Unix, Perl and Python

Perl for Bioinformatics

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`http://jura.wi.mit.edu/bio/education/hot_topics/Unix_Perl_Python/`

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Perl for Bioinformatics

- Introduction
- Data types
- Input and output
- Functions
- Control structures
- Comparisons
- Sample script

Objectives

- write, modify, and run simple Perl scripts

- design customized and streamlined data manipulation and analysis pipelines with Perl scripts

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Why Perl?

- Good for text processing (sequences and data)
- Easy to learn and quick to write
- Built from good parts of lots of languages/tools
- Lots of bioinformatics tools available
- Open source and free for Unix, Windows, and Mac

A first Perl program

- Create this program and call it hey.pl

```perl
#!/usr/local/bin/perl -w
# The Perl "Hey" program
print "What is your name? ";
chomp ($name = <STDIN>);
print "Hey, $name, welcome to the
  BaRC course.\n";
```

- To run: **perl hey.pl**   *or*
- To run: **chmod +x hey.pl**
               ./hey.pl

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Scalar data

- Describe one thing
- Start with $
- Can be numbers or text (a "string")
- Strings need single or double quotes

```perl
$numSeq = 5;          # number; no quotes
$seqName = "GAL4";    # "string"; use quotes
$level = -3.75;       # numbers can be decimals too
print "The level of $seqName is $level\n";
```

- Perl has some strange-looking "special variables" too:

```perl
$_                 default input variable
$.                 input line number
```

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Array

- An ordered list of scalar variables
- The entire list is indicated by a @

```perl
@genes = ("BMP2", "GATA-2", "Fez1");
@orfLengths = (395, 475, 431);
@info = (12, "student", 5.0e-05, "comic books");
```

- One item of the list is accessed like $foo[2]
- The first item is actually the 0th item

```perl
print "The ORF of $genes[0] is $orfLengths[0] nt.";
```

Prints out: **The ORF of BMP2 is 395 nt.**

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Hash

- An unordered pair ("keys" and "values") of lists
- Each key points to a corresponding value.
- The entire list is indicated by a %

```perl
%geneToLength = ();      # Create an empty hash
```

- An item of the hash is accessed like $foo{key}

```perl
$geneToLength{"BMP2"} = 395;
$gene = "BMP2";
print "The ORF of $gene is $geneToLength{$gene} nt.";
```

- Prints out: **The ORF of BMP2 is 395 nt.**

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Perl input and output

- Types of input:
  - keyboard (STDIN)
  - files
- Types of output:
  - screen (STDOUT)
  - files
- Unix redirection can be very helpful
  ex: ./**hey.pl > hey_output.txt**

Filehandles

To read from or write to a file in Perl, it first needs to be opened.
In general,   **open(filehandle, filename);**

Filehandles can serve at least three purposes:
```
open(IN, $inFile);            # Open for input
open(OUT, ">$outFile");       # Open for output
open(OUT, ">>$outFile");      # Open for appending
```

Then, get data all at once **@lines = <IN>;**
or one line at a time
```
while (<IN>) {
    $line = $_; do stuff with this line;
    print OUT "This line: $line"; }
```

Perl functions – a sample

print	opendir	closedir	open	close
chomp	mkdir	split	join	die
length	chdir	readdir	chmod	sort
substr	push	unlink	rename	use
m//	s///	tr///	lc	uc

Description of command: slides   exercises

Control Structures 1

```
if (condition)      # note that 0, "", and (undefined) are false
{
    print "If statement is true";
}
else      # optional; 'if' can be used alone; elsif also possible
{
    print "If statement is false";
}


if ($exp >= 2)         # gene is up-regulated
{
  print "The gene $seq is up-regulated ($exp)";
}
```

Control Structures 2

```
while (condition)
{
    print "condition is true";
    # Do interesting things...
}


open(DATA, "myData.txt");  # Open a file to read
while (<DATA>)
{
    # Split by tabs and make an array
    @dataThisRow = split /\t/, $_;
    # Print first field followed by "\n" (line end)
    print "$dataThisRow[0]\n";
}
```

Control Structures 3

```
for ( initialize; test; increment )
{
    # Do something interesting with this value
}


# Go through an array (@seqs) where
#    $#seqs = index of the last element in @seqs

for ($i = 0; $i <= $#seqs; $i++)
{   # Print elements of @seqs and @orf on a line
    print "$seqs[$i]\t";
    print "$orf[$i]\n";
}
```

Arithmetic & numeric comparisons

- Arithmetic operators: **+ - / * %**
- Notation: **$i = $i + 1; $i += 1; $i++;**
- Comparisons: $>, <, <=, >=, ==, !=$

```
if ($num1 != $num2) # If these are different
{
    print "$num1 and $num2 are different";
}
```

- Note that $==$ is very different from $=$
    $==$ used as a test: if ($num == 50)
    $=$ used to assign a variable: $num = 50$

String comparisons

- Choices: **eq** (equals), **ne** (not equal to)

```
if ($gene1 ne $gene2)
{
    print "$gene1 and $gene2 are different";
}
else
{
    print "$gene1 and $gene2 are the same";
}
```

Multiple comparisons

- AND **&&**
- OR **||**

```
if (($exp > 2) || ($exp > 1.5 && $numExp > 10))
{
  print "Gene $gene is up-regulated";
}
```

Embedding shell commands

- use backquotes (`) around shell command
- example using EMBOSS to reverse-complement:
  `` `revseq mySeq.fa mySeq_rc.fa`; ``

- Capture stdout from shell command if desired
- EMBOSS qualifier "-filter" prints to stdout
  ```
  $date = `date`;
  $rev_comp = `revseq mySeq.fa -filter`;
  print $date;
  print "Reverse complement:\n$rev_comp\n";
  ```

Perl modules

- "a unit of software reuse"
- adds a collection of commands related to a specific task
- see https://tak.wi.mit.edu/trac/wiki/Perl to find Perl modules installed on tak
- BioPerl is a collection of bioinformatics tasks
- Example of a descriptive statistics module:

```
use Statistics::Lite qw(:all);
@nums = (324, 456, 876, 678, 654, 789);
$mean = mean(@nums);
print "The mean of my numbers is $mean\n";
```

Programming issues

- What <u>should</u> the program do? What <u>does</u> it do?
- Who will be using/updating your software?
  - Reusability
  - Commenting
  - Error checking
- Development vs. execution time
- Debugging tools: printing and commenting
- Beware of OBOBs ("off-by-one bugs")

Example: align_pairs.pl

```perl
#!/usr/local/bin/perl -w
# Automatically do lots of pairwise sequence alignments
$seqs = $ARGV[0];    # Get first argument (word after command)
$hs = "human";       # directory with human proteins
$mm = "mouse";       # directory with mouse proteins
open(SEQ_LIST, $seqs);    # Open file for reading
while(<SEQ_LIST>)         # Read one line at a time
{
   $seq = chomp($_);     # trim end-of-line character
   print STDERR "Aligning $seqFile…\n";
   # Create EMBOSS command for S-W (optimal) alignment
   $CMD = "water $hs/$seq $mm/$seq -outfile $seq.aligned";
   # Execute the command (needs EMBOSS package)
   `$CMD`;
}
print "All done with alignments\n";
```

| BMP7 |
| GATA4 | *Example file* |
| LIN28A |

To run: **./align_pairs.pl SeqList.txt**

Summary

- Input/output
- Variables (scalars and arrays)
- Functions (brief look)
- Control structures
- Comparisons
- Sample script: align_pairs.pl

Books with more information

- O'Reilly books at http://proquest.safaribooksonline.com/search/perl
  - *Thanks to the MIT Libraries*
  - Learning Perl   (Schwartz et al.)
  - Programming Perl   (Wall, Christiansen, and Orwant)

- Beginning Perl for Bioinformatics – Tisdall

- 'Using Perl to Facilitate Biological Analysis' (Stein) in *Bioinformatics* (Baxevanis & Ouellette)

- 'Bioinformatics Programming using Perl and Perl Modules' in *Bioinformatics: Sequence and Genome Analysis, 2nd ed.* (Mount)

  AND several good web sites (see course page)

Demo scripts:
http://iona.wi.mit.edu/bio/bioinfo/scripts/
and /nfs/BaRC_Public/BaRC_code/

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Perl scripts for Bioinformatics

[Go to Unix commands for Bioinformatics]

Script name	Description	Sample input	Sample output	Download
hey.pl	Test Perl on your system			download
rev_comp.pl	Reverse and complement a fasta sequence using EMBOSS's 'revseq' command			download
oligos.pl	Extract oligos from a sequence and analyze them			download
patscan_batch.pl	Run patscan (to search for a pattern) on every sequence in a directory			download
puzzle_helper.html	Web-based interface for the puzzle.cgi script			NA
parse_genbank.pl	Simple GenBank nucleotide report parser using regular expressions	input	output	download
get_web_data.pl	Use LWP to automate web file access	input	output	download
draw_figure.pl	Draw a PNG figure using the GD module	input	output	download

Exercises

- Parsing a SAM short-read alignment file into a BED file

- Retrieving and aligning a list of human-mouse orthologs

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