BINF2111 – Introduction to Bioinformatics Computing

UNIX 101 part trois (grep regrex and sed)

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RAW Lab

Lecture 4 - Thursday Aug 31st, 2023

Learning Objectives

- Review quiz and bonus

- Regular expressions in grep

- Sed

- Regular expressions in sed

- Quiz 4

grep vs. python vs. rust

```
>seq1
ATACTCATATCAT
>seq2
ATCTGCTCGCTAG
>seq3
AGCTCGATCAGCG
```

Linux terminal (bash) commands:

```
grep '>' one.fasta | wc -l
Or:
grep -c '>' one.fasta
```

Python Script:

```python
#!/usr/bin/env python

import sys

count = 0
with open(sys.argv[1]) as reader:
    for line in reader:
        if line.startswith('>'):
            count += 1
print(count)
```

Rust

```rust
use std::env;
use std::fs::File;
use std::io::{BufReader, Read};

fn main() -> Result<(), Box<dyn std::error::Error>> {
    // Get the command-line arguments
    let args: Vec<String> = env::args().collect();

    // Check if an argument (FASTA file path) is provided
    if args.len() != 2 {
        eprintln!("Usage: {} <fasta_file>", args[0]);
        std::process::exit(1);
    }

    let filename = &args[1];
    let file = File::open(filename)?;

    let mut reader = BufReader::new(file);
    let mut buffer = [0u8; 8192]; // Read in 8KB chunks

    let mut count = 0;
    let mut in_header = false;

    loop {
        let bytes_read = reader.read(&mut buffer)?;
        if bytes_read == 0 {
            break;
        }

        for &byte in buffer.iter().take(bytes_read) {
            match byte {
                b'>' => {
                    if !in_header {
                        count += 1;
                        in_header = true;
                    }
                }
                b'\n' => {
                    in_header = false;
                }
                _ => {}
            }
        }
    }

    println!("Number of '>' symbols: {}", count);

    Ok(())
}
```

grep vs. python vs. rust

```
(base) drrichardallenwhiteiii@system76-pc:~/fasta_counter$ time ./fastacounter example.fasta
Number of '>' symbols: 3

real    0m0.002s
user    0m0.002s
sys     0m0.000s
(base) drrichardallenwhiteiii@system76-pc:~/fasta_counter$ time grep ">" -c example.fasta
3

real    0m0.002s
user    0m0.002s
sys     0m0.000s
(base) drrichardallenwhiteiii@system76-pc:~/fasta_counter$ time python count.py example.fasta
3

real    0m0.020s
user    0m0.020s
sys     0m0.000s
```

grep vs. python vs. rust

```
sys     0m0.000s
(base) drrichardallenwhiteiii@system76-pc:~/fasta_counter$ time python count.py example.fasta
3

real    0m0.020s
user    0m0.020s
sys     0m0.000s
(base) drrichardallenwhiteiii@system76-pc:~/fasta_counter$ time python count.py example.fasta
3

real    0m0.019s
user    0m0.015s
sys     0m0.004s
(base) drrichardallenwhiteiii@system76-pc:~/fasta_counter$ time python count.py example.fasta
3

real    0m0.019s
user    0m0.018s
sys     0m0.000s
(base) drrichardallenwhiteiii@system76-pc:~/fasta_counter$ time python count.py example.fasta
3

real    0m0.019s
user    0m0.015s
sys     0m0.004s
(base) drrichardallenwhiteiii@system76-pc:~/fasta_counter$ time python count.py example.fasta
3

real    0m0.019s
user    0m0.018s
sys     0m0.000s
```

grep vs. python vs. rust

```
sys     0m0.000s
(base) drrichardallenwhiteiii@system76-pc:~/fasta_counter$ time ./fastacounter example.fasta
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real    0m0.002s
user    0m0.002s
sys     0m0.000s
(base) drrichardallenwhiteiii@system76-pc:~/fasta_counter$
```

Quiz 3 answers

Command 1

echo “ATATCCC” | grep -c "AT"

Command 2

echo “ATATCCC” | grep "AT" | wc -l

How many AT repeats does it count?

Quiz 3 answers

Command 1
echo “ATATCCC” | grep -c "AT"

Command 2
echo “ATATCCC” | grep "AT" | wc -l

How many AT repeats does it count?

One each

Quiz 3 answers

Command 1
echo “ATATCCC” | grep -c "AT"

Command 2
echo “ATATCCC” | grep "AT" | wc -l

How many AT repeats does it count?

How would I count both AT’s?

Quiz 3 answers

How would I count both AT's?

Command 1

echo "ATATCCC" | grep -o "AT" | wc -l

Is there another way?

Quiz 3 answers

How would I count both AT's?

Command 1

echo "ATATCCC" | grep -o "AT" | wc -l

Is there another way?

Command 2

echo "ATATCCC" | grep -o "AT" | grep -c ""

Another way?

Quiz 3 answers

How would I count both AT's?

```
echo “ATATCCC” | grep -o "AT" | wc -l
echo “ATATCCC” | grep -o "AT" | grep -c “”
```

Another way?

```
echo "ATATCC" | grep -o "AT\|AT" | grep -c "AT"
```

or

Quiz 3 answers

How would I count both AT's?

```
echo “ATATCCC” | grep -o "AT" | wc -l
echo “ATATCCC” | grep -o "AT" | grep -c “”
```

Another way?

```
echo "ATATCC" | grep -o "AT\|AT" | grep -c "AT"
```

or

```
echo -n "ATATCC" | tr -d '\n' | grep -o "AT" | wc -l
```

Quiz 3 answers

head file.txt
Kite rats kite cash REd kite
kite rats kite red caSh rats

grep ‘^[Kk]ite’ file.txt | wc -l

The grep command does what?

Quiz 3 answers

head file.txt
Kite rats kite cash REd kite
kite rats kite red caSh rats

grep ‘^[Kk]ite’ file.txt | wc -l

The grep command does what?

Counts K or k (upper/lower case) at the beginning of each line, which counts 2 in the file.

Quiz 3 answers

- echo “ATCCGCGCGCGCGGGGCGCGCGCGTT” | grep -c “AT”

Does the command count all AT's in this sequence string?

T or F

Quiz 3 answers

- echo “ATCCGCGCGCGCGGGGCGCGCGCGTT” | grep -c “AT”

Does the command count all AT's in this sequence string?

T or F

Quiz 3 answers

- grep -c “AT” example.fasta command is able to count all AT's in this line?

ATCCGCGCGCGGCGCGCGCGGCGCGTT

T or F

Quiz 3 answers

- grep -c “AT” example.fasta command is able to count all AT's in this line?

ATCCGCGCGCGCGGCGCGCGCGCGGCGCG
CGCGTT

T or F

New question

- grep -c “AT” example.fasta command is able to count all AT's in this line?

ATCCGCGCGCGGCGCGCGCGGCGCG
CGCGTTAT

T or F

New question

- grep -c “AT” example.fasta command is able to count all AT's in this line?

ATCCGCGCGCGCGGCGCGCGCGCGGCGCG
CGCGTTAT

T or F

New question

- grep -c “AT” example.fasta command is able to count all AT's in this line?

ATCCGCGCGCGCGGCGCGCGCGCGCGGCGCG
CGCGTTAT

How would you count it?

New question

- grep -c “AT” example.fasta command is able to count all AT's in this line?

ATCCGCGCGCGGCGCGCGCGGCGCG
CGCGTTAT

What this work?
grep -c “AT” example.fasta

New question

- grep -c “AT” example.fasta command is able to count all AT's in this line?

ATCCGCGCGCGGCGCGCGCGGCGCG
CGCGTTAT

What this work?
grep -o -c “AT” example.fasta or
grep -oc “AT” example.fasta

New question

- grep -c “AT” example.fasta command is able to count all AT's in this line?

ATCCGCGCGCGGCGCGCGCGGCGCG
CGCGTTAT

What this work?
grep -Eo “AT” example.fasta --color
grep -o “AT” example.fasta

New question

- grep -c “AT” example.fasta command is able to count all AT's in this line?

ATCCGCGCGCGGCGCGCGCGGCGCG
CGCGTTAT

What this work?
grep -Eo “AT” example.fasta | wc -l
grep -o “AT” example.fasta | wc -l

New question

- grep -c “AT” example.fasta command is able to count all AT's in this line?

ATCCGCGCGCGGCGCGCGCGGCGCG
CGCGTTAT

What this work?
grep -o “^AT|AT$” example.fasta

New question

- grep -c “AT” example.fasta command is able to count all AT's in this line?

ATCCGCGCGCGGCGCGCGCGGCGCG
CGCGTTAT

What this work?
grep -Eo “^AT|AT$” example.fasta | wc -l
egrep -o “^AT|AT$” example.fasta | wc -l

Bonus 3

- For the example.fasta file count both the number of AT and GC in one grep command
and in another command print the line number which they appear?

Command 1
grep -Eo "GC|AT" example.fasta | wc -l
egrep -o "GC|AT" example.fasta | wc -l

Command 2
grep -nEo "GC|AT" example.fasta --color >>file.txt
egrep -no "GC|AT" example.fasta --color >>file.txt

Bonus 3 extra questions

- For the example.fasta file count both the number of AT and GC in one grep command
and in another command print the line number which they appear?

How many GC and AT's are present count?
Number here:
command:

And, how many are GC and AT's individually?
Commands here:
Number here:

Bonus 3 extra questions

- For the example.fasta file count both the number of AT and GC in one grep command
and in another command print the line number which they appear?

How many GC and AT's are present count?
Number here: 15
command: egrep -o "GC|AT" example.fasta | wc -l

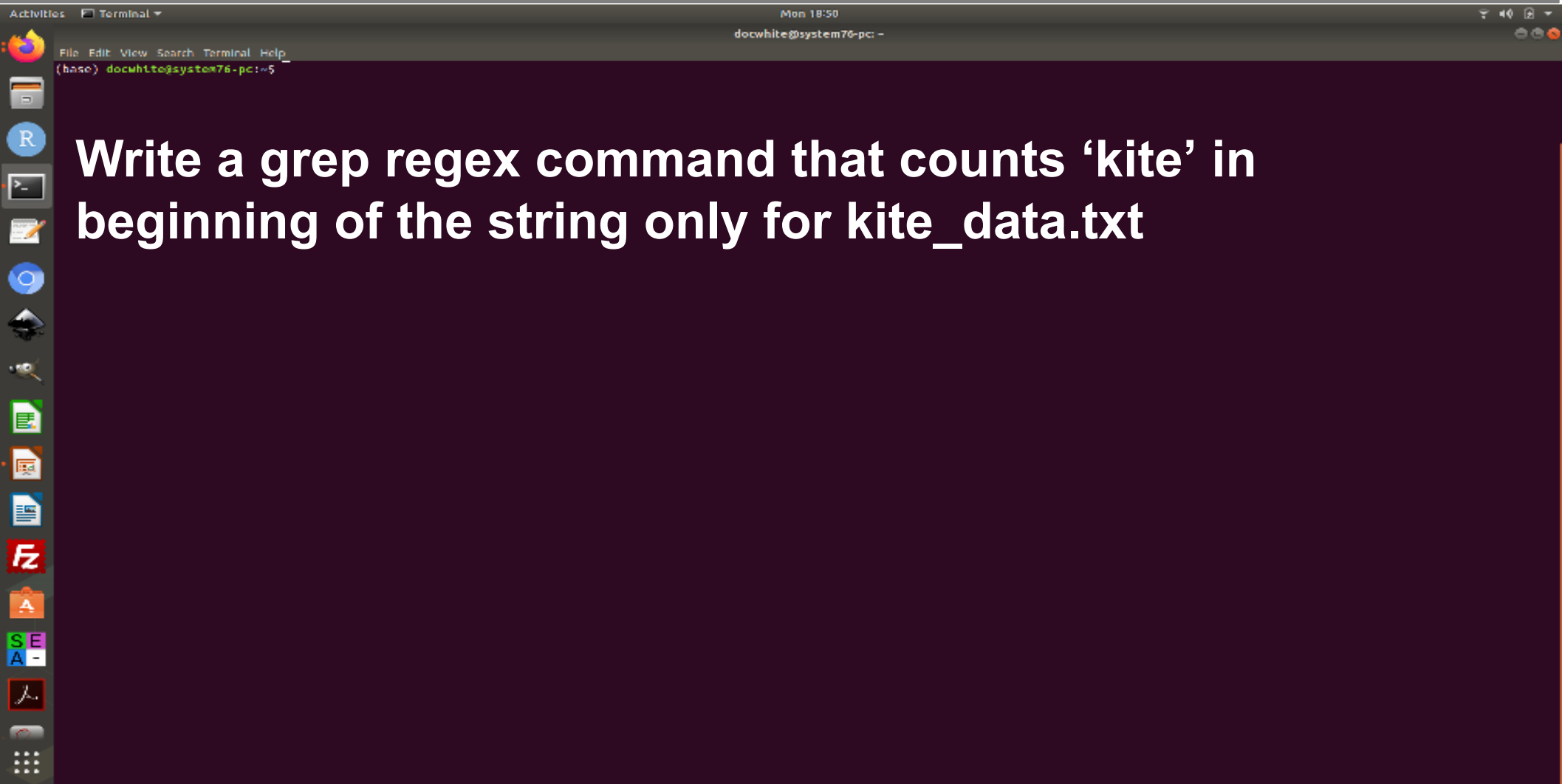
And, how many are GC and AT's individually?
Commands here: egrep -o "GC" example.fasta | wc -l
egrep -o "AT" example.fasta | wc -l
Number here: GC = 8 and AT = 7

grep – syntax to hands of UNIX

grep [option] pattern file

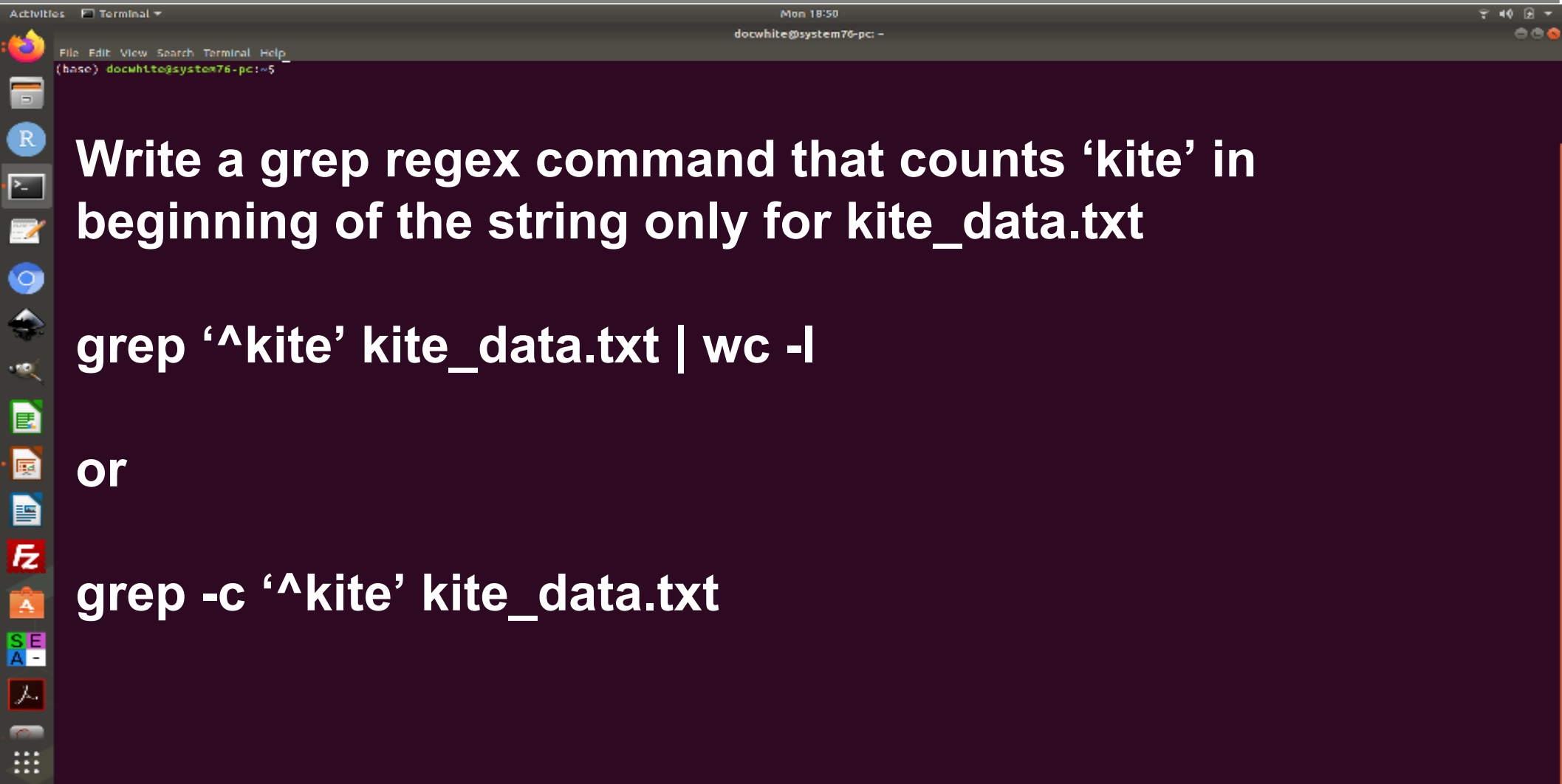
Understanding Regular Expressions:
^ (Caret) match expression at the start of a line, as in ^A.
$ (Question) match expression at the end of a line, as in A$.
\ (Back Slash) turn off the special meaning of the next character, as in \^. To look for a Caret "^" at the start of a line, the expression is ^\^.
[ ] (Brackets) match any one of the enclosed characters, as in [aeiou]. Use Hyphen "-" for a range, as in [0-9].
[^] match any one character except those enclosed in [ ], as in [^0-9].
. (Period) match a single character of any value, except end of line. So b.b will match "bob", "bib", "b-b", etc.
* (Asterisk) match zero or more of the preceding character or expression. An asterisk matches zero or more of what precedes it. Thus [A-Z]* matches any number of upper-case letters, including none, while [A-Z][A-Z]* matches one or more upper-case letters.

grep examples



Write a grep regex command that counts ‘kite’ in beginning of the string only for kite_data.txt

grep examples



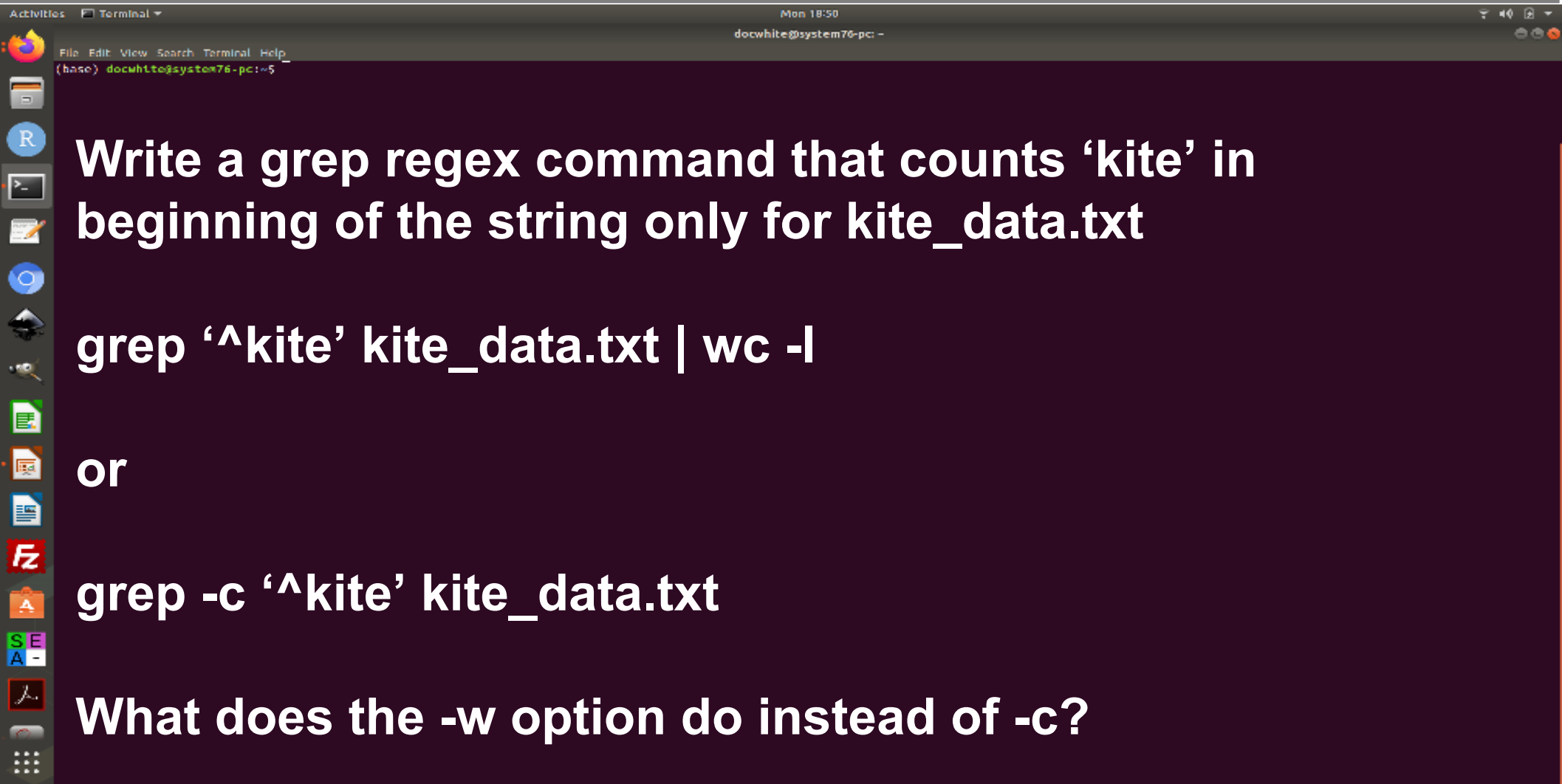
Write a grep regex command that counts ‘kite’ in beginning of the string only for kite_data.txt

grep ‘^kite’ kite_data.txt | wc -l

or

grep -c ‘^kite’ kite_data.txt

grep examples



Write a grep regex command that counts ‘kite’ in beginning of the string only for kite_data.txt

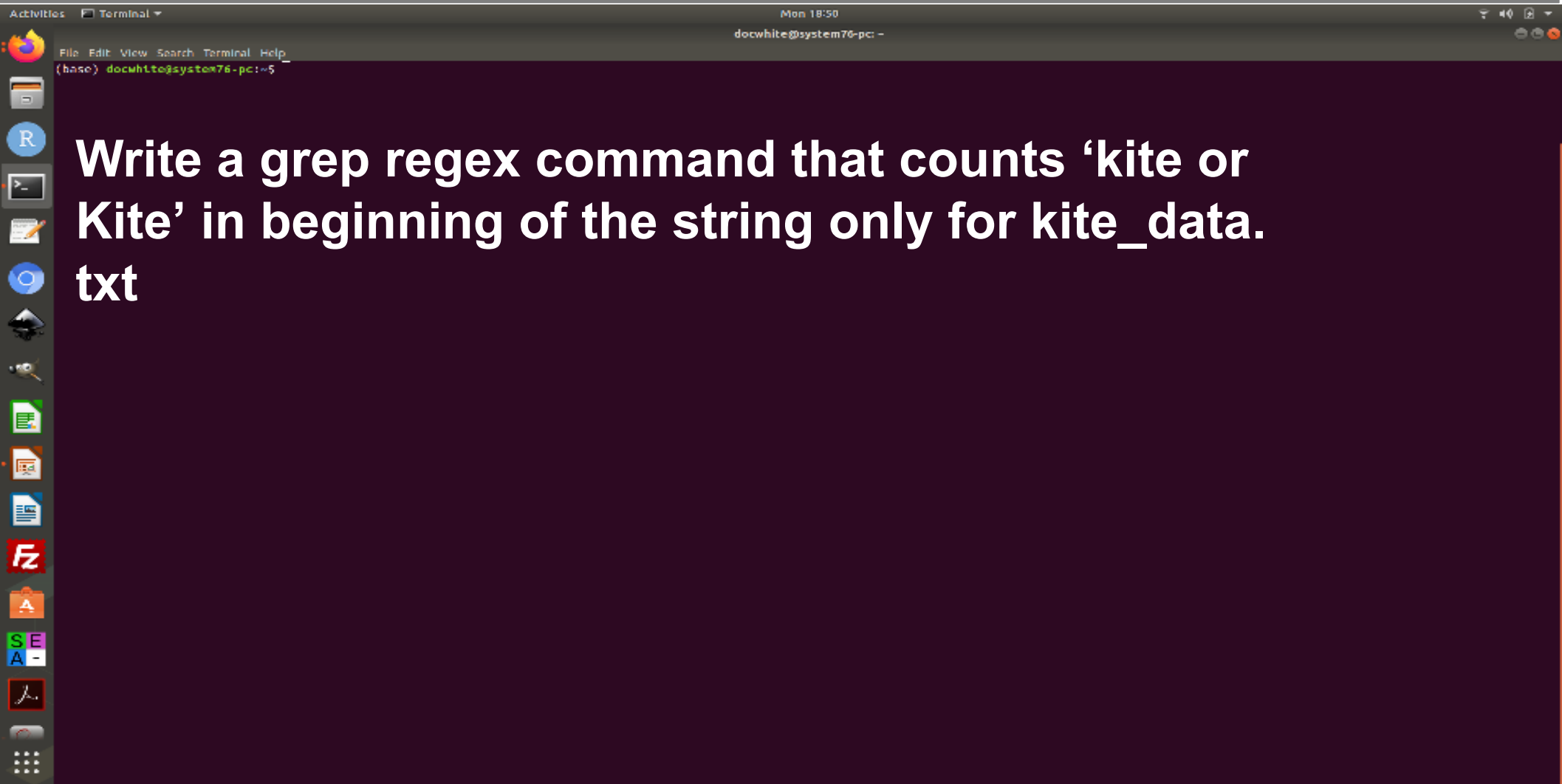
grep ‘^kite’ kite_data.txt | wc -l

or

grep -c ‘^kite’ kite_data.txt

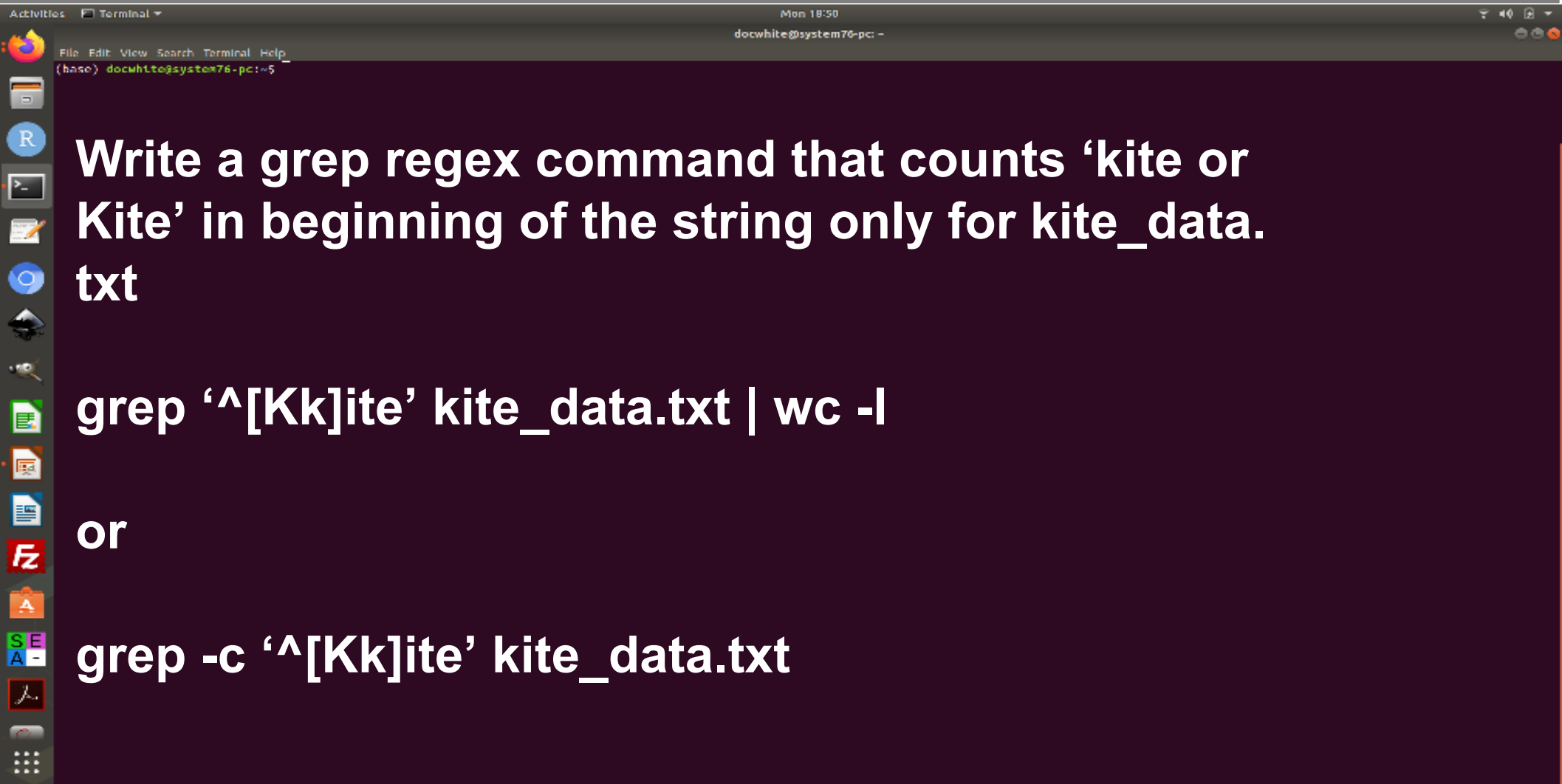
What does the -w option do instead of -c?

grep examples



Write a grep regex command that counts ‘kite or Kite’ in beginning of the string only for kite_data.txt

grep examples



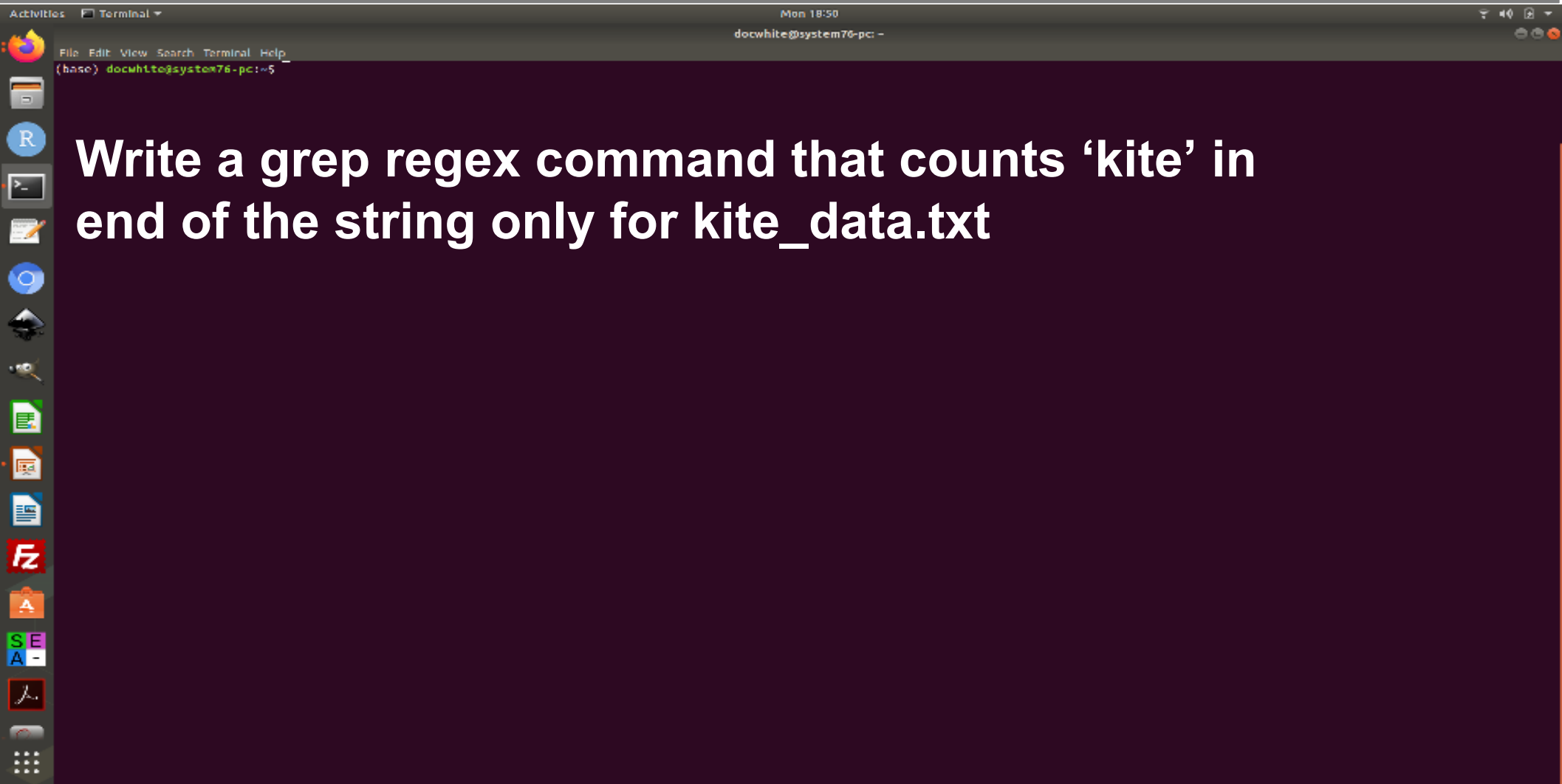
Write a grep regex command that counts ‘kite or Kite’ in beginning of the string only for kite_data.txt

grep ‘^[Kk]ite’ kite_data.txt | wc -l

or

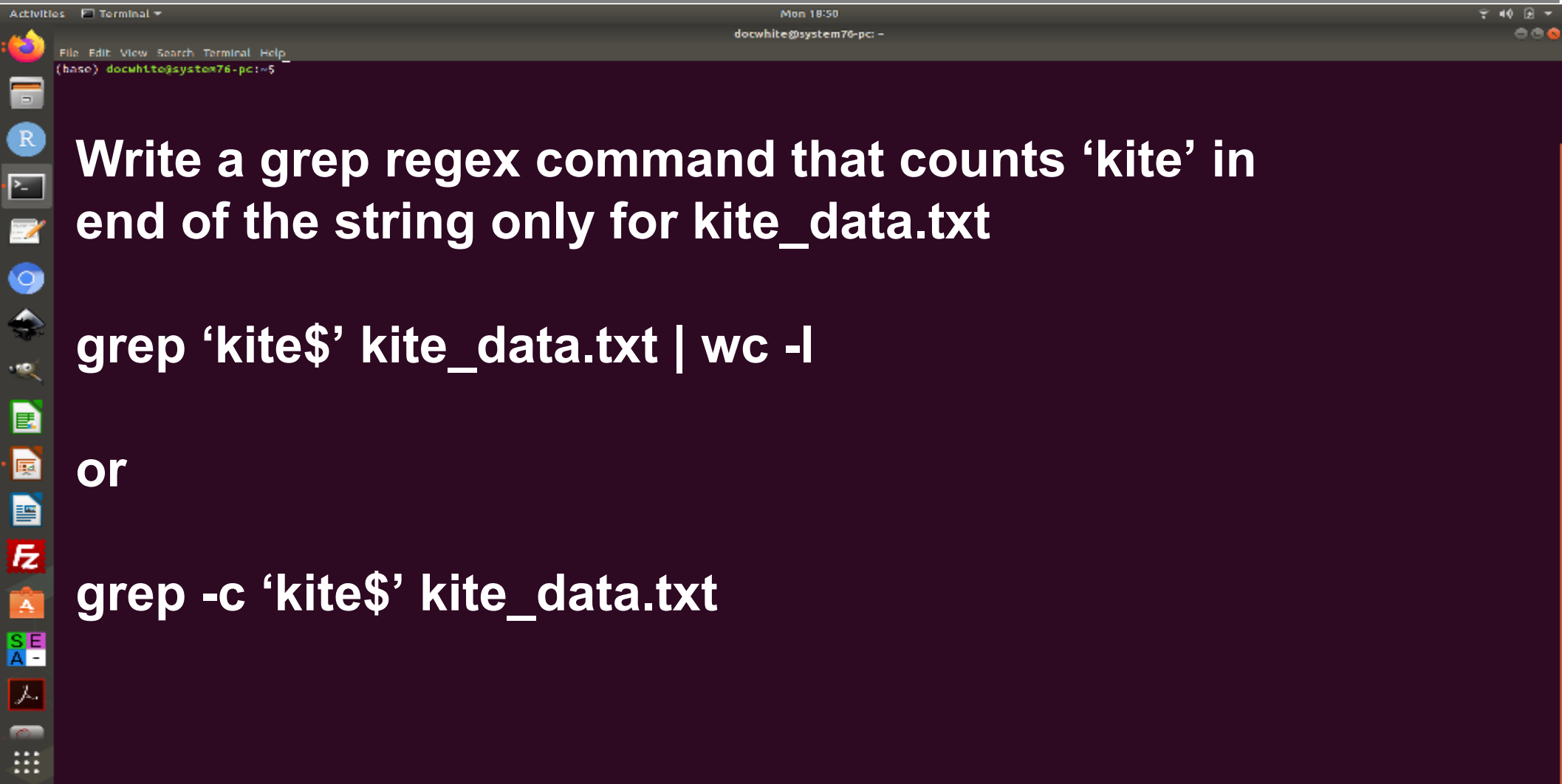
grep -c ‘^[Kk]ite’ kite_data.txt

grep examples



Write a grep regex command that counts ‘kite’ in end of the string only for kite_data.txt

grep examples



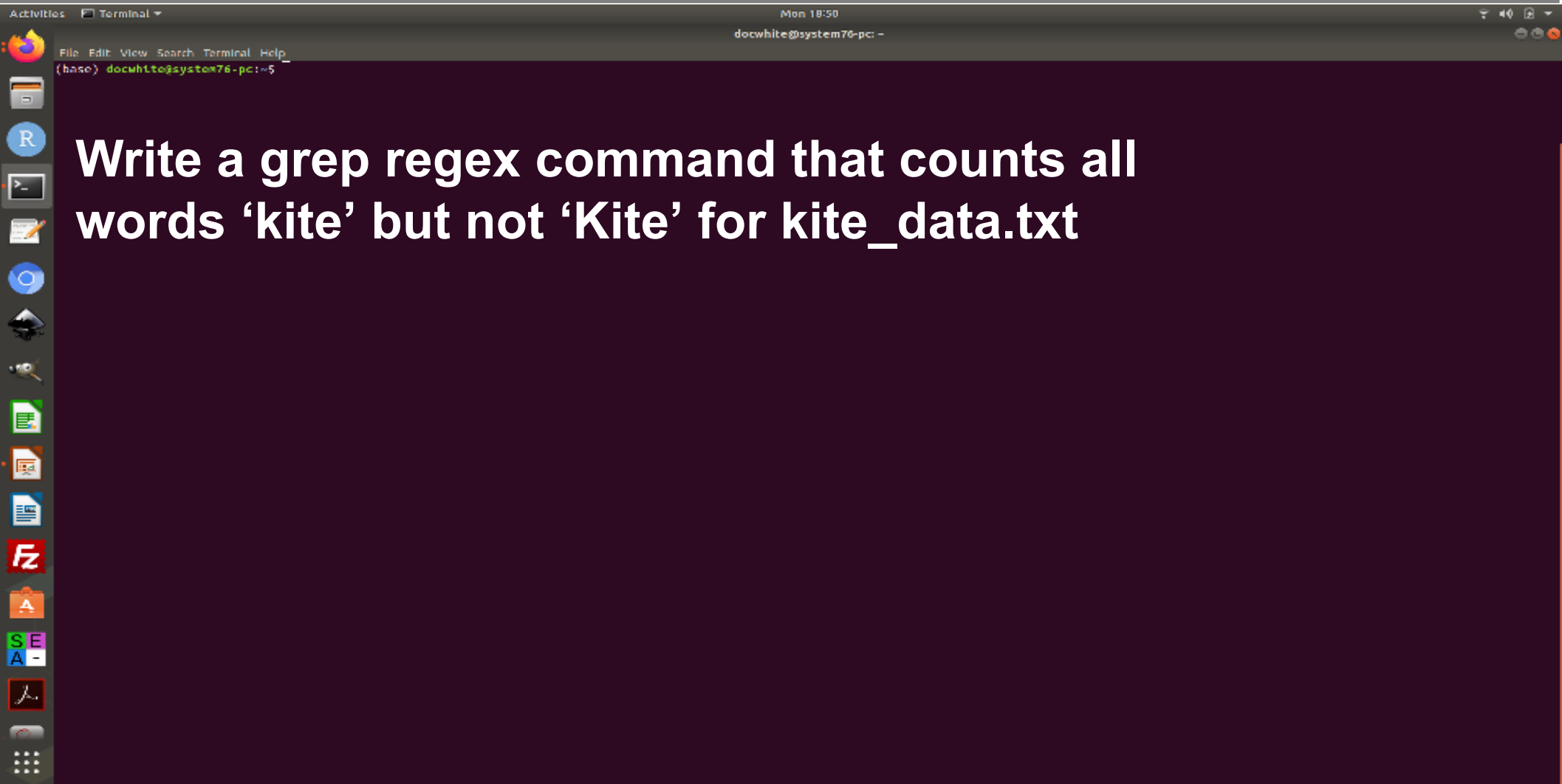
Write a grep regex command that counts ‘kite’ in end of the string only for kite_data.txt

grep ‘kite$’ kite_data.txt | wc -l

or

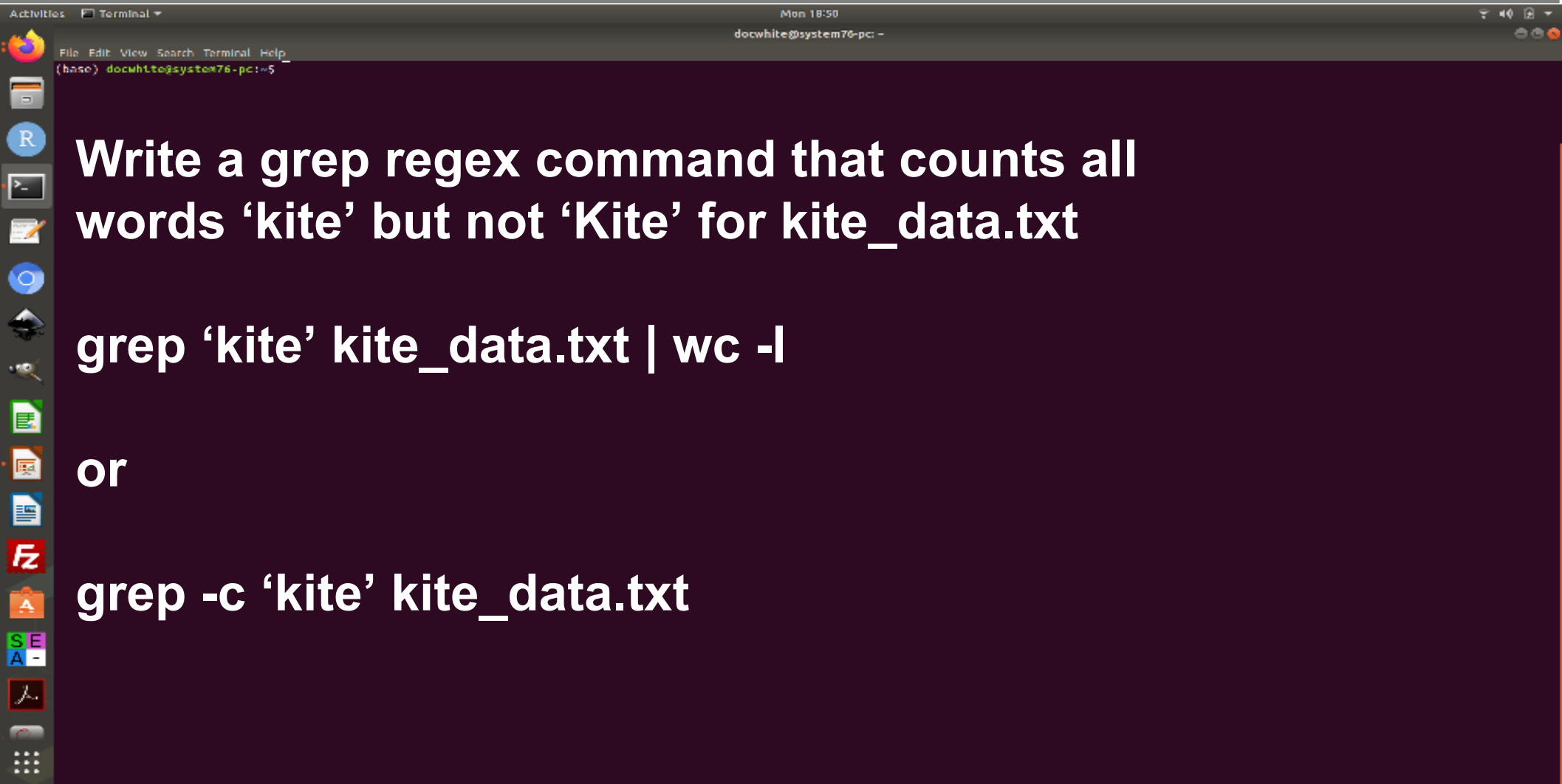
grep -c ‘kite$’ kite_data.txt

grep examples



Write a grep regex command that counts all words ‘kite’ but not ‘Kite’ for kite_data.txt

grep examples



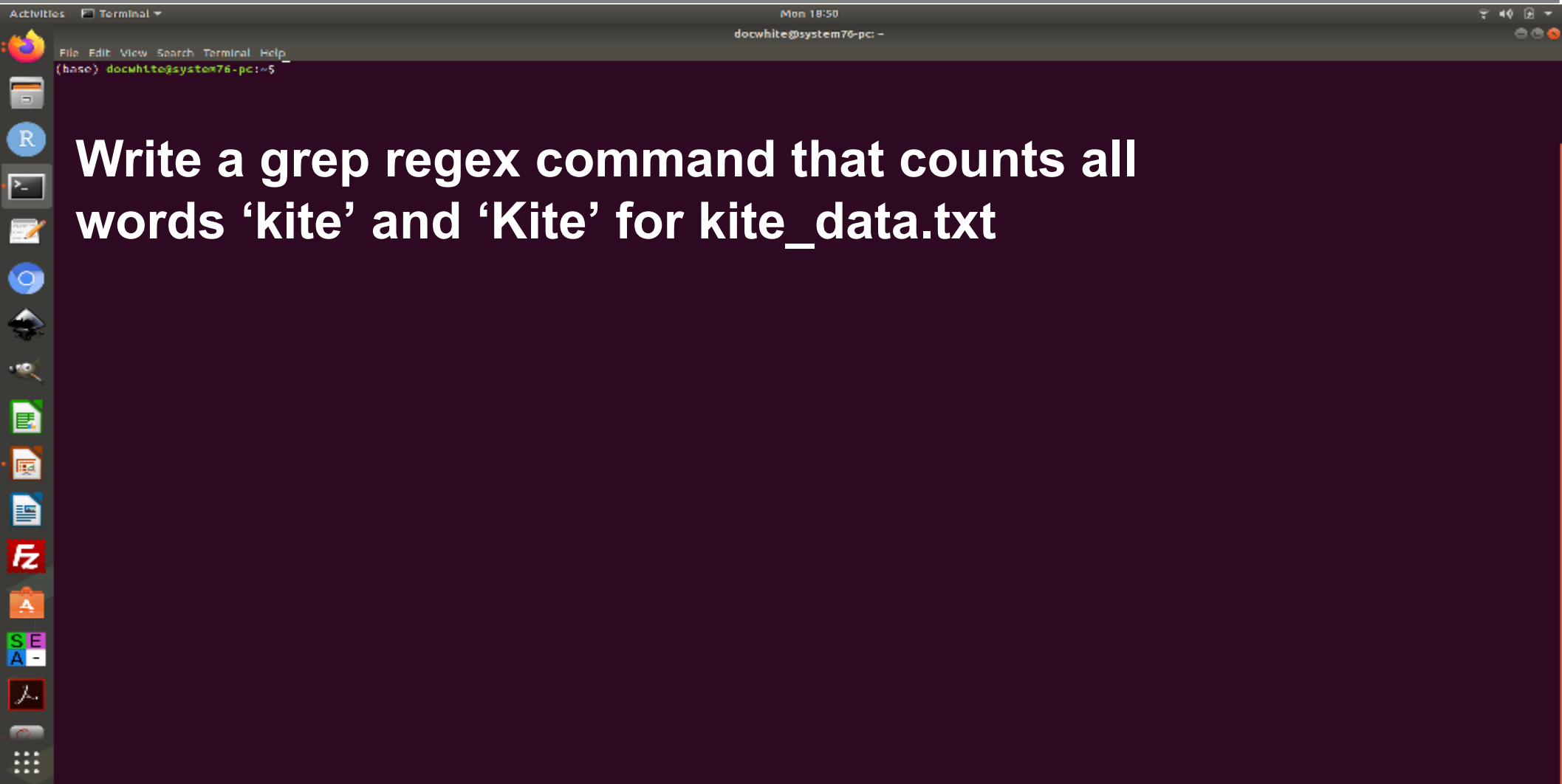
Write a grep regex command that counts all words ‘kite’ but not ‘Kite’ for kite_data.txt

grep ‘kite’ kite_data.txt | wc -l

or

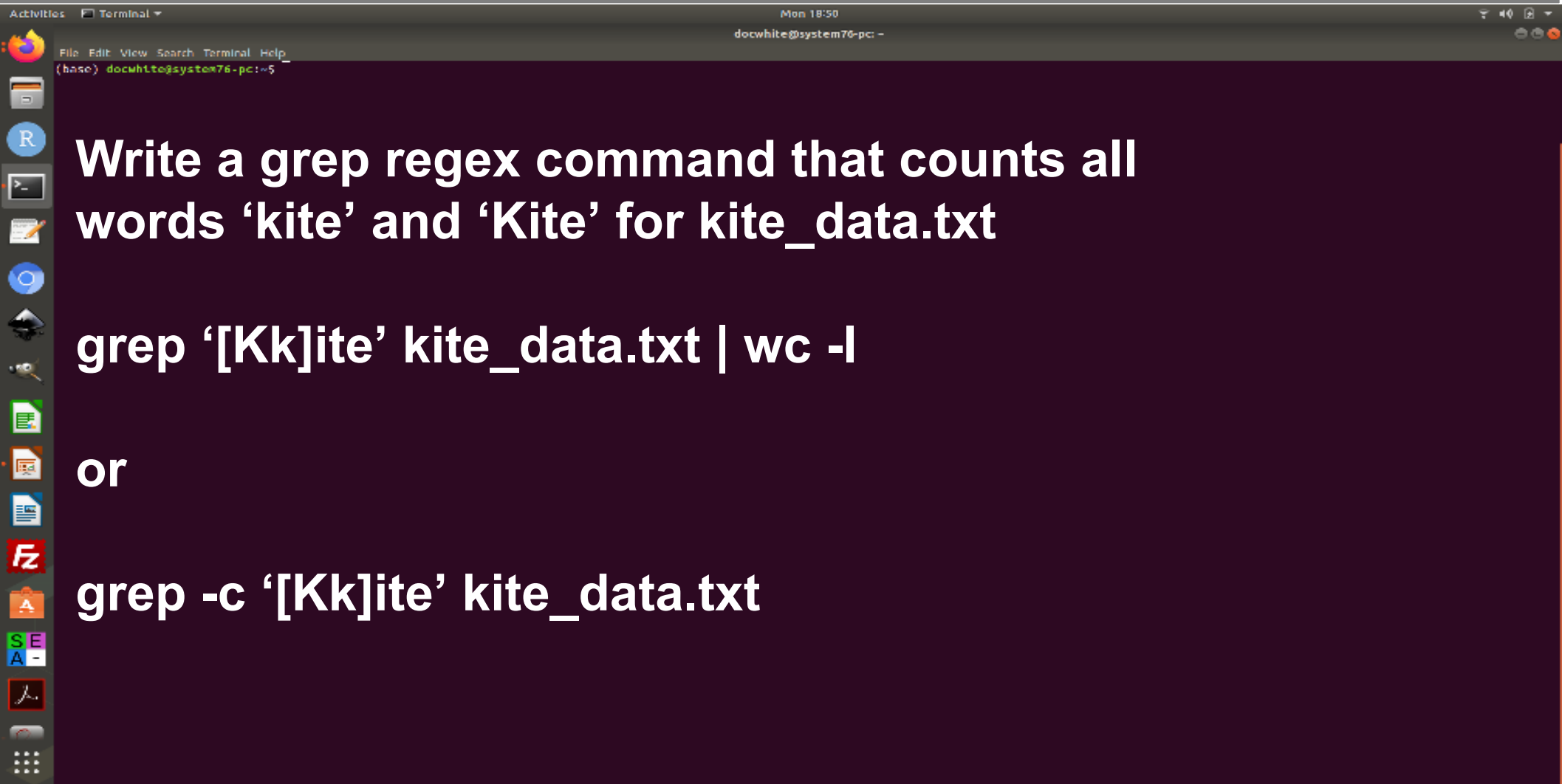
grep -c ‘kite’ kite_data.txt

grep examples



Write a grep regex command that counts all words ‘kite’ and ‘Kite’ for kite_data.txt

grep examples



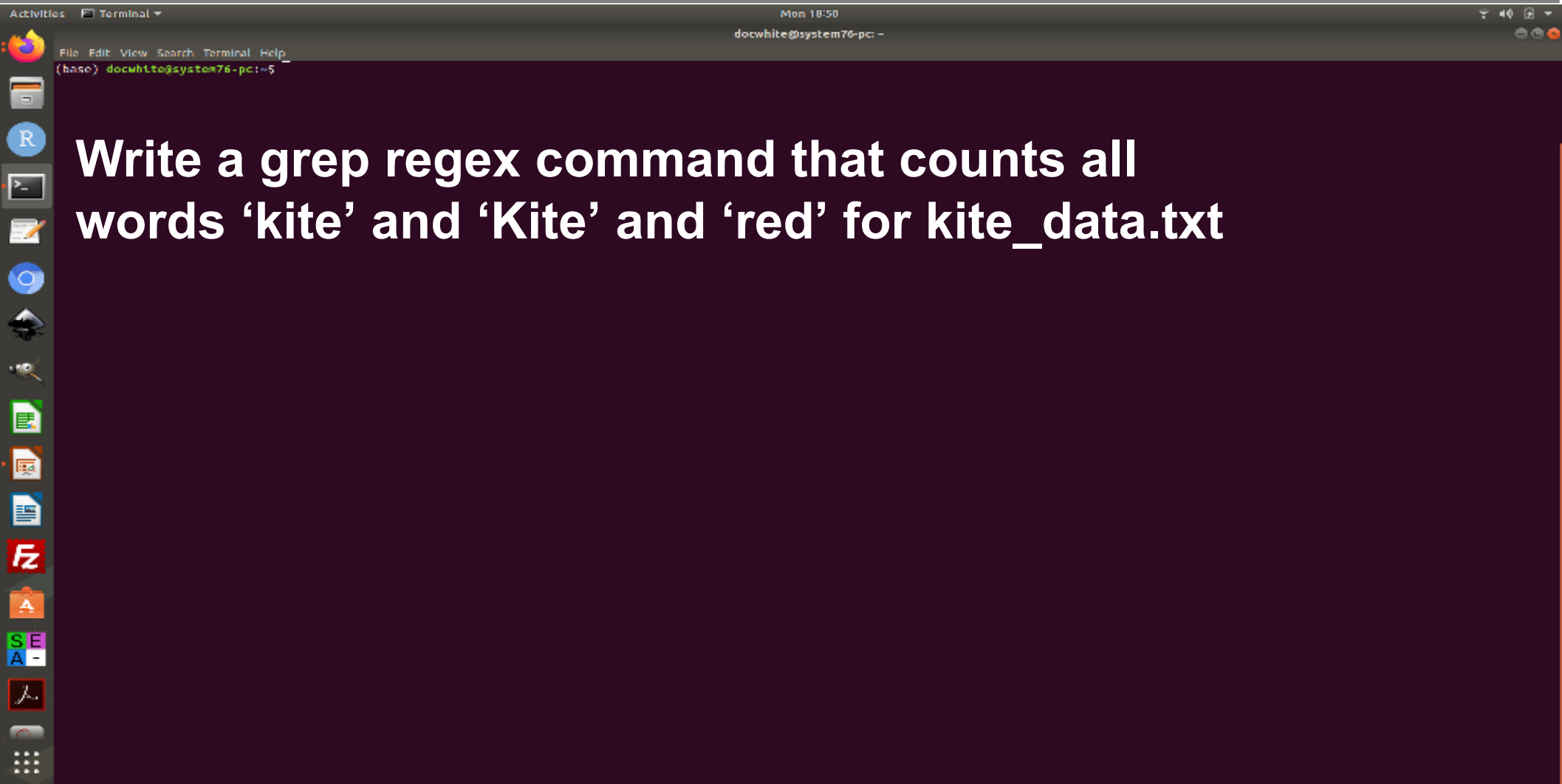
Write a grep regex command that counts all words ‘kite’ and ‘Kite’ for kite_data.txt

grep ‘[Kk]ite’ kite_data.txt | wc -l

or

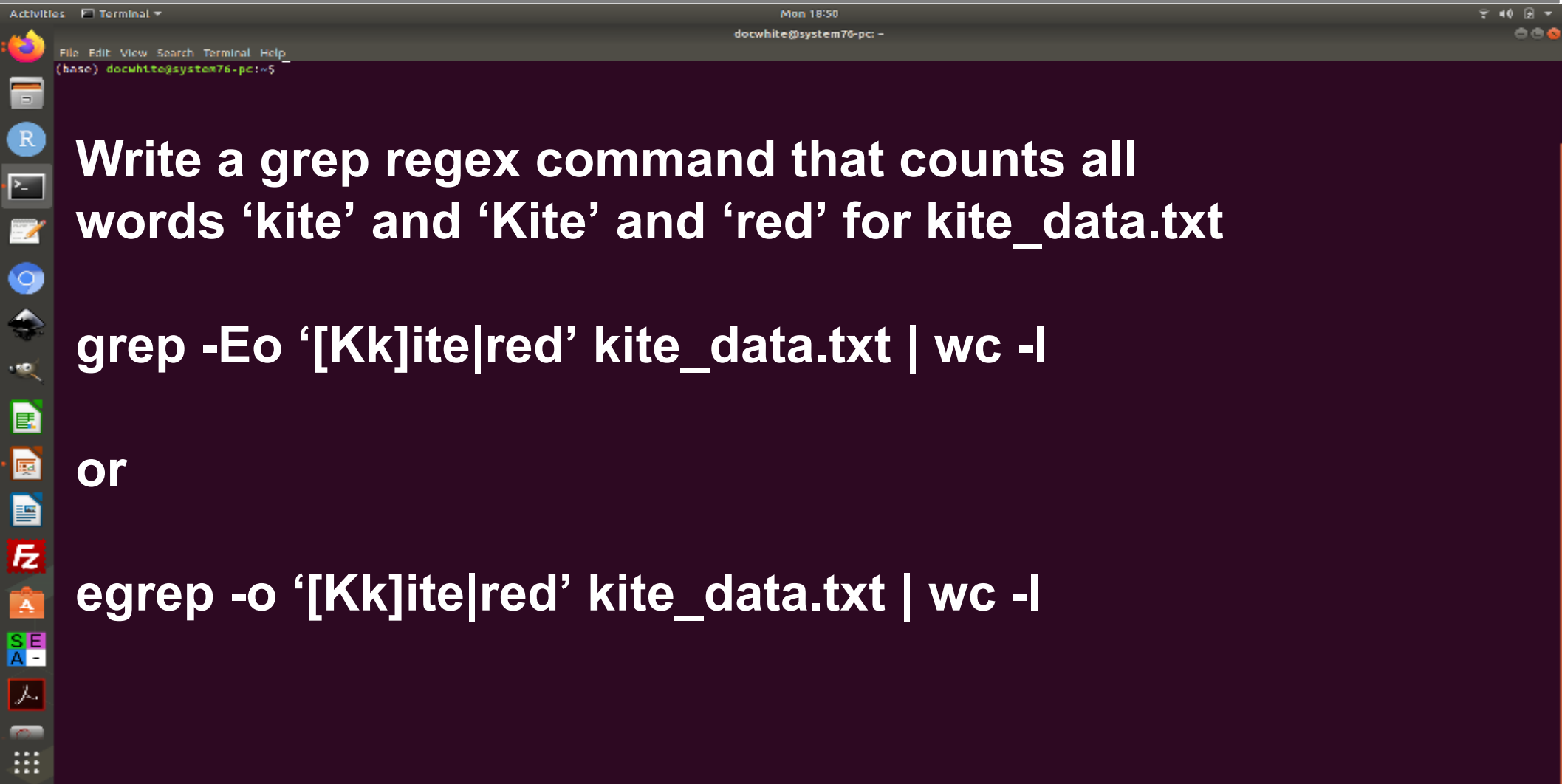
grep -c ‘[Kk]ite’ kite_data.txt

grep examples



Write a grep regex command that counts all words ‘kite’ and ‘Kite’ and ‘red’ for kite_data.txt

grep examples



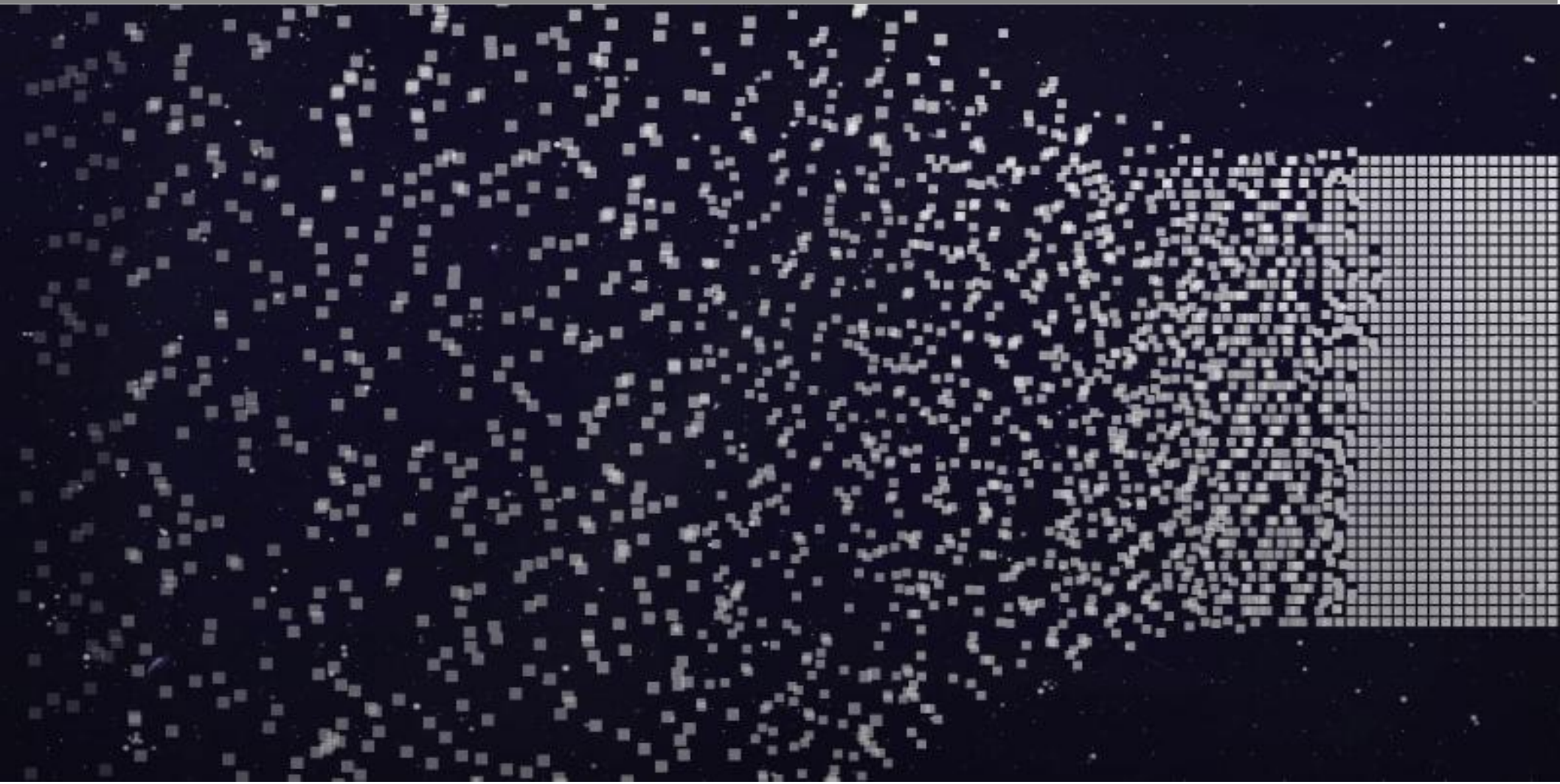
Write a grep regex command that counts all words ‘kite’ and ‘Kite’ and ‘red’ for kite_data.txt

grep -Eo ‘[Kk]ite|red’ kite_data.txt | wc -l

or

egrep -o ‘[Kk]ite|red’ kite_data.txt | wc -l

Data science



Data science

Sed - Stream Editor

sed ("stream editor") is a Unix utility that parses and transforms text, using a simple, compact programming language. sed was developed from 1973-1974 by Lee E. McMahon of Bell Labs

Lee E. McMahon

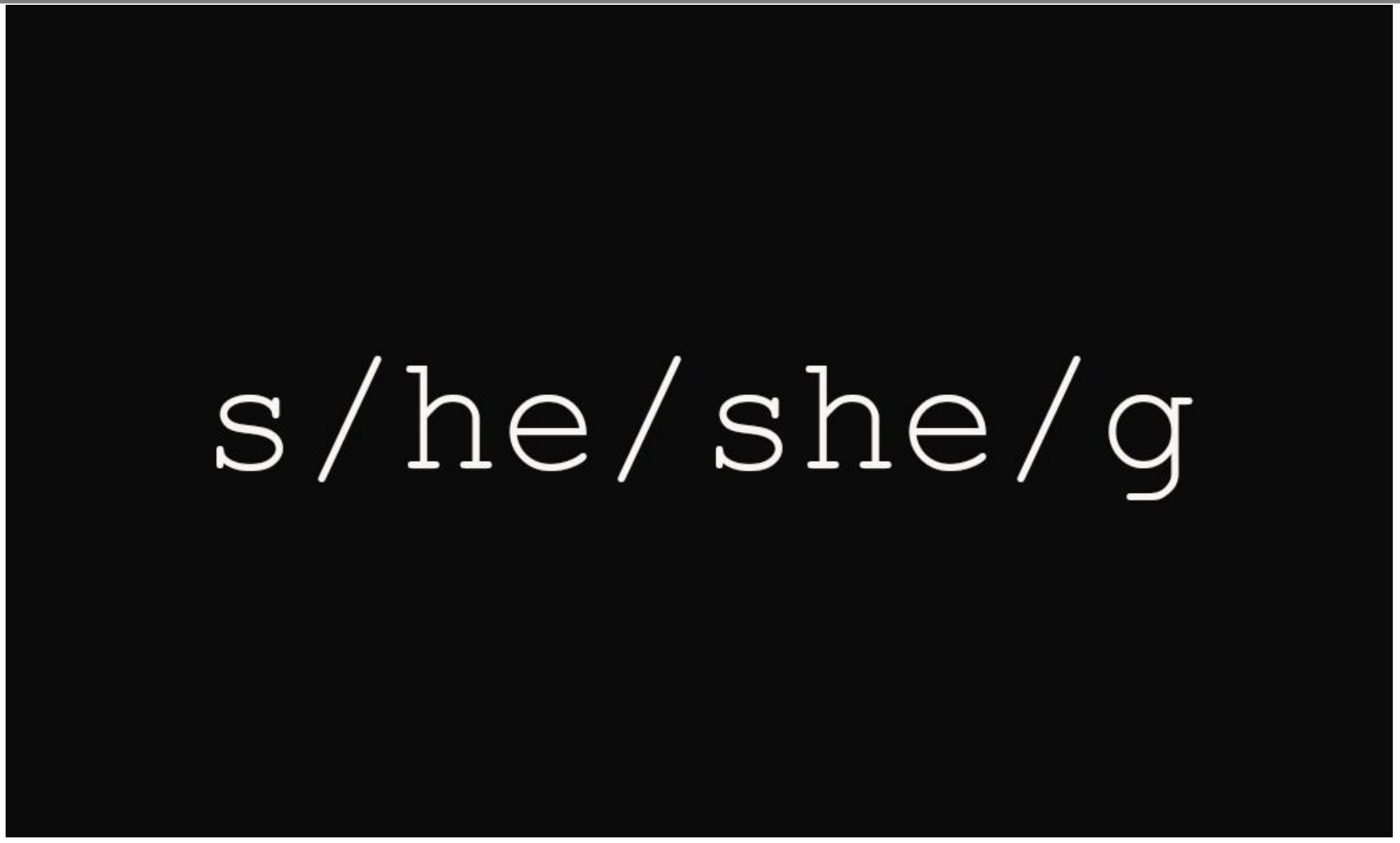
Sed - Stream Editor

sed ("stream editor") is sed was one of the earliest tools to support regular expressions, and remains in use for text processing, most notably with the substitution command. Written in C www.gnu.org/software/sed/

Sed - Stream Editor

Popular alternative tools for plaintext string manipulation and "stream editing" include AWK and Perl.

Sed - Stream Editor



Sed - Stream Editor

sed OPTIONS... [SCRIPT] [INPUTFILE…]

--version (Print out the version of sed)

--help (help page)

-n, --quiet, --silent (suppress automatic printing of pattern space)

--debug

-e script, --expression=script (Add the commands in script to the set of commands to be run)

-i [SUFFIX], –in-place[=SUFFIX] (This option specifies that files are to be edited in-place)

Sed - Stream Editor

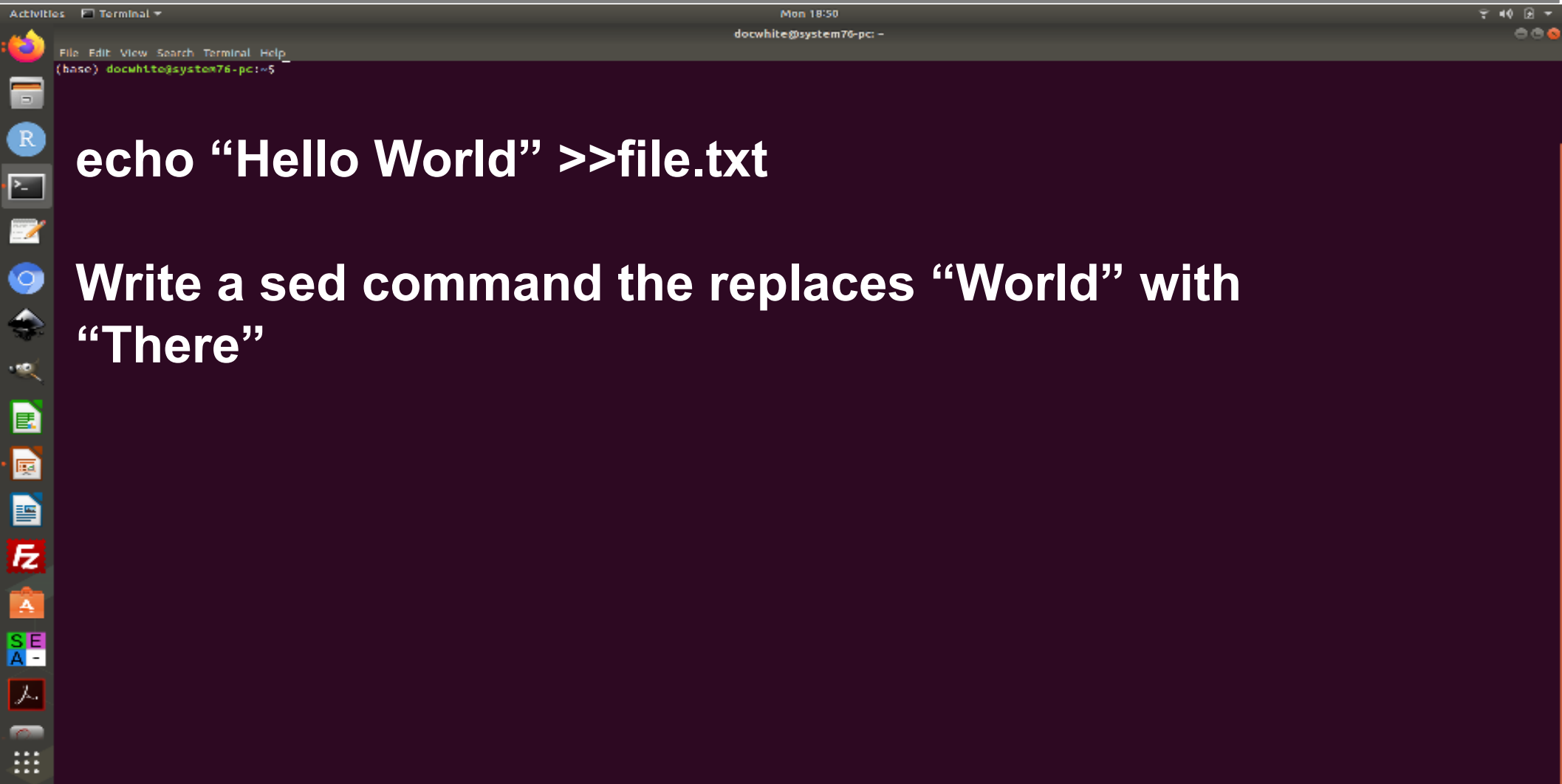
Substitution command

S command swiss army knife

sed 's/regexp/replacement/g' inputFileName > outputFileName

The **s** stands for substitute, while the **g** stands for global, which means that all matching occurrences in the line would be replaced.

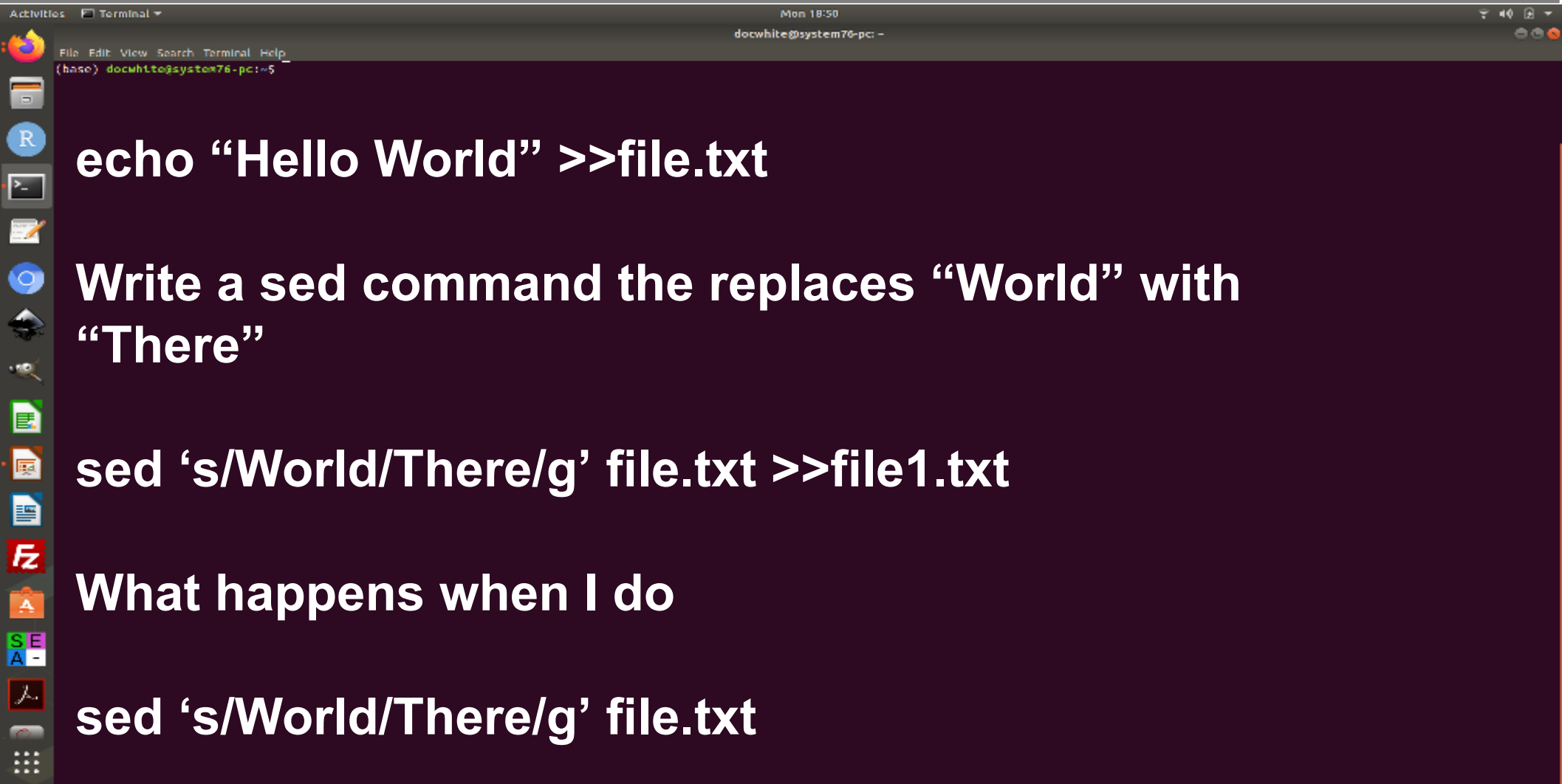
sed examples



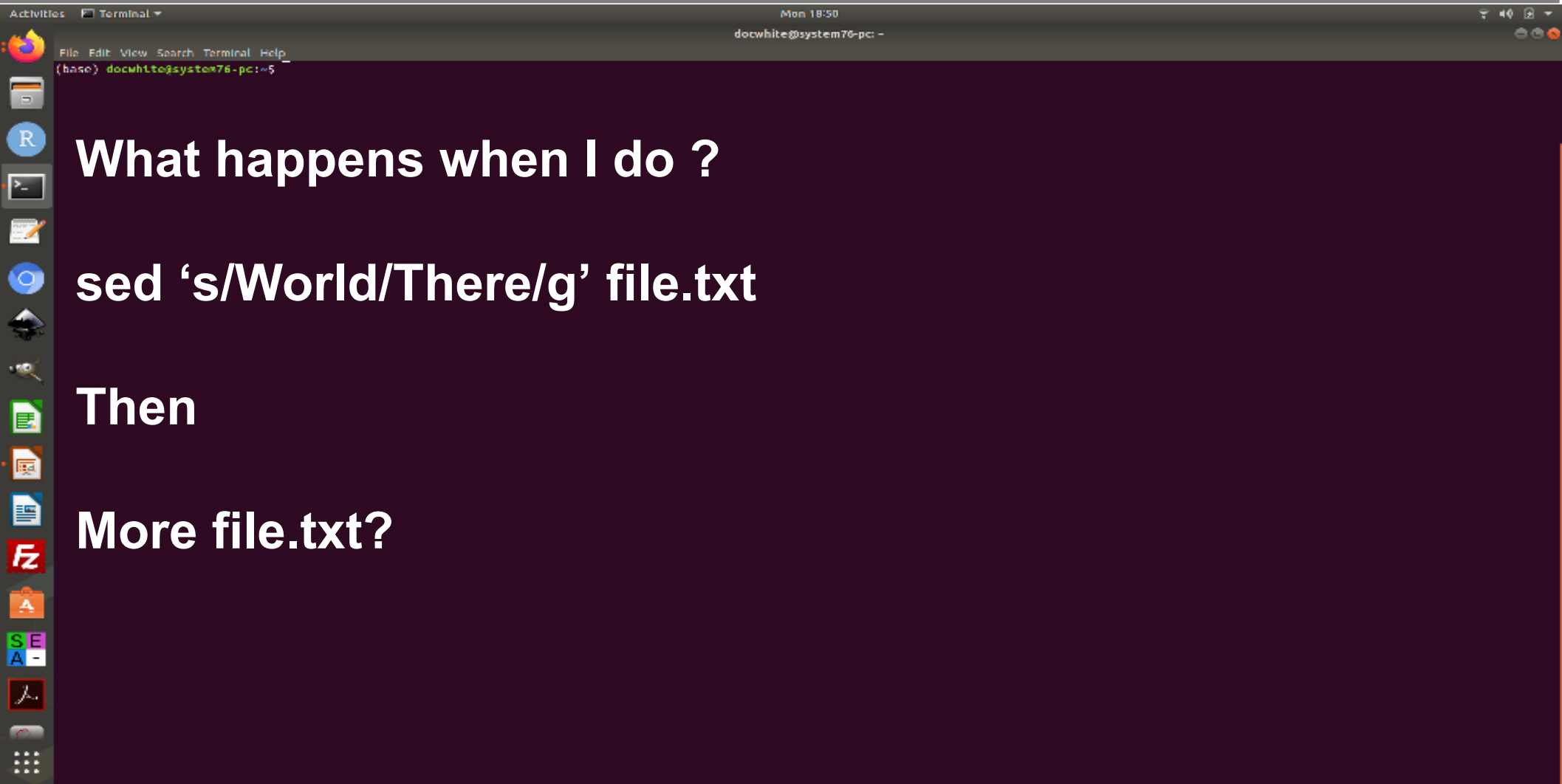
echo “Hello World” >>file.txt

Write a sed command the replaces “World” with “There”

sed examples



sed examples



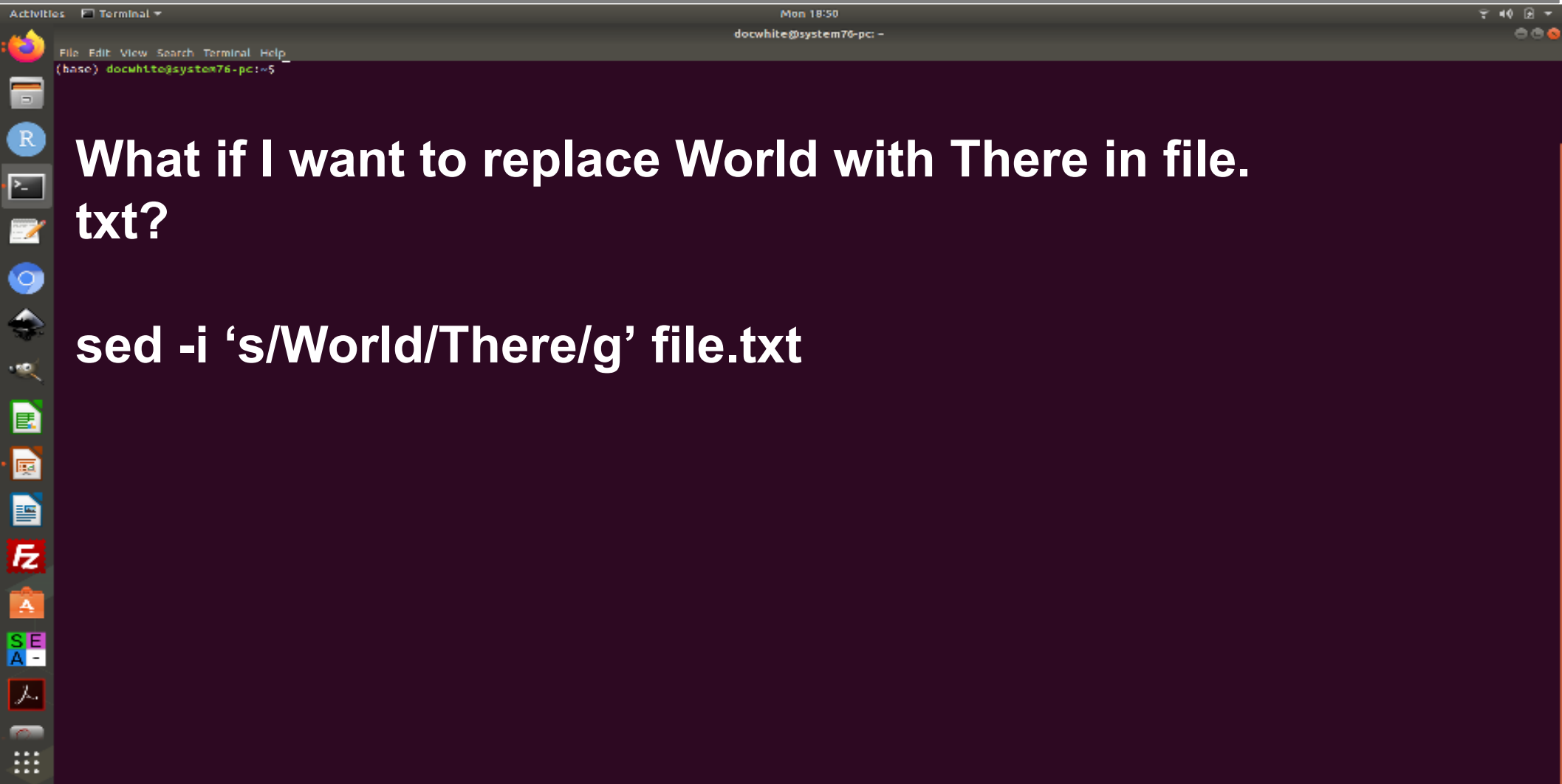
What happens when I do ?

sed ‘s/World/There/g’ file.txt

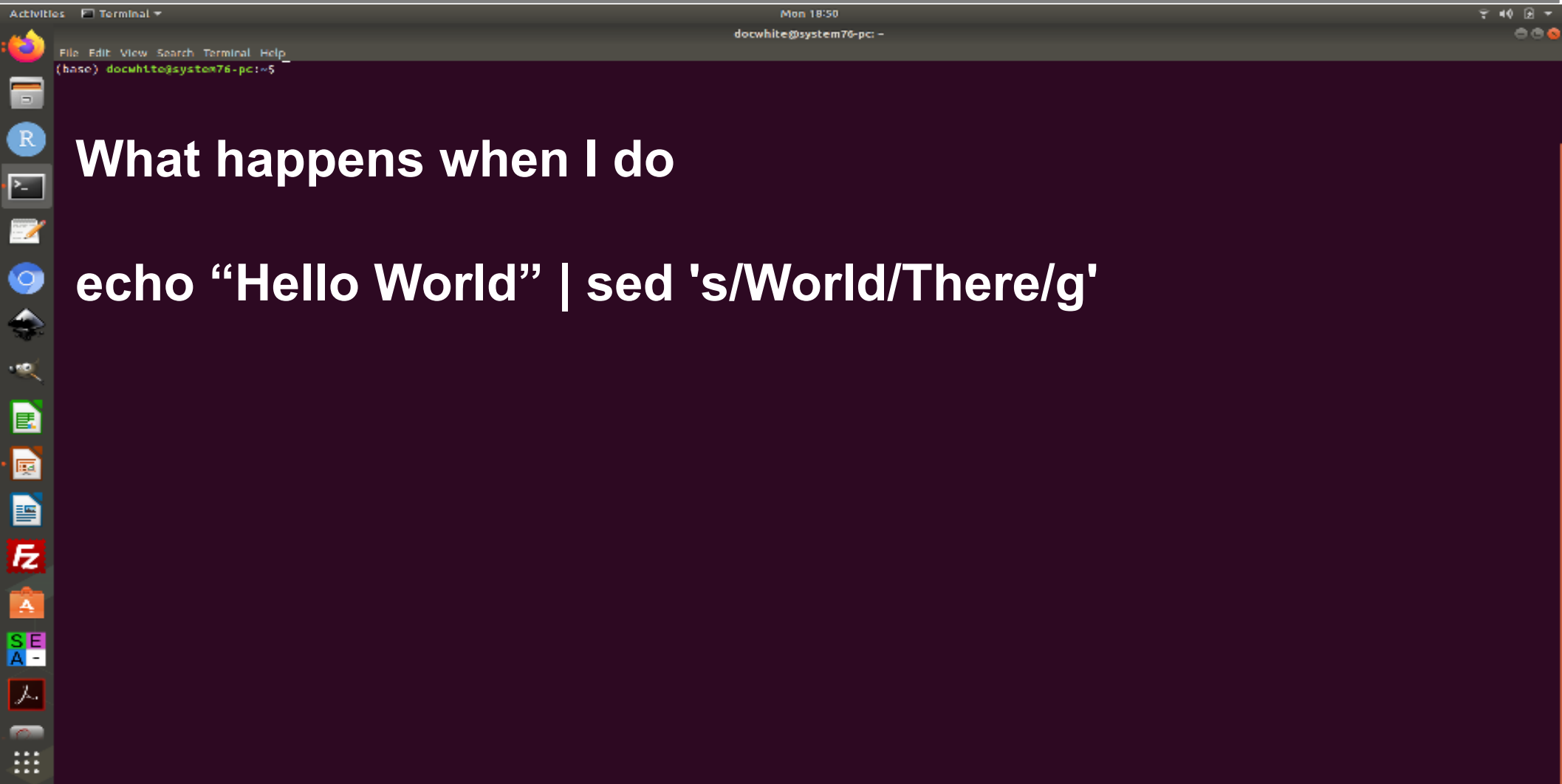
Then

More file.txt?

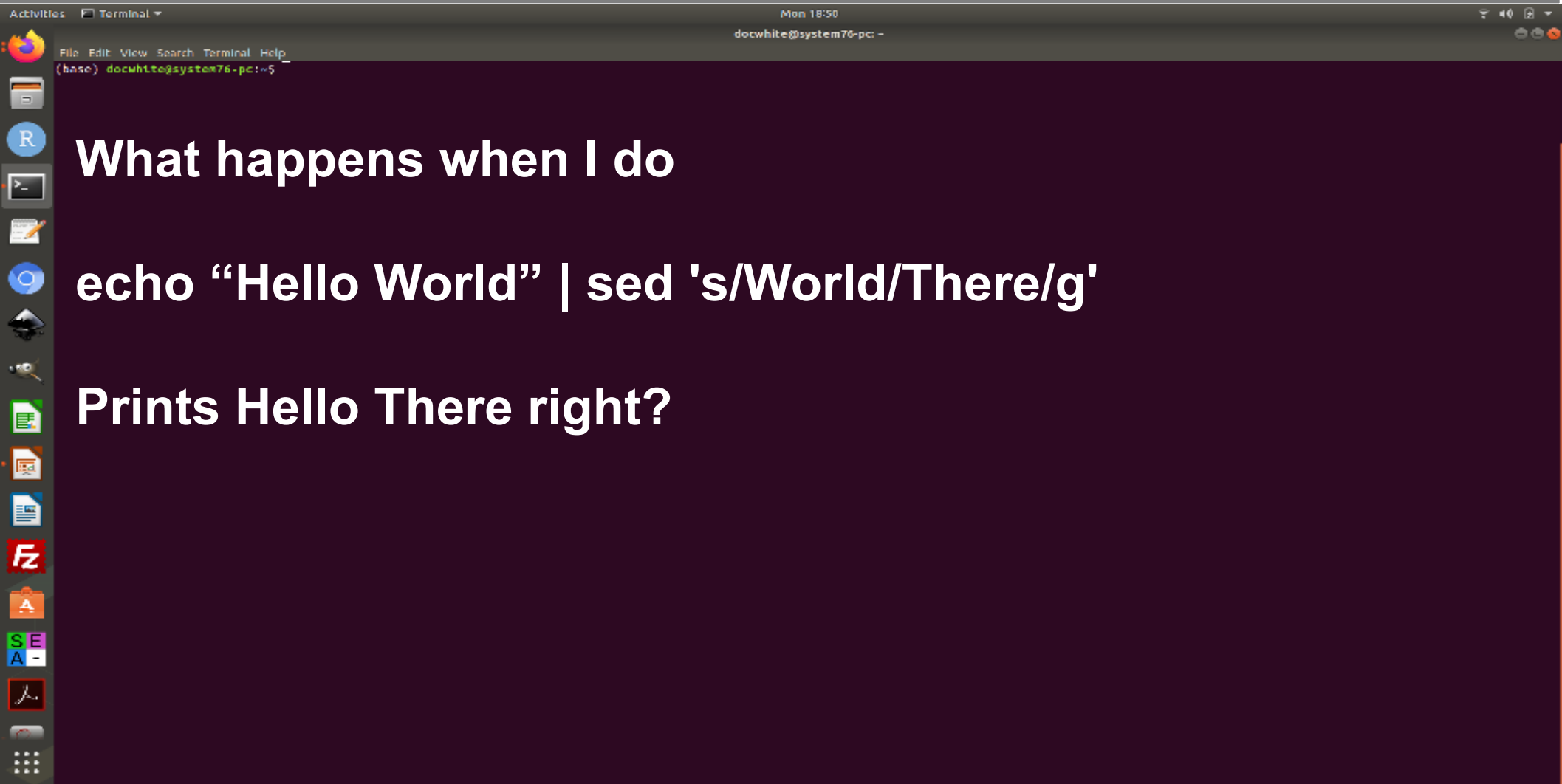
sed examples



sed examples



sed examples



What happens when I do

echo “Hello World” | sed 's/World/There/g'

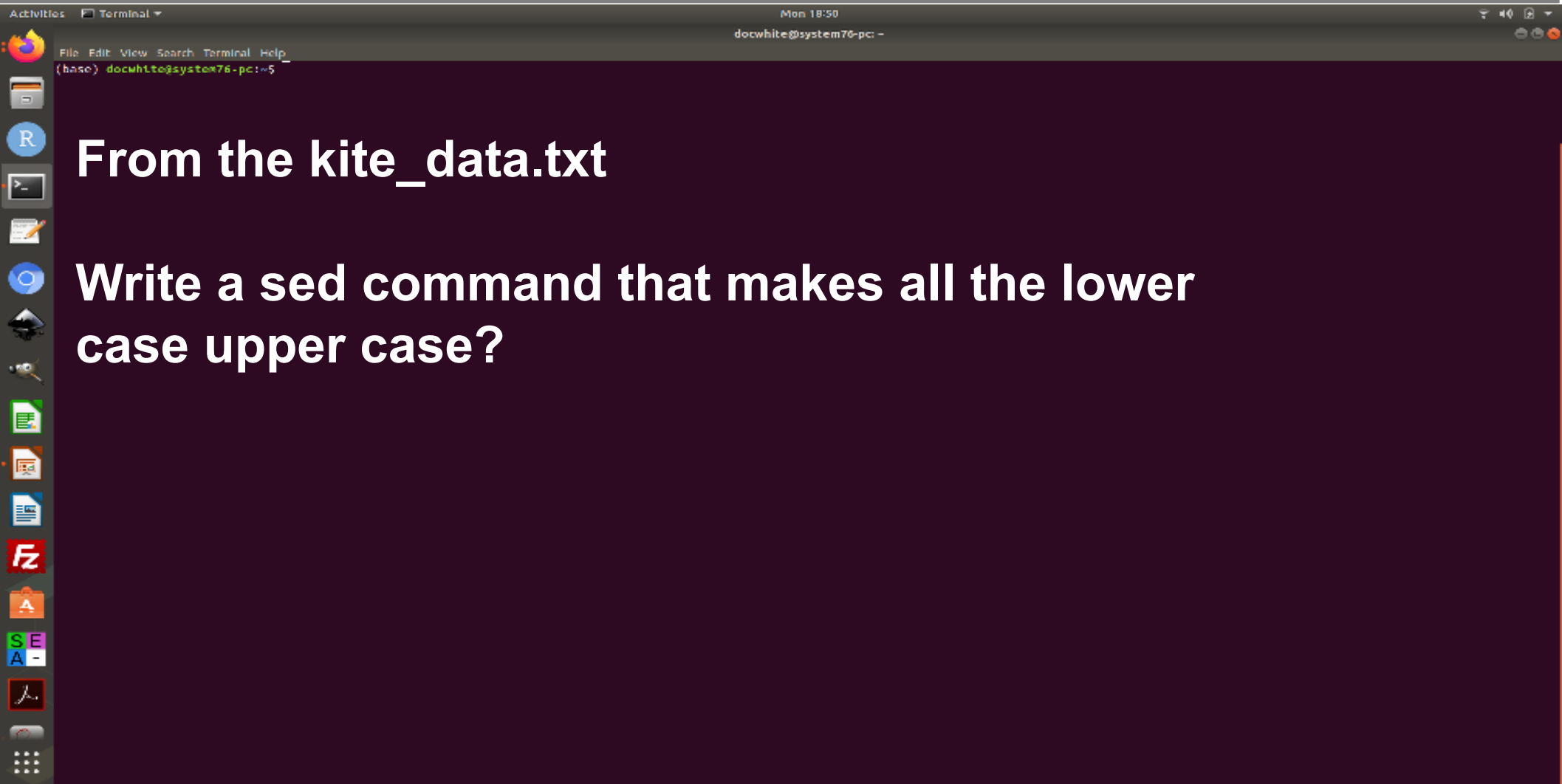
Prints Hello There right?

Sed – S swiss army knife

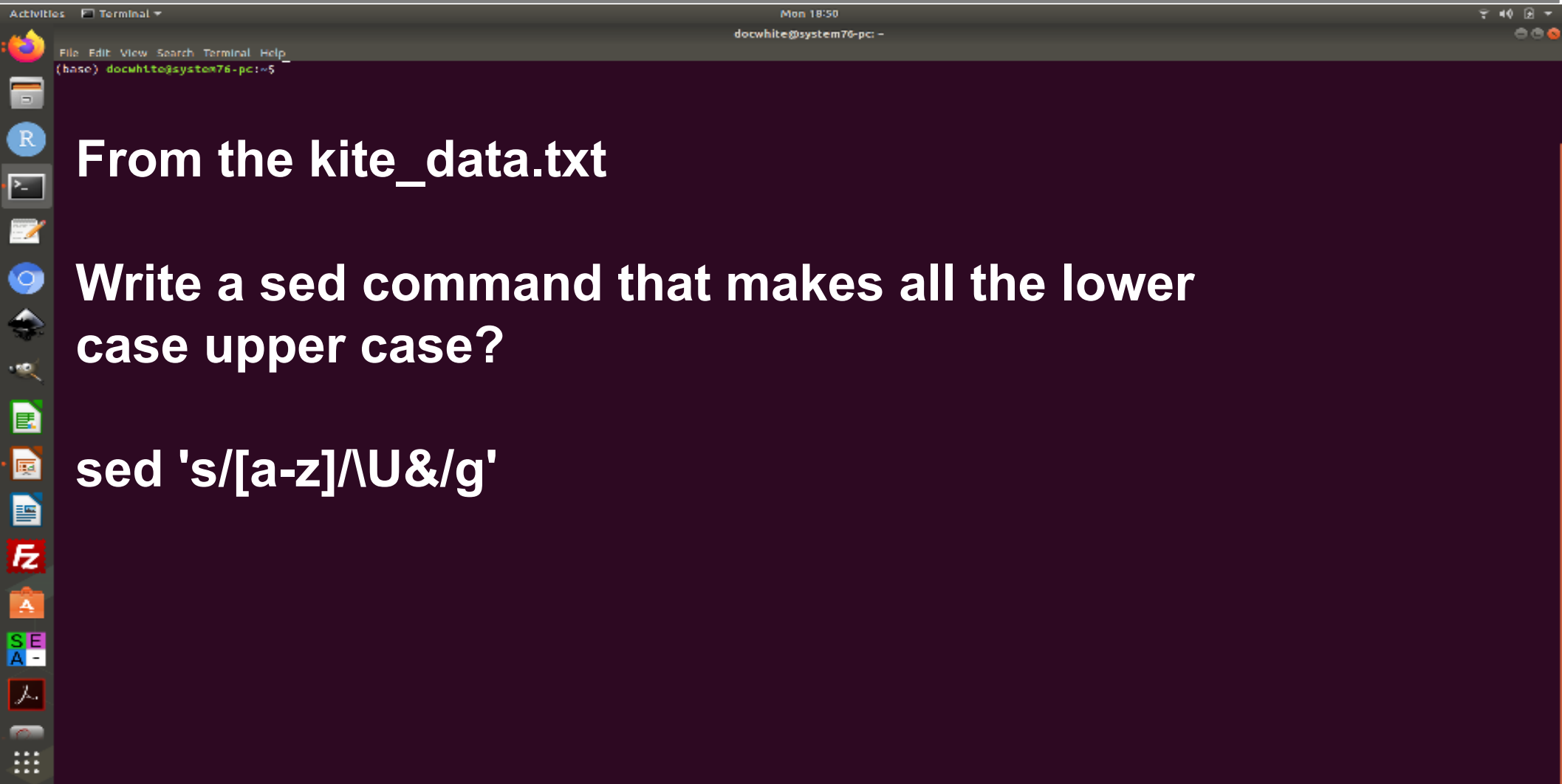
sed ‘s/regexp/replacement/flags’.

\L - Turn the replacement to lowercase until a \U or \E is found
\l - Turn the next character to lowercase,
\U - Turn the replacement to uppercase until a \L or \E is found,
\u -Turn the next character to uppercase,
\E - Stop case conversion started by \L or \U.
g - Apply the replacement to all matches to the regexp, not just the first.
d - Delete the pattern space; immediately start next cycle.
a comment, until the next newline.

sed examples



sed examples

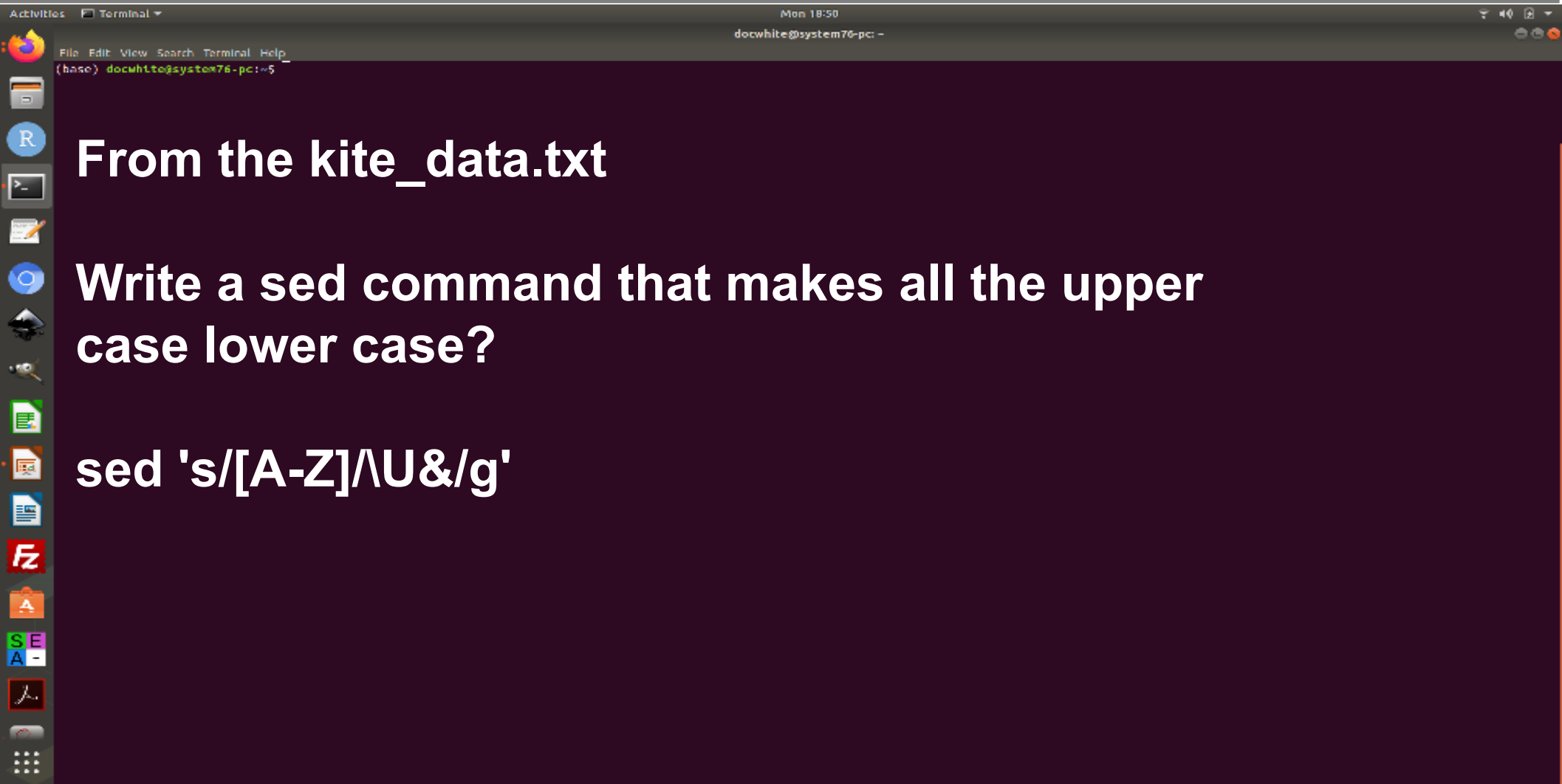


From the kite_data.txt

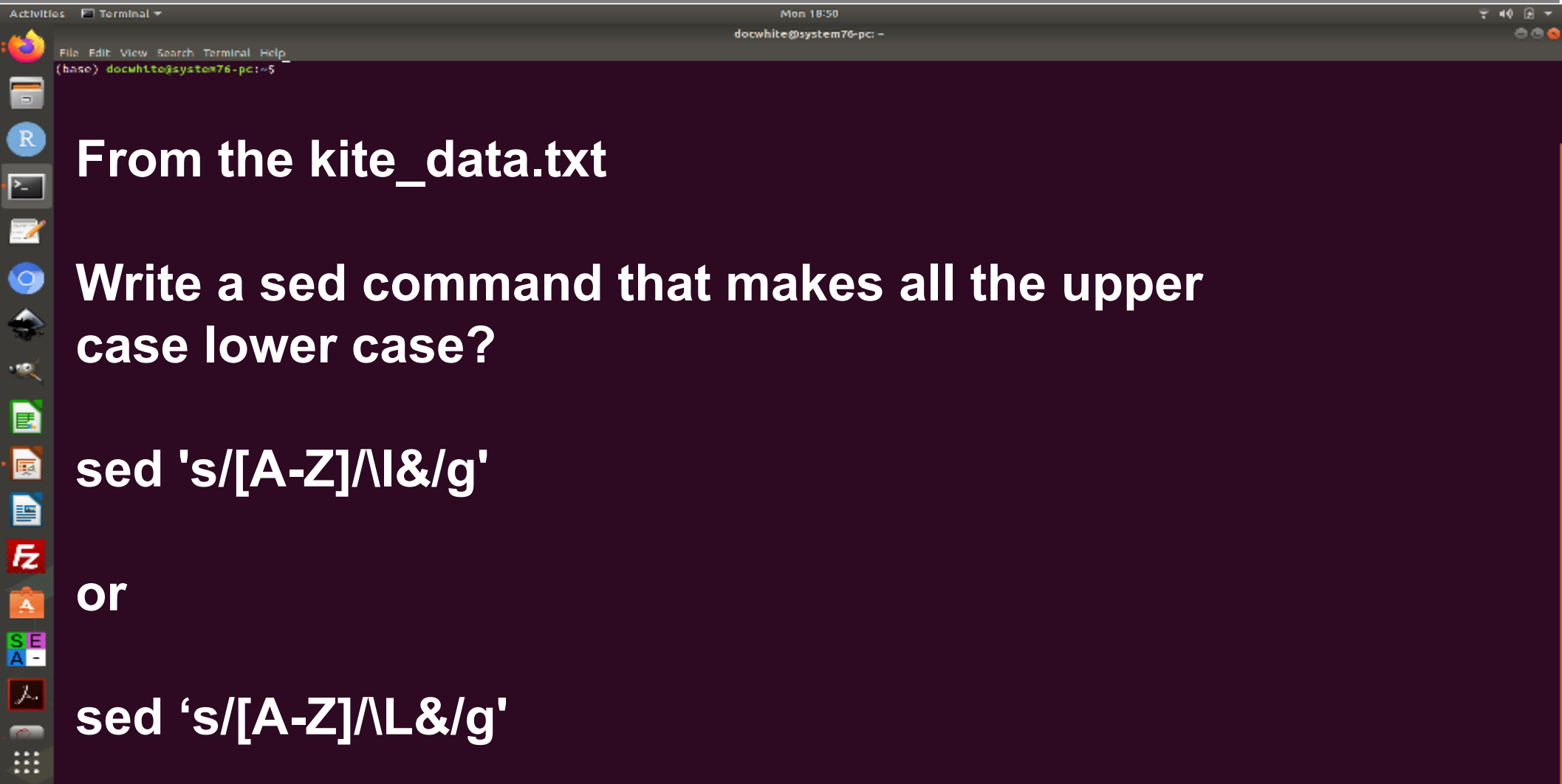
Write a sed command that makes all the lower case upper case?

sed 's/[a-z]/\U&/g'

sed examples



sed examples

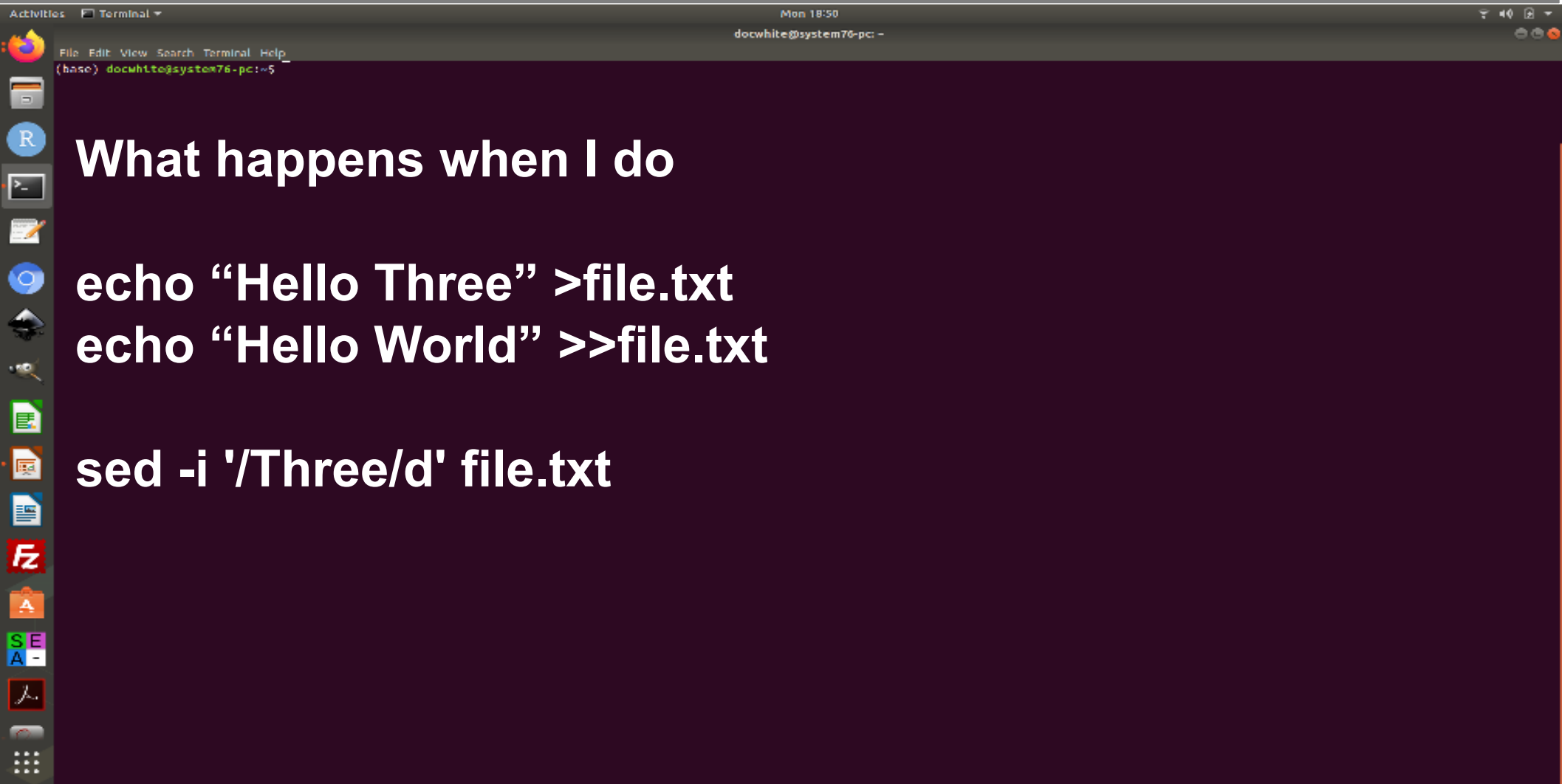


Sed – delete

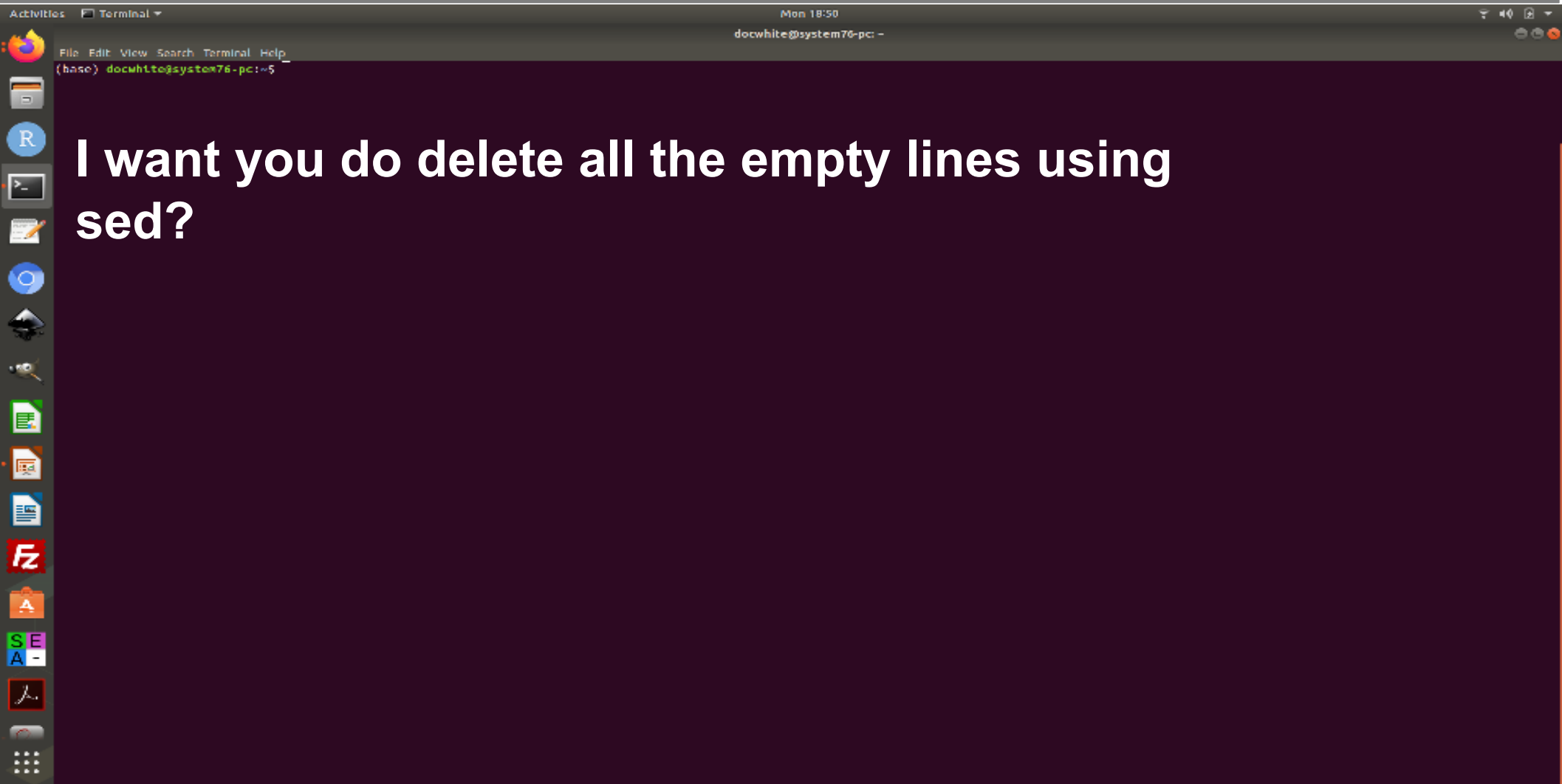
sed '/^ *$/d' inputFileName.

- The caret (^) matches the beginning of the line.
- The dollar sign ($) matches the end of the line.
- The asterisk (*) matches zero or more occurrences of the previous character.
- The plus (+) matches one or more occurrence(s) of the previous character.
- The question mark (?) matches zero or one occurrence of the previous character.
- The dot (.) matches exactly one character.

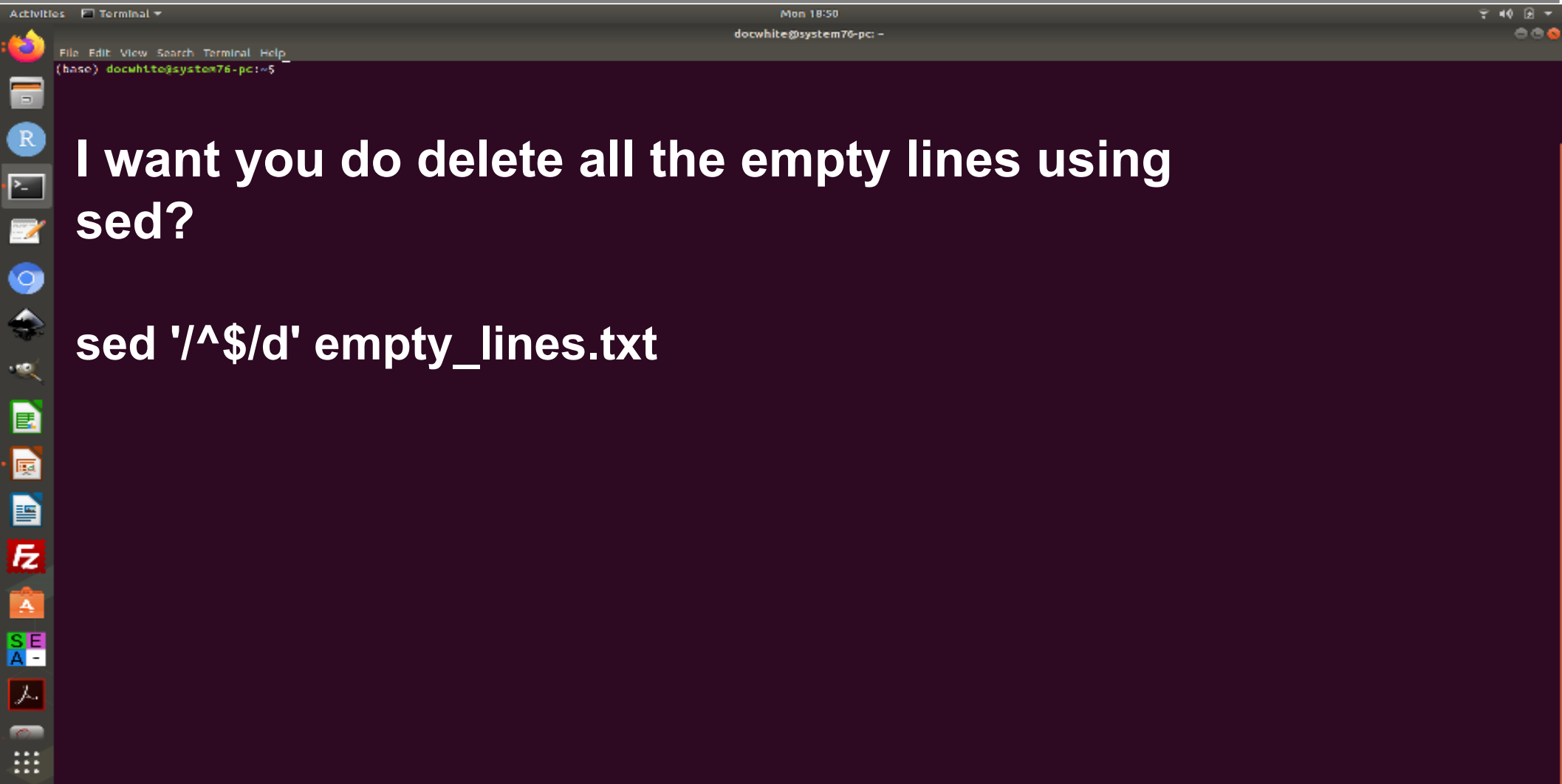
sed examples



sed examples



sed examples



Bonus 4

- Delete all the empty lines in the empty lines file with
→ grep
→ awk

- Delete all the ‘all white space’ with grep
→ grep
→ awk

Also, in python (think Pandas)

Quiz 4

- On canvas now