

Unix, Perl and Python

Perl for Bioinformatics

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





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

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 #!/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

Scalar data

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

```
$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:

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

Array

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

```
@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

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

Prints out: The ORF of BMP2 is 395 nt.

Hash

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

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

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

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

Prints out: The ORF of BMP2 is 395 nt.

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";
                                               13
```

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
                                                15
```

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 should the program do? What does 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

```
#!/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
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`;
                                         BMP7
                                               Example
print "All done with alignments\n";
                                               file
```

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

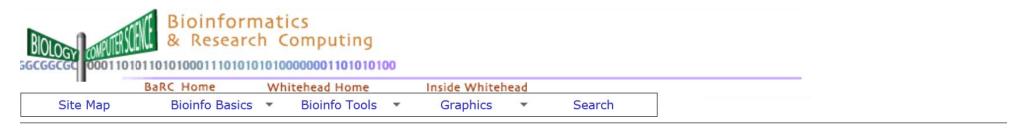
Books with more information

- 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/



BaRC > Bioinformatics > Script library

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 humanmouse orthologs