ZHANG Youchi (张又驰)'s TA report for assignment05
SID: 12132603
Github: https://github.com/yzydlc/ESE5023_Assignments_12132603
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Grade: 30

Assignment 5

Great! Happy to see your improvement. Pls keep on

1.

First, I change my directory to ~ by using command cd ~.

1.1

use man to learn

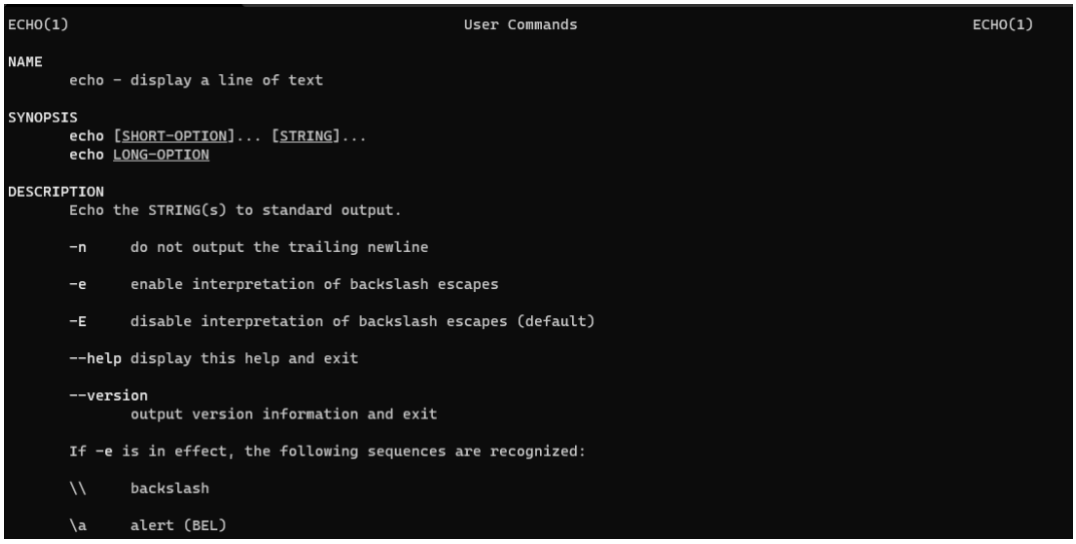
```
LN(1)                                   User Commands                                   LN(1)

NAME
       ln - make links between files

SYNOPSIS
       ln [OPTION]... [-T] TARGET LINK_NAME
       ln [OPTION]... TARGET
       ln [OPTION]... TARGET... DIRECTORY
       ln [OPTION]... -t DIRECTORY TARGET...

DESCRIPTION
       In the 1st form, create a link to TARGET with the name LINK_NAME.  In the 2nd form, create a link to TARGET in
       the current directory.  In the 3rd and 4th forms, create links to each TARGET in DIRECTORY.  Create hard links
       by  default,  symbolic  links with --symbolic.  By default, each destination (name of new link) should not al-
       ready exist.  When creating hard links, each TARGET must exist.  Symbolic links can hold  arbitrary  text;  if
       later resolved, a relative link is interpreted in relation to its parent directory.

       Mandatory arguments to long options are mandatory for short options too.

       --backup[=CONTROL]
              make a backup of each existing destination file

       -b     like --backup but does not accept an argument

       -d, -F, --directory
              allow  the  superuser  to  attempt to hard link directories (note: will probably fail due to system re-
              strictions, even for the superuser)
```

The result

```
[ese-zhangych@login02 ~]$ ln -s data_demo/ data_demo_link
[ese-zhangych@login02 ~]$ ll
total 2
drwxr-xr-x 2 ese-zhangych ese-ouycc 4096 Dec  8 15:09 data_demo
lrwxrwxrwx 1 ese-zhangych ese-ouycc   10 Dec  8 15:08 data_demo_link -> data_demo/
drwxr-xr-x 2 ese-zhangych ese-ouycc 4096 Nov  2 18:48 exam
drwxr-xr-x 2 ese-zhangych ese-ouycc 4096 Nov 24 20:19 TEST
[ese-zhangych@login02 ~]$
```

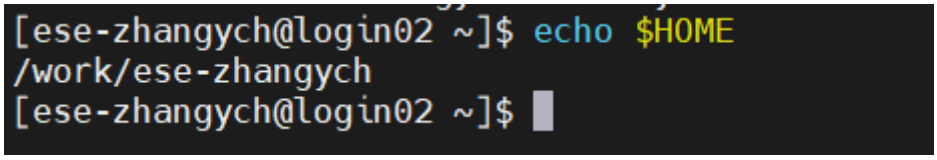
1. 2

use man to learn



```
ECHO(1)                                  User Commands                                  ECHO(1)

NAME
       echo - display a line of text

SYNOPSIS
       echo [SHORT-OPTION]... [STRING]...
       echo LONG-OPTION

DESCRIPTION
       Echo the STRING(s) to standard output.

       -n     do not output the trailing newline

       -e     enable interpretation of backslash escapes

       -E     disable interpretation of backslash escapes (default)

       --help display this help and exit

       --version
              output version information and exit

       If -e is in effect, the following sequences are recognized:

       \\     backslash

       \a     alert (BEL)
```

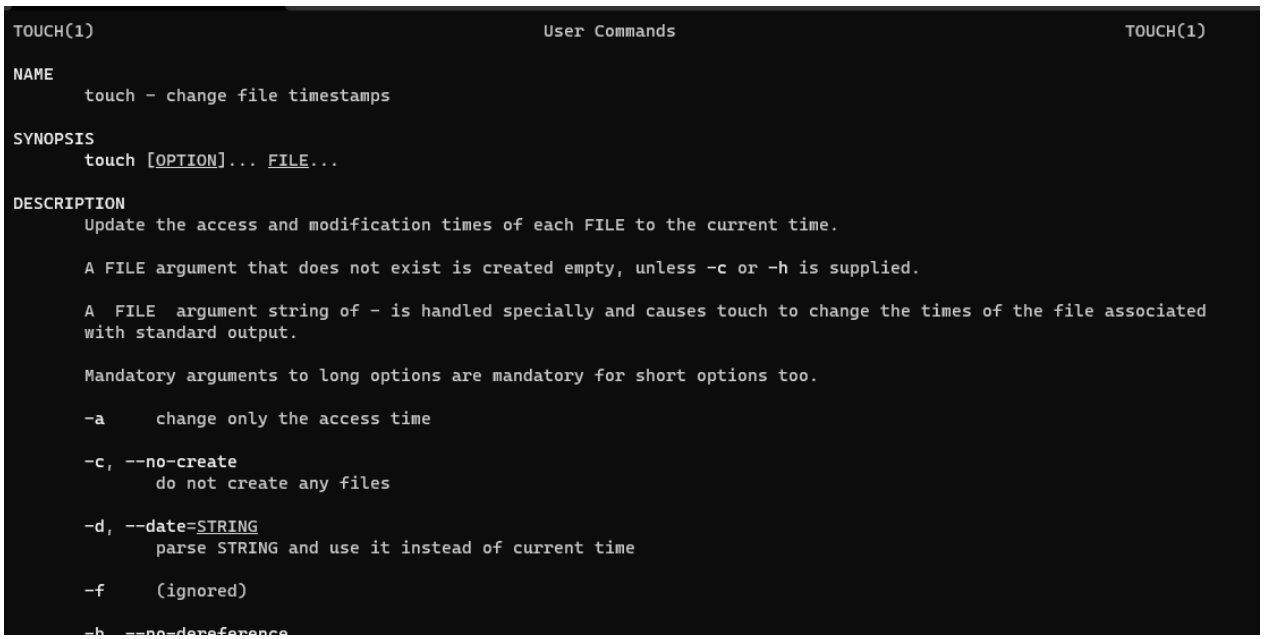
The result



```
[ese-zhangych@login02 ~]$ echo $HOME
/work/ese-zhangych
[ese-zhangych@login02 ~]$
```

1. 3

use man to learn



```
TOUCH(1)                                 User Commands                                  TOUCH(1)

NAME
       touch - change file timestamps

SYNOPSIS
       touch [OPTION]... FILE...

DESCRIPTION
       Update the access and modification times of each FILE to the current time.

       A FILE argument that does not exist is created empty, unless -c or -h is supplied.

       A  FILE  argument string of - is handled specially and causes touch to change the times of the file associated
       with standard output.

       Mandatory arguments to long options are mandatory for short options too.

       -a     change only the access time

       -c, --no-create
              do not create any files

       -d, --date=STRING
              parse STRING and use it instead of current time

       -f     (ignored)

       -h, --no-dereference
```

The result

```
[ese-zhangych@login02 ~]$ touch test.pdb
[ese-zhangych@login02 ~]$ ls
data_demo  data_demo_link  exam  TEST  test.pdb
[ese-zhangych@login02 ~]$
```

1. 4

Use man to learn

```
WC(1)                                   User Commands                                   WC(1)

NAME
       wc - print newline, word, and byte counts for each file

SYNOPSIS
       wc [OPTION]... [FILE]...
       wc [OPTION]... --files0-from=F

DESCRIPTION
       Print  newline,  word,  and byte counts for each FILE, and a total line if more than one FILE is specified.  A
       word is a non-zero-length sequence of characters delimited by white space.

       With no FILE, or when FILE is -, read standard input.

       The options below may be used to select which counts are printed, always  in  the  following  order:  newline,
       word, character, byte, maximum line length.

       -c, --bytes
              print the byte counts

       -m, --chars
              print the character counts

       -l, --lines
              print the newline counts

       --files0-from=F
              read  input  from the files specified by NUL-terminated names in file F; If F is - then read names from
```

```
FIND(1)                                 General Commands Manual                                 FIND(1)

NAME
       find - search for files in a directory hierarchy

SYNOPSIS
       find [-H] [-L] [-P] [-D debugopts] [-Olevel] [starting-point...] [expression]

DESCRIPTION
       This manual page documents the GNU version of find.  GNU find searches the directory tree rooted at each given
       starting-point by evaluating the given expression from left to right, according to  the  rules  of  precedence
       (see  section OPERATORS), until the outcome is known (the left hand side is false for and operations, true for
       or), at which point find moves on to the next file name.  If no starting-point is specified, `.' is assumed.

       If you are using find in an environment where security is important (for example if you are using it to search
       directories  that  are  writable by other users), you should read the `Security Considerations' chapter of the
       findutils documentation, which is called Finding Files and comes with findutils.  That document also  includes
       a  lot  more  detail and discussion than this manual page, so you may find it a more useful source of informa-
       tion.

OPTIONS
       The -H, -L and -P options control the treatment of symbolic links.  Command-line arguments following these are
       taken  to  be  names of files or directories to be examined, up to the first argument that begins with `-', or
       the argument `(' or `!'.  That argument and any following arguments are taken to be the expression  describing
       what is to be searched for.  If no paths are given, the current directory is used.  If no expression is given,
       the expression -print is used (but you should probably consider using -print0 instead, anyway).

       This manual page talks about `options' within the expression list.  These options  control  the  behaviour  of
       find  but  are  specified immediately after the last path name.  The five `real' options -H, -L, -P, -D and -O
```

The result

```
[ese-zhangych@login02 ~]$
[ese-zhangych@login02 ~]$ find /work/ese-zhangych/data_demo/data/elements/ -type f | wc -l
103
[ese-zhangych@login02 ~]$
```

1.5

Use man to learn

```
GNU(1)                                  User Commands                                  GNU(1)

NAME
       GNU diff - compare files line by line

SYNOPSIS
       diff [OPTION]... FILES

DESCRIPTION
       Compare FILES line by line.

       Mandatory arguments to long options are mandatory for short options too.

       --normal
              output a normal diff (the default)

       -q, --brief
              report only when files differ

       -s, --report-identical-files
              report when two files are the same

       -c, -C NUM, --context[=NUM]
              output NUM (default 3) lines of copied context

       -u, -U NUM, --unified[=NUM]
              output NUM (default 3) lines of unified context

       -e, --ed
```

The result

```
[ese-zhangych@login02 ~]$ diff data_demo/data/pdb/ethane.pdb data_demo/data/pdb/ethanol.pdb
1,11c1,12
< COMPND      ETHANE
< AUTHOR      DAVE WOODCOCK  95 12 18
< ATOM      1  C           1      -0.752   0.001  -0.141  1.00  0.00
< ATOM      2  C           1       0.752  -0.001   0.141  1.00  0.00
< ATOM      3  H           1      -1.158   0.991   0.070  1.00  0.00
< ATOM      4  H           1      -1.240  -0.737   0.496  1.00  0.00
< ATOM      5  H           1      -0.924  -0.249  -1.188  1.00  0.00
< ATOM      6  H           1       1.158  -0.991  -0.070  1.00  0.00
< ATOM      7  H           1       0.924   0.249   1.188  1.00  0.00
< ATOM      8  H           1       1.240   0.737  -0.496  1.00  0.00
< TER       9              1
---
> COMPND      ETHANOL
> AUTHOR      DAVE WOODCOCK  96 01 03
> ATOM      1  C           1      -0.426  -0.115  -0.147  1.00  0.00
> ATOM      2  O           1      -0.599   1.244  -0.481  1.00  0.00
> ATOM      3  H           1      -0.750  -0.738  -0.981  1.00  0.00
> ATOM      4  H           1      -1.022  -0.351   0.735  1.00  0.00
> ATOM      5  H           1      -1.642   1.434  -0.689  1.00  0.00
> ATOM      6  C           1       1.047  -0.383   0.147  1.00  0.00
> ATOM      7  H           1       1.370   0.240   0.981  1.00  0.00
> ATOM      8  H           1       1.642  -0.147  -0.735  1.00  0.00
> ATOM      9  H           1       1.180  -1.434   0.405  1.00  0.00
> TER      10              1
[ese-zhangych@login02 ~]$
```

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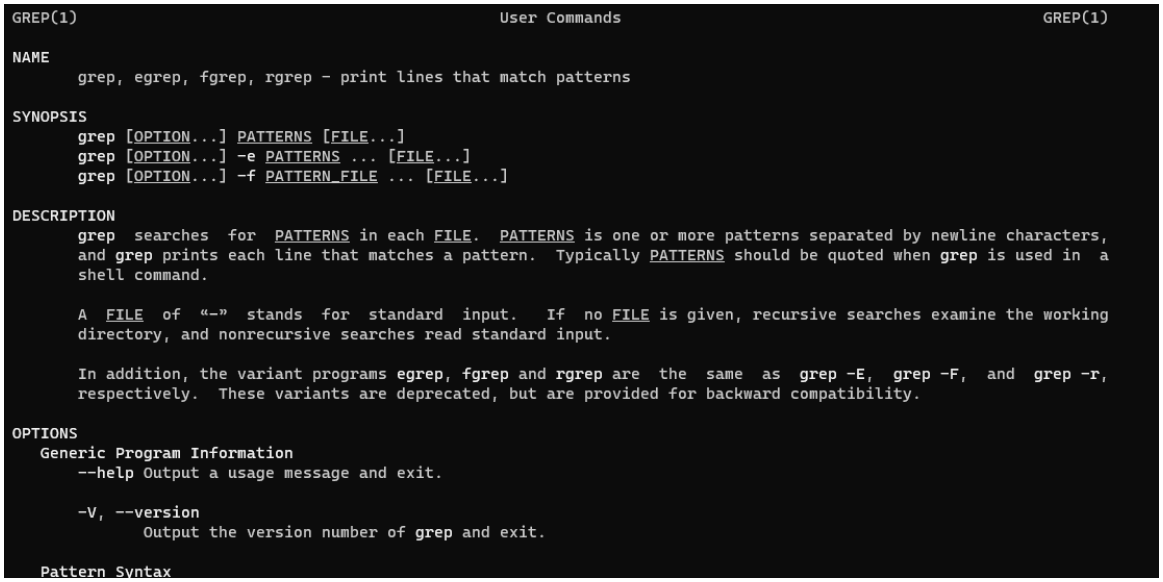
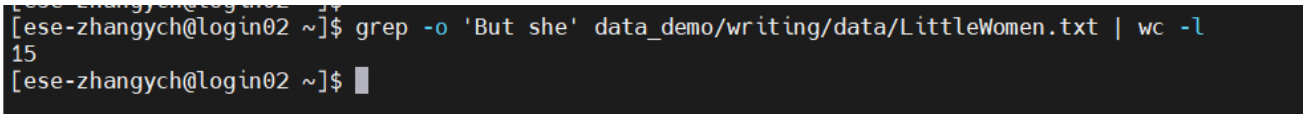
Use man to learn



```
GREP(1)                                    User Commands                                    GREP(1)

NAME
       grep, egrep, fgrep, rgrep - print lines that match patterns

SYNOPSIS
       grep [OPTION...] PATTERNS [FILE...]
       grep [OPTION...] -e PATTERNS ... [FILE...]
       grep [OPTION...] -f PATTERN_FILE ... [FILE...]

DESCRIPTION
       grep  searches  for  PATTERNS in each FILE.  PATTERNS is one or more patterns separated by newline characters,
       and grep prints each line that matches a pattern.  Typically PATTERNS should be quoted when grep is used in  a
       shell command.

       A  FILE  of  “-”  stands  for  standard  input.   If  no FILE is given, recursive searches examine the working
       directory, and nonrecursive searches read standard input.

       In addition, the variant programs egrep, fgrep and rgrep are  the  same  as  grep -E,  grep -F,  and  grep -r,
       respectively.  These variants are deprecated, but are provided for backward compatibility.

OPTIONS
   Generic Program Information
       --help Output a usage message and exit.

       -V, --version
              Output the version number of grep and exit.

   Pattern Syntax
```

The result



```
[ese-zhangych@login02 ~]$ grep -o 'But she' data_demo/writing/data/LittleWomen.txt | wc -l
15
[ese-zhangych@login02 ~]$
```

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Use man to learn

```
DU(1)                                      User Commands                                      DU(1)

NAME
       du - estimate file space usage

SYNOPSIS
       du [OPTION]... [FILE]...
       du [OPTION]... --files0-from=F

DESCRIPTION
       Summarize disk usage of the set of FILEs, recursively for directories.

       Mandatory arguments to long options are mandatory for short options too.

       -0, --null
              end each output line with NUL, not newline

       -a, --all
              write counts for all files, not just directories

       --apparent-size
              print  apparent sizes, rather than disk usage; although the apparent size is usually smaller, it may be
              larger due to holes in ('sparse') files, internal fragmentation, indirect blocks, and the like

       -B, --block-size=SIZE
              scale sizes by SIZE before printing them; e.g., '-BM' prints sizes in units  of  1,048,576  bytes;  see
              SIZE format below

       -b, --bytes
```

The result

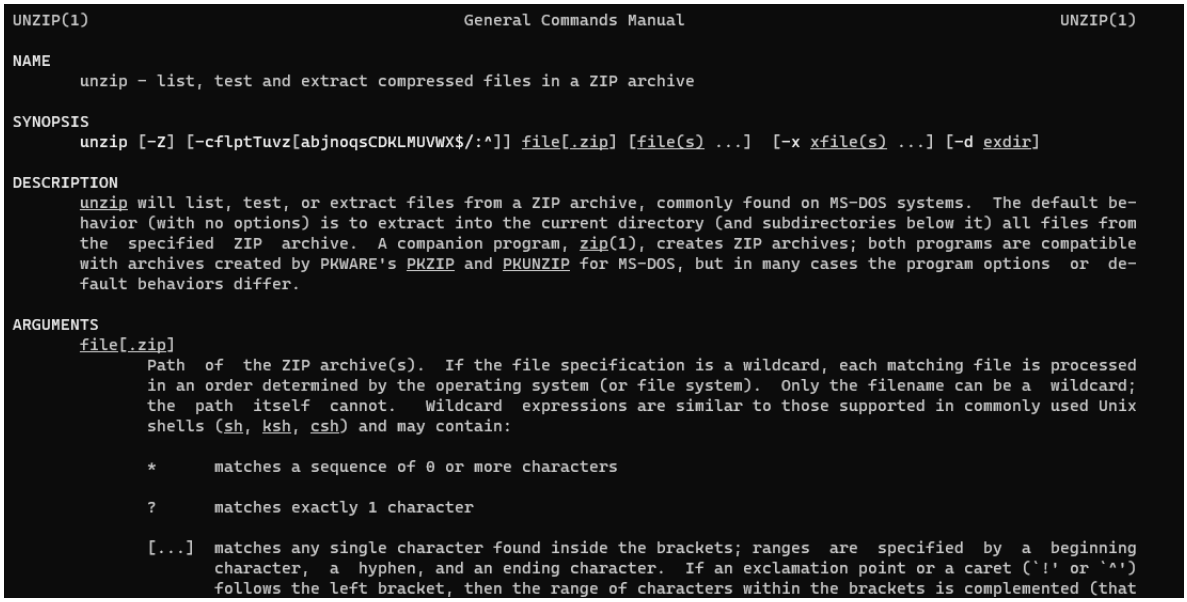
```
[ese-zhangych@login02 ~]$ du -h -c data_demo/data/
409K    data_demo/data/pdb
52K     data_demo/data/elements
1.0K    data_demo/data/animal-counts
721K    data_demo/data/
721K    total
[ese-zhangych@login02 ~]$
```

1.8

Use man to learn

```
CP(1)                                   User Commands                                   CP(1)

NAME
       cp - copy files and directories

SYNOPSIS
       cp [OPTION]... [-T] SOURCE DEST
       cp [OPTION]... SOURCE... DIRECTORY
       cp [OPTION]... -t DIRECTORY SOURCE...

DESCRIPTION
       Copy SOURCE to DEST, or multiple SOURCE(s) to DIRECTORY.

       Mandatory arguments to long options are mandatory for short options too.

       -a, --archive
              same as -dR --preserve=all

       --attributes-only
              don't copy the file data, just the attributes

       --backup[=CONTROL]
              make a backup of each existing destination file

       -b     like --backup but does not accept an argument

       --copy-contents
              copy contents of special files when recursive
```

```
ZIP(1)                                General Commands Manual                                ZIP(1)

NAME
       zip - package and compress (archive) files

SYNOPSIS
       zip  [-aABcdDeEfFghjklLmoqrRSTuvVwXyz!@$]  [--longoption  ...]  [-b  path] [-n suffixes] [-t date] [-tt date]
       [zipfile [file ...]]  [-xi list]

       zipcloak (see separate man page)

       zipnote (see separate man page)

       zipsplit (see separate man page)

       Note:  Command line processing in zip has been changed to support long options and handle all options and  ar-
       guments  more  consistently.  Some old command lines that depend on command line inconsistencies may no longer
       work.

DESCRIPTION
       zip is a compression and file packaging utility for Unix, VMS, MSDOS, OS/2, Windows  9x/NT/XP,  Minix,  Atari,
       Macintosh,  Amiga,  and  Acorn RISC OS.  It is analogous to a combination of the Unix commands tar(1) and com-
       press(1) and is compatible with PKZIP (Phil Katz's ZIP for MSDOS systems).

       A companion program (unzip(1)) unpacks zip archives.  The zip and unzip(1) programs  can  work  with  archives
       produced  by  PKZIP  (supporting  most PKZIP features up to PKZIP version 4.6), and PKZIP and PKUNZIP can work
       with archives produced by zip (with some exceptions, notably streamed archives, but recent changes in the  zip
       file  standard  may  facilitate better compatibility).  zip version 3.0 is compatible with PKZIP 2.04 and also
       supports the Zip64 extensions of PKZIP 4.5 which allow archives as well as files to exceed the previous  2  GB
```



```
UNZIP(1)                                General Commands Manual                                UNZIP(1)

NAME
       unzip - list, test and extract compressed files in a ZIP archive

SYNOPSIS
       unzip [-Z] [-cflptTuvz[abjnoqsCDKLMUVWX$/:^]] file[.zip] [file(s) ...]  [-x xfile(s) ...] [-d exdir]

DESCRIPTION
       unzip will list, test, or extract files from a ZIP archive, commonly found on MS-DOS systems.  The default be-
       havior (with no options) is to extract into the current directory (and subdirectories below it) all files from
       the  specified  ZIP  archive.  A companion program, zip(1), creates ZIP archives; both programs are compatible
       with archives created by PKWARE's PKZIP and PKUNZIP for MS-DOS, but in many cases the program options  or  de-
       fault behaviors differ.

ARGUMENTS
       file[.zip]
              Path  of  the ZIP archive(s).  If the file specification is a wildcard, each matching file is processed
              in an order determined by the operating system (or file system).  Only the filename can be a  wildcard;
              the  path  itself  cannot.   Wildcard  expressions are similar to those supported in commonly used Unix
              shells (sh, ksh, csh) and may contain:

              *      matches a sequence of 0 or more characters

              ?      matches exactly 1 character

              [...]  matches any single character found inside the brackets; ranges  are  specified  by  a  beginning
                     character,  a  hyphen, and an ending character.  If an exclamation point or a caret (`!' or `^')
                     follows the left bracket, then the range of characters within the brackets is complemented (that
```

The result

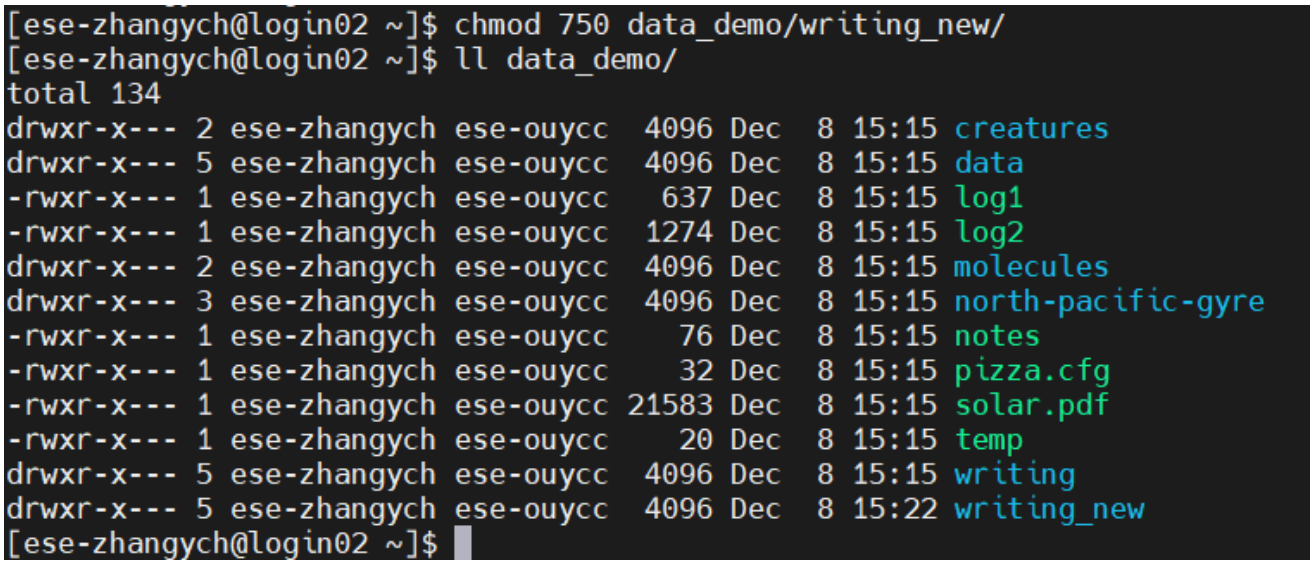
```
[ese-zhangych@login02 ~]$ cp -r data_demo/writing/ data_demo/writing_new/
[ese-zhangych@login02 ~]$ zip -r wn.zip data_demo/writing_new/*
  adding: data_demo/writing_new/data/ (stored 0%)
  adding: data_demo/writing_new/data/one.txt (deflated 53%)
  adding: data_demo/writing_new/data/LittleWomen.txt (deflated 61%)
  adding: data_demo/writing_new/data/two.txt (deflated 59%)
  adding: data_demo/writing_new/haiku.txt (deflated 29%)
  adding: data_demo/writing_new/thesis/ (stored 0%)
  adding: data_demo/writing_new/thesis/empty-draft.md (stored 0%)
  adding: data_demo/writing_new/tools/ (stored 0%)
  adding: data_demo/writing_new/tools/stats (stored 0%)
  adding: data_demo/writing_new/tools/old/ (stored 0%)
  adding: data_demo/writing_new/tools/old/oldtool (stored 0%)
  adding: data_demo/writing_new/tools/format (deflated 13%)
[ese-zhangych@login02 ~]$ unzip wn.zip -d test/
Archive:  wn.zip
   creating: test/data_demo/writing_new/data/
  inflating: test/data_demo/writing_new/data/one.txt
  inflating: test/data_demo/writing_new/data/LittleWomen.txt
  inflating: test/data_demo/writing_new/data/two.txt
  inflating: test/data_demo/writing_new/haiku.txt
   creating: test/data_demo/writing_new/thesis/
 extracting: test/data_demo/writing_new/thesis/empty-draft.md
   creating: test/data_demo/writing_new/tools/
 extracting: test/data_demo/writing_new/tools/stats
   creating: test/data_demo/writing_new/tools/old/
 extracting: test/data_demo/writing_new/tools/old/oldtool
  inflating: test/data_demo/writing_new/tools/format
[ese-zhangych@login02 ~]$
```

1.9

Use man to learn

```
CHMOD(1)                          User Commands                          CHMOD(1)

NAME
       chmod - change file mode bits

SYNOPSIS
       chmod [OPTION]... MODE[,MODE]... FILE...
       chmod [OPTION]... OCTAL-MODE FILE...
       chmod [OPTION]... --reference=RFILE FILE...

DESCRIPTION
       This  manual page documents the GNU version of chmod.  chmod changes the file mode bits of each given file ac-
       cording to mode, which can be either a symbolic representation of changes to make, or an octal  number  repre-
       senting the bit pattern for the new mode bits.

       The  format  of  a  symbolic mode is [ugoa...][[-+=][perms...]...], where perms is either zero or more letters
       from the set rwxXst, or a single letter from the set ugo.  Multiple symbolic modes can be given, separated  by
       commas.

       A  combination of the letters ugoa controls which users' access to the file will be changed: the user who owns
       it (u), other users in the file's group (g), other users not in the file's group (o), or all  users  (a).   If
       none  of  these  are given, the effect is as if (a) were given, but bits that are set in the umask are not af-
       fected.

       The operator + causes the selected file mode bits to be added to the existing file mode bits of each  file;  -
       causes them to be removed; and = causes them to be added and causes unmentioned bits to be removed except that
       a directory's unmentioned set user and group ID bits are not affected.

       The letters rwxXst select file mode bits for the affected users: read (r), write (w), execute (or  search  for
```

The result



```
[ese-zhangych@login02 ~]$ chmod 750 data_demo/writing_new/
[ese-zhangych@login02 ~]$ ll data_demo/
total 134
drwxr-x--- 2 ese-zhangych ese-ouycc  4096 Dec  8 15:15 creatures
drwxr-x--- 5 ese-zhangych ese-ouycc  4096 Dec  8 15:15 data
-rwxr-x--- 1 ese-zhangych ese-ouycc   637 Dec  8 15:15 log1
-rwxr-x--- 1 ese-zhangych ese-ouycc  1274 Dec  8 15:15 log2
drwxr-x--- 2 ese-zhangych ese-ouycc  4096 Dec  8 15:15 molecules
drwxr-x--- 3 ese-zhangych ese-ouycc  4096 Dec  8 15:15 north-pacific-gyre
-rwxr-x--- 1 ese-zhangych ese-ouycc    76 Dec  8 15:15 notes
-rwxr-x--- 1 ese-zhangych ese-ouycc    32 Dec  8 15:15 pizza.cfg
-rwxr-x--- 1 ese-zhangych ese-ouycc 21583 Dec  8 15:15 solar.pdf
-rwxr-x--- 1 ese-zhangych ese-ouycc    20 Dec  8 15:15 temp
drwxr-x--- 5 ese-zhangych ese-ouycc  4096 Dec  8 15:15 writing
drwxr-x--- 5 ese-zhangych ese-ouycc  4096 Dec  8 15:22 writing_new
[ese-zhangych@login02 ~]$
```

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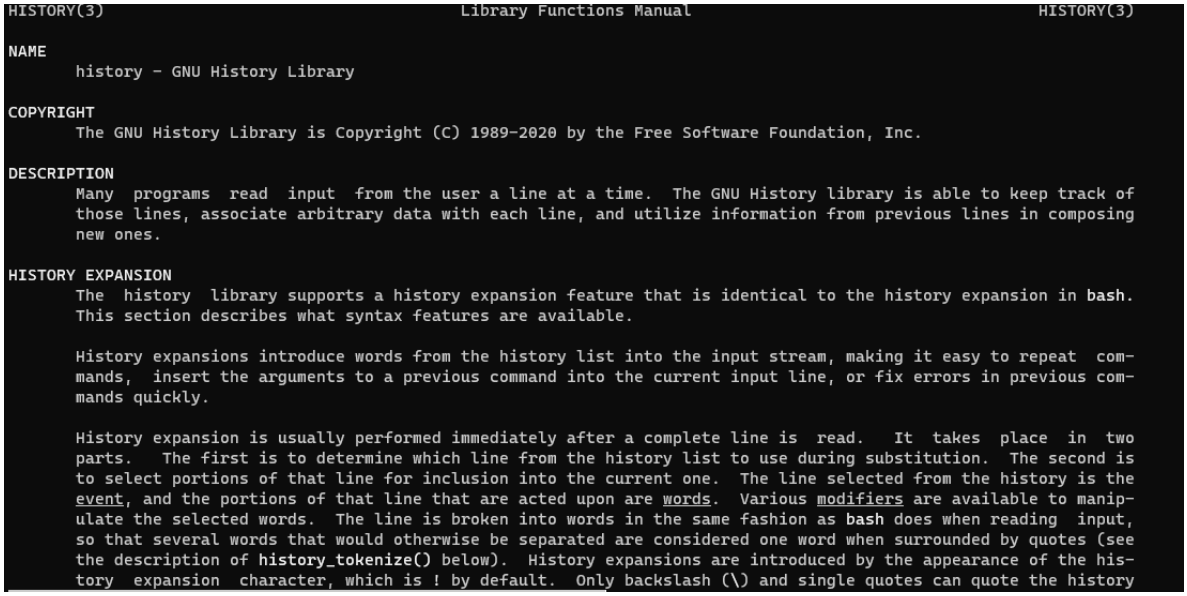
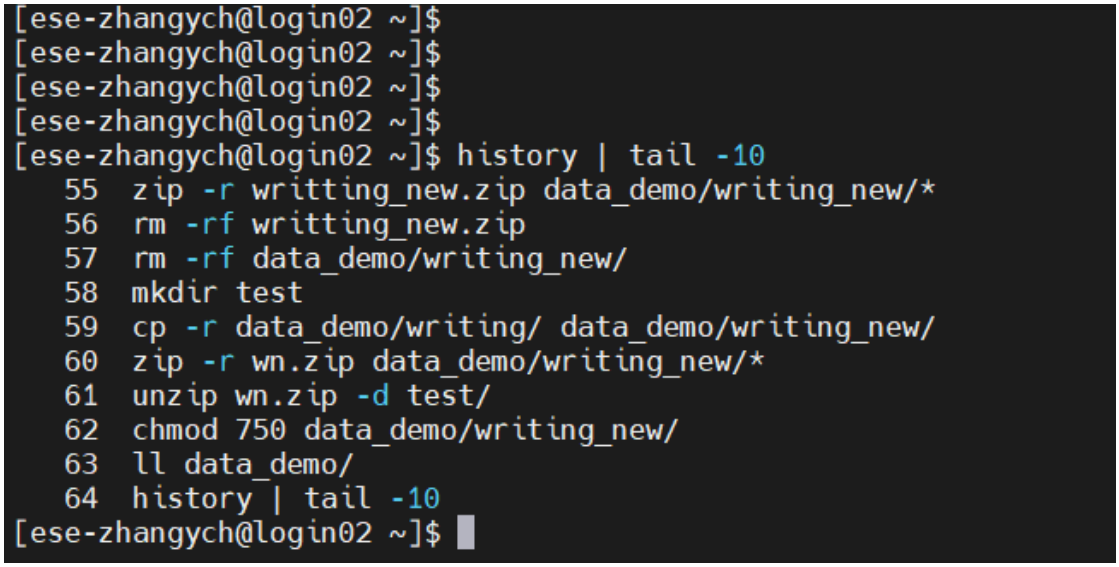
Use man to learn



```
HISTORY(3)                  Library Functions Manual                  HISTORY(3)

NAME
       history - GNU History Library

COPYRIGHT
       The GNU History Library is Copyright (C) 1989-2020 by the Free Software Foundation, Inc.

DESCRIPTION
       Many  programs  read  input  from the user a line at a time.  The GNU History library is able to keep track of
       those lines, associate arbitrary data with each line, and utilize information from previous lines in composing
       new ones.

HISTORY EXPANSION
       The  history  library supports a history expansion feature that is identical to the history expansion in bash.
       This section describes what syntax features are available.

       History expansions introduce words from the history list into the input stream, making it easy to repeat  com-
       mands,  insert the arguments to a previous command into the current input line, or fix errors in previous com-
       mands quickly.

       History expansion is usually performed immediately after a complete line is  read.   It  takes  place  in  two
       parts.   The first is to determine which line from the history list to use during substitution.  The second is
       to select portions of that line for inclusion into the current one.  The line selected from the history is the
       event, and the portions of that line that are acted upon are words.  Various modifiers are available to manip-
       ulate the selected words.  The line is broken into words in the same fashion as bash does when reading  input,
       so that several words that would otherwise be separated are considered one word when surrounded by quotes (see
       the description of history_tokenize() below).  History expansions are introduced by the appearance of the his-
       tory  expansion  character, which is ! by default.  Only backslash (\) and single quotes can quote the history
```

The result



```
[ese-zhangych@login02 ~]$
[ese-zhangych@login02 ~]$
[ese-zhangych@login02 ~]$
[ese-zhangych@login02 ~]$
[ese-zhangych@login02 ~]$ history | tail -10
   55  zip -r writting_new.zip data_demo/writing_new/*
   56  rm -rf writting_new.zip
   57  rm -rf data_demo/writing_new/
   58  mkdir test
   59  cp -r data_demo/writing/ data_demo/writing_new/
   60  zip -r wn.zip data_demo/writing_new/*
   61  unzip wn.zip -d test/
   62  chmod 750 data_demo/writing_new/
   63  ll data_demo/
   64  history | tail -10
[ese-zhangych@login02 ~]$
```

2

the shell script:

```
#!/bin/sh
for f in ~/data_demo/data/pdb/*.pdb; do
echo "$f"
done
"p2.sh" 4L, 65C
```

the result:

```
[ese-zhangych@login02 ~]$ bash p2.sh
/work/ese-zhangych/data_demo/data/pdb/aldrin.pdb
/work/ese-zhangych/data_demo/data/pdb/ammonia.pdb
/work/ese-zhangych/data_demo/data/pdb/ascorbic-acid.pdb
/work/ese-zhangych/data_demo/data/pdb/benzaldehyde.pdb
/work/ese-zhangych/data_demo/data/pdb/camphene.pdb
/work/ese-zhangych/data_demo/data/pdb/cholesterol.pdb
/work/ese-zhangych/data_demo/data/pdb/cinnamaldehyde.pdb
/work/ese-zhangych/data_demo/data/pdb/citronellal.pdb
/work/ese-zhangych/data_demo/data/pdb/codeine.pdb
/work/ese-zhangych/data_demo/data/pdb/cubane.pdb
/work/ese-zhangych/data_demo/data/pdb/cyclobutane.pdb
/work/ese-zhangych/data_demo/data/pdb/cyclohexanol.pdb
/work/ese-zhangych/data_demo/data/pdb/cyclopropane.pdb
/work/ese-zhangych/data_demo/data/pdb/ethane.pdb
/work/ese-zhangych/data_demo/data/pdb/ethanol.pdb
/work/ese-zhangych/data_demo/data/pdb/ethylcyclohexane.pdb
/work/ese-zhangych/data_demo/data/pdb/glycol.pdb
/work/ese-zhangych/data_demo/data/pdb/heme.pdb
/work/ese-zhangych/data_demo/data/pdb/lactic-acid.pdb
/work/ese-zhangych/data_demo/data/pdb/lactose.pdb
/work/ese-zhangych/data_demo/data/pdb/lanoxin.pdb
/work/ese-zhangych/data_demo/data/pdb/lsd.pdb
/work/ese-zhangych/data_demo/data/pdb/maltose.pdb
/work/ese-zhangych/data_demo/data/pdb/menthol.pdb
/work/ese-zhangych/data_demo/data/pdb/methane.pdb
/work/ese-zhangych/data_demo/data/pdb/methanol.pdb
/work/ese-zhangych/data_demo/data/pdb/mint.pdb
/work/ese-zhangych/data_demo/data/pdb/morphine.pdb
/work/ese-zhangych/data_demo/data/pdb/mustard.pdb
/work/ese-zhangych/data_demo/data/pdb/nerol.pdb
/work/ese-zhangych/data_demo/data/pdb/norethindrone.pdb
/work/ese-zhangych/data_demo/data/pdb/octane.pdb
/work/ese-zhangych/data_demo/data/pdb/pentane.pdb
/work/ese-zhangych/data_demo/data/pdb/piperine.pdb
/work/ese-zhangych/data_demo/data/pdb/propane.pdb
/work/ese-zhangych/data_demo/data/pdb/pyridoxal.pdb
/work/ese-zhangych/data_demo/data/pdb/quinine.pdb
/work/ese-zhangych/data_demo/data/pdb/strychnine.pdb
/work/ese-zhangych/data_demo/data/pdb/styrene.pdb
/work/ese-zhangych/data_demo/data/pdb/sucrose.pdb
```