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Xenopus Bioinformatics: AWK+

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Advanced UNIX Topics

Command line editing

- Control-A (^A): Move cursor to beginning of line. Mnemonic: A is first letter of alphabet
- ^E: **E**nd of line

(^Z was already taken for something else).

- ^D: **D**elete character currently under the cursor.
- ^K: **K**ill (cut) from the cursor to end of line. (Deleted text goes to a clipboard)
- ^Y: **Y**ank (paste) the clipboard text back onto the command line

File/Directory Permissions

- Every file and directory has an owner (a user) and a group
- `groups lp28` – groups I belong to
- `ls -l` shows each file's owner/group
- `chown`, `chgrp` changes these values

```
botka@portal.77% ls -la
total 64
drwxrwxr-x    2 botka    botka        4096 Feb 25 08:06 ./
drwxrwx---   48 botka    cgradmin    45056 Feb 25 08:02 ../
-rw-rw-r--    1 botka    botka        5332 Feb 25 08:02 moreseqs
-rw-rw-r--    1 botka    botka        1102 Feb 25 08:06 opsd_human.fasta
-rw-rw-r--    1 botka    botka        1247 Feb 25 08:02 seqs
```

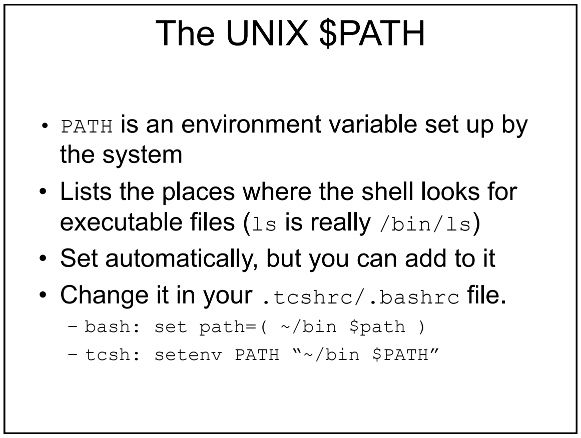
Permissions II

- `ls -l` says who can do what to a file/directory:
  - r: read, w: write (or delete), x: execute a file, see inside a directory
  - categories: **u**ser, **g**roup, **o**ther
- `chmod` changes these values
  - `chmod o+w seqs` (now others can edit the file)
  - `chmod 644 seqs` (magic to set permissions: see chmod man page)

```
botka@portal.77% ls -la
total 64
drwxrwxr-x    2 botka    botka        4096 Feb 25 08:06 ./
drwxrwx---   48 botka    lp28        45056 Feb 25 08:02 ../
-rw-rw-r--    1 botka    botka        5332 Feb 25 08:02 moreseqs
-rw-rw-r--    1 botka    botka        1102 Feb 25 08:06 opsd_human.fasta
-rw-rw-r--    1 botka    botka        1247 Feb 25 08:02 seqs
```

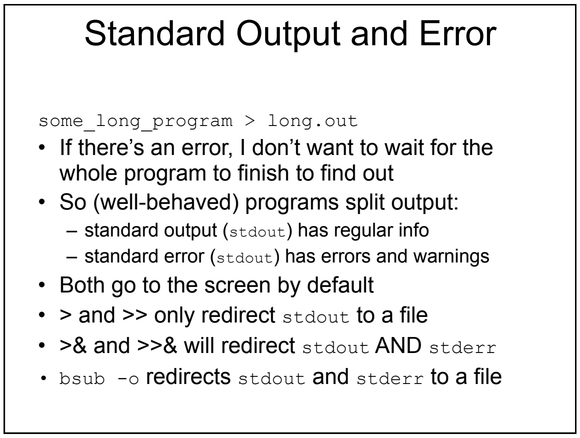
Environment Variables

- Information about your account
- Preferences for your account
- Locations of databases, files, programs
- `tcsh:`
  - `setenv BLASTDB ~/my_blastdbs`
  - `printenv BLASTDB`
- `bash:`
  - `Set BLASTDB = ~/my_blastdbs`
  - `echo $BLASTDB`



The UNIX $PATH

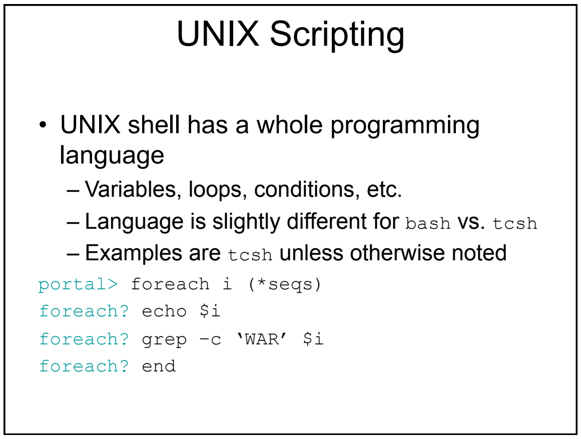
- `PATH` is an environment variable set up by the system
- Lists the places where the shell looks for executable files (`ls` is really `/bin/ls`)
- Set automatically, but you can add to it
- Change it in your `.tcshrc/.bashrc` file.
  - `bash: set path=( ~/bin $path )`
  - `tcsh: setenv PATH "~/bin $PATH"`



Standard Output and Error

```
some_long_program > long.out
```

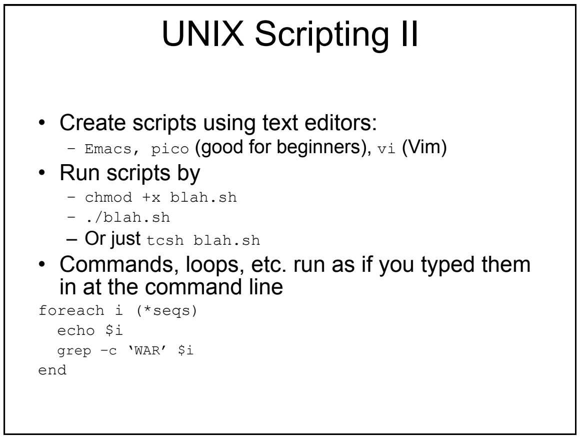
- If there's an error, I don't want to wait for the whole program to finish to find out
- So (well-behaved) programs split output:
  - standard output (`stdout`) has regular info
  - standard error (`stdout`) has errors and warnings
- Both go to the screen by default
- > and >> only redirect `stdout` to a file
- >& and >>& will redirect `stdout` AND `stderr`
- `bsub -o` redirects `stdout` and `stderr` to a file



UNIX Scripting

- UNIX shell has a whole programming language
  - Variables, loops, conditions, etc.
  - Language is slightly different for `bash` vs. `tcsh`
  - Examples are `tcsh` unless otherwise noted

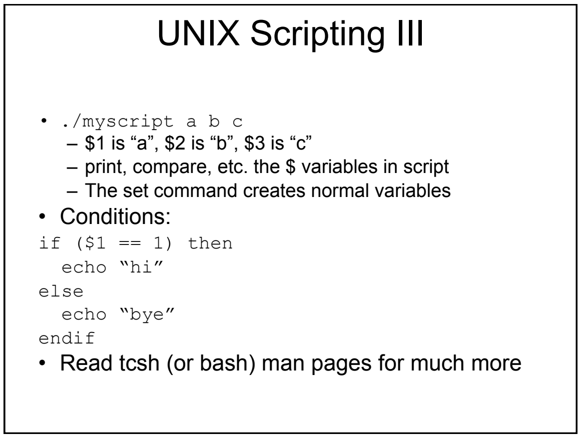
```
portal> foreach i (*seqs)
foreach? echo $i
foreach? grep -c 'WAR' $i
foreach? end
```



UNIX Scripting II

- Create scripts using text editors:
  - `Emacs, pico` (good for beginners), `vi` (Vim)
- Run scripts by
  - `chmod +x blah.sh`
  - `./blah.sh`
  - Or just `tcsh blah.sh`
- Commands, loops, etc. run as if you typed them in at the command line

```
foreach i (*seqs)
  echo $i
  grep -c 'WAR' $i
end
```

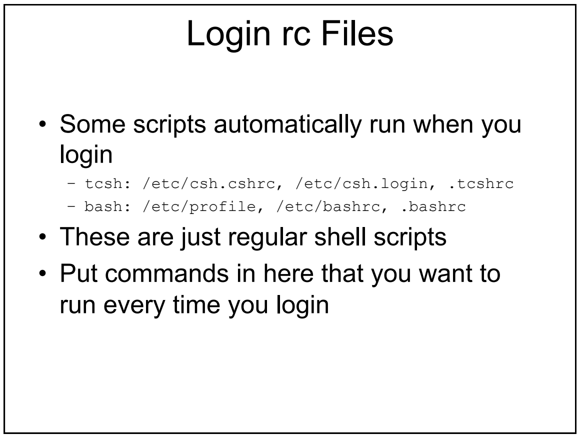


UNIX Scripting III

- `./myscript a b c`
  - $1 is "a", $2 is "b", $3 is "c"
  - print, compare, etc. the $ variables in script
  - The set command creates normal variables
- Conditions:

```
if ($1 == 1) then
  echo "hi"
else
  echo "bye"
endif
```

- Read tcsh (or bash) man pages for much more



Login rc Files

- Some scripts automatically run when you login
  - `tcsh: /etc/csh.cshrc, /etc/csh.login, .tcshrc`
  - `bash: /etc/profile, /etc/bashrc, .bashrc`
- These are just regular shell scripts
- Put commands in here that you want to run every time you login

More Shortcuts: Aliases and Links

- `ln -s ../../some/far/away/file ./here`
  - In is just like cp, but it makes a link instead
  - more here will more the far away file, etc.
- `alias cdd ‘cd some/far/away/dir’`
  - put this in your .tcshrc so you always have it
- alias can also use variables!
  - `alias lastlog ‘set lastlog=`ls -dtr /usr/local/adm/log/updatedb/{\!:*}* | tail -n 1`; echo “Most recent \!:* log: $lastlog”; more $lastlog`

More commands

- /bin has 81 commands
  - And then there’s /usr/bin, /usr/local/bin...
- Data manipulation: sort, cut, paste, join, tr
- File filters: sed, awk
- Real programming languages: Perl, Python

AWK Program

```
gawk 'BEGIN{RS="//";FS="AUTHORS|TITLE|JOURNAL"}
{n=split($2,a," ");c[a[n]]++}END{for (i in c) print i"\t"c[i]}'
cDNA-GenBank-format-Xl-MB-UNIX.txt | sort -rnk2 | more
```

Running An AWK Program

awk [-Ffs] [*‘program’*|-f progfile] [datafile...]

fs	field separator
‘program’	AWK program entered on cmd line
progfile	text file containing AWK program
datafile	data you want to pass through your AWK program (“-” is stdin)

```
gb|AAN86046.2| rhodopsin [Sminthopsis crassicaudata]              617   e-177
gb|AAP35089.1|AF425072_1 RH1 opsin [Oncorhynchus mykiss]   553   e-158
dbj|BAC76806.1| green-sensitive opsin 1 [Cyprinus carpio]          508   e-144
dbj|BAC76807.1| green-sensitive opsin 2 [Cyprinus carpio]          500   e-142
gb|AAP35093.1|AF425076_1 RH2 opsin [Oncorhynchus mykiss]   441   e-124
gb|AAO38746.1| green rod opsin [Xenopus laevis]              356   1e-98
gb|AAP35092.1|AF425075_1 SWS2 opsin [Oncorhynchus mykiss]          322   2e-88
gb|AAP35091.1|AF425074_1 SWS1 opsin [Oncorhynchus mykiss]          292   3e-79
gb|AAP37944.1| short wave-sensitive opsin 1 [Macropus eugenii]       287   8e-78
gb|AAP30082.1| opsin [Parus caeruleus]                    284   7e-77
gb|AAP37945.1| medium wave-sensitive opsin 1 [Macropus eugenii]      266   2e-71
gb|AAP35090.1|AF425073_1 LWS opsin [Oncorhynchus mykiss]           255   4e-68
gb|AAP30087.1| opsin [Luscinia svecica]                   247   1e-65
gb|AAM77793.1| vertebrate ancient opsin long isoform [Rutilus ru...   243   1e-64
gb|AAP30084.1| opsin [Parus palustris]                    240   1e-63
gb|AAP30085.1| opsin [Euplectes afer]                     238   6e-63
gb|AAM77794.1| vertebrate ancient opsin short isoform [Rutilus r...   232   2e-61
gb|AAP30088.1| opsin [Luscinia calliope]                  231   5e-61
gb|AAP30083.1| opsin [Parus major]                        224   9e-59
gb|AAP30086.1| opsin [Euplectes orix]                     220   1e-57
```

Internal Variables

```
$ cat data1
one
two two
three three three oops
four four four four
$
$ awk '{print NR,$0,"FIELD COUNT:",NF}' data1
1 one FIELD COUNT: 1
2 two two FIELD COUNT: 2
3 three three three oops FIELD COUNT: 4
4 four four four four FIELD COUNT: 4
```

Internal Variables Continued

NF	**field count for current record**
NR	**count of records read so far**
FNR	**count of records read from current file**
FS	**input field separator**
RS	**input record separator**
OFS	**output field separator**
ORS	**output record separator**
$0	**entire input line**
$1	**first field, $2 is second field ....**

Even More About Internal Variables

NF **is an integer**
(the number of fields in this record)

$NF **is the contents of the last**
field in the record

$NR **the contents of the NRth field in**
this record

```
$ cat data2
a b c d e
f g h i j
k l m n o p
q r s t u
v w x y z
$
$ awk '{print $NR}' data2
a
g
m
t
z
```

```
$ cat data2
a b c d e
f g h i j
k l m n o p
q r s t u
v w x y z
$
$ awk '{print $NF}' data2
e
j
p
u
z
```

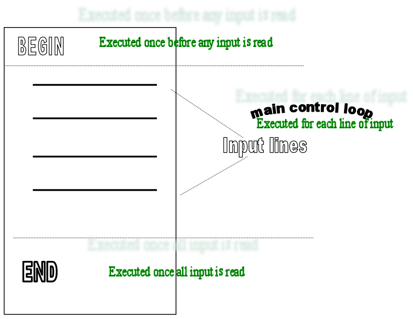
AWK Program Structure

PATTERN {action}
PATTERN {action}
.
.
.

PATTERNS

BEGIN
END
/regular_expression/
$1 ~ /regular_expression/
$1 !~ /regular_expression/
NF != 3
$2 == 5
$1 == “literal_string”
$2 >= 4 || $3 <= 20

awk



BEGIN

Executed once before any input is read

main control loop

Executed for each line of input

Input lines

END

Executed once all input is read

Regular Expressions

^	**beginning of line**
$	**end of line**
.	**any single character**
[ ]	**character class**
|	**alternation**
*****	**closure (zero or more)**
+	**positive closure (one or more)**
?	**zero or one**
( )	**grouping**
\	**escapes meaning of meta character**

Regular Expression Examples

(BOZO|COOKIE|WIZZO)(UP|DOWN)(TO|YESTER)DAY

BOZO UP TODAY
COOKIE DOWN YESTERDAY
COOKIE UP YESTERDAY

(AB)+c

ABc
ABABc
ABABABc

/^(\+|-)?[0-9]+\.?[0-9]*$/

!

Pattern Ranges

/BOZO/,/PROFANDY/

BOZO tricks COOKIE
WIZZO botches magic trick
PROFANDY plays music
PROFANDY gets cream pie
BOZO chases COOKIE with pie
BOZO sings to audience
PROFANDY talks with GOLLY
WIZZO performs magic trick
WIZZO receives cream pie

Actions

- Output
- Data Manipulation
- Flow Control

Output

print **basic output**

quoted strings are output verbatim
comma-separated arguments are output with the OFS between them

printf **formatted output (works just like C)**

first argument is format string
other arguments are the values to substitute

print

one two three

```
BEGIN       { OFS=”|”}
            { print $1 $2 ”test”,$3,”wow”}
```

onetwotest|three|wow

printf

one two three

```
BEGIN{ OFS=”|”}
      { printf(“%s%s%s%s\n”,$1,$3,OFS,”wow”}
```

onethree|wow

printf format strings

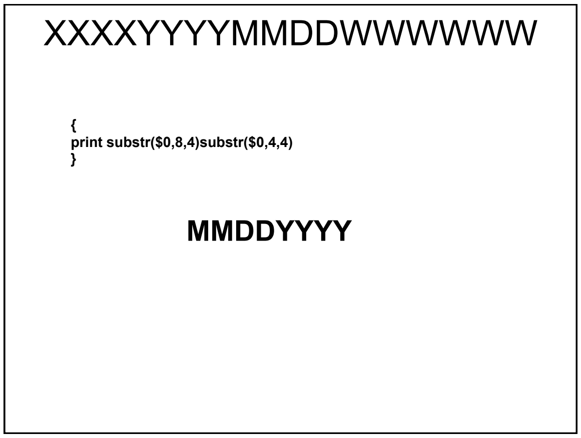
```
                              |1234567890|
printf(“|%c|”,100)            |d|
printf(“|%5d”,100)            |  100|
printf(“|%7.2f|,100.5)        |  100.5|
printf(“|%s|”,”MySystm”)      |MySystm|
printf(“|%-10s|”,”MySystm”)   |MySystm   |
printf(“|%10s|”,”MySystm”)    |   MySystm|
printf(“|%5s|”,”MySystm”)          |MySystm|
                              |1234567890|
```

Data Manipulation

- Built-In Functions
  - String
  - Numeric
- Operators

Built-In Functions (String)

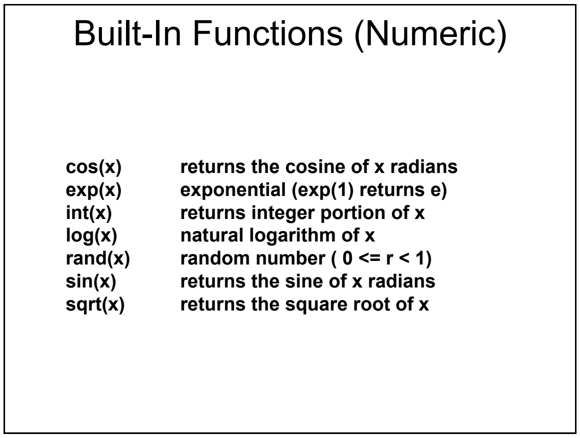
gsub(r,s,t) **substitue s for r in string t**
index(s,t) **return first postition of t in s**
length(s) **number of characters in string s**
split(s,a,fs) **split s into array a on field separator fs; returns field count**
sub(r,s,t) **substitute s for the leftmost longest substring of t matched by r**
substr(s,p,n) **return substring of s of length n starting at position p**



XXXXYYYYMMDDWWWWWW

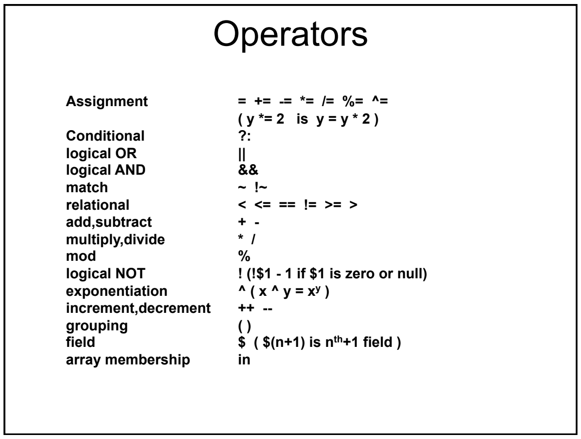
```
{
print substr($0,8,4)substr($0,4,4)
}
```

MMDDYYYY



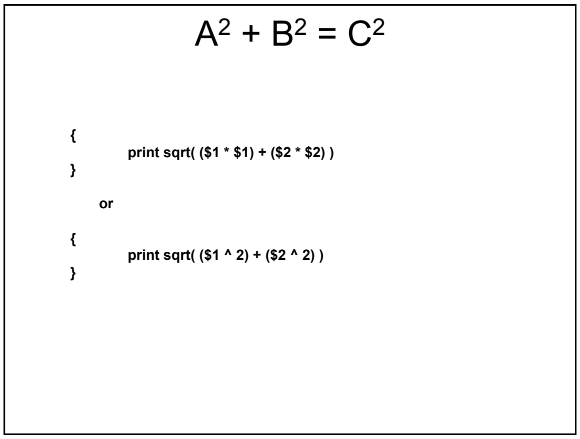
Built-In Functions (Numeric)

cos(x)	**returns the cosine of x radians**
exp(x)	**exponential (exp(1) returns e)**
int(x)	**returns integer portion of x**
log(x)	**natural logarithm of x**
rand(x)	**random number (0 <= r < 1)**
sin(x)	**returns the sine of x radians**
sqrt(x)	**returns the square root of x**



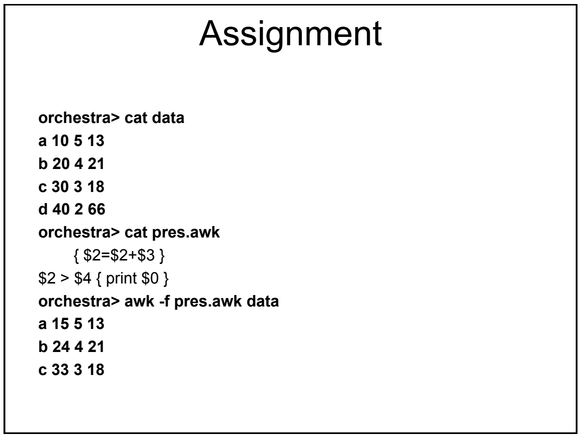
Operators

Assignment	**= += -= *= /= %= ^=** **(y *= 2 is y = y * 2)**
Conditional	**?:**
logical OR	**||**
logical AND	**&&**
match	**~ !~**
relational	**< <= == != >= >**
add,subtract	**+ -**
multiply,divide	*** /**
mod	**%**
logical NOT	**! (!$1 - 1 if $1 is zero or null)**
exponentiation	**^ (x ^ y = x^y)**
increment,decrement	**++ --**
grouping	**( )**
field	**$ ($(n+1) is nth+1 field)**
array membership	**in**



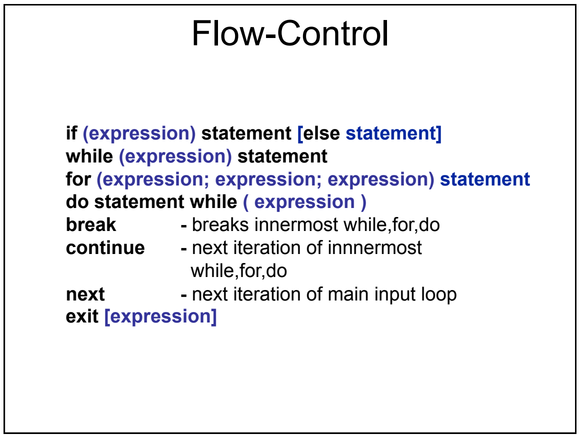
$A^2 + B^2 = C^2$

```
{
        print sqrt( ($1 * $1) + ($2 * $2) )
}

    or

{
        print sqrt( ($1 ^ 2) + ($2 ^ 2) )
}
```



Assignment

```
orchestra> cat data
a 10 5 13
b 20 4 21
c 30 3 18
d 40 2 66
orchestra> cat pres.awk
      { $2=$2+$3 }
$2 > $4 { print $0 }
orchestra> awk -f pres.awk data
a 15 5 13
b 24 4 21
c 33 3 18
```



Flow-Control

if (expression) **statement** [**else** statement]
while (expression) **statement**
for (expression; expression; expression) statement
do statement while (expression)
break - breaks innermost while,for,do
continue - next iteration of innnermost while,for,do
next - next iteration of main input loop
exit [expression]

```
BEGIN  {
       maxwidth=79
       }

       {
       if ( $1 <= maxwidth )
            {
            for (i=$1;i > 0; i--) printf(“*”)
            printf(”\n”)
            }
       else
            {
            printf(“Value %d at line %d > %d\n”,$1,NR,maxwidth)
            }
       }
```

Command Line Variables

```
awk -f prog.awk a=- c=2 d=3 data0 a=k b=y c=x data1 data2

          data0  a=-     b=““    c=2    d=3
          data1  a=k     b=y     c=x    d=3
          data2  a=k     b=y     c=x    d=3
```

Arrays

- Declaration not necessary
- Subscripts are strings
- Multi-dimensional obtained by subscript concatenation
- Element Occurrance (“in”)

Arrays (reverse.gawk)

```
# Output lines of file in reverse order
        {
        array[NR]=$0
        }

END     {
        for (i=NR;i>0;i--) print array[i]
        }
```

Arrays (primaries.gawk)

```
BEGIN  {
       primaries[“red”]=1
       primaries[“blue”]=2
       primaries[“yellow”]=3
       }

       {
       if ( $1 in primaries ) print $1,”is a primary color”
       else print $1,”is NOT a primary color”
       }
```

Arrays Continued

```
        { cntarray[$3]=cntarray[$3]+1 }
END     { for ( i in cntarray ) print i,
  cntarray[i]}

             totals[$1","hour","$3]=
```

Multiple-Line Records

DATA(mlr.fasta)

```
>prot1
RKRKRKRKRKRKR
KRKRKRKRKRKRKRKR

>prot100
SVLIVLSISLIVSLIVSLIVLSIV
SVLISVLISVLISVLISVLSIV
SVLISLIVSLIVSLVI

>prot10000
EVILEVILEVILEVILEEVILEILEVIEL
```

Program(mlr.awk)

```
BEGIN   {
        RS=““
        FS=“\n”
        }

        {
        print $1
        }
```

RUN

```
$ awk -f mlr.awk mlr.fasta
>prot1
>prot100
>prot10000
$
```

CONCLUSION

- experiment
- walk before you run
- you might find AWK useful for:
  - making sure every record of a file has the same field count
  - manipulating numeric information
  - creating reports from raw data
  - gathering specific information from reports
  - data conversions

Useful AWK One-Liners

```
{ print $NF }       # Last field on every line
--------------------------------------------------------------
        { if ( NF > mfields ) mfields = NF }
END     { print “MOST FIELDS =“,mfields}
--------------------------------------------------------------
        { if ( length($0) > wideline ) wideline = length($0) }
END     { print “WIDEST LINE =“,wideline }
--------------------------------------------------------------
{ print $($1) } # print the field referenced by first field
--------------------------------------------------------------
NF > 0 { print $0 } # removes blank lines
--------------------------------------------------------------
{ print NR":",$0 } # numbers the lines in a file
```

More Useful AWK One-Liners

```
NF != 5 { print NR,NF,$0 } # If a line does not have exactly 5 fields
                           # print the line number, the number of
                           # fields found and the line itself
--------------------------------------------------------------------
          { total=total + $2 }
END       { print total }    # total of field two
--------------------------------------------------------------------
$3 > max          { max = $3 ; maxline = $0 }
END               { print maxline } # find the maximum value for
                                    # field three and print the line
--------------------------------------------------------------------
{
  for (i=NF;i>0;i--) printf("%s ",$i)
  printf("\n")
} # reverse the order of fields on each line
```

Still More AWK One-Liners

```
####### potential orphaned processes
ps -ef | awk ‘$3 == 1 { print $0 }’
--------------------------------------------------------------
####### Center Lines of Text (need to pass width)
        {
         format=sprintf("%%%ds", width/2 - length($0)/2)
        printf(format"%s\n", " ", $0)
        }
--------------------------------------------------------------
####### total each input line
{
total=0
for (i=NF;i>0;i--) total=total+$i
print total
}
```

REFERENCES

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