

Welcome to BCB/EEOB 5460!

Computational Skills for Biological Data

Instructors:

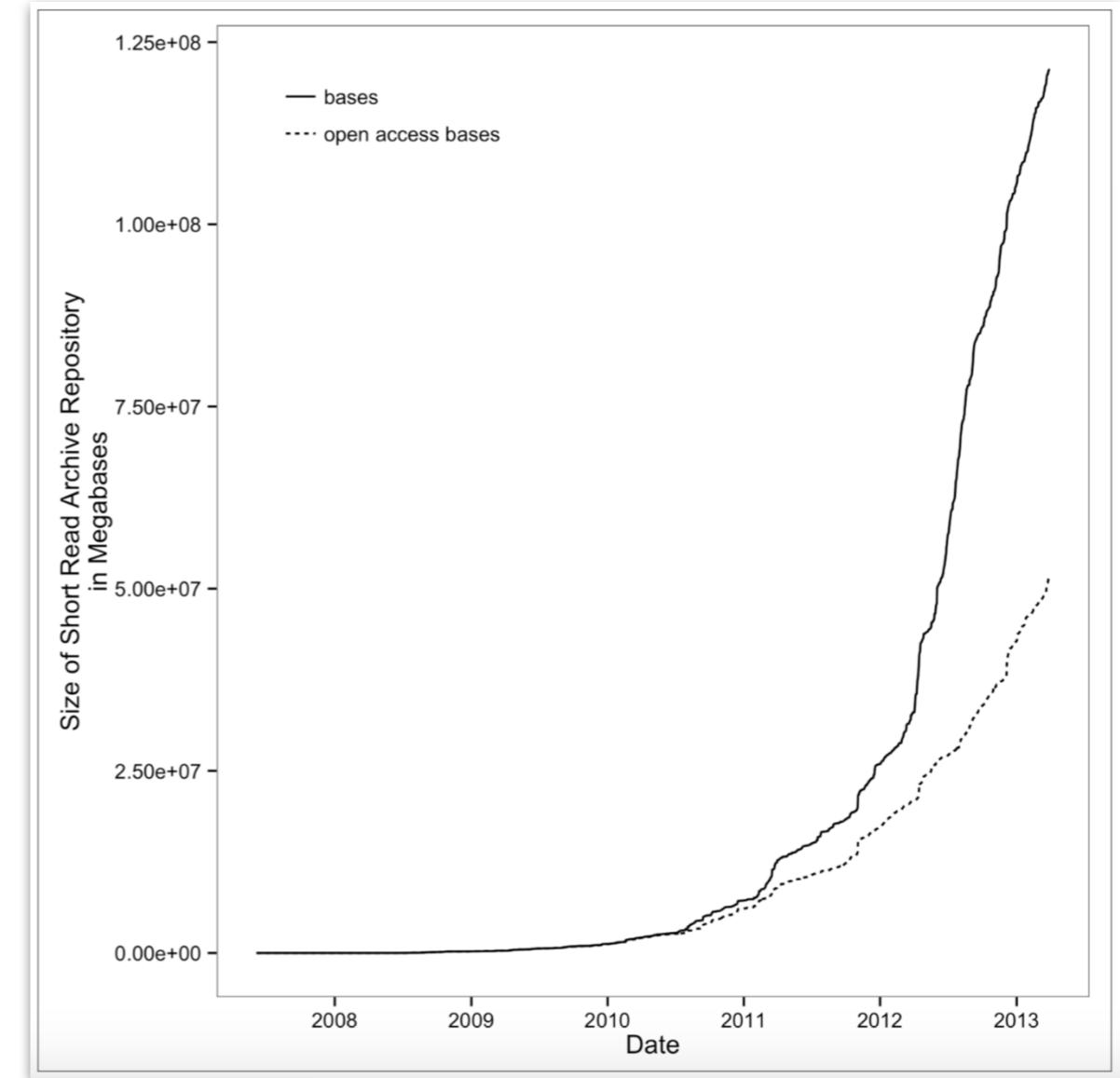
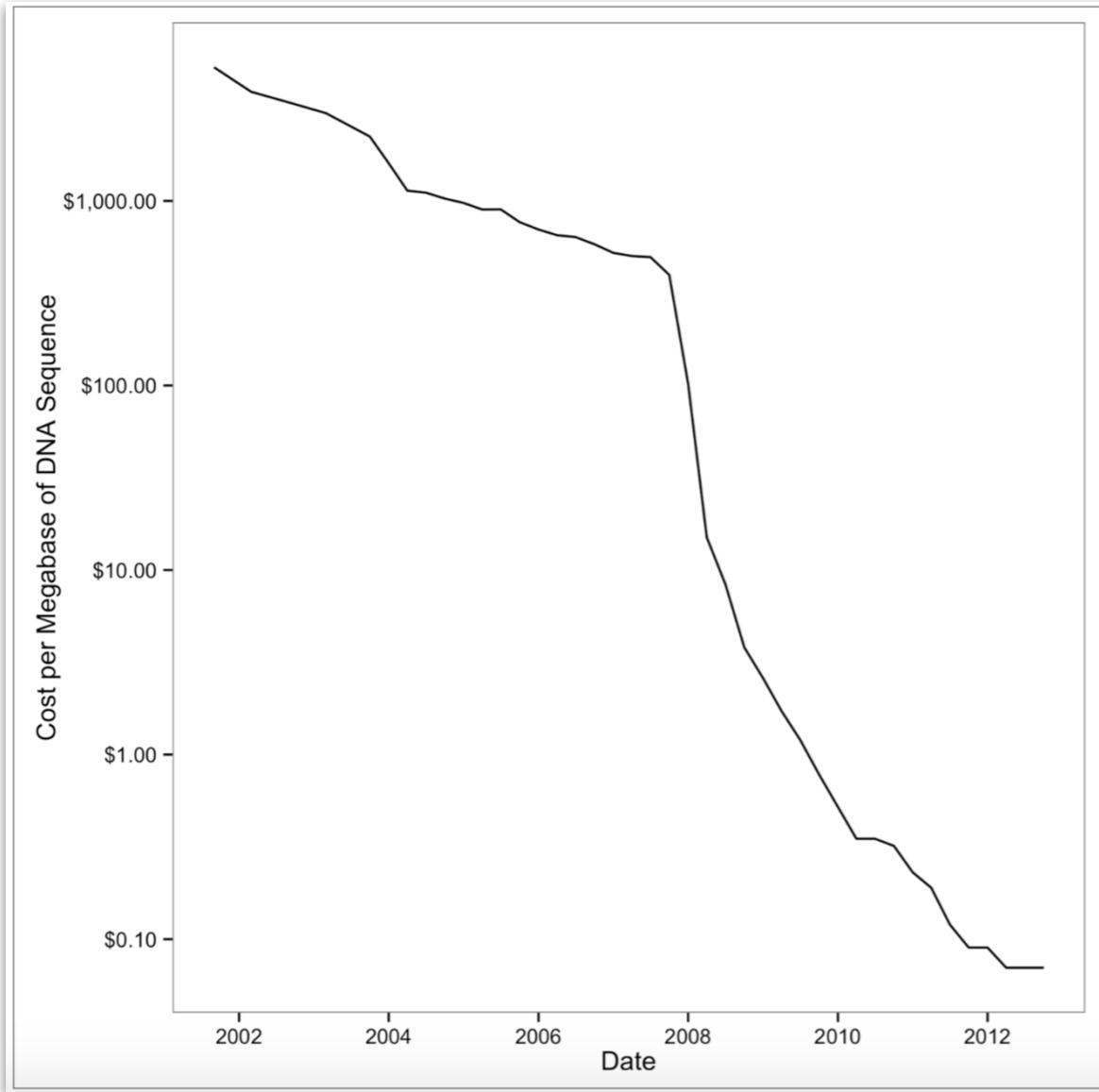
Matt Hufford

Corrinne Grover

Dennis Lavrov

Introduction and Basic Unix

What motivated us to teach this class?



Introduction and Basic Unix

What motivated you to take this class?

- ♦ Many of you likely have interest in more specific applications (e.g., transcriptomics, formal sequence analysis, GWAS, etc...)
- ♦ This course will focus on basic skills that will be necessary for working with large data sets and will be useful in these applications...it's a first step
- ♦ You all are drinking from the data firehose!

Introduction and Basic Unix

Our Objectives

By the end of this course, you should:

- Navigate through your computer, create and modify files and directories, and process data using basic Unix commands
- Become familiar with basic R syntax and data structures and implement these in data analysis and plotting.
- Utilize the Python scripting language for more sophisticated data processing.

Introduction and Basic Unix

Our Objectives

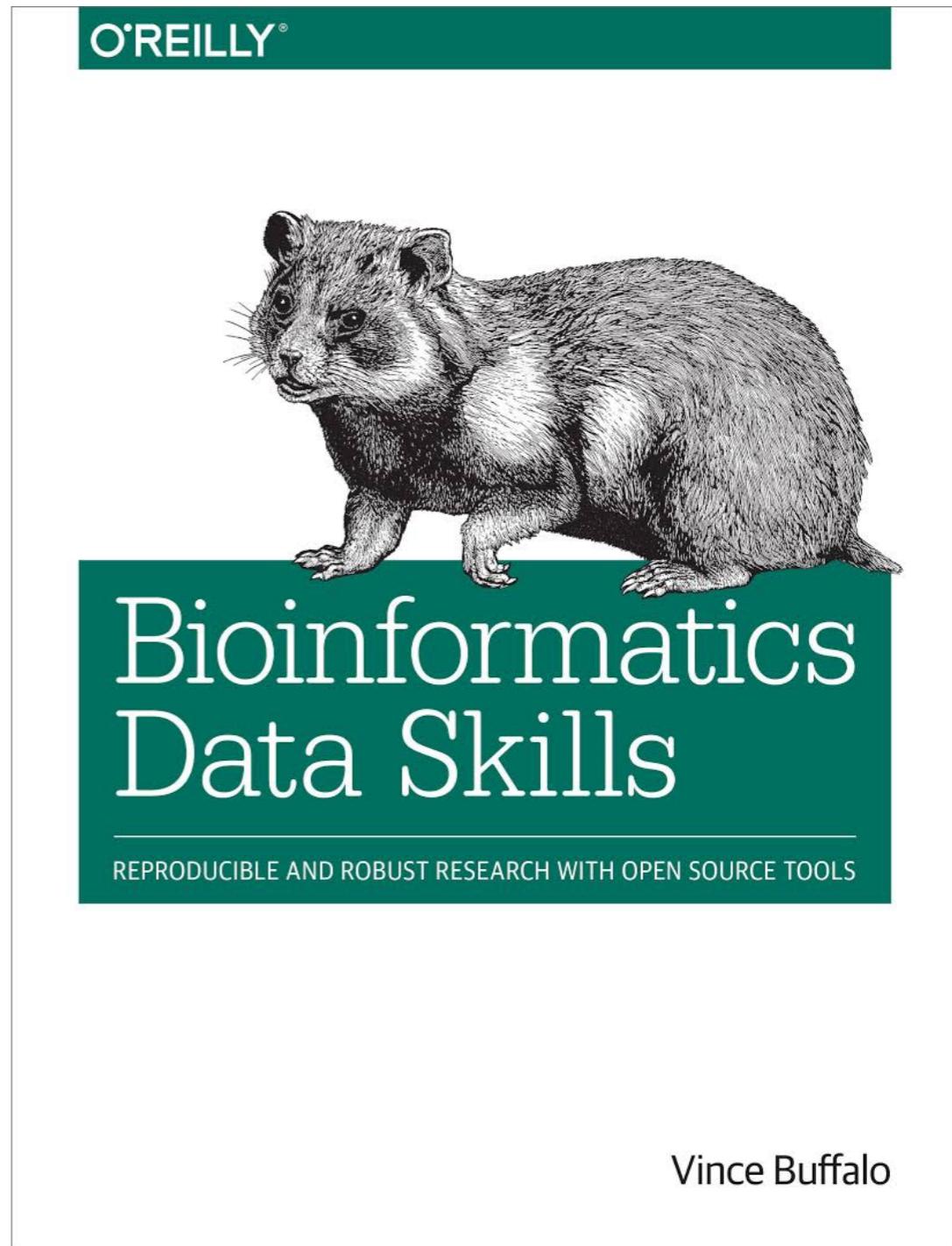
By the end of this course, you should:

- Become familiar with various genomic data types (range, sequence, and alignment data) and learn how to write scripts and analysis pipelines for working with these data.
- Become familiar with high performance computing resources at Iowa State as well as how and when to employ these resources.
- Explore additional resources/topics in computational biology including manuscript preparation in LaTeX and Overleaf and creation of NSF-style Data Management Plans.

Introduction and Basic Unix

Our Textbooks

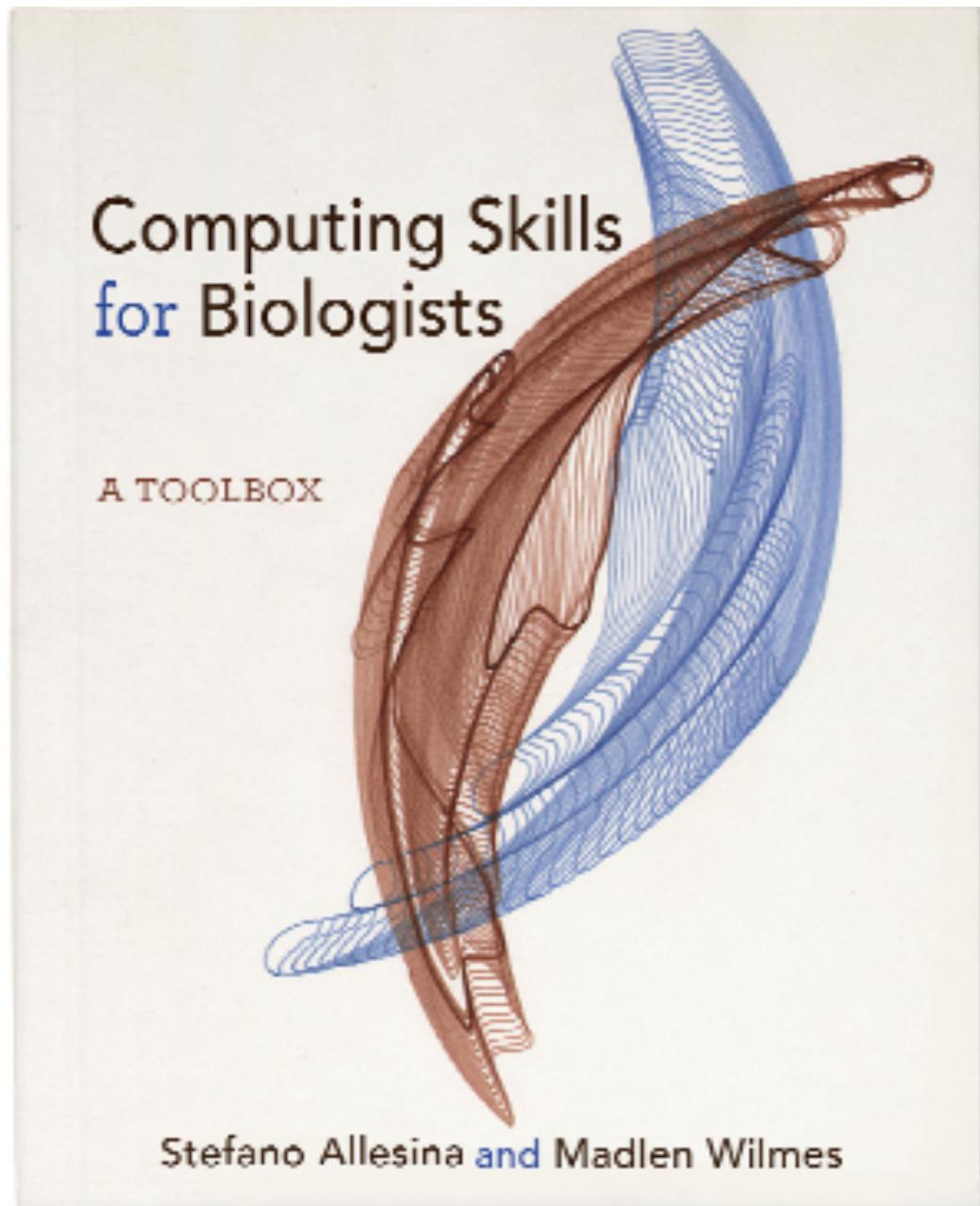
- ♦ Written to help address sudden need in biology to be able to handle Big Data
- ♦ Available through Amazon (hard copy), O'Reilly (hard copy and eBook), and ISU Library (eBook, FREE!!)



Vince Buffalo

Introduction and Basic Unix

Our Textbooks

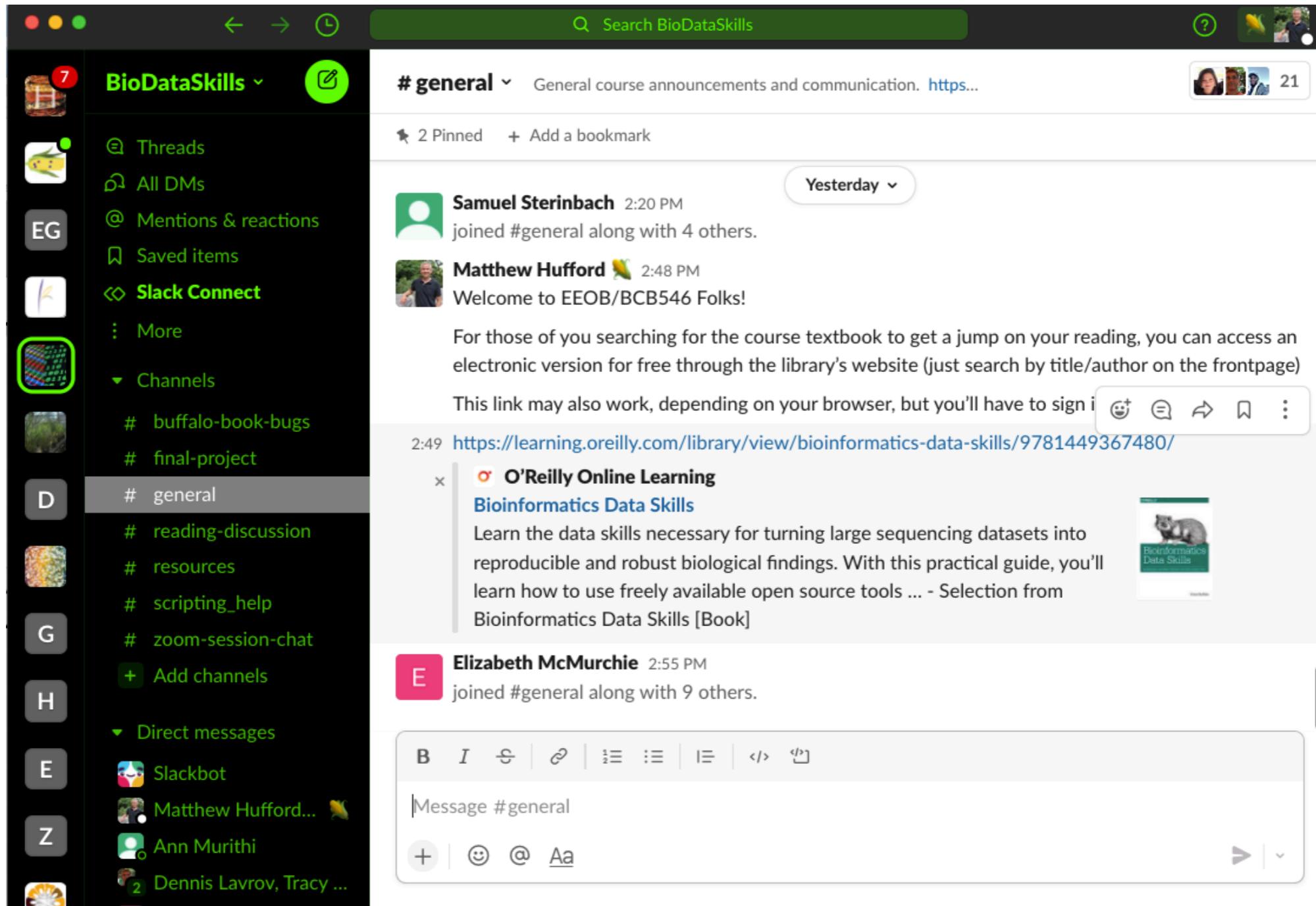


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Introduction and Basic Unix

How will we communicate?

Slack



Introduction and Basic Unix

What is our schedule?

Google Sheet

<https://docs.google.com/spreadsheets/d/1dIJyk07rNC-L6VrhlefbLCJ65Ytw96SOwukjhgl5cY/edit?usp=sharing>

Introduction and Basic Unix

How will grades be assigned?

Grading:

Assignment 1: Unix	15%
Assignment 2: R	15%
Assignment 3: Python	15%
Assignment 4: Data Management Plan	15%
Group Project and Presentation	40%

Chapter I

- ♦ Our two main goals in bioinformatics are to have research that is *reproducible* and *robust*
- ♦ How can we make our analysis reproducible?
- ♦ How can we make our analysis robust?

Chapter I

- ♦ Writing code for humans makes it reproducible, but it must still be readable by your computer

```

#!/usr/bin/perl
# PathHaps.pl by Matthew Hufford
use strict;
use warnings;

open AF, "<AllFreq.txt" or die "fail!\n\n";
my %data;
while (<AF>) {
    chomp;
    my $AllFreq = $_;
    my ($locus, $allele, $freq) = split("\t", $AllFreq);
    $data{$locus}->{$allele}=$freq;
}
close AF;

#define a hash of allele frequencies from the bulked seed

open PG, "<PatGenosIN(-9).txt" or die "fail\n\n";
my ($patallele_id, @genos) = <PG>; #first line turned into string, rest of file turned into an array
close PG;
print `cp Pools2Format.txt outfile.txt`;
my @patallele_id = split("\t", $patallele_id); #creating array of loci names from string of first line
open OUT, ">outfile.txt";
print (OUT "\n");

foreach my $dad (@genos) {
    chomp $dad;
    my ($dadID, @linedata) = split ("\t", $dad); #splitting paternal ID from array of genotypes
    print (OUT "$dadID\t0\t0\t");
    #printing dad ID with a tab

    for my $a (0..$#linedata) { #creating a list from 0 to the number of scalars in each line of the array; the $# notation indicates the total number in array
        my $allele=$linedata[$a]; #putting list into the array and creating a string of allele calls that are at those positions.

        if ($allele =~ m/&/) { #matching all alleles that contain an ampersand
            my ($allele1, $allele2) = split ("&", $allele); #creating an array of the two possible alleles
            my $freq1=$data{$patallele_id[$a]}->{$allele1}; #creating frequency scalar for each allele 1
            my $freq2=$data{$patallele_id[$a]}->{$allele2}; #creating frequency scalar for each allele 2

            if (rand()<($freq1/($freq1+$freq2))) { #assessing whether random number between 0 and 1 is less than freq 1
                print (OUT "$allele1\t-9\t");
            }
            else {
                print (OUT "$allele2\t-9\t");
            }
        }
    }
}

```

Chapter I

- ♦ Adding in tests for your code helps avoid the dreaded silent errors and makes your research more robust

```
def add(x, y):  
    """Add two things together.""" return x + y  
  
def test_add():  
    """Test that the add() function works for a variety of numeric types."""  
    assert(add(2, 3) == 5)  
    assert(add(-2, 3) == 1)  
    assert(add(-1, -1) == -2)  
    assert(abs(add(2.4, 0.1) - 2.5) < EPS)
```

Chapter I

- ♦ If a library already exists for what you want to do, why not use it?
- ♦ Do not modify your raw data directly (treat as “Read Only”)
- ♦ If you’re going to use a script multiple times, turn it into a tool:
 - ♦ document it
 - ♦ create versions
 - ♦ make your command-line arguments clear
 - ♦ sharing in a version-controlled repository

Chapter I

- ♦ Publish both your scripts and data
- ♦ Also publish your documentation and document everything!
- ♦ *What's the difference between documenting a script and a project? How might we do both?*
- ♦ Make an analysis and the figures showing the results of an analysis the product of a script

Intro. to Computational Methods

UNIX

- ♦ UNIX is an operating system originally developed by AT&T's Bell Labs in the 1960's (then Novell, then The Open Group)
- ♦ “Operating System” = Suite of programs that make your computer work
- ♦ macOS is one flavor of UNIX; others are Linux, Solaris, BSD

Intro. to Computational Methods

UNIX

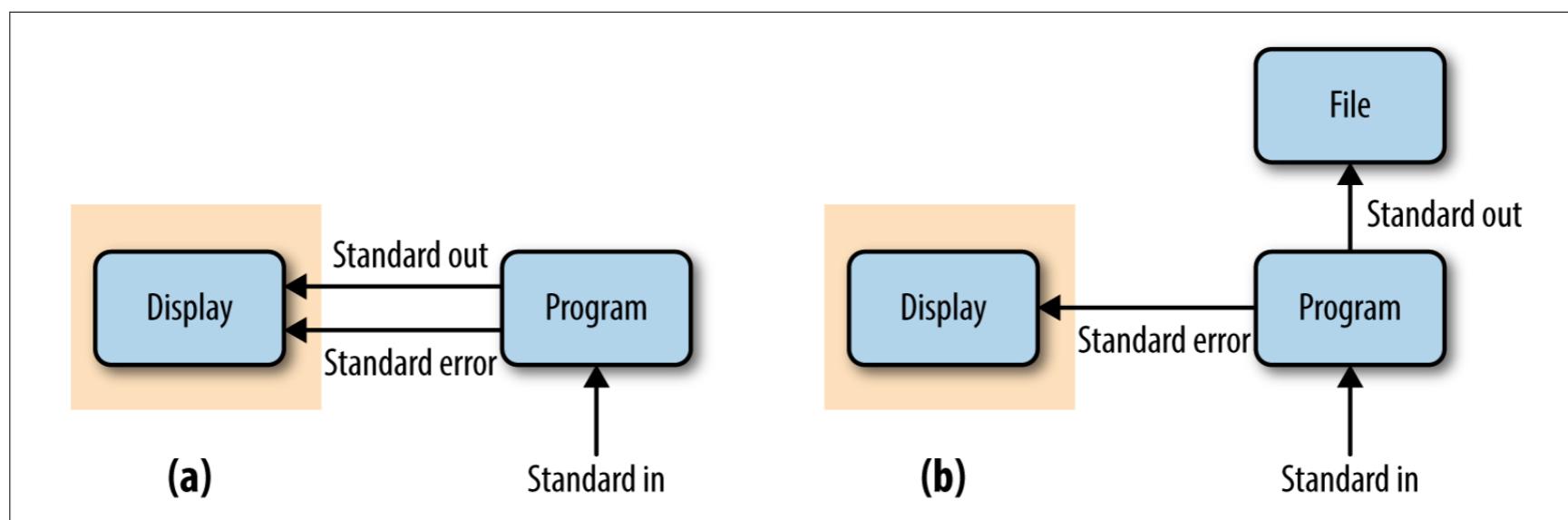
The UNIX OS has three components:

- (1) The Kernel: OS Hub; allocates memory and time
- (2) The Shell: Interface between user and the kernel; the shell searches for command files called by user and passes requests to the kernel
- (3) Programs: Commands called by the user

Intro. to Computational Methods

UNIX

- ♦ UNIX is modular: **What does this mean?**
- ♦ UNIX handles data as a stream
- ♦ A given program generates standard output and standard error streams: **What is the difference?**
- ♦ How can we redirect streams?



Introduction and Basic Unix

Our Computational Goals for Today

- I. Make sure everyone has a Shell solution
2. Installation of GitBash if necessary
3. Clone the Git repository for the textbook and the course
4. Work through a Basic Unix example

Introduction and Basic Unix

Where to from here?

- I. If the basic Unix commands in our example were all new (and even if they weren't!), you should consider working through the Unix portions of these tutorials :
<https://sites.google.com/site/eeob563/computer-labs/Lab-I>

http://korflab.ucdavis.edu/Unix_and_Perl/

2. If you haven't already, read Chapters 1-3 of Buffalo
 - For Chapter 1, create a text snippet in Slack with a few favorite points and any questions on points that were not clear, and we'll discuss these on Friday
 - We'll also discuss and work through examples from Chapter 3 on Friday