excercise

use the test_scores.csv file to calculate the average score (colum 4) for each sex (column 2)

4.11.3 sys.argv

The sys module contains many objects and functions for dealing with how python was compiled or called when executed. Most significantly is argv, which is a list containing all the parameters passed on the command line when python executed, including the name of the python program in position 0. Note that all the elements of sys.argv are *strings* - if you want a number, you will have to convert it using `int()` or `float()`. For example, if you want to assign the argument at position 1 as an integer variable, you can use `n = int(sys.argv[1])`.

```
import sys
if len(sys.argv) > 1:
  print sys.argv
else:
  print 'no arguments passed'
```

```
[jacob@moku ~]$ python argv_example.py foo bar baz
['argv_example.py', 'foo', 'bar', 'baz']
```

sys.argv exercise

write a program that takes two arguments, your first name, and your age, and then prints out your name and the year you were born.

4.11.4 glob module

The *glob* module proves the glob function to perform file globbing similar to what the unix shell provides

```
In [1]: import glob

In [2]: for file in glob.glob('./*.txt'):
   ...:     print file
   ...:
C.txt
B.txt
A.txt
hamlet.txt
```

4.11.5 math module

The *math* module provides common algebra and trigonometric function along with several math constants. Note that the trigonometric functions work in *radians* rather than degrees. You can convert from radians to degrees with `math.degrees` and vice versa with `math.radians`.

```
In [1]: import math

In [2]: math.e
Out[2]: 2.718281828459045

In [3]: math.pi
Out[3]: 3.141592653589793
```

```
In [4]: math.log10(100)
Out[4]: 2.0

In [5]: math.log(math.e)
Out[5]: 1.0

In [7]: math.cos(math.pi)
Out[7]: -1.0

In [10]: math.exp(1)
Out[10]: 2.7182818284590455

In [11]: math.pow(5,2)
Out[11]: 25.0

In [12]: math.sin(math.pi)
Out[12]: 1.2246467991473532e-16
```

for those wondering about line 12, see floats

4.11.6 re (regular expressions)

The *re* module provides access to powerful regular expressions. Use *re.search* to determine if a pattern exists in a string, or use *re.findall* to search for all instances of a pattern in a string.

```
In [1]: import re

In [2]: m = re.search('games', 'all fun and games')

In [3]: m.group()
Out[3]: 'games'

In [4]: re.findall('[1234567890]+','12 drummers drumming, 11 pipers piping, 10 lords a-leaping')
Out[4]: ['12', '11', '10']
```

4.11.7 datetime and time

The *datetime* module provides *time* and *datetime* objects, allowing easy comparison of times and dates.

```
In [1]: import datetime

In [2]: a = datetime.time(8,30)

In [3]: b = datetime.time(9,45)

In [4]: b>a
```

The *time* module provides simple estimates for how long a command takes.

```
In [1]: import time

In [2]: a = time.time()

In [3]: time.sleep(10)

In [4]: b = time.time()
```

```
In [5]: print b-a
10.743445158
```

4.11.8 pickling and unpickling

The *pickle* module provides a way to save python objects to a file that you can unpickle later in a different program. This allows the saving and loading of complex objects such as classes, dictionaries etc.

```
In [1]: import pickle

In [2]: adict = {'a': [1,2,3], 'b' : [4,5,6]}

# pickle.dump takes as arguments the object to be pickled and a file handler
In [3]: pickle.dump(adict, open('adict.pic', 'w'))

# delete adict to see if loading from a pickled file works
In [4]: del adict

# adict has been deleted, so we get an error message
In [5]: adict
---------------------------------------------------------------------------
NameError                                 Traceback (most recent call last)
/Users/cliburn/hg/pcfb/<ipython-input-5-5f470a13239f> in <module>()
----> 1 adict

NameError: name 'adict' is not defined

# load adict from pickled file
In [6]: adict = pickle.load(open('adict.pic'))

In [7]: adict
Out[7]: {'a': [1, 2, 3], 'b': [4, 5, 6]}
```

4.11.9 pypi (formerly cheese shop)

The python community maintains a database of third party python packages. This database lives at pypi. Many of these packages can be installed using *pip* or *easy_install*. In the example below, I first use easy_install to install pip, then use pip to install xlrd (a module for reading XLS files). The `-U` flag means that the program should *update* the installation if the module is already installed. Finally, we can also use pip to uninstall modules (but not easy_install, which is why we prefer to use pip).

```
iMac:pcfb cliburn$ easy_install -U pip
Searching for pip
<SNIP>
Installed /Users/cliburn/Library/Python/2.7/site-packages/pip-1.1-py2.7.egg
Processing dependencies for pip
Finished processing dependencies for pip

iMac:pcfb cliburn$ pip install -U xlrd
Downloading/unpacking xlrd from
<SNIP>
Successfully installed xlrd
Cleaning up...

iMac:pcfb cliburn$ pip uninstall xlrd
```

```
Uninstalling xlrd:
  /Users/cliburn/Library/Python/2.7/site-packages/xlrd
  /Users/cliburn/Library/Python/2.7/site-packages/xlrd-0.7.7-py2.7.egg-info
  /Users/cliburn/bin/runxlrd.py
Proceed (y/n)? y
  Successfully uninstalled xlrd
```

4.11.10 Exercise

Write a program that takes a number on the command line and calculates the log, square, sin and cosine, and writes them out in a csv file.

4.12 NumPy and Matplotlib

4.12.1 NumPy - numeric computing

NumPy is the *de facto* standard for numerical computing in Python. It is highly optimized and extremely useful for working with matrices. The standard matrix class in NumPy is called an array. We will first get comfortable with working with arrays the we will cover a number of useful functions. Then we will touch on the linear algebra capabilities of NumPy and finally we will use a few examples to tie together key concepts.

NumPy - arrays

Contents

The main object in NumPy is the *homogeneous*, *multidimensional* array. An array is a table of elements. An example is a matrix x

$$x = \begin{pmatrix} 1 & 2 & 3 \\ 4 & 5 & 6 \\ 7 & 8 & 9 \end{pmatrix}$$

can be represented as

```
>>> import numpy as np
>>> x = np.array([[1,2,3],[4,5,6],[7,8,9]])
>>> x
array([[1, 2, 3],
       [4, 5, 6],
       [7, 8, 9]])
>>> x.shape
(3, 3)
```

The array x has 2 dimensions. In NumPy the number of dimensions is referred to as **rank**. The ndim is the same as the number of axes or the length of the output of x.shape

```
>>> x.ndim
2

>>> x.size
9
```

Arrays are convenient because of built in methods.

```
>>> x.sum(axis=0)
array([12, 15, 18])
>>> x.sum(axis=1)
array([ 6, 15, 24])

>>> x.mean(axis=0)
array([ 4.,  5.,  6.])
>>> x.mean(axis=1)
array([ 2.,  5.,  8.])
```

But arrays are also useful because they interact with other NumPy functions as well as being central to other package functionality. To make a sequence of numbers, similar to *range* in the Python standard library, we use arange.

```
>>> np.arange(10)
array([0, 1, 2, 3, 4, 5, 6, 7, 8, 9])
>>> np.arange(5,10)
array([5, 6, 7, 8, 9])
>>> np.arange(5,10,0.5)
array([ 5. ,  5.5,  6. ,  6.5,  7. ,  7.5,  8. ,  8.5,  9. ,  9.5])
```

Also we can recreate the first matrix by **reshaping** the output of arange.

```
>>> x = np.arange(1,10).reshape(3,3)
>>> x
array([[1, 2, 3],
       [4, 5, 6],
       [7, 8, 9]])
```

Another similar function to arange is linspace which fills a vector with evenly spaced variables for a specified interval.

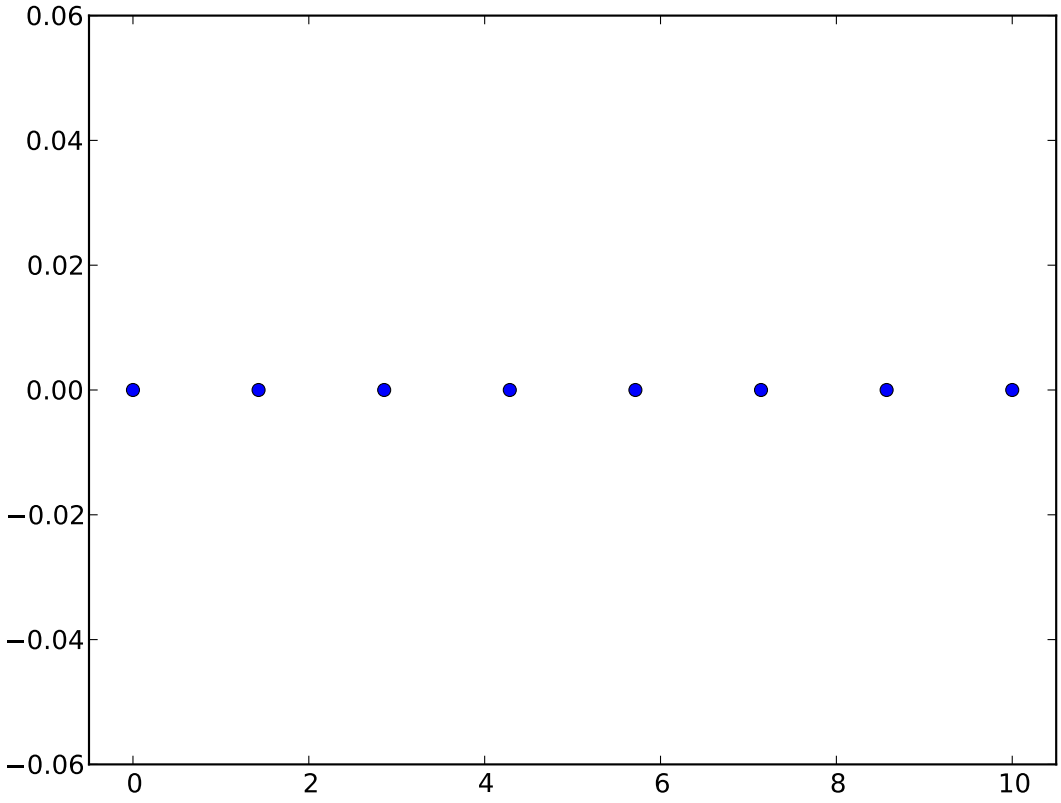
```
>>> x = np.linspace(0,5,5)
>>> x
array([ 0.  ,  1.25,  2.5 ,  3.75,  5.  ])
```

As a reminder you may access the documentation at anytime using

```
~$ pydoc numpy.linspace
```

Visualizing linspace...

```
import numpy as np
import matplotlib.pyplot as plt
fig = plt.figure()
ax = fig.add_subplot(111)
N = 8
y = np.zeros(N)
x1 = np.linspace(0, 10, N, endpoint=True)
p1 = plt.plot(x1, y, 'o')
ax.set_xlim([-0.5,10.5])
plt.show()
```



Arrays may be made of different types of data.

```
>>> x = np.array([1,2,3])
>>> x.dtype
dtype('int64')
>>> x = np.array([0.1,0.2,0.3])
>>> x
array([ 0.1,  0.2,  0.3])
>>> x.dtype
dtype('float64')
>>> x = np.array([1,2,3],dtype='float64')
>>> x.dtype
dtype('float64')
```

There are several convenience functions for making arrays that are worth mentioning:

- zeros
- ones

```
>>> x = np.zeros([3,4])
>>> x
array([[ 0.,  0.,  0.,  0.],
       [ 0.,  0.,  0.,  0.],
       [ 0.,  0.,  0.,  0.]])
>>> x = np.ones([3,4])
>>> x
```

```
array([[ 1.,  1.,  1.,  1.],
       [ 1.,  1.,  1.,  1.],
       [ 1.,  1.,  1.,  1.]])
```

Exercise

1. Create the following array (1 line)

$$a = \begin{pmatrix} 1 & 2 & \cdots & 10 \\ 11 & 12 & \cdots & 20 \\ \vdots & \ddots & \ddots & \vdots \\ 91 & 92 & \cdots & 100 \end{pmatrix}$$

2. Use the array object to get the number of elements, rows and columns
3. Get the mean of the rows and columns
4. What do you get when you do this?

```
>>> a[4,:]
```

5. **[extra] If you have time you can get familiar try**
    - np.log(a)
    - np.cumsum(a)
    - np.rank(a)
    - np.power(a,2)
6. [extra] How do you create a vector that has exactly 50 points and spans the range 11 to 23

NumPy - basics

Quick reference

Here we provide a quick reference guide to the commonly used functions from the NumPy package along with several frequently encountered examples.

NumPy command	Note
a.ndim	returns the num. of dimensions
a.shape	returns the num. of rows and colums
arange(start,stop,step)	returns a sequence vector
linspace(start,stop,steps)	returns a evenly spaced sequence in the specificed interval
dot(a,b)	matrix multiplication
vstack([a,b])	stack arrays a and b vertically
hstack([a,b])	stack arrays a and b horizontally
where(a>x)	returns elements from an array depending on condition
argsort(a)	returns the sorted indices of an input array

Basic operations

Arithmetic operators in NumPy work elementwise.

```
>>> a = np.array([3,4,5])
>>> b = np.ones(3)
>>> a - b
array([ 2.,  3.,  4.])
```

Something that can be tricky for people familar with other programming languages is that the * operator **does not** carry out a matrix product. This is done with the dot function.

```
>>> a = np.array([[1,2],[3,4]])
>>> b = np.array([[1,2],[3,4]])
>>> a
array([[1, 2],
       [3, 4]])
>>> b
array([[1, 2],
       [3, 4]])
>>> a * b
array([[ 1,  4],
       [ 9, 16]])
>>> np.dot(a,b)
array([[ 7, 10],
       [15, 22]])
```

Special addition and multiplication operators

```
>>> a = np.zeros((2,2),dtype='float')
>>> a += 5
>>> a
array([[ 5.,  5.],
       [ 5.,  5.]])
>>> a *= 5
>>> a
array([[ 25.,  25.],
       [ 25.,  25.]])
>>> a + a
array([[ 50.,  50.],
       [ 50.,  50.]])
```

Concatenation

```
>>> a = np.array([1,2,3])
>>> b = np.array([4,5,6])
>>> c = np.array([7,8,9])
>>> np.hstack([a,b,c])
array([1, 2, 3, 4, 5, 6, 7, 8, 9])
>>> np.vstack([a,b,c])
array([[1, 2, 3],
       [4, 5, 6],
       [7, 8, 9]])
```

Sorting arrays

```
>>> x.sort()
>>> x
array([0, 0, 1, 3, 4, 5])
>>> x = np.array(([1,3,4,0,0,5]))
array([3, 4, 0, 1, 2, 5])
```

```
>>> np.argsort(x)
array([3, 4, 0, 1, 2, 5])
```

Common math functions

```
>>> x = np.arange(1,5)
>>> np.sqrt(x) * np.pi
array([ 3.14159265,  4.44288294,  5.44139809,  6.28318531])
>>> 2**4
16
>>> np.power(2,4)
16
>>> np.log(np.e)
1.0
>>> x = np.arange(5)
>>> x.max() - x.min()
4
```

Basic operations excercise

Exercise

In the following table we have expression values for 5 genes at 4 time points. These are completely made up data. Although, some of the questions can be easily answered by looking at the data, microarray data generally come in much larger tables and if you can figure it out here the same code will work for an entire gene chip.

Gene name	4h	12h	24h	48h
A2M	0.12	0.08	0.06	0.02
FOS	0.01	0.07	0.11	0.09
BRCA2	0.03	0.04	0.04	0.02
CPOX	0.05	0.09	0.11	0.14

1. create a single array for the data (4x4)
2. find the mean expression value *per gene*
3. find the mean expression value *per time point*
4. which gene has the maximum mean expression value?
5. sort the gene names by the max expression value

Tip:

```
>>> geneList = np.array(["A2M", "FOS", "BRCA2","CPOX"])
>>> values0  = np.array([0.12,0.08,0.06,0.02])
>>> values1  = np.array([0.01,0.07,0.11,0.09])
>>> values2  = np.array([0.03,0.04,0.04,0.02])
>>> values3  = np.array([0.05,0.09,0.11,0.14])
```

Additional NumPy

Indexing and Slicing 1D arrays can be indexed in the same way a Python list can.

```
>>> a = np.arange(10)
>>> a[2:4]
array([2, 3])
>>> a[:10:2]
array([0, 2, 4, 6, 8])
>>> a[::-1]
array([9, 8, 7, 6, 5, 4, 3, 2, 1, 0])
```

Multidimensional arrays can have one index per axis

```
>>> x = np.arange(12).reshape(3,4)
>>> x
array([[ 0,  1,  2,  3],
       [ 4,  5,  6,  7],
       [ 8,  9, 10, 11]])
>>> x[2,3]
11
>>> x[:,1]                          # everything in the second row
array([1, 5, 9])
>>> x[1,:]                          # everything in the second column
array([4, 5, 6, 7])
>>> x[1:3,:]                        # second and third rows
array([[ 4,  5,  6,  7],
       [ 8,  9, 10, 11]])
```

Where

```
>>> a = np.array([1,1,1,2,2,2,3,3,3])
>>> a[a>1]
array([2, 2, 2, 3, 3, 3])
>>> a[a==3]
array([3, 3, 3])
>>> np.where(a<3)
(array([0, 1, 2, 3, 4, 5]),)
>>> np.where(a<3)[0]
array([0, 1, 2, 3, 4, 5])
>>> np.where(a>9)
(array([], dtype=int64),)
```

Printing

```
>>> for row in x:
...     print row
...
[0 1 2 3]
[4 5 6 7]
[ 8  9 10 11]

>>> for element in x.flat:
...     print element
...
0
1
2
3
4
5
6
```

```
7
8
9
10
11
```

Copying

```
>>> a = np.array(['a','b','c'])
>>> b = a
>>> b[1] = 'z'
>>> a
array(['a', 'z', 'c'],
      dtype='|S1')

>>> a = np.array(['a','b','c'])
>>> b = a.copy()
>>> b[1] = 'z'
>>> a
array(['a', 'b', 'c'],
      dtype='|S1')
```

Missing data

```
>>> import numpy as np
>>> from scipy.stats import nanmean
>>> a = np.array([[1,2,3],[4,5,np.nan],[7,8,9]])
>>> a
array([[  1.,   2.,   3.],
       [  4.,   5.,  nan],
       [  7.,   8.,   9.]])
>>> columnMean = nanmean(a,axis=0)
>>> columnMean
array([ 4.,  5.,  6.])
>>> rowMean = nanmean(a,axis=1)
>>> rowMean
array([ 2. ,  4.5,  8. ])
```

Generating random numbers

```
>>> np.random.randint(0,10,5)       # random integers from a closed interval
array([2, 8, 3, 7, 8])
>>> np.random.normal(0,1,5)         # random numbers from a Gaussian
array([ 1.44660159, -0.35625249, -2.09994545,  0.7626487 ,  0.36353648])
>>> np.random.uniform(0,2,5)        # random numbers from a uniform distribution
array([ 0.07477679,  0.36409135,  1.42847035,  1.61242304,  0.54228665])
```

There are many useful functions in random however we are showing only a few so that they will be familar when we get to plotting.

NumPy - linear algebra

Linear algebra is a branch of mathematics concerned with vector spaces and the mappings between those spaces. NumPy has a package called linalg. This page is meant only to familiarize you with the NumPy's linear algebra functions for those who are interested.

A $1 \times N$ dimensional vector x

$$x = \begin{pmatrix} x_1 \\ x_2 \\ \vdots \\ x_N \end{pmatrix}$$

and its transpose $\mathbf{x}^T = (x_1, x_2, \ldots, x_N)$ can be expressed in python as

```
>>> import numpy as np
>>> x = np.array([[1,2,3]]).T
>>> xt = x.T
>>> x.shape
(3, 1)
>>> xt.shape
(1, 3)
```

A **column matrix** in NumPy.

$$x = \begin{pmatrix} 3 \\ 4 \\ 5 \\ 6 \end{pmatrix}$$

```
>>> x = np.array([[3,4,5,6]]).T
```

A **row matrix** in NumPy.

$$x = \begin{pmatrix} 3 & 4 & 5 & 6 \end{pmatrix}$$

```
>>> x = np.array([[3,4,5,6]])
```

General matrices you are *already familiar with*.

$$A_{m,n} = \begin{pmatrix} a_{1,1} & a_{1,2} & \cdots & a_{1,n} \\ a_{2,1} & a_{2,2} & \cdots & a_{2,n} \\ \vdots & \vdots & \ddots & \vdots \\ a_{m,1} & a_{m,2} & \cdots & a_{m,n} \end{pmatrix}$$

Common tasks

Matrix determinant

```
>>> a = np.array([[3,-9],[2,5]])
>>> np.linalg.det(a)
33.000000000000014
```

Matrix inverse

```
>>> A = np.array([[-4,-2],[5,5]])
>>> A
array([[-4, -2],
       [ 5,  5]])
>>> invA = np.linalg.inv(A)
```

```
>>> invA
array([[-0.5, -0.2],
       [ 0.5,  0.4]])

>>> np.round(np.dot(A,invA))
array([[ 1.,  0.],
       [ 0.,  1.]])
```

Because $AA^{-1} = A^{-1}A = I$.

Eigenvalues and Eigenvectors

```
>>> a = np.diag((1, 2, 3))
>>> a
array([[1, 0, 0],
       [0, 2, 0],
       [0, 0, 3]])
>>> w,v = np.linalg.eig(a)
>>> w;v
array([ 1.,  2.,  3.])
array([[ 1.,  0.,  0.],
       [ 0.,  1.,  0.],
       [ 0.,  0.,  1.]])
```

This is by no means a complete list—also the SciPy package has additional functions if this is an area of interest.

Bibliographic notes

1. Duda, R. O., Hart, P. E. & Stork, D. G. Pattern Classification, John Wiley & Sons, Inc., 2001.

Useful links

- NumPy homepage
- Official NumPy tutorial
- NumPy for MATLAB users

4.12.2 Matplotlib - plotting in Python

Matplotlib - basics

Introduction

The most frequently used plotting package in Python, matplotlib, is written in pure Python and is heavily dependent on NumPy. The main webpage introduction itemizes what John Hunter (mpl creator) was looking for in a plotting toolkit.

- Plots should look great - publication quality. One important requirement for me is that the text looks good (antialiased, etc.)
- Postscript output for inclusion with TeX documents
- Embeddable in a graphical user interface for application development
- Code should be easy enough that I can understand it and extend it

- Making plots should be easy

Matplotlib is conceptually divided into three parts:

1. pylab interface (similar to MATLAB) – pylab tutorial
2. Matplotlib **frontend** or API – artist tutorial
3. **backends** – drawing devices or renderers

Essentials

The Axes class is the most important class in mpl. The following three lines are used to get an axes class ready for use.

```
>>> import matplotlib.pyplot as plt
>>> fig = plt.figure()
>>> ax = fig.add_subplot(2,1,1)
```

If you need a freehand axis then

```
>>> fig2 = plt.figure()
>>> ax2 = fig2.add_axes([0.15, 0.1, 0.7, 0.3])    # [left, bottom, width, height]
```

After a figure is drawn you may save it and or plot it with the following.

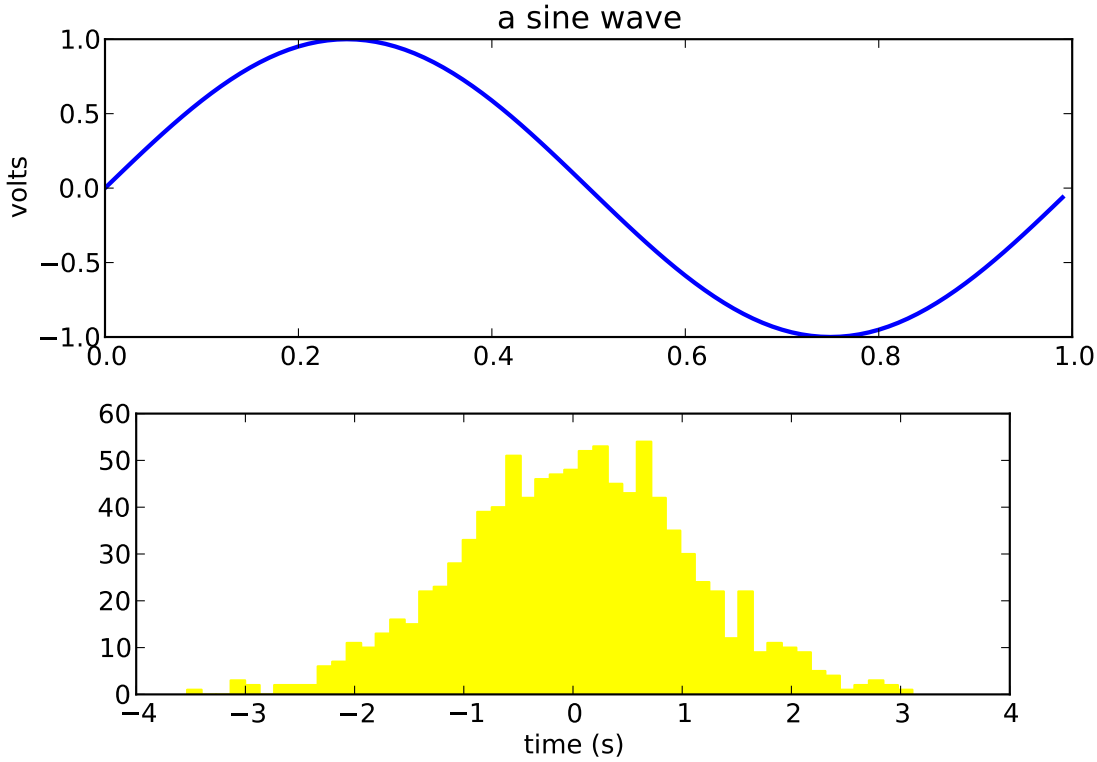
```
>>> fig.saveas('foo.png',dpi=200)
>>> plt.show()
```

The DPI argument is optional and we can save to a bunch of formats like: JPEG, PNG, TIFF, PDF and EPS.

Here is the example from the artist tutorial.

An example

```
import numpy as np
import matplotlib.pyplot as plt

fig = plt.figure()
fig.subplots_adjust(top=0.8)
ax1 = fig.add_subplot(211)
ax1.set_ylabel('volts')
ax1.set_title('a sine wave')

t = np.arange(0.0, 1.0, 0.01)
s = np.sin(2*np.pi*t)
line, = ax1.plot(t, s, color='blue', lw=2)

ax2 = fig.add_axes([0.15, 0.1, 0.7, 0.3])
n, bins, patches = ax2.hist(np.random.randn(1000), 50,
    facecolor='yellow', edgecolor='yellow')
ax2.set_xlabel('time (s)')
```

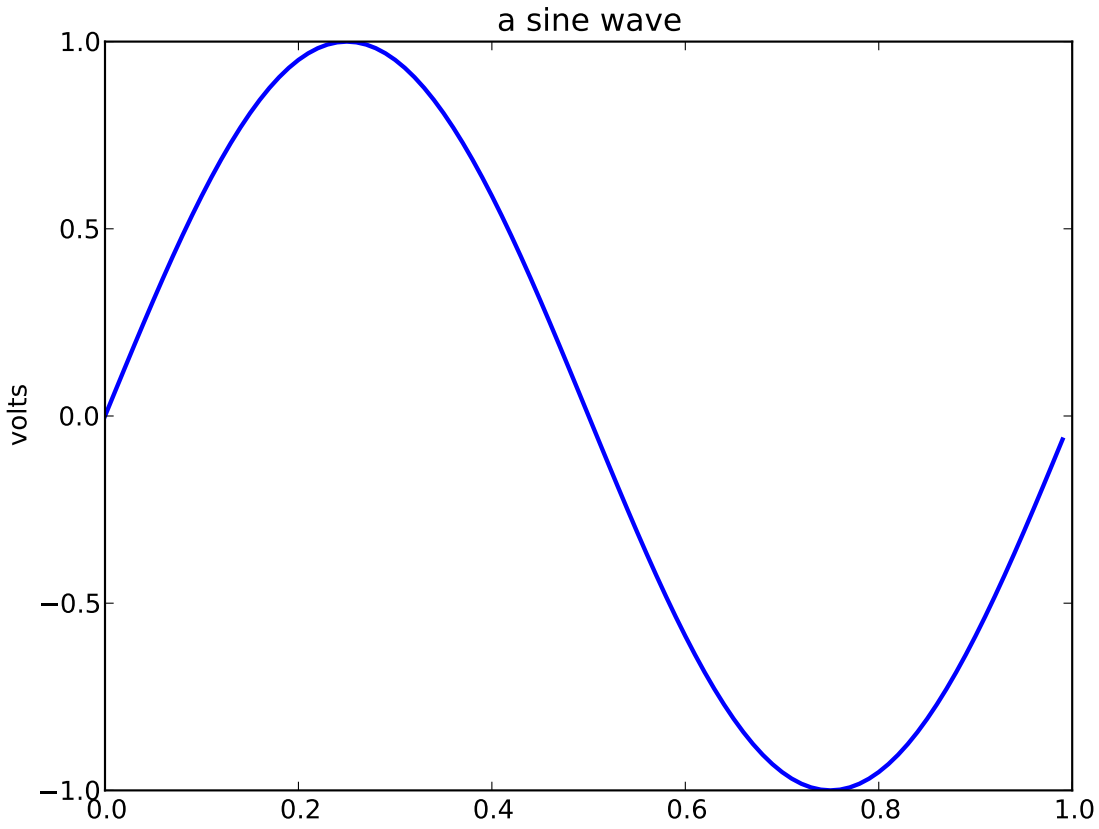


Matplotlib - line and box plots

- *Simple line plot*
- *Lines with markers*
- *Box plots*

Simple line plot

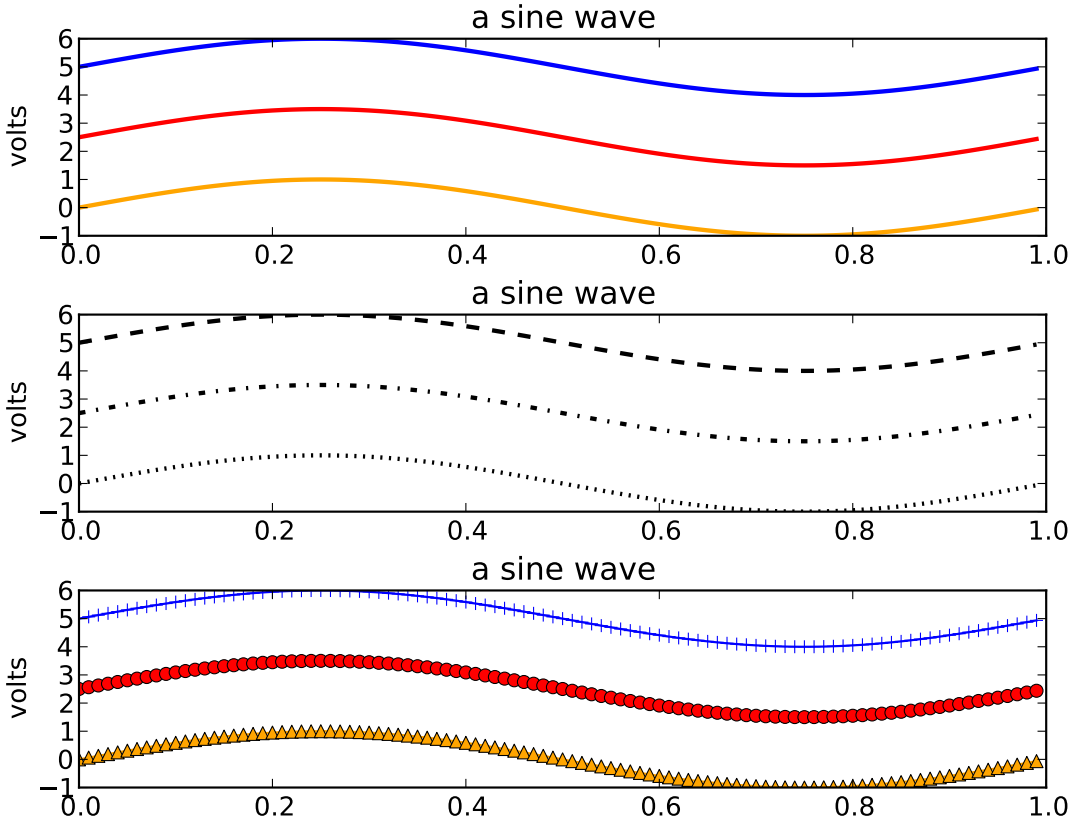
```
import numpy as np
import matplotlib.pyplot as plt

## initialize the axes
fig = plt.figure()
ax = fig.add_subplot(111)

## format axes
ax.set_ylabel('volts')
ax.set_title('a sine wave')

t = np.arange(0.0, 1.0, 0.01)
s = np.sin(2*np.pi*t)
line, = ax.plot(t, s, color='blue', lw=2)
```



Lines with markers

```
import numpy as np
import matplotlib.pyplot as plt

## initialize the figure
fig = plt.figure()


## the data
t = np.arange(0.0, 1.0, 0.01)
s = np.sin(2*np.pi*t)

## the top axes
ax1 = fig.add_subplot(3,1,1)
ax1.set_ylabel('volts')
ax1.set_title('a sine wave')

line1 = ax1.plot(t, s+5.0, color='blue', lw=2)
line2 = ax1.plot(t, s+2.5, color='red', lw=2)
line3 = ax1.plot(t, s, color='orange', lw=2)

## the middle axes
ax2 = fig.add_subplot(3,1,2)
```

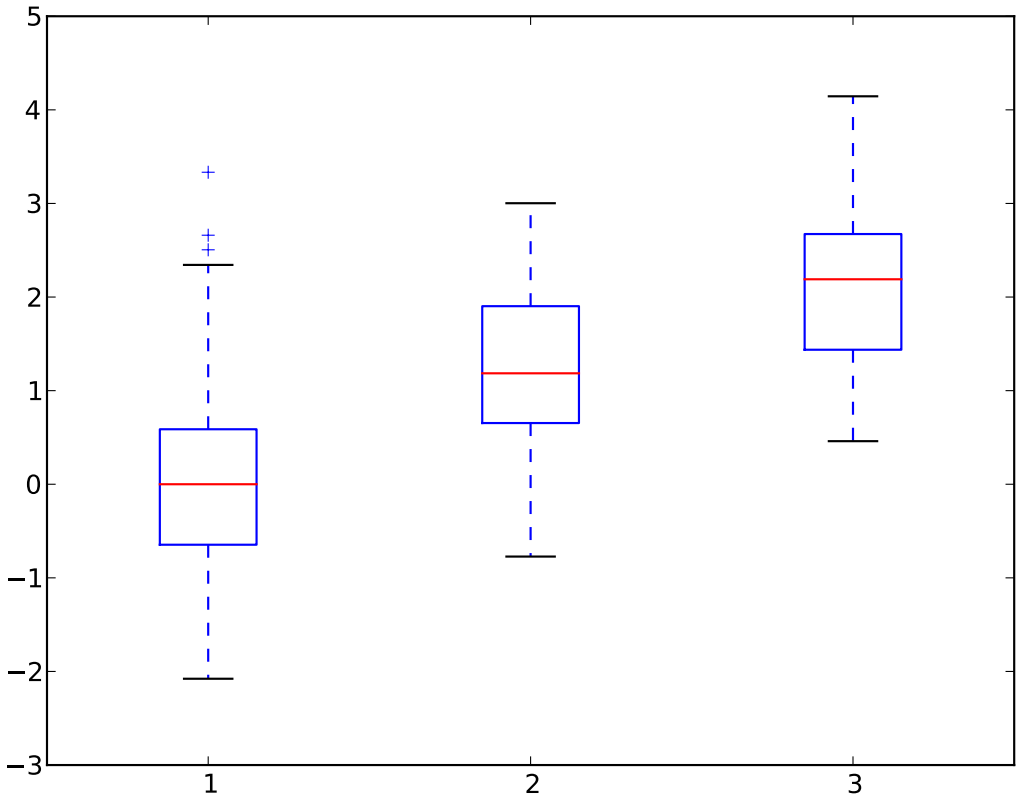
```
ax2.set_ylabel('volts')
ax2.set_title('a sine wave')

line1 = ax2.plot(t, s+5.0, color='black', lw=2,linestyle="--")
line2 = ax2.plot(t, s+2.5, color='black', lw=2,linestyle="-.")
line3 = ax2.plot(t, s, color='#000000', lw=2,linestyle=":")

## the thrid axes
ax3 = fig.add_subplot(3,1,3)
ax3.set_ylabel('volts')
ax3.set_title('a sine wave')

line1 = ax3.plot(t,s+5.0, color='blue', marker="+")
line2 = ax3.plot(t,s+2.5, color='red', marker="o")
line3 = ax3.plot(t,s, color='orange', marker="^")

## adjust the space between plots
plt.subplots_adjust(wspace=0.2,hspace=.4)
```



Box plots

For more information on box plots try the demo

```
import numpy as np
import matplotlib.pyplot as plt


fig = plt.figure()
ax = fig.add_subplot(111)

x1 = np.random.normal(0,1,50)
x2 = np.random.normal(1,1,50)
x3 = np.random.normal(2,1,50)

ax.boxplot([x1,x2,x3])
plt.show()
```

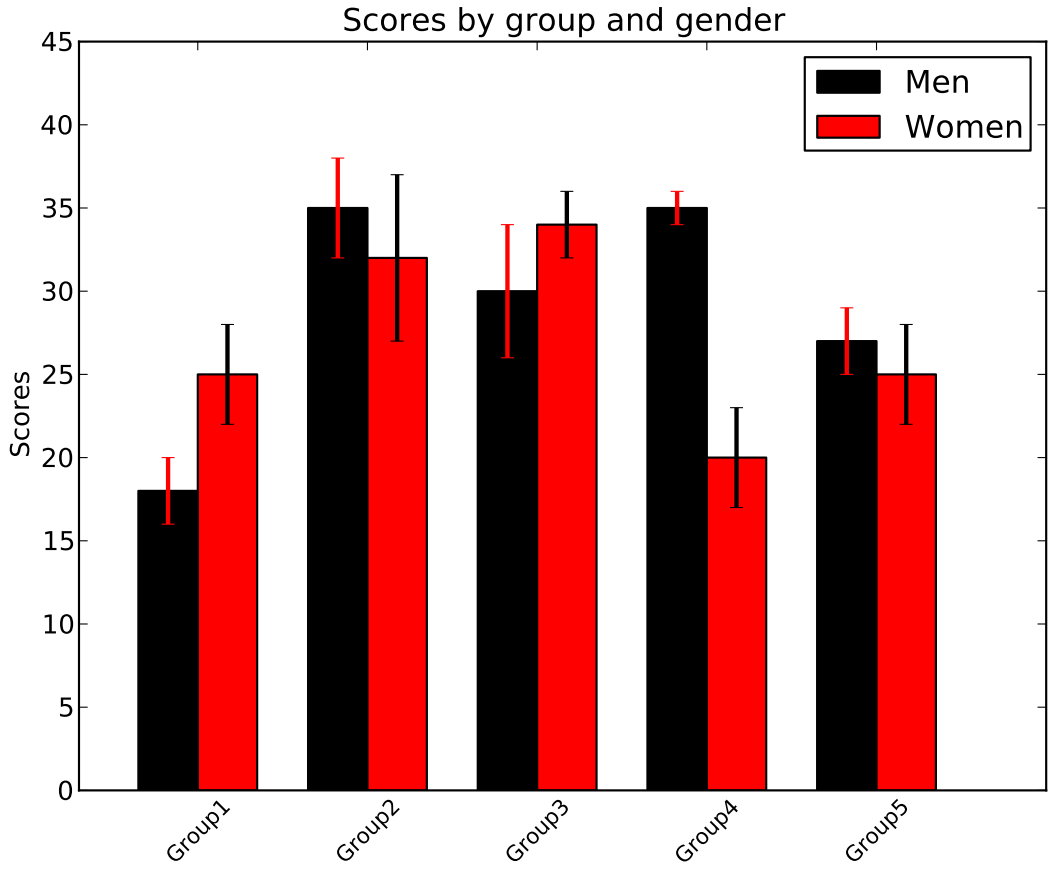


Matplotlib - bar,scatter and histogram plots

- *Simple bar plot*
- *Another bar plot*
- *Scatter plot*

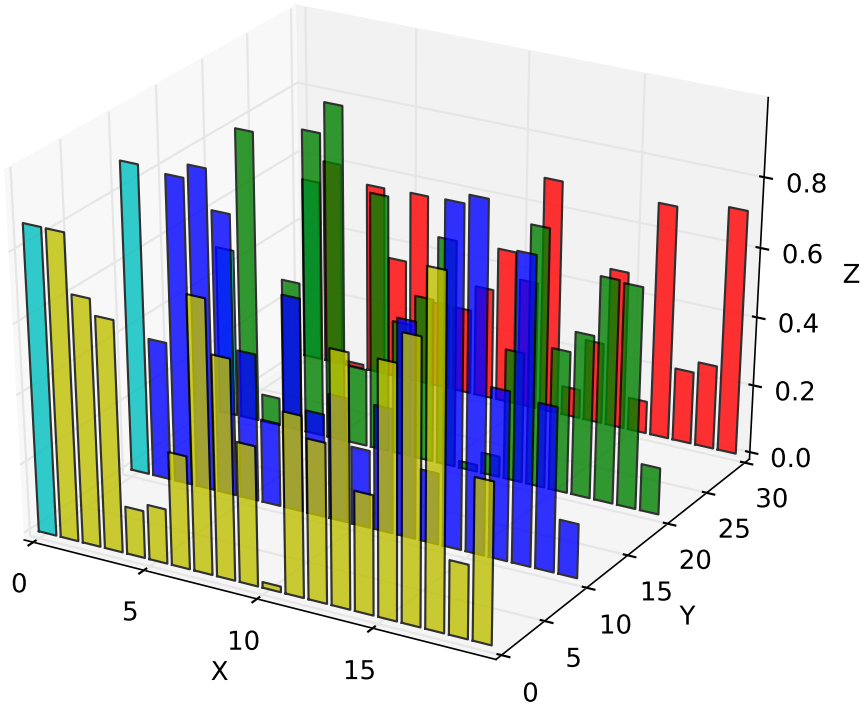
Simple bar plot

```
import numpy as np
import matplotlib.pyplot as plt

fig = plt.figure()
ax = fig.add_subplot(111)

## the data
N = 5
menMeans = [18, 35, 30, 35, 27]
menStd =   [2, 3, 4, 1, 2]
womenMeans = [25, 32, 34, 20, 25]
womenStd =   [3, 5, 2, 3, 3]

## necessary variables
ind = np.arange(N)                # the x locations for the groups
width = 0.35                      # the width of the bars

## the bars
rects1 = ax.bar(ind, menMeans, width,
                color='black',
                yerr=menStd,
                error_kw=dict(elinewidth=2,ecolor='red'))

rects2 = ax.bar(ind+width, womenMeans, width,
                    color='red',
                    yerr=womenStd,
                    error_kw=dict(elinewidth=2,ecolor='black'))

# axes and labels
ax.set_xlim(-width,len(ind)+width)
ax.set_ylim(0,45)
ax.set_ylabel('Scores')
ax.set_title('Scores by group and gender')
xTickMarks = ['Group'+str(i) for i in range(1,6)]
ax.set_xticks(ind+width)
xtickNames = ax.set_xticklabels(xTickMarks)
plt.setp(xtickNames, rotation=45, fontsize=10)

## add a legend
ax.legend( (rects1[0], rects2[0]), ('Men', 'Women') )

plt.show()
```



Another bar plot

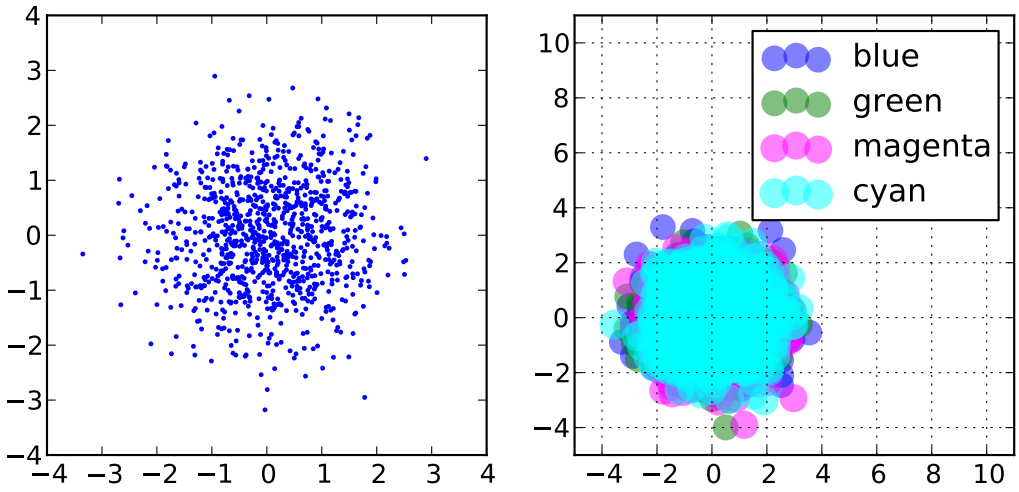
```
from mpl_toolkits.mplot3d import Axes3D
import matplotlib.pyplot as plt
import numpy as np

fig = plt.figure()
ax = fig.add_subplot(111,projection='3d')
for c, z in zip(['r', 'g', 'b', 'y'], [30, 20, 10, 0]):
    xs = np.arange(20)
    ys = np.random.rand(20)

    # You can provide either a single color or an array. To demonstrate this,
    # the first bar of each set will be colored cyan.
    cs = [c] * len(xs)
    cs[0] = 'c'
    ax.bar(xs, ys, zs=z, zdir='y', color=cs, alpha=0.8)

ax.set_xlabel('X')
ax.set_ylabel('Y')
ax.set_zlabel('Z')

plt.show()
```



Scatter plot

```
#!/usr/bin/env python
import matplotlib.pyplot as plt
import numpy as np

fig = plt.figure()
ax1 = fig.add_subplot(121)

## the data
N=1000
x = np.random.randn(N)
y = np.random.randn(N)

## left panel
ax1.scatter(x,y,color='blue',s=5,edgecolor='none')
ax1.set_aspect(1./ax1.get_data_ratio()) # make axes square


## right panel
ax2 = fig.add_subplot(122)
props = dict(alpha=0.5, edgecolors='none' )

handles = []
```

```
colors = ['blue', 'green', 'magenta', 'cyan']
for color in colors:
    x = np.random.randn(N)
    y = np.random.randn(N)
    s = np.random.randint(50,200)
    handles.append(ax2.scatter(x, y, c=color, s=s, **props))

ax2.set_ylim([-5,11])
ax2.set_xlim([-5,11])

ax2.legend(handles, colors)
ax2.grid(True)
ax2.set_aspect(1./ax2.get_data_ratio())
plt.show()
```

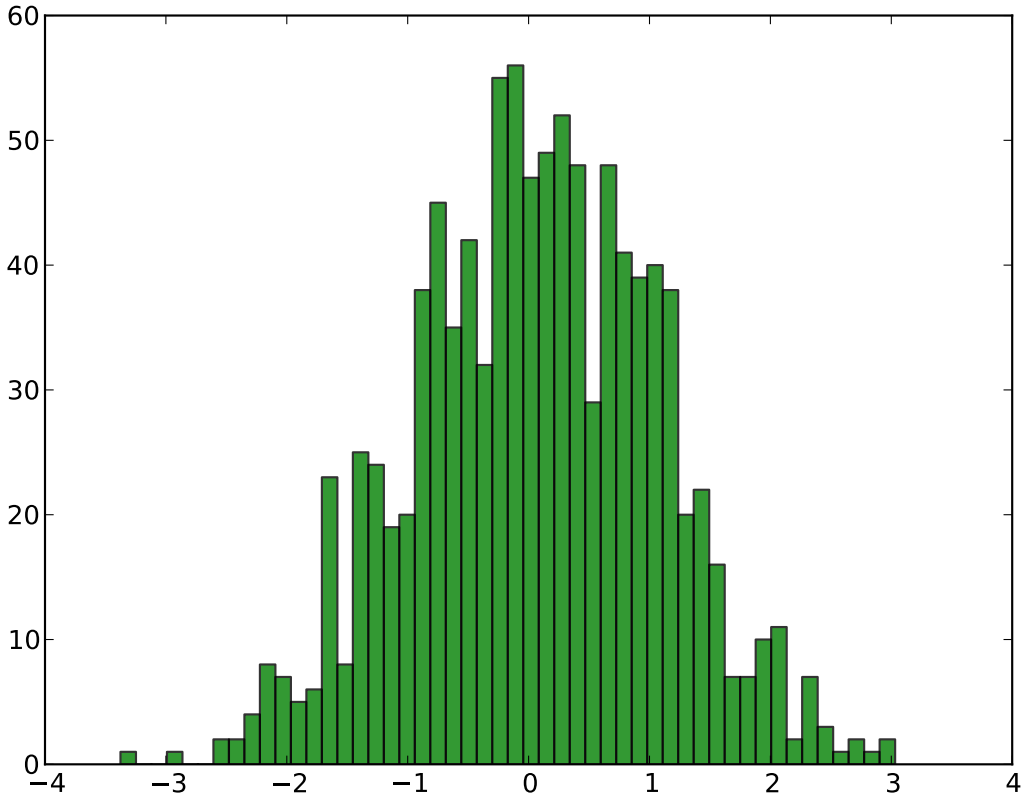


Histogram plot

Here is the matplotlib histogram demo

```
import numpy as np
import matplotlib.pyplot as plt


fig = plt.figure()
ax = fig.add_subplot(111)
```

```
x = np.random.normal(0,1,1000)
numBins = 50
ax.hist(x,numBins,color='green',alpha=0.8)
plt.show()
```



Matplotlib - exercises

Yeast cell cycle data

`File download`

The data were originally downloaded from the Yeast Cell Cycle Analysis Project Page. These data [1] by Spellman and Sherlock have likely been used in over a hundred papers.

1. look at the file so you know what you are getting into (less,wc)
2. copy this script into an editor and lets go over it

```
#!/usr/bin/env python

import csv,os,sys,pickle
import numpy as np

## read the file once to get numRows and numCols
txtFilePath = os.path.join("..","data","cellcycle.txt")
```

```
numRows = 0
reader = csv.reader(open(txtFilePath, 'r'),delimiter='\t')
expListIDs = reader.next()
expListIDs = np.array(expListIDs[1:])
for linja in reader:
    numRows+=1

## populate a matrix and name vectors with file info
numColumns = len(expListIDs)
exprMat = np.zeros([numRows,numColumns])
reader = csv.reader(open(txtFilePath, 'r'),delimiter='\t')
header = reader.next()
rowInd = 0
geneList = []

for linja in reader:
    row = np.array(linja[1:])
    newRow = np.zeros(len(row),)
    nanInds = np.where(row == '')
    goodInds = np.where(row != '')
    newRow[nanInds] = np.nan
    newRow[goodInds] = [float(element) for element in row[goodInds]]
    exprMat[rowInd,:] = newRow
    rowInd +=1
    geneList.append(linja[0])
geneList = np.array(geneList)

## print out info
print "..............."
print "matrix of size (%s,%s)  created..."%(exprMat.shape)
print "gene list size - %s"%geneList.size
print "exp list size  - %s"%expListIDs.size
print "..............."

## write the data to a file
outFilePath = os.path.join(".","excercise-np.pickle")
tmp = open(outFilePath,'w')
pickle.dump([geneList,expListIDs,exprMat],tmp)
tmp.close()
```

3. save the file using your editor to a directory and use it to read cellcycle.txt. To do this you will need to change at least one line?
4. create your own script(s) that does the following
    - opens the pickle file
    - calculates mean expression value for a gene
    - plot expression values for a given gene in a histogram
    - [extra] for a given gene create a lineplot that shows expression values for all the conditions
    - [extra] make plot that has boxplots for the 5 genes with the greatest expression mean
    - [extra] create a scatter plot (1 condition) where the negative expression values are green and positive ones are red

Note that:

```
>>> a = np.array([1,2,3,np.nan])
>>> a.max()
nan
>>> a.min()
nan
>>> a.mean()
nan
>>> np.where(np.isnan(a)==False)[0]
array([0, 1, 2])
```

Also, note that we do not transform, normalize or otherwise process the data in this example. We are using this data set as a learning tool. The missing data difficulties that arise are common in the biological sciences.

Bibliographic notes

1. Spellman P T, Sherlock, G, Zhang, M Q, Iyer, V R, Anders, K, Eisen, M B, Brown, P O, Botstein, D, Futcher, B. Comprehensive identification of cell cycle-regulated genes of the yeast Saccharomyces cerevisiae by microarray hybridization. *Molecular biology of the cell*, Vol. 9 (12): 3273-97, 1998. PubMed.

Useful links

- Matplotlib homepage
- Matplotlib gallery

4.13 Biopython I

From the Biopython:

Biopython is a set of freely available tools for biological computation written in Python by an international team of developers. It is a distributed collaborative effort to develop Python libraries and applications which address the needs of current and future work in bioinformatics. The source code is made available under the Biopython License, which is extremely liberal and compatible with almost every license in the world.

4.13.1 Biopython - basics

Introduction

From the biopython website their goal is to "make it as easy as possible to use Python for bioinformatics by creating high-quality, reusable modules and scripts." These modules use the biopython tutorial as a template for what you will learn here. Here is a list of some of the most common data formats in computational biology that are supported by biopython.

Uses	Note
Blast	finds regions of local similarity between sequences
ClustalW	multiple sequence alignment program
GenBank	NCBI sequence database
PubMed and Medline	Document database
ExPASy	SIB resource portal (Enzyme and Prosite)
SCOP	Structural Classification of Proteins (e.g. 'dom','lin')
UniGene	computationally identifies transcripts from the same locus
SwissProt	annotated and non-redundant protein sequence database

Some of the other principal functions of biopython.

- A standard sequence class that deals with sequences, ids on sequences, and sequence features.
- Tools for performing common operations on sequences, such as translation, transcription and weight calculations.
- Code to perform classification of data using k Nearest Neighbors, Naive Bayes or Support Vector Machines.
- Code for dealing with alignments, including a standard way to create and deal with substitution matrices.
- Code making it easy to split up parallelizable tasks into separate processes.
- GUI-based programs to do basic sequence manipulations, translations, BLASTing, etc.

Getting started

```
>>> import Bio
>>> Bio.__version__
'1.58'
```

Some examples will also require a working internet connection in order to run.

```
>>> from Bio.Seq import Seq
>>> my_seq = Seq("AGTACACTGGT")
>>> my_seq
Seq('AGTACACTGGT', Alphabet())
>>> aStringSeq = str(my_seq)
>>> aStringSeq
'AGTACACTGGT'
>>> my_seq_complement = my_seq.complement()
>>> my_seq_complement
Seq('TCATGTGACCA', Alphabet())
>>> my_seq_reverse = my_seq.reverse()
>>> my_seq_rc = my_seq.reverse_complement()
>>> my_seq_rc
Seq('ACCAGTGTACT', Alphabet())
```

There is so much more, but first before we get into it we should figure out how to get sequences in and out of python.

`File download`

FASTA formats are the standard format for storing sequence data. Here is a little reminder about sequences.

Nucleic acid code	Note	Nucleic acid code	Note
A	adenosine	K	G/T (keto)
T	thymidine	M	A/C (amino)
C	cytidine	R	G/A (purine)
G	guanine	S	G/C (strong)
N	A/G/C/T (any)	W	A/T (weak)
U	uridine	B	G/T/C
D	G/A/T	Y	T/C (pyrimidine)
H	A/C/T	V	G/C/A

Here is quickly a bit about how biopython works with sequences

```
>>> for seq_record in SeqIO.parse(os.path.join("data","ls_orchid.fasta"), "fasta"):
...     print seq_record.id
...     print repr(seq_record.seq)
...     print len(seq_record)
...
```

```
gi|2765658|emb|Z78533.1|CIZ78533
Seq('CGTAACAAGGTTTCCGTAGGTGAACCTGCGGAAGGATCATTGATGAGACCGTGG...CGC', SingleLetterAlphabet())
740
```

4.13.2 Biopython - sequences and alphabets

The Sequence object

Some examples will also require a working internet connection in order to run.

```
>>> from Bio.Seq import Seq
>>> from Bio.Alphabet import IUPAC
>>> my_seq = Seq("AGTACACTGGT", IUPAC.unambiguous_dna)
>>> my_seq
Seq('AGTACACTGGT', IUPACUnambiguousDNA())
>>> my_seq.alphabet
IUPACUnambiguousDNA()
```

A *Seq* object in python acts like a normal python string.

```
>>> for letter in my_seq:
...     print letter
>>> len(my_seq)
>>> my_seq[4:12]
>>> my_seq[::-1]
>>> str(my_seq)
```

Nucleotide counts, transcription, translation

```
>>> my_seq.count("A")
3
```

to get the GC nucleotide content.

```
>>> from Bio.SeqUtils import GC
>>> GC(my_seq)
45.45454545454545
```

transcription and translation

```
>>> my_mRNA = my_seq.transcribe()
Seq('AGUACACUGGU', IUPACUnambiguousRNA())
>>> my_seq.translate()
Seq('STL', IUPACProtein())
```

complement and reverse complement

```
>>> str(my_seq)
'AGTACACTGGT'
>>> my_seq.complement()
Seq('TCATGTGACCA', IUPACUnambiguousDNA())
>>> my_seq.reverse_complement()
Seq('ACCAGTGTACT', IUPACUnambiguousDNA())
```

You can translate directly from the DNA coding sequence or you can use the mRNA directly.

```
>>> from Bio.Seq import Seq
>>> from Bio.Alphabet import IUPAC
>>> messenger_rna = Seq("AUGGCCAUUGUAAUGGGCCGCUGAAAGGGUGCCCGAUAG", IUPAC.unambiguous_rna)
>>> messenger_rna
Seq('AUGGCCAUUGUAAUGGGCCGCUGAAAGGGUGCCCGAUAG', IUPACUnambiguousRNA())
>>> messenger_rna.translate()
Seq('MAIVMGR*KGAR*', HasStopCodon(IUPACProtein(), '*'))
```

Now, you may want to translate the nucleotides up to the first in frame stop codon, and then stop (as happens in nature):

```
>>> coding_dna.translate()
Seq('MAIVMGR*KGAR*', HasStopCodon(IUPACProtein(), '*'))
>>> coding_dna.translate(to_stop=True)
Seq('MAIVMGR', IUPACProtein())
```

Exercise

1. There is so much stuff available in biopython. What happens if you do this?

   ```
   >>> from Bio.Data import CodonTable
   >>> standard_table = CodonTable.unambiguous_dna_by_id[1]
   >>> mito_table = CodonTable.unambiguous_dna_by_id[2]
   >>> print standard_table
   >>> print mito_table
   ```

The Sequence record object

The *SeqRecord* objects are the basic data type for the *SeqIO* objects and they are very similar to *Seq* objects,however, there are a few additional attributes.

- **seq** - The sequence itself, typically a Seq object.
- **id** - The primary ID used to identify the sequence – a string. In most cases this is something like an accession number.
- **name** - A 'common' name/id for the sequence – a string. In some cases this will be the same as the accession number, but it could also be a clone name. Analagous to the LOCUS id in a GenBank record.
- **description** - A human readable description or expressive name for the sequence – a string.

We can think of the *SeqRecord* as a container that has the above attributes including the *Seq*.

Exercise

1. Copy the following script into an editor and save as 'BioSequences.py'
2. Open a terminal window and cd into the appropriate directory.
3. Fill in the missing lines with code

```
from Bio.Seq import Seq
from Bio.SeqRecord import SeqRecord

## create a simple SeqRecord object
simple_seq = Seq("GATCAGGATTAGGCC")
simple_seq_r = SeqRecord(simple_seq)
simple_seq_r.id = "AC12345"
```

```
simple_seq_r.description = "I am not a real sequence"

## print summary
print simple_seq_r.id
print simple_seq_r.description
print str(simple_seq_r.seq)
print simple_seq_r.seq.alphabet

## translate the sequence
translated_seq = simple_seq_r.seq.translate()
print translated_seq

# exercise 1 -- translate the sequence only until the stop codon


# exercise 2 -- get the reverse complement of the sequence


# exercise 3 -- get the reverse of the sequence (just like for lists)


# exercise 4 -- get the GC nucleotide content
```

The Sequence IO object

There is one more object that we have to discuss and this the *SeqIO* object is like a container for multiple *SeqRecord* objects.

```
import os
from Bio import SeqIO

'''
We use a list here to save the gene records from a FASTA file
If you have many records a dictionary will make the program faster.

'''

## save the sequence records to a list
allSeqRecords = []
allSeqIDs     = []
pathToFile = os.path.join("..","data","ls_orchid.fasta")
for seq_record in SeqIO.parse(pathToFile, "fasta"):
    allSeqRecords.append(seq_record)
    allSeqIDs.append(seq_record.id.split("|")[1])
    print seq_record.id
    print str(seq_record.seq)
    print len(seq_record)

## print out fun stuff about the sequences
print "We found ", len(allSeqIDs), "sequences"
print "information on the third sequence:"
ind = 2
seqRec = allSeqRecords[ind]
print "\t", "GI number     ", allSeqIDs[ind]
print "\t", "full id       ", seqRec.id
print "\t", "num nucleo.   ", len(seqRec.seq)
print "\t", "1st 10 nucleo.", seqRec.seq[:10]
```

Just as easy as it is to read a set of files we can save modified versions (i.e. QA). Also, it is almost the exact same code as above to parse sequences from a GenBank (.gb) file.

There is really way to much to cover in the time we have, but if you have Next Generation Sequencing data then refer to sections 4.8, 16.1.7 and 16.1.8 of the biopython tutorial. There is even support for binary formats (i.e. SFF).

4.13.3 Bibliographic notes

3. Cock, P J A and Antao, Tiago and Chang, J T and Chapman, B A and Cox, C J and Dalke, A and Friedberg, I and Hamelryck, T and Kauff, F and Wilczynski B and de Hoon, M J L, Biopython: freely available Python tools for computational molecular biology and bioinformatics, *Bioinformatics*, Jun, 2009, 25, 11, 1422-3. PubMed.

4.14 Biopython II

4.14.1 Biopython - Entrez databases

NCBI's Guidelines

Taken from the tutorial.

Before using Biopython to access the NCBI's online resources (via Bio.Entrez or some of the other modules), please read the NCBI's Entrez User Requirements. If the NCBI finds you are abusing their systems, they can and will ban your access!

To paraphrase: For any series of more than 100 requests, do this at weekends or outside USA peak times. This is up to you to obey. Use the http://eutils.ncbi.nlm.nih.gov address, not the standard NCBI Web address. Biopython uses this web address. Make no more than three requests every seconds (relaxed from at most one request every three seconds in early 2009). This is automatically enforced by Biopython. Use the optional email parameter so the NCBI can contact you if there is a problem. You can either explicitly set this as a parameter with each call to Entrez (e.g. include email="A.N.Other@example.com" in the argument list), or as of Biopython 1.48, you can set a global email address:

```
>>> from Bio import Entrez
>>> Entrez.email = "A.N.Other@example.com"
```

Bio.Entrez will then use this email address with each call to Entrez. The example.com address is a reserved domain name specifically for documentation (RFC 2606). Please DO NOT use a random email – it's better not to give an email at all. The email parameter will be mandatory from June 1, 2010. In case of excessive usage, NCBI will attempt to contact a user at the e-mail address provided prior to blocking access to the E-utilities.

If you are using Biopython within some larger software suite, use the tool parameter to specify this. You can either explicitly set the tool name as a parameter with each call to Entrez (e.g. include tool="MyLocalScript" in the argument list), or as of Biopython 1.54, you can set a global tool name:

```
>>> from Bio import Entrez
>>> Entrez.tool = "MyLocalScript"
```

The tool parameter will default to Biopython. For large queries, the NCBI also recommend using their session history feature (the WebEnv session cookie string, see Section 8.15). This is only slightly more complicated.

What databases do I have access to?

```
>>> from Bio import Entrez
>>> Entrez.email = "adam.richards@stat.duke.edu"
>>> handle = Entrez.einfo()
>>> record = Entrez.read(handle)
>>> record["DbList"]
['pubmed', 'protein', 'nuccore', 'nucleotide', 'nucgss', 'nucest', 'structure', 'genome',
'genomeprj', 'bioproject', 'biosample', 'biosystems', 'blastdbinfo', 'books', 'cdd', 'clone',
'gap', 'gapplus', 'dbvar', 'epigenomics', 'gene', 'gds', 'geo', 'geoprofiles', 'homologene',
'journals', 'mesh', 'ncbisearch', 'nlmcatalog', 'omia', 'omim', 'pmc', 'popset', 'probe',
'proteinclusters', 'pcassay', 'pccompound', 'pcsubstance', 'pubmedhealth', 'seqannot', 'snp',
'sra', 'taxonomy', 'toolkit', 'toolkitall', 'unigene', 'unists', 'gencoll', 'gcassembly',
'assembly']
```

What if I want info about a database?

```
>>> handle = Entrez.einfo(db="pubmed")
>>> record = Entrez.read(handle)
>>> record["DbInfo"]["Description"]
'PubMed bibliographic record'
>>> record["DbInfo"]["Count"]
'21827335'
```

How do I search a db for a given term?

```
>>> handle = Entrez.esearch(db="pubmed", term="biopython")
>>> record = Entrez.read(handle)
>>> record["IdList"]
['22399473', '21666252', '21210977', '20015970', '19811691', '19773334', '19304878',
'18606172', '21585724', '16403221', '16377612', '14871861', '14630660', '12230038']
```

Other databases?

```
>>> handle = Entrez.esearch(db="nucleotide",term="Cypripedioideae[Orgn] AND matK[Gene]")
>>> record = Entrez.read(handle)
>>> record["Count"]
'75'
```

Get all journals that have 'computational' as a term

```
>>> handle = Entrez.esearch(db="journals", term="computational")
>>> record = Entrez.read(handle)
>>> record["Count"]
'54'
>>> record["IdList"]
['39206', '37505', '37511', '37435', '37518', '36366', '39786', '34878', '30367', '38517', '33843', '
```

Ok I have a term now I want the item itself

```
>>> from Bio import Entrez, SeqIO
>>> handle = Entrez.efetch(db="nucleotide", id="186972394",rettype="gb", retmode="text")
>>> record = SeqIO.read(handle, "genbank")
```

```
>>> handle.close()
>>> print record
ID: EU490707.1
Name: EU490707
Description: Selenipedium aequinoctiale maturase K (matK) gene, partial cds; chloroplast.
Number of features: 3
/sequence_version=1
/source=chloroplast Selenipedium aequinoctiale
/taxonomy=['Eukaryota', 'Viridiplantae', 'Streptophyta', 'Embryophyta', 'Tracheophyta', 'Spermatophyt
/keywords=['']
/references=[Reference(title='Phylogenetic utility of ycf1 in orchids: a plastid gene more variable t
/accessions=['EU490707']
/data_file_division=PLN
/date=15-JAN-2009
/organism=Selenipedium aequinoctiale
/gi=186972394
Seq('ATTTTTTACGAACCTGTGGAAATTTTTGGTTATGACAATAAATCTAGTTTAGTA...GAA', IUPACAmbiguousDNA())

>>> handle = Entrez.efetch(db="pubmed", id="21210977")
>>> print handle.read()
```

4.15 Data management and relational databases

4.15.1 The (very) Basics of SQL

Databases are a very large and complex topic. Classes typically cover weeks, so in our short time we will only scratch the surface of the basics of selecting, inserting, and joining selects.

Data in relational databases are organized into tables, containing fixed columns of specified data types. For our example we will use two tables, people and experiment, described below.

```
create table people (
         id integer primary key,
   name varchar,
   position varchar,
   phone varchar,
   office varchar
);

create table experiment (
   id integer primary key,
   name varchar,
   researcher integer,
   description text,
   foreign key(researcher) references people(id)
);
```

Select

the select command retrieves data from the database.

```
sqlite> select * from people;
0|Alice|Research Director|555-123-0001|4b
1|Bob|Research assistant|555-123-0002|17
```

```
2|Charles|Research assistant|555-123-0001|24
3|David|Research assistant|555-123-0001|8

sqlite> select * from experiment;
0|EBV Vaccine trial|0|A vaccine trial
1|Flu antibody study|2|Study of the morphology of flu antibodies
```

The * in the *select* statement says to select all columns. If you only need a few of the columns you can select them by name.

```
sqlite> select name, phone from people;
Alice|555-123-0001
Bob|555-123-0002
Charles|555-123-0001
David|555-123-0001

sqlite> select name, description from experiment;
EBV Vaccine trial|A vaccine trial
Flu antibody study|Study of the morphology of flu antibodies
```

You can also limit the returned results to rows that match specified information using the *where* directive.

```
sqlite> select * from people where name == 'Alice';
0|Alice|Research Director|555-123-0001|4b

sqlite> select position from people where name == 'David';
Research assistant
```

Insert

Adding values to the database is done by using the *insert* statement.

```
sqlite> insert into people values ( Null, 'Edward', 'Toadie', 'None', 'Basement');
sqlite> select * from people where name == 'Edward';
4|Edward|Toadie|None|Basement
```

Update

You can also change existing rows once they've been inserted. *update* takes a table name as it's first argument followed by *set* column = value. With out a where clause this will set all row's values. You there for will almost always use the where clause so that you get specific row/rows values updated.

```
sqlite> select * from people;
0|Alice|Research Director|555-123-0001|4b
1|Bob|Research assistant|555-123-0002|17
2|Charles|Research assistant|555-123-0001|24
3|David|Research assistant|555-123-0001|8
4|Edward|Toadie|None|Basement
sqlite> update people set name='Eddie' where id=4;
sqlite> select * from people;
0|Alice|Research Director|555-123-0001|4b
1|Bob|Research assistant|555-123-0002|17
2|Charles|Research assistant|555-123-0001|24
3|David|Research assistant|555-123-0001|8
4|Eddie|Toadie|None|Basement
```

Delete

Similar to updating you can *delete* rows from the database. The argument again will most likely want a where clause to prevent deleting all rows in a table.

```
sqlite> select * from people;
0|Alice|Research Director|555-123-0001|4b
1|Bob|Research assistant|555-123-0002|17
2|Charles|Research assistant|555-123-0001|24
3|David|Research assistant|555-123-0001|8
4|Eddie|Toadie|None|Basement
sqlite> delete from people where name='Eddie';
sqlite> select * from people;
0|Alice|Research Director|555-123-0001|4b
1|Bob|Research assistant|555-123-0002|17
2|Charles|Research assistant|555-123-0001|24
3|David|Research assistant|555-123-0001|8
```

Joins

The power of relational databases lies in recording relations (the foreign key in the table declaration). To join two tables you use the *join* keyword in the select statement and provide a relation to join the two tables. Note, that since both the people and experiment tables have a column called name we must cast the tables using the as statement.

```
sqlite> select p.name, e.name from people as p join experiment as e where e.researcher == p.id;
Alice|EPV Vaccine trial
Charles|Flu antibody study
```

4.15.2 Python and DBI

Working with relational databases is fairly simple with python,

1. Create a connection object
2. Execute a SQL statement
3. Iterate over results

```
In [1]: import sqlite3

In [2]: con = sqlite3.connect('pcfb.sqlite')

In [3]: r = con.execute('select * from people')

In [4]: for i in r:
   ...:     print i

(0, u'Alice', u'Research Director', u'555-123-0001', u'4b')
(1, u'Bob', u'Research assistant', u'555-123-0002', u'17')
(2, u'Charles', u'Research assistant', u'555-123-0001', u'24')
(3, u'David', u'Research assistant', u'555-123-0001', u'8')
(4, u'Edward', u'Toadie', u'None', u'Basement')

In [5]: r = con.execute('select p.name, e.name from people as p join experiment as e where e.research

In [6]: for i in r:
   ...:     print 'Name: %s\n\tExperiment: %s' % (i[0],i[1])
```

```
   ...:
Name: Alice
   Experiment: EPV Vaccine trial
Name: Charles
   Experiment: Flu antibody study
```

4.15.3 Exercise:

Write a script to a add a new user and experiment to the database, remove Alice, and reassign her experiments to the new user. Then have it print out all the experiment names with who owns each experiment.

4.16 Data analysis with Python

We have seen how to perform *data munging* with regular expressions and Python. For a refresher, here is a Python program using regular expressions to munge the `Ch3observations.txt` file that we did on day 1 using TextWrangler.

```
import re

find = r'(\d+)\s+(\w{3})[\w\,\.]*\s+(\d+)\sat\s(\d+):(\d+)\s+([-\d\.]+)\s+([-\d\.]+).*'
replace = r'\3\t\2.\t\1\t\4\t\5\t\6\t\7'

for line in open('examples/Ch3observations.txt'):
    newline = re.sub(find, replace, line)
    print newline,
```

which when run produces this output

```
eris:pcfb cliburn$ python examples/regex.py
1752    Jan.    13      13      53      -1.414  5.781
1961    Mar.    17      03      46      14      3.6
2002    Oct.    1       18      22      36.51   -3.4221
1863    Jul.    20      12      02      1.74    133
```

This session will introduce you to the next stage of *data analysis* and *data visualization*. Because it is impossible to do any justice to these areas in a few hours, the aim of this session is to provide a taste of what analysis and visualization in Python look like, and a tour of some of the many modules available for scientific computation in Python.

4.16.1 Curve Fitting

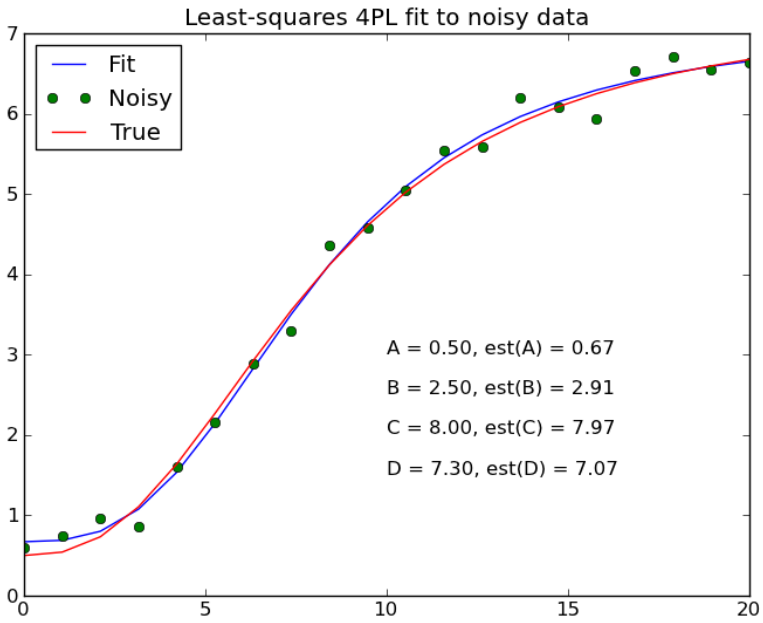
One common analysis task performed by biologists is *curve fitting*. For example, we may want to fit a 4 parameter logistic (4PL) equation to ELISA data. The usual formula for the 4PL model is

$$f(x) = \frac{A - D}{1 + (x/C)^B} + D$$

where x is the concentration, A is the minimum asymptote, B is the steepness, C is the inflection point and D is the maximum asymptote.

```
import numpy as np
import numpy.random as npr
import matplotlib.pyplot as plt
from scipy.optimize import leastsq
```

```
def logistic4(x, A, B, C, D):
    """4PL lgoistic equation."""
    return ((A-D)/(1.0+((x/C)**B))) + D

def residuals(p, y, x):
    """Deviations of data from fitted 4PL curve"""
    A,B,C,D = p
    err = y-logistic4(x, A, B, C, D)
    return err

def peval(x, p):
    """Evaluated value at x with current parameters."""
    A,B,C,D = p
    return logistic4(x, A, B, C, D)

# Make up some data for fitting and add noise
# In practice, y_meas would be read in from a file
x = np.linspace(0,20,20)
A,B,C,D = 0.5,2.5,8,7.3
y_true = logistic4(x, A, B, C, D)
y_meas = y_true + 0.2*npr.randn(len(x))

# Initial guess for parameters
p0 = [0, 1, 1, 1]

# Fit equation using least squares optimization
plsq = leastsq(residuals, p0, args=(y_meas, x))

# Plot results
plt.plot(x,peval(x,plsq[0]),x,y_meas,'o',x,y_true)
plt.title('Least-squares 4PL fit to noisy data')
plt.legend(['Fit', 'Noisy', 'True'], loc='upper left')
for i, (param, actual, est) in enumerate(zip('ABCD', [A,B,C,D], plsq[0])):
    plt.text(10, 3-i*0.5, '%s = %.2f, est(%s) = %.2f' % (param, actual, param, est))
plt.savefig('logistic.png')
```



It will be straightforward to modify this code to use, for example, a five parameter logistic or other equation, offering a flexibility rarely available with standard analysis software.

4.16.2 Simulation-based statistics

With increasing computational power, it is now feasible to run many, many simulations to estimate parameters instead of, or in addition to, the traditiional parameteric statistial methods. Most of these methods are based on some form of *resampling* of the data available to estimate the null distribution, with well known examples being the *bootstrap* and *permuation resampling*.

Before we do this, we need to understand a little about how to get random numbers. The `numpy.random` module has random number generators for a variety of common probabiltiy distributions. These numbers are then used to simulate the generation of new random samples. If the samples are chosen in a certain way, the statistics of the randomly drawn samples can provide useful information about the properties of our original data sample. Here are some examples of random number generation in `iptyhon`.

```
In [1]: import numpy.random as npr

In [2]: npr.random(5)
Out[2]: array([ 0.93946009,  0.47060219,  0.10922504,  0.70776782,  0.41784061])

In [3]: npr.random((3,4))
Out[3]:
array([[ 0.29302404,  0.9372624 ,  0.36149538,  0.59367473],
       [ 0.42932372,  0.20717542,  0.18447385,  0.91159639],
       [ 0.83125219,  0.85109042,  0.32720074,  0.33453366]])

In [4]: npr.normal(5, 1, 4)
Out[4]: array([ 3.45966714,  3.99815107,  5.0191997 ,  5.93739408])

In [5]: npr.randint(1, 7, 10)
Out[5]: array([6, 4, 1, 5, 6, 6, 1, 3, 4, 2])
```

```
In [6]: npr.uniform(1, 7, 10)
Out[6]:
array([ 3.55239006,  5.45862348,  1.77176392,  5.91184323,  2.49197674,
        6.23527185,  2.51701757,  3.96170981,  6.43878462,  4.57074553])

In [7]: npr.binomial(n=10, p=0.2, size=(4,4))
Out[7]:
array([[5, 0, 4, 2],
       [1, 1, 0, 2],
       [3, 2, 0, 2],
       [0, 1, 2, 4]])

In [8]: x =  [1,2,3,4,5,6]

In [9]: npr.shuffle(x)

In [10]: x
Out[10]: [2, 1, 5, 6, 4, 3]

In [11]: npr.permutation(10)
Out[11]: array([2, 7, 4, 1, 6, 5, 8, 9, 3, 0])
```

For example, choosing a new sample with replacement from an existing sample (i.e. we draw one item from the data, record what it is, then replace it in the data and repeat to get a new sample) can be done efficiently in this way:

```
In [1]: import numpy as np

In [2]: import numpy.random as npr

In [3]: data = np.array(['tom', 'jerry', 'mickey', 'minnie', 'pocahontas'])

In [4]: idx = npr.randint(0, len(data), (4,len(data)))

In [5]: idx
 Out[5]:
array([[3, 0, 2, 1, 0],
       [4, 2, 3, 4, 4],
       [4, 0, 0, 0, 3],
       [2, 2, 3, 1, 4]])

In [6]: samples_with_replacement = data[idx]

In [7]: samples_with_replacement
 Out[7]:
array([['minnie', 'tom', 'mickey', 'jerry', 'tom'],
       ['pocahontas', 'mickey', 'minnie', 'pocahontas', 'pocahontas'],
       ['pocahontas', 'tom', 'tom', 'tom', 'minnie'],
       ['mickey', 'mickey', 'minnie', 'jerry', 'pocahontas']],
      dtype='|S10')
```

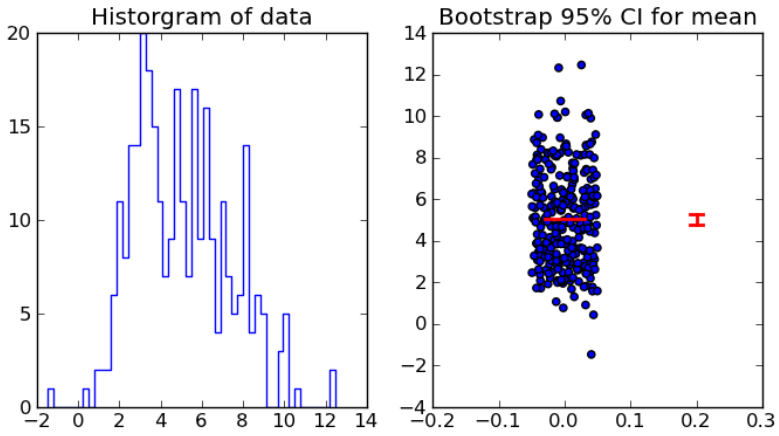
In the next version of numpy (1.7.0), a new function `choice` is available in `numpy.random` to do the same thing with a nicer syntax. Version 1.7.0 is only currently available from the git repository as source code that you must compile yourself, but should be available for easy_install/pip installation soon.

```
In [1]: import numpy.random as npr

In [2]: data = ['tom', 'jerry', 'mickey', 'minnie', 'pocahontas']
```

```
# only availlable if you install numpy 1.7.0 from the git repository
In [3]: npr.choice(data, size=(4, len(data)), replace=True)
---------------------------------------------------------------------------
AttributeError                            Traceback (most recent call last)
/Volumes/HD3/hg/pcfb/<ipython-input-3-84e7d179a607> in <module>()
----> 1 npr.choice(data, size=(4, len(data)), replace=True)

AttributeError: 'module' object has no attribute 'choice'
```

Moving on our first simulation example - if we want to plot the 95% confidence interval for the mean of our data samples, we can use the bootstrap to do so. The basic idea is simple - draw many, many samples with replacement from the data available, estimate the mean from each sample, then rank order the means to estimate the 2.5 and 97.5 percentile values for 95% confidence interval. Unlike using normal assumptions to calculate 95% CI, the results generated by the bootstrap are robust even if the underlying data are very far from normal.

```
import numpy as np
import numpy.random as npr
import pylab

def bootstrap(data, num_samples, statistic, alpha):
    """Returns bootstrap estimate of 100.0*(1-alpha) CI for statistic."""
    n = len(data)
    idx = npr.randint(0, n, (num_samples, n))
    samples = x[idx]
    stat = np.sort(statistic(samples, 1))
    return (stat[int((alpha/2.0)*num_samples)],
            stat[int((1-alpha/2.0)*num_samples)])

if __name__ == '__main__':
    # data of interest is bimodal and obviously not normal
    x = np.concatenate([npr.normal(3, 1, 100), npr.normal(6, 2, 200)])

    # find mean 95% CI and 100,000 bootstrap samples
    low, high = bootstrap(x, 100000, np.mean, 0.05)

    # make plots
    pylab.figure(figsize=(8,4))
    pylab.subplot(121)
    pylab.hist(x, 50, histtype='step')
    pylab.title('Historgram of data')
    pylab.subplot(122)
    pylab.plot([-0.03,0.03], [np.mean(x), np.mean(x)], 'r', linewidth=2)
    pylab.scatter(0.1*(npr.random(len(x))-0.5), x)
    pylab.plot([0.19,0.21], [low, low], 'r', linewidth=2)
    pylab.plot([0.19,0.21], [high, high], 'r', linewidth=2)
    pylab.plot([0.2,0.2], [low, high], 'r', linewidth=2)
    pylab.xlim([-0.2, 0.3])
    pylab.title('Bootstrap 95% CI for mean')
    pylab.savefig('examples/boostrap.png')
```



Note that the bootstrap function is a *higher order* function, and will return the boostrap CI for any valid statistical function, not just the mean. For example, to find the 95% CI for the standard deviation, we only need to change `np.mean` to `np.std` in the arguments:

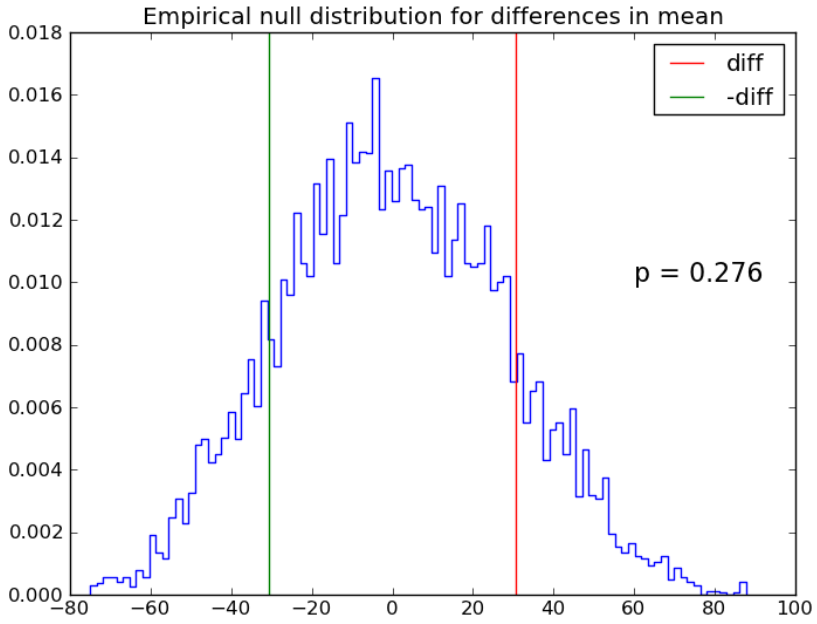
```
# find standard deviation 95% CI bootstrap samples
low, high =  bootstrap(x, 100000, np.std, 0.05)
```

The function is also highly optimized, and takes under 2 seconds to calculate the boostrap mean for a data sample of size 300 using 100,000 bootstrap samples on a 4 year old MacBook Pro with 2.4 GHz Intel Core 2 Duo processor.

Permutation-resampling is another form of simulation-based statistical calculation, and is often used to evaluate the p-value for the difference between two groups, under the null hypothesis that the groups are invariant under label permutation. For example, in a case-control study, it can be used to find the p-value that hypothesis that the mean of the case group is different from that of the control group, and we cannot use the t-test because the distributions are highly skewed.

```
import numpy as np
import numpy.random as npr
import pylab

def permutation_resampling(case, control, num_samples, statistic):
    """Returns p-value that statistic for case is different
    from statistc for control."""

    observed_diff = abs(statistic(case) - statistic(control))
    num_case = len(case)

    combined = np.concatenate([case, control])
    diffs = []
    for i in range(num_samples):
        xs = npr.permutation(combined)
        diff = np.mean(xs[:num_case]) - np.mean(xs[num_case:])
        diffs.append(diff)

    pval = (np.sum(diffs > observed_diff) +
            np.sum(diffs < -observed_diff))/float(num_samples)
    return pval, observed_diff, diffs

if __name__ == '__main__':
    # make up some data
    case = [94, 38, 23, 197, 99, 16, 141]
    control = [52, 10, 40, 104, 51, 27, 146, 30, 46]
```

```
# find p-value by permutation resampling
pval, observed_diff, diffs = \
      permutation_resampling(case, control, 10000, np.mean)

# make plots
pylab.title('Empirical null distribution for differences in mean')
pylab.hist(diffs, bins=100, histtype='step', normed=True)
pylab.axvline(observed_diff, c='red', label='diff')
pylab.axvline(-observed_diff, c='green', label='-diff')
pylab.text(60, 0.01, 'p = %.3f' % pval, fontsize=16)
pylab.legend()
pylab.savefig('examples/permutation.png')
```



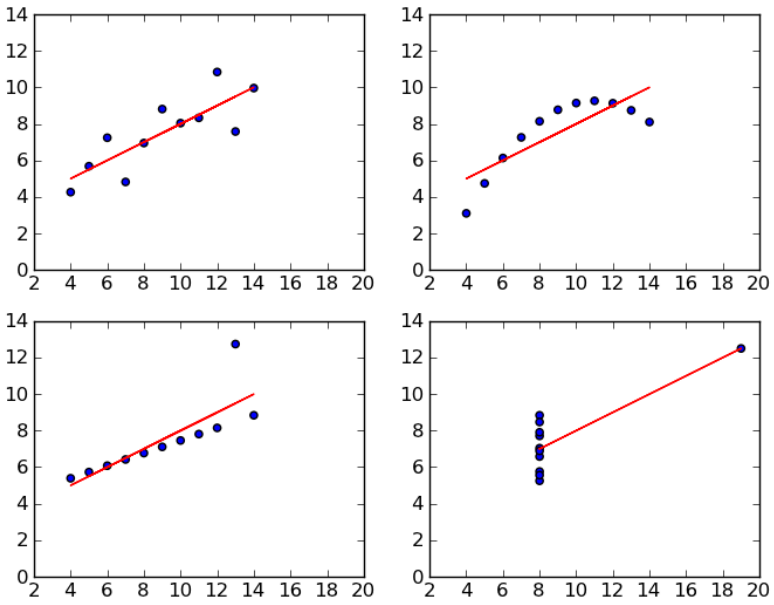
4.16.3 Data visualization

Data visualization is important for *exploratory data analysis* as well as for communication of scientific results. Using `ipython` with the `-- pylab` option provides an interarctive environment that is ideal for exploratory data analysis. The classic Anscombe data set illustrates the importance of visualization when analysing data. The Anscombe data set consists of 4 different sets of (x,y) values, with esentially *identical* values for the

1. mean of x
2. variance of x
3. mean of y
4. variance of y
5. correlation between x and y
6. linear regression intercept and slope

Plotting the actual data sets quickly shows that the data sets are not as similar as suggested by the summary stattstics!

```
import numpy as np
import pylab

xs = np.loadtxt('anscombe.txt')
for i in range(4):
    x = xs[:,i*2]
    y = xs[:,i*2+1]
    A = np.vstack([x, np.ones(len(x))]).T
    m, c = np.linalg.lstsq(A, y)[0]

    pylab.subplot(2,2,i+1)
    pylab.scatter(x, y)
    pylab.plot(x, m*x+c, 'r')
    pylab.axis([2,20,0,14])

pylab.savefig('anscombe.png')
```



For communication of results, matplotlib offers a huge range of graphics. We have only scratched the surface of what the package has to offer. The fastest way to get a custom graphic to communicate your results is to look at the thumbnails at http://matplotlib.sourceforge.net/gallery.html. If one of the graphics looks appropirate for your needs, just click on the thumbnail to get the source code. You should now know enough Python to customize the graphic to your specific needs.

4.17 Vector graphics with Inkscape

4.17.1 Graphical concepts

A quote from the text (PCFB).

No longer can you submit a photo that looks right; it has to be a "CMYK image, with 300 DPI at printed dimension, saved as a TIFF with LZW compression". The goal here is to introduce a software that can help with some of these

requirements. Please refer to Chapter 17 for further depth than we go into here on graphics.

Vector and **pixel** images are probably concepts most biologists are familiar with. Pixel images (bitmap, raster) are a uniform grid of colored dots. In vector art a line can be defined by two endpoints. The vector representation has the advantage of being often easier to store. Also, the amount of information for vector art stays the same no matter how large the plot and as you zoom in vector art stays the same.

File formats that store vector based images include: PDF, EPS, SVG and AI. File formats that store pixel-based images are JPEG, PNG, TIFF, BMP and PSD. PDF, EPS and AI can store embedded pixel information (hybrid images).

It is always possible to go from vector to pixel art, but it is not so easy to go the other way. Another advantage of vector art is that pixel text is not easily retrieved by a machine.

Pixel art is everywhere (photos, machine output), however if we have to create a completely plot then there are a number of reasons to do so using vector graphics. Vector art is covered in chapter 18 of the book.

4.17.2 Inkscape

Inkscape uses the SVG (Scalable Vector Graphics) format for its files. SVG is an open standard widely supported by graphic software.

Inkscape basics

QuickRef

NumPy command	Note
Ctrl+arrow	pan or scroll the canvas
Ctrl+B	hides scrollbars
"-" "+" "="	zoom zoom zoom
Ctrl+N	create a new inkscape documents
Ctrl+O	opens an exisiting svg file
Ctrl+S	saves the current file
holding Alt	restricts movement in the move mode
holding Ctrl	preserves the original height/width ratio during resize
space or F1	activates the selector
"[" and "]"	rotate an object
arrows	move objects
Alt+< and Alt+>	resize and object. "<" and ">" work too
tom	bombadil
hold Shift + click	selects multiple objects

Getting familiar

1. open a new inkscape document
2. select the square shape and create a square or rectangle by pressing the mouse button once on your canvas dragging the mouse a little then letting go of the mouse. (try the control squares and circle)
3. Hit the spacebar to go into *move/resize* mode (try holding Ctrl)
4. Click on the rectangle again to change into *rotate/skew* mode. (try holding Ctrl) (try '[','],'<','>')

Inkscape tutorials

Since there are people that make their living by working with inkscape I figured there were better tutorials already available on the web than what I could come up with.

Contents

One of the most common issues in inkscape is making arrows. Although, it is a little work once you have made one then you can save it and use it for all future derivative arrows.

- Arrow tutorial

One nice aspect of inkscape is how easy it is to trace a bitmap.

- Bitmap tracing tutorial
- Try having a look at the Donate button tutorial you can download the svg and open it in inkscape.

Additional tutorials

Now that you are a pro

- The coffee cup tutorial
- The shiny clock face

Uses

- Inkscape can import other formats (e.g. PNG or EPS) then convert.
- One could create a image in matplotlib (SVG,PDF etc) and import then annotate

- Resizing of images
- Adding text or shapes or colors to a bitmap

Additional Resources

- The inkscape documentation
- Nice set of tutorials
- Very nice gallery of wallpapers
- Python effects tutorial

4.18 Capstone Example

4.18.1 Analysing cytokine array data

In this final example, we will write a program to extract potentially useful summaries of data from a cytokine assay kindly donated by Herman Staats. You can download the file from the *Data Samples* page. As you can see, real world data analysis is far more messy than we have let on so far. Suppose we want to do two things - display the distribution of each cytokine on diffeerent days to see changes over time, and generate some QC summaries on what errors are associated with what samples. Doing this manually in Excel will certainly be painful - what if Herman had stashed away hundreds of such files and wanted to perform the analysis on every single one of them? A manual analysis might take weeks and will likely be ridden with errors as we grow increasingly bored and frustrated with the task.

So we will write a program to do this instead. The program will be quite challenging to write - we have broken the task down into subtasks, and your job is to write functions to execute each subtask. Please ask for help if you get stuck at any point - we recognize that this will be an extemely challenging problem for most of you. OK - let's begin ...

First, we need to convert the spreadsheet into a plain text format by exporting it within Excel. The *Data Samples* page provides a tab delimited version exported from Excel; exporting to csv format is also fine if you prefer. (Note that Python modules to read and write Excel files are available - see http://www.python-excel.org/ and http://packages.python.org/openpyxl/ but as these were not covered in the workshop, we will continue to work with exported plain text files).

Notice that the data is arranged as a nice rectangular grid, with row 1 giving the header information, column 1 the sample names, and the rest the actual data values or various error messages. This suggests that we can use numpy arrays to manipulate the data, which will lead to a shorter program than the use of the csv module to parse every item. Notice also that there is a mixture of strings and numbers in the spreadsheet, and numpy only works with arrays of all the same type. Since strings can represent numbers but not vice versa, we will first load the data as an array of strings using the numpy loadtxt function. Our strategy is then to manipulate the data so that apart from the header (row 1) and sample (column 1) information, everything else is converted to an array of floats for statistical analysis and visualization.

Our first task is to read the file and convert to an array of strings, which can be done with the `loadtxt` function. We first see what `loadtxt` does:

```
In [4]: import numpy as np

In [5]: help(np.loadtxt);
```

4.18.2 Exercise

Write a function called `read_table` to load a tab delimited file as a numpy array using the numpy `loadtxt` function. The function should take a filename and an optional delimiter (e.g. 't' for TDL and ',' for CSV) as arguments, and return a numpy array of strings:

```
def read_table(filename, delimiter='\t'):
    # your code goes here and should return a numpy array of strings
```

Now that we have the table as a numpy array, let's focus on converting the middle "data" portion into an array of floats. We need to somehow convert all those error or warning messages into numbers. One simple way to do thiis is to encode each unique message as a number that cannot be mistaken for a data value. Since concentrations are never negative, we will use the negative integers to encode the errors. But in order to do the encoding, we first need to find out what types of messages exist in the data set.

4.18.3 Exercise

Write a function that finds all the warnings in the table returned by the previous `read_table` function and returns a dictionary of {warning : code} where warning is a string (e.g. 'Bead Issues' or 'UN') and code is a negative number. Each unique warning should be given a different negative number. Basically we want to find all strings in the "data" part of the table, i.e. table[1:, 1:], and everytime we find a string, we shove it into the dictionary if it is not already there with a new negative number code:

```
def parse_warnings(table):
    # your code goes here and should return a dictionary of warnings
```

Next, let's deal with the sample information in column 1, excluding row 1, column 1. We notice that the same sample name can occur on multiple rows - let's create a dictionary whose key is the sample name, and whose value is the row number minus one (minus one because we want row number = 0 to index the first data row, not the header information).

4.18.4 Exercise

Complete the function:

```
def parse_samples(table):
    # your code goes here and should return a dictionary of lists of row numbers for each sample
```

Parsing the header information is slightly more challenging. We notice that two different pieces of information are provided by each cell in the header - the cytokine name (e.g. IL-2 beta) and the day the sample was taken (e.g. day 3). Each cytokine is sampled on multple days (0, 3 and 28). We want to create a dictionary that will tell us what column we can find the values for a given cytokine, day combination. One way to deal with the fact that the same cytokine is sampled on multiple days is to use a *dictionary of dictionaries*. In particular, we will construct a dictionary whose key is a cytokine name, and whose value is another dictionary. This other dictionary has a key representing the day, and a value representing the column number minus one for the (cytokine, day) combination.

4.18.5 Exercise

Complete the function:

```
def parse_headers(table):
    # your code goes here and should return a dictionary of dictionaries as described in the text
```

We finally get to convert the data from an array of strings to an array of floats. Replace all the warning messages with the code numbers, and return a new array of floats comprising the following subarray - table[1:, 1:].

4.18.6 Exercise

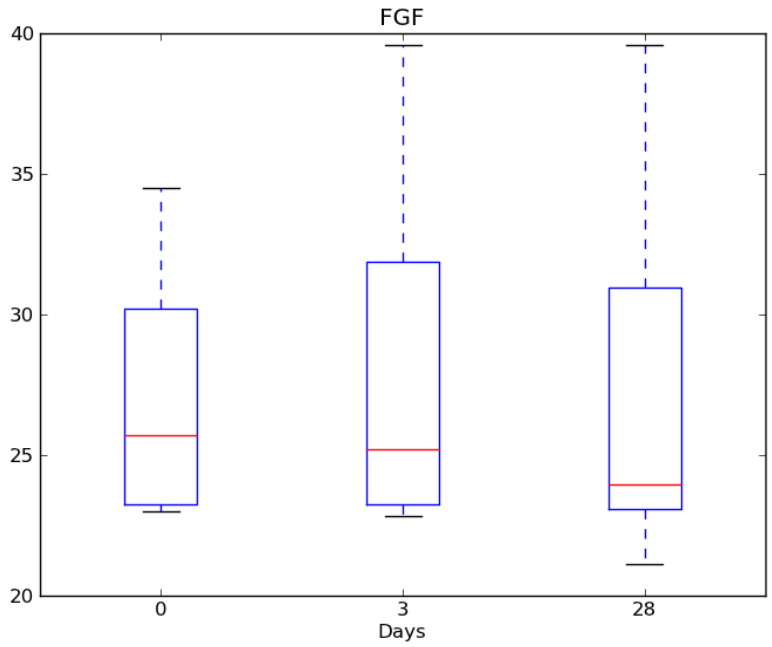
Complete the function:

```
def parse_data(table, warning_dict):
  # your code goes here and should return an array of floats containing values for the entries in tab
```

Let's consolidate all the above functions into a single function that when given a filename, reads the file and breaks it down into a sample dictionary, a cytokine dicitonary and a data array. My function is shown below - you only have to change the names to match the structures that you created:

```
def parse_cytokine_table(filename):
    # extract data and sample and cytokine mapping dictinaries from table
    table = read_table(filename)

    warning_dict = parse_warnings(table)
    sample_mapper = parse_samples(table)
    cytokine_mapper = parse_headers(table)
    data = parse_data(table, warning_dict)
    return warning_dict, sample_mapper, cytokine_mapper, data
```

Well done! The most difficult part of the program is now complete. We next see how we can use the structures we have created to make summaries of the data. First, let's use a box-and-whiskers plot to show the distribution of each cytokine over days 0, 3 and 28. Generate one such figure for each such cytokine - it should look something like this.



4.18.7 Exercise

Write the function to generate the box-and -whiskers plots. Remember that the negative numbers are not really cytokine concentrations and should not be used for plotting:

```
def plot_cytokine(cytokine, cytokine_mapper, data, save=False, directory='.'):
  # generate plots like the one shown
```

```
  # if save is False, don't save but simply show each figure
  # if save if True, save to disk with savefig(directory/filename)
```

Finally, let's write the QC data to file. There seem to be an enormous number of errors in this file - let's summarize them so that Herman can figure out what is going on! Generate one text file per unique warning, where each row has two columns - the sample name, and the number of that type of warning associated with the sample. For instance, the `Bead_Issues.txt` file will contain the following values:

```
0921-X-2-2    2
1059-X-2-2    12
0273-X-2-2    2
0740-X-2-2    4
0263-X-2-2    18
0175-X-2-2    2
0012-X-2-2    4
0108-X-2-2    1
0066-X-2-2    2
0057-X-2-2    12
0313-X-2-2    7
0103-X-2-2    25
0685-X-2-2    2
0799-X-2-2    4
0749-X-2-2    16
0693-X-2-2    1
1023-X-2-2    6
0300-X-2-2    2
```

Complete the function:

```
def write_qc(qc, directory='.'):
    # write QC reports as described
    # save to the directory given and use the mesage name + '.txt' as the filename
```

That wraps up the coding part of this final capstone example.

4.18.8 Final Exercise

Now that you know how to think like a programmer, don't create such spreadsheets in the future if possible! Design spreadsheets so that the information is "machine-friendly". What are some of the ways you can make the original spreadsheet more "machine-friendly" if you could change the design?

The full program that for parsing the cytokne assay file:

```
"""Intermediate example of data munging using numpy.
Task: Summarize the change in concentration over time for each cytokine.
Input: An Excel worksheet exported as a tab delimited file
Output: Figures summarizing concentrations of individual cytokines over time.
"""

import numpy
import pylab
import os

def parse_cytokine_table(filename):
    # extract data and sample and cytokine mapping dictinaries from table
    table = read_table(filename)

    warning_dict = parse_warnings(table)
```

```
    sample_mapper = parse_samples(table)
    cytokine_mapper = parse_headers(table)
    data = parse_data(table, warning_dict)
    return warning_dict, sample_mapper, cytokine_mapper, data

def read_table(filename, delimiter='\t'):
    # read data into an array of strings
    # this can also be done by standard data munging techniques
    # but would be more painful
    return numpy.loadtxt(filename, dtype='string', delimiter=delimiter)

def parse_warnings(table):
    # create a dictionary to convert missing data codes into numeric codes
    data = table[1:, 1:]
    warning_dict = {}
    idx = -1
    for x in data.ravel():
        try:
            float(x)
        except:
            if x not in warning_dict:
                warning_dict[x] = idx
                idx -= 1
    return warning_dict

def parse_samples(table):
    # create a dictionary that returns the rows where each sample has data
    samples = table[1:,0]
    sample_mapper = {}
    for i, sample in enumerate(samples):
       sample_mapper.setdefault(sample, []).append(i)
    return sample_mapper

def parse_headers(table):
    # get header information in first row
    headers = table[0,:]
    # parse header informtion to find columns for each cytokine/day combination
    cytokine_mapper = {}
    for i, label in enumerate(headers[1:]):
        cytokine, day = label.split('day')
        cytokine_mapper.setdefault(cytokine.strip(), {})[int(day)] = i
    return cytokine_mapper

def parse_data(table, warning_dict):
    # convert missing data from strings to code numbers for analysis
    data = table[1:, 1:]
    for warning in warning_dict:
        data[data==warning] = warning_dict[warning]
    data = data.astype('float')
    return data

def plot_cytokine(cytokine, cytokine_mapper, data, save=False, directory='.'):
    # generate box and whiskers plot for distribution of a single cytokine
    idx_dict = cytokine_mapper[cytokine]
    xs = data[:, sorted(idx_dict.values())]

    # collect measured values for each day in a list ignoring missing values
    ys = []
```

```
    for i in range(xs.shape[1]):
        col = xs[:,i]
        ys.append(col[col >= 0])

    # if there are any measured values, visualize the data disbution
    if numpy.sum(len(y) for y in ys) > 0:
        pylab.figure()
        pylab.boxplot(ys)
        pylab.xticks(range(1, len(idx_dict.keys())+1), idx_dict.keys())
        pylab.xlabel('Days')
        pylab.title(cytokine)

    if save:
        if not os.path.exists(directory):
            os.makedirs(directory)
        pylab.savefig(os.path.join(directory, cytokine + '.png'))

def sample_qc(warning_dict, sample_mapper, data):
    # generate a dictionary whose keys are warning labels
    # and whose values are lists of (sample, number of warnings) pairs
    qc = {}
    for warning in warning_dict:
        for sample in sample_mapper:
            idx = sample_mapper[sample]
            xs = data[idx, :]
            num_warnings =  numpy.sum(xs==warning_dict[warning])
            qc.setdefault(warning, []).append((sample, num_warnings))
    return qc

def write_qc(qc, directory='.'):
    if not os.path.exists(directory):
        os.makedirs(directory)

    for k in sorted(qc):
        filename = k.replace(' ', '_').replace('/', '-') + '.txt'
        fo = open(os.path.join(directory, filename), 'w')
        sample_list = qc[k]
        for sample in sample_list:
            if sample[1] != 0:
                fo.write('%s\t%d' % sample + '\n')
        fo.close()

if __name__ == '__main__':
    # parse the file
    warning_dict, sample_mapper, cytokine_mapper, data = parse_cytokine_table(
        'Cytokine_assay_31Dec08PAD.txt')

    # visualize cytokine distributions
    for cytokine in cytokine_mapper:
        plot_cytokine(cytokine, cytokine_mapper, data,
                      save=True, directory='figures')

    # Save errors by sample for QC to output files
    qc = sample_qc(warning_dict, sample_mapper, data)
    write_qc(qc, directory='qc_reports')
```

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