# 8.3 File Analysis

## 8.3.1 Regular Expressions

## **Regular Expressions**

A **regular expression (regex)** is a sequence of characters that define a pattern, which can be used for searching text. The most basic regular expression is a word. To illustrate the concept of regular expressions, patterns and matches of regular expressions to the following text will be shown:

Apples are a fruit. An apple a day keeps the doctor away.

To search this piece of text for occurrences of the word "apple" in lower case, the regular expression would simply be "apple". The matches of the regular expression are shown in the text below:

Apples are a fruit. An apple a day keeps the doctor away.

A more complex regular expression could search for the word "apple" and match all occurrences that start with an upper or lower case "A". The regular expression for this task is "[Aa]pple". The matches are shown in the text below:

Apples are a fruit. An apple a day keeps the doctor away.

As you can see, the whole word does not need to match the regex in order for there to be a match. A regular expression can be written to match any 5-letter character sequence containing no spaces, numbers, or symbols. The regular expression for this task is " $[A-Za-z]{5}$ ". The matches are shown in the text below:

Apples are a fruit. An apple a day keeps the doctor away.

The rules of writing a regular expression are complex. In this course, regular expressions will not be covered in depth, further information can be found online

The two basic aspects of writing a regular expression are defining what to match and how many times to match it. The following tables describe some of the basic symbols for writing regular expressions:

## **Representations of Multiple Characters**

0-9	Any Number
A-Z	Any uppercase letters
a-z	Any lowercase letters
•	Any character

#### Quantification of Occurrences

*	Zero or more occurrences
+	One or more occurrences
?	Zero or one occurrence
{N}	N occurrences

In regular expressions, square brackets [] are used to denote a set of characters to match.

To understand how to put these symbols into a regular expression, below are descriptions of patterns that can be used to find matches, along with the regular expression.

Example 1: match the number 8004

**Pattern:** one occurrence of the number 8, followed by two occurrences of the

number 0, followed by one occurrence of the number 4.

Regular expression: 8004

Example 2: Match any number from 8000-8999

Pattern: one occurrence of the number 8, followed by 3 occurrences of any number

from 0 to 9.

**Regular expression:** 8 [ 0 – 9 ] { 3 }

**Example 3:** Match any word that starts with a capital letter

Pattern: one occurrence of any capital letter from "A" to "Z", followed by zero or

more occurrences of any lowercase letter from "a" to "z".

**Regular expression:** [A-Z][a-z]\*

In example 1, the pattern needs to describe an exact match to the number 8004, thus the regular expression is the exact number. Any time an exact set of characters is being matched the regular expression is simply the set of characters.

In example 2, [0-9] represents the set of numbers. This is directly followed by  $\{3\}$ , indicating that three occurrences of characters that belong to the set [0-9] need to be present for a match. The symbols used to define the quantification of occurrences only apply to the character or set of characters directly to the left of the quantification symbol. For example, the regular expression ab+ matches one "a" followed by one or more "b"s (+ indicates 1 or more occurrences). The expression ab+ will match ab or abbbb but will not match aaab.

In example 3, [A-Z] represents the set of capital letters and [a-z] represents the set of lowercase letters. [A-Z] is not followed by any symbols defining the expected number of occurrences meaning that exactly one occurrence is expected. [a-z] is followed by an asterisk (\*) indicating that zero or more occurrences of lowercase letters can be present. The asterisk is not applied to the set of uppercase letters as it is only applied to the set directly to the left.

Below are three more examples of regular expressions along with a subset of possible matches and non-matches, these examples are not exhaustive, there are hundreds to thousands of possible matches for each regular expression and even more non-matches.

**Regular expression:** [xyz]+

The regular expression will match one or more occurrence of the letters "x", "y", and "z". By putting the letters within square brackets, it becomes a set. Therefore, one or more occurrences of any combination of the letters within the set will match.

Matches: xxxx, yyy, zzzzz, zzyx, xyz, x, y, z

Non-matches: aazzyx, abc, ccyc, dd

**Regular expression:** pt [A-Za-z0-9]\*

The regular expression will match "pt\_" followed by 0 or more occurrences of uppercase letters, lowercase letters, and numbers. Multiple ranges can put into one set.

```
Matches: pt_8xdC7, pt_, pt_100, pt_A, pt_onehundred Non-matches: pt89cD, t_8xdC7, pt_one_hundred, 100
```

```
Regular expression: [0-9]\{2\} [A-Z]?
```

The regular expression will match two numbers, followed by an underscore "\_",

followed by 0 or 1 occurrence of an uppercase letter.

```
Matches: 13_C, 78_, 94_X, 00_
Non-matches: 3_C, 13C, 94_XB, C_13
```

## The grep Command

Regular expressions can be used with the grep command.

```
grep [OPTION]... PATTERN [FILE]...
```

The grep command searches for matches to a specified pattern in a file. The PATTERN argument is a regular expression.

The directory Week.8/8.3.File.Analysis contains a file called test\_grep.txt with 5 lines, each containing 4 lowercase letters:

```
j:~$ cd Week.8/8.3.File.Analysis
j:~/Week.8/8.3.File.Analysis$ cat test_grep.txt
aaaa
aazz
yyxz
xxxx
abcd
j:~/Week.8/8.3.File.Analysis$
```

By default, the grep command will return all lines that contain a match to the PATTERN anywhere in the line. For example, if the pattern is "a", all lines containing a single occurrence of the letter "a" will be output.

```
j:~/Week.8/8.3.File.Analysis$ grep "a" test_grep.txt
aaaa
aazz
abcd
j:~/Week.8/8.3.File.Analysis$
```

Comparing back to the full contents of the file above, the  $1^{st}$ ,  $2^{nd}$ , and  $5^{th}$  lines contain at least one lowercase "a" and were output.

The grep command has many useful options. One important option is the -P (--perl-regexp) option which allows one to use more complex regular expressions. Some special regular expression characters are not recognized by standard grep, but are recognized by Perl regular expressions, including: ?, +,  $\{$ ,  $\t$ .

```
-P, --perl-regexp PATTERNS are Perl regular expression
```

To search for matches to the regular expression "[xyz]+", the -P option is required. As a reminder, this regular expression will match one or more occurrence of the letters "x", "y", and "z".

```
j:~/Week.8/8.3.File.Analysis$ grep -P "[xyz]+" test_grep.txt
aazz
yyxz
xxxx
j:~/Week.8/8.3.File.Analysis$
```

Notice that because grep searches for matches to the pattern within each line, the line aazz is output because zz matches the pattern.

The −o option returns only the part of the line that matches the pattern.

```
-o, --only-matching show only nonempty parts of lines that match
```

In 8.2.1 using multiple options is introduced. For a command that has the options -a, -b, and -c, if none of the options take arguments, there are two ways to use the options together:

```
command -a -b -c ARGUMENTS command -abc ARGUMENTS
```

When multiple options without arguments are used they can be combined without spaces after a single hyphen.

To output only the parts of test\_grep.txt that match the pattern "[xyz]+", both the – P and the –O option are required:

```
j:~/Week.8/8.3.File.Analysis$ grep -oP "[xyz]+" test_grep.txt
zz
yyxz
xxxx
j:~/Week.8/8.3.File.Analysis$
```

Using the −o option, only the zz from the line containing aazz is output.

The -x option only returns a line with a match if the whole line matches the pattern.

```
-x, --line-regexp match only whole lines
```

Using the -x option, the line containing aazz is not returned at all as only part of the line matches the pattern.

```
j:~/Week.8/8.3.File.Analysis$ grep -xP "[xyz]+" test_grep.txt
yyxz
xxxx
j:~/Week.8/8.3.File.Analysis$
```

There are many other options to use with grep, including:

```
-n, --line-number print line number with output lines
-v, --invert-match select non-matching lines
```

Output lines that match the pattern "[xyz]+" along with their line numbers:

```
j:~/Week.8/8.3.File.Analysis$ grep -nP "[xyz]+" test_grep.txt
2:aazz
3:yyxz
4:xxxx
j:~/Week.8/8.3.File.Analysis$
```

Output lines that DO NOT match the pattern "[xyz]+" along with their line numbers:

```
j:~/Week.8/8.3.File.Analysis$ grep -nvP "[xyz]+" test_grep.txt
1:aaaa
5:abcd
j:~/Week.8/8.3.File.Analysis$
```

Combining the -n and -o options will return all the unique occurrences of a pattern along with their line numbers. For example, using the pattern "a":

```
j:~/Week.8/8.3.File.Analysis$ grep -no "a" test_grep.txt
1:a
1:a
1:a
2:a
2:a
5:a
j:~/Week.8/8.3.File.Analysis$
```

There are four matches to "a" on line 1, two on line 2, and one on line 5.

#### Patterns in Biological Data

The grep command is very useful for gathering information from biological data files in the command line. For example, grep can be used to learn about the tab delimited file cancer\_pts.txt. The file has 4 columns: patient.ID, sex, age, and cancer.type.

```
j:~/Week.8/8.3.File.Analysis$ head cancer pts.txt
patient.ID
               sex
                       age
                               cancer.type
DO49528 Male
               54
                       Acute myeloid leukemia
DO49529 Male
               54
                       Acute myeloid leukemia
DO49531 Male
               49
                       Acute myeloid leukemia
DO49532 Female 39
                       Acute myeloid leukemia
               39
DO49533 Male
                       Acute myeloid leukemia
DO49536 Male
               46
                       Acute myeloid leukemia
```

```
DO49537 Female 50 Acute myeloid leukemia
DO52732 Female 75 Acute myeloid leukemia
DO52739 Female 66 Acute myeloid leukemia
j:~/Week.8/8.3.File.Analysis$
```

For example, all the lines in cancer\_pts.txt that contain the word neoplasm (capitalized or all lowercase) can be found using the regular expression "[Nn]eoplasm":

```
j:~/Week.8/8.3.File.Analysis$ grep "[Nn]eoplasm" cancer pts.txt | head
DO49137 Female 67
                       Intraductal papillary mucinous neoplasm
DO49172 Female 60
                       Intraductal papillary mucinous neoplasm
DO33488 Male
               61
                       Intraductal papillary mucinous neoplasm
DO6428 Female 78
                       Mature B-Cell Neoplasms
                       Mature B-Cell Neoplasms
DO7018 Male
               60
               16
DO27847 Male
                       Mature B-Cell Neoplasms
DO51967 Female 54
                       Mature B-Cell Neoplasms
DO51989 Female 61
                       Mature B-Cell Neoplasms
DO51992 Female 42
                       Mature B-Cell Neoplasms
DO52651 Female 72
                       Mature B-Cell Neoplasms
j:~/Week.8/8.3.File.Analysis$
```

The output contains patients with the cancer type "Intraductal papillary mucinous neoplasm", as well as patients with the cancer type "Mature B-Cell Neoplasms". The <code>[Nn]</code> in the regular expression allows the command to return patients with both types of cancer.

In the output of the grep command above, patients IDs vary in length. Each starts with the letters "D0" followed by numbers. The regular expression "D0 [0-9] {3}" will retrieve all the lines containing D0 followed by 3 numbers. Note that use of curly braces requires the -P option.

```
j:~/Week.8/8.3.File.Analysis$ grep -P "DO[0-9]{3}" cancer pts.txt | head
DO49528 Male
               54
                      Acute myeloid leukemia
               54
DO49529 Male
                      Acute myeloid leukemia
DO49531 Male 49
                      Acute myeloid leukemia
DO49532 Female 39
                      Acute myeloid leukemia
               39
DO49533 Male
                      Acute myeloid leukemia
DO49536 Male
               46
                      Acute myeloid leukemia
DO49537 Female 50
                      Acute myeloid leukemia
DO52732 Female 75
                       Acute myeloid leukemia
DO52739 Female
               66
                       Acute myeloid leukemia
               45
DO52740 Male
                       Acute myeloid leukemia
j:~/Week.8/8.3.File.Analysis$
```

The patient IDs in the output do not contain only three numbers. This is because grep with the pattern "DO[0-9] {3}" will return lines that contain the pattern anywhere in the line, even if it is followed directly by more numbers. To get the lines that have patient IDs with ONLY three numbers there are two possibilities.

Firstly, because this is a tab-delimited file, the patient ID will always be followed by a tab. Extending the regular expression "DO[0-9]{3}\t" will find "DO", followed by three letters, followed directly by a tab:

```
j:~/Week.8/8.3.File.Analysis$ grep -P "DO[0-9]{3}\t" cancer pts.txt |
head
DO472
                53
        Male
                        Bladder Cancer
        Male
                79
DO477
                        Bladder Cancer
                34
        Male
                        Bladder Cancer
DO479
DO483
        Female
                67
                        Bladder Cancer
DO496
        Female
                53
                        Bladder Cancer
DO498
        Male
                84
                        Bladder Cancer
DO522
        Female
                64
                        Bladder Cancer
D0536
        Male
                65
                        Bladder Cancer
                57
DO548
        Male
                        Bladder Cancer
DO555
        Female 79
                        Bladder Cancer
j:~/Week.8/8.3.File.Analysis$
```

Secondly, one can use the same pattern as was used originally ("DO[0-9]  $\{3\}$ ") along with the grep option -w:

```
-w, --word-regexp match only whole words
```

This option only outputs matches that are preceded by a space, a tab, or the beginning of a line and followed by a space, a tab, or the end of a line.

```
j:~/Week.8/8.3.File.Analysis$ grep -wP "DO[0-9]{3}" cancer_pts.txt |
head
DO472
        Male
                53
                        Bladder Cancer
DO477
        Male
                79
                        Bladder Cancer
                34
DO479
        Male
                        Bladder Cancer
DO483
        Female
                67
                        Bladder Cancer
DO496
        Female
                53
                        Bladder Cancer
DO498
        Male
                84
                        Bladder Cancer
DO522
        Female
                64
                        Bladder Cancer
DO536
        Male
                65
                        Bladder Cancer
DO548
        Male
                57
                        Bladder Cancer
        Female 79
DO555
                        Bladder Cancer
j:~/Week.8/8.3.File.Analysis$
```

## 8.3.2 Counting Occurrences

### **Line Counts**

The wc command counts the number of lines, words, and/or bytes in a file.

```
wc [OPTION]... [FILE]...
```

Used without options, it returns the counts for lines, words, and bytes, in that order:

```
j:~/Week.8/8.3.File.Analysis$ wc cancer_pts.txt
2344 12318 86042 cancer_pts.txt
j:~/Week.8/8.3.File.Analysis$
```

The file cancer\_pts.txt has 2,344 lines, 12,318 words, and 86042 characters. Remember that the number of bytes is the number of characters including line ends, spaces, and tabs.

The wc command can also be used with one of the following options to only output the number of bytes, words, or lines:

```
-c, --bytes print the byte counts
-m, --chars print the character counts
-l, --lines print the newline counts

j:~/Week.8/8.3.File.Analysis$ wc -l cancer pts.txt
```

```
2344 cancer_pts.txt
j:~/Week.8/8.3.File.Analysis$
```

Used with the wildcard, the number of lines in all files in the PWD that end with .txt can be output, as well as the total number of lines in all the .txt files:

```
j:~/Week.8/8.3.File.Analysis$ wc -l *.txt
2344 cancer_pts.txt
5 test_grep.txt
2349 total
j:~/Week.8/8.3.File.Analysis$
```

By piping the output of a grep command to the wc command, the number of lines containing a specific pattern in a file can be identified. For example, count the number of lines in cancer pts.txt that contain the word "Glioma":

```
j:~/Week.8/8.3.File.Analysis$ grep "Glioma" cancer_pts.txt | wc -1
48
j:~/Week.8/8.3.File.Analysis$
```

By piping the output of a grep command to the wc command, the number of lines containing a specific pattern in a file can be identified. For example, count the number of lines in cancer pts.txt that contain the word "Glioma":

```
j:~/Week.8/8.3.File.Analysis$ grep "Glioma" cancer_pts.txt | wc -1
48
j:~/Week.8/8.3.File.Analysis$
```

### **Sorting Files**

The sort command will sort a file based on a full line or one more fields (columns).

```
sort [OPTION]... [FILE]...
```

By default, the sort command sorts a file based on the full line in increasing alphabetical order. For example, sort the cancer pts.txt file.

The -r option tells the sort command to sort in reverse (decreasing) order:

```
-r, --reverse reverse the result of comparisons
```

```
j:~/Week.8/8.3.File.Analysis$ sort -r cancer pts.txt | head -n 5
patient.ID
               sex
                       age
                               cancer.type
DO9940 Female
               78
                       Colorectal Cancer
       Male
               75
DO9876
                       Colorectal Cancer
DO9788 Female 73
                       Colorectal Cancer
DO9732 Female 78
                       Colorectal Cancer
j:~/Week.8/8.3.File.Analysis$
```

The -k option tells the sort command to sort based on a "key". This is the number of the field to sort on.

```
-k, --key=KEYDEF sort via a key; KEYDEF gives location and type
```

For example, to sort the <code>cancer\_pts.txt</code> file based on the patient cancer type, the -k option is used with the argument 4, because cancer type is in the  $4^{th}$  column/field.

```
j:~/Week.8/8.3.File.Analysis$ sort -k 4 cancer pts.txt | head -n 5
                               Acute myeloid leukemia
DO221548
               Female 35
DO49528 Male
               54
                        Acute myeloid leukemia
DO49529 Male
               54
                       Acute myeloid leukemia
DO49531 Male
               49
                        Acute myeloid leukemia
DO49532 Female 39
                       Acute myeloid leukemia
j:~/Week.8/8.3.File.Analysis$
```

By default, sort uses alphabetical order which can cause problems when sorting with numbers. Although 9 is a smaller number than 10, in alphabetical order the number 10 comes before the number 9, because it begins with 1. The cancer\_pts.txt file contains 77 patients under the age of 10, however, when sorted by column 3 the output shows 10-year-old patients first:

This can be corrected by using the -g option:

```
-g, --general-numeric-sort compare according to general numerical value
```

This compares numbers based on numerical value instead of alphabetical value. Sorting the cancer pts.txt file on field 3 again with the -g option changes the output.

```
j:~/Week.8/8.3.File.Analysis$ sort -g -k 3 cancer_pts.txt | head -n 5
D01013 Female NA Breast Cancer
D01014 Female NA Breast Cancer
D01015 Female NA Breast Cancer
D01016 Female NA Breast Cancer
D01076 Female NA Breast Cancer
j:~/Week.8/8.3.File.Analysis$
```

A number of patients do not have an associated age and instead have an "NA" value in place of the patient age. Using the grep command with the  $\neg v$  option we can remove these patients from the output.

```
j:~/Week.8/8.3.File.Analysis$ sort -g -k 3 cancer pts.txt | grep -v "NA"
| head -n 5
patient.ID
               sex
                       age
                              cancer.type
               1
D035566 Male
                       Medulloblastoma
DO35574 Female 1
                       Medulloblastoma
               2
                       Medulloblastoma
DO35620 Male
DO35622 Male
            2
                       Embryonal Tumor
j:~/Week.8/8.3.File.Analysis$
```

Now patients are in order of age, starting with 1. The patients can also be output in reverse order of age:

### **Unique Lines**

The uniq command outputs unique adjacent lines.

```
uniq [OPTION]... [FILE]...
```

The uniq command outputs a single line for every set of adjacent lines that are exactly the same. If applied to a file containing the following lines:

aaaaaa bbbbbb bbbbbb bbbbbb

The uniq command would output:

aaaaaa bbbbbb

Each unique line in the file is output. However, if the uniq command was applied to a file containing the following lines:

aaaaaa bbbbbb bbbbbb bbbbb aaaaaa

The uniq command would output:

aaaaaa bbbbbb aaaaaa

This is because the in the second file, the two lines containing aaaaaa are not adjacent to one another. For example, these are the first 10 lines of the  $2^{nd}$  column of cancer pts.txt:

```
j:~/Week.8/8.3.File.Analysis$ cut -f 2 cancer_pts.txt | head
sex
Male
Male
Male
Female
Male
Female
Female
Female
Female
Female
j:~/Week.8/8.3.File.Analysis$
```

Only three unique values are present: "sex", "Male", and "Female". Applying the uniq command to these 10 lines:

```
j:~/Week.8/8.3.File.Analysis$ cut -f 2 cancer_pts.txt | head | uniq
sex
Male
Female
Male
Female
j:~/Week.8/8.3.File.Analysis$
```

To prevent this issue, the uniq command should always be used with the sort command:

```
j:~/Week.8/8.3.File.Analysis$ cut -f 2 cancer_pts.txt | head | sort |
uniq
Female
Male
sex
j:~/Week.8/8.3.File.Analysis$
```

When the sort command is used all of the identical lines will be adjacent to one another.

The -c option tells the uniq command to count the number of lines that have each unique value:

```
-c, --count prefix lines by the number of occurrences
```

For example, to get the number of patients in <code>cancer\_pts.txt</code> that have each type of cancer, the 4<sup>th</sup> column (cancer.type) can be extracted with the <code>cut</code> command, then the <code>sort</code> and <code>uniq</code> commands can be applied:

```
j:~/Week.8/8.3.File.Analysis$ cut -f 4 cancer pts.txt | sort | uniq -c
     13 Acute myeloid leukemia
    23 Bladder Cancer
    47 Bone Cancer
    209 Breast Cancer
     1 cancer.type
    20 Cervical Cancer
    52 Colorectal Cancer
    120 Embryonal Tumor
     20 Endometrial Cancer
    165 Esophagogastric Cancer
    13 Essential Thrombocythemia
    48 Glioma
    56 Head and Neck Cancer
    348 Hepatobiliary Cancer
     6 Intraductal papillary mucinous neoplasm
    38 Lung Cancer
     1 Mastocytosis
    103 Mature B-cell lymphoma
    93 Mature B-Cell Neoplasms
    21 Medulloblastoma
    11 Myelodysplastic/Myeloproliferative Neoplasms
    46 Non-Small Cell Lung Cancer
     99 Ovarian Cancer
```

```
305 Pancreatic Cancer
194 Prostate Cancer
186 Renal Cell Carcinoma
34 Soft Tissue Sarcoma
48 Thyroid Cancer
24 Uterine Endometrioid Carcinoma
j:~/Week.8/8.3.File.Analysis$
```

Similarly, the number of patients of each sex can counted:

```
j:~/Week.8/8.3.File.Analysis$ cut -f 2 cancer_pts.txt | sort | uniq -c
    1053 Female
    1290 Male
    1 sex
j:~/Week.8/8.3.File.Analysis$
```

Note that in the last two commands, a line with the value of the header file was returned (cancer.type & sex). The tail command can be used to get all lines in a file after the first line without having to calculate the number of lines in a file. The following command returns every line in a file except for the first line:

```
tail -n +2 FILE
```

Re-running the above command to get the number of patients of each sex with the tail command, the header row can be ignored:

```
j:~/Week.8/8.3.File.Analysis$ tail -n +2 cancer_pts.txt | cut -f 2 |
sort | uniq -c
    1053 Female
    1290 Male
j:~/Week.8/8.3.File.Analysis$
```

#### **Applying Commands to Answer Questions**

Below are a number of example commands that answer questions about the information in the cancer\_pts.txt file by combining the commands from this module and module 8.2.

What is the age of the youngest patient with breast cancer?

```
j:~/Week.8/8.3.File.Analysis$ grep "Breast Cancer" cancer_pts.txt | sort
-g -k 3 | grep -v "NA" | head -n 1
D01257 Female 30 Breast Cancer
j:~/Week.8/8.3.File.Analysis$
```

What is the age of the oldest patient with ovarian cancer?

```
j:~/Week.8/8.3.File.Analysis$ grep "Ovarian Cancer" cancer_pts.txt |
sort -gr -k 3 | grep -v "NA" | head -n 1
DO28093 Female 81    Ovarian Cancer
j:~/Week.8/8.3.File.Analysis$
```

How many patients are 75 years old?

```
j:~/Week.8/8.3.File.Analysis$ cut -f 3 cancer_pts.txt | grep -w "75" |
wc -l
49
j:~/Week.8/8.3.File.Analysis$
```

What types of cancer do patients under 10 have? (Note: grep -w "[0-9]" gets lines that contain a single number in one of the fields, i.e. 1 digit ages.)

```
j:~/Week.8/8.3.File.Analysis$ grep -w "[0-9]" cancer_pts.txt | cut -f 4
| sort | uniq
Embryonal Tumor
Mature B-cell lymphoma
Medulloblastoma
j:~/Week.8/8.3.File.Analysis$
```

How many female and male hepatobiliary cancer patients are there?