# BINF2111 – Introduction to Bioinformatics Computing

## UNIX 101 – enter the coding zone

UNIX

Richard Allen White III, PhD

RAW Lab

Lecture 5 - Tuesday Sep 3rd, 2024

## Learning Objectives

- Review bonus

- Comments about data and formats

- Sort/uniq/cut commands

- PATHS

- Quiz 5

## Bonus 4

- Delete all the empty lines in the empty lines file with

- Delete all the ‘all white space’ with grep

Also, in python (think Pandas)

## Bonus 4

- Delete all the empty lines in the empty lines file with
→ grep: grep -v -e '^$' file

- Delete all the ‘all white space’ with grep

Also, in python (think Pandas)

# Bonus 4

- Delete all the empty lines in the empty lines file with

→ grep: grep -v -e '^$' file

→ awk:  awk '!/^$/' file

- Delete all the ‘all white space’ with grep

Also, in python (think Pandas)

## Bonus 4

- Delete all the empty lines in the empty lines file with

→ grep: grep -v -e '^$' file

→ awk:  awk '!/^$/' file

- Delete all the ‘all white space’ with grep

→ grep: grep -v -e '^[[:space:]]*$' file

Also, in python (think Pandas)

## Bonus 4

- Delete all the empty lines in the empty lines file with
→ grep: grep -v -e '^$' file or egrep -v '^$' file
→ awk:  awk '!/^$/' file

- Delete all the ‘all white space’ with grep
→ grep: grep -v -e '^[[:space:]]*$' file
→ awk: awk 'NF > 0' file
→ sed '/^[[:space:]]*$/d'

Also, in python (think Pandas)
**Any one try in Python Pandas.**

## Bonus 4 – Python Pandas

- First use sed to convert from tsv (tab delim) to csv (column delim)

```
import pandas as pd

df = pd.read_csv('data.csv')
new_df = df.dropna()  or df.dropna(inplace = True)
print(new_df.to_string()) or print(df.to_string())
```

# Quiz 4

**Expression 1**
^[A-Z]

**Expression 2**
[A-Z]$

**A regular expression would do what to this file?**

```
head file.txt
line 1 bat cat RAT
line 2 RAT cat bat
line 3 rat cat bat
```

A) expression 1 acts on line 1, expression 2 acts on line 3.

B) expression 1 acts on line 2, expression 2 acts on line 1.

C) expression 1 acts on line 1, expression 2 acts on line 2.

# Quiz 4

**Expression 1**
^[A-Z]

**Expression 2**
[A-Z]$

**A regular expression would do what to this file?**

```
head file.txt
line 1 bat cat RAT
line 2 RAT cat bat
line 3 rat cat bat
```

A) expression 1 acts on line 1, expression 2 acts on line 3.

**B) expression 1 acts on line 2, expression 2 acts on line 1.**

C) expression 1 acts on line 1, expression 2 acts on line 2.

# Quiz 4

**Expression 1**
^[A-Z]

**Expression 2**
[A-Z]$

**A regular expression would do what to this file?**

```
head file.txt
line 1 bat cat RAT
line 2 RAT cat bat
line 3 rat cat bat
```

A) expression 1 acts on line 1, expression 2 acts on line 3.

**B) expression 1 acts on line 2, expression 2 acts on line 1.**

C) expression 1 acts on line 1, expression 2 acts on line 2.

# Quiz 4

**Expression 1**
^[A-Z]

**Expression 2**
[A-Z]$

**A regular expression would do what to this file?**

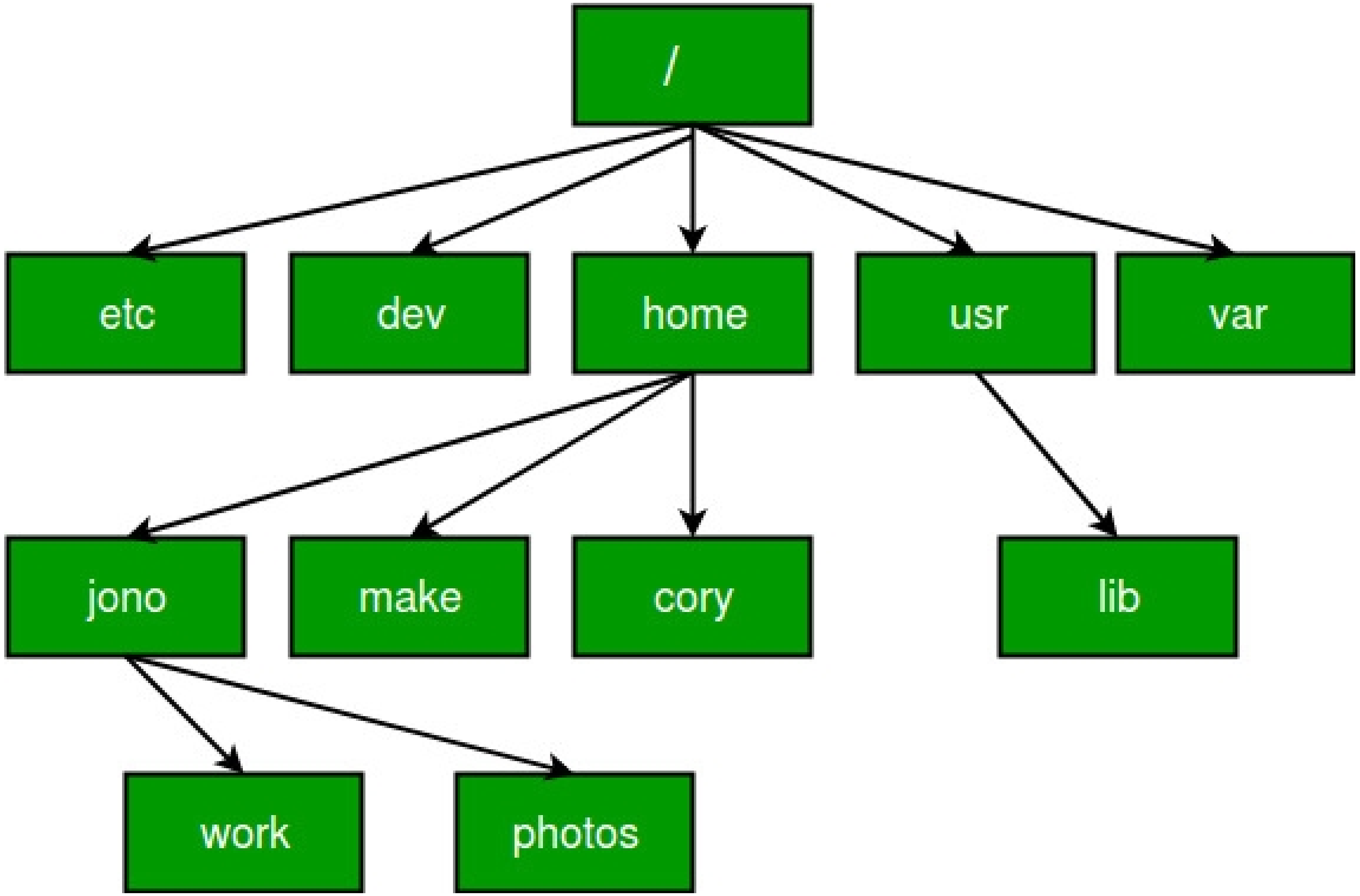
```
head file.txt
line 1 bat cat RAT
line 2 RAT cat bat
line 3 rat cat bat
```

A) expression 1 acts on line 1, expression 2 acts on line 3.

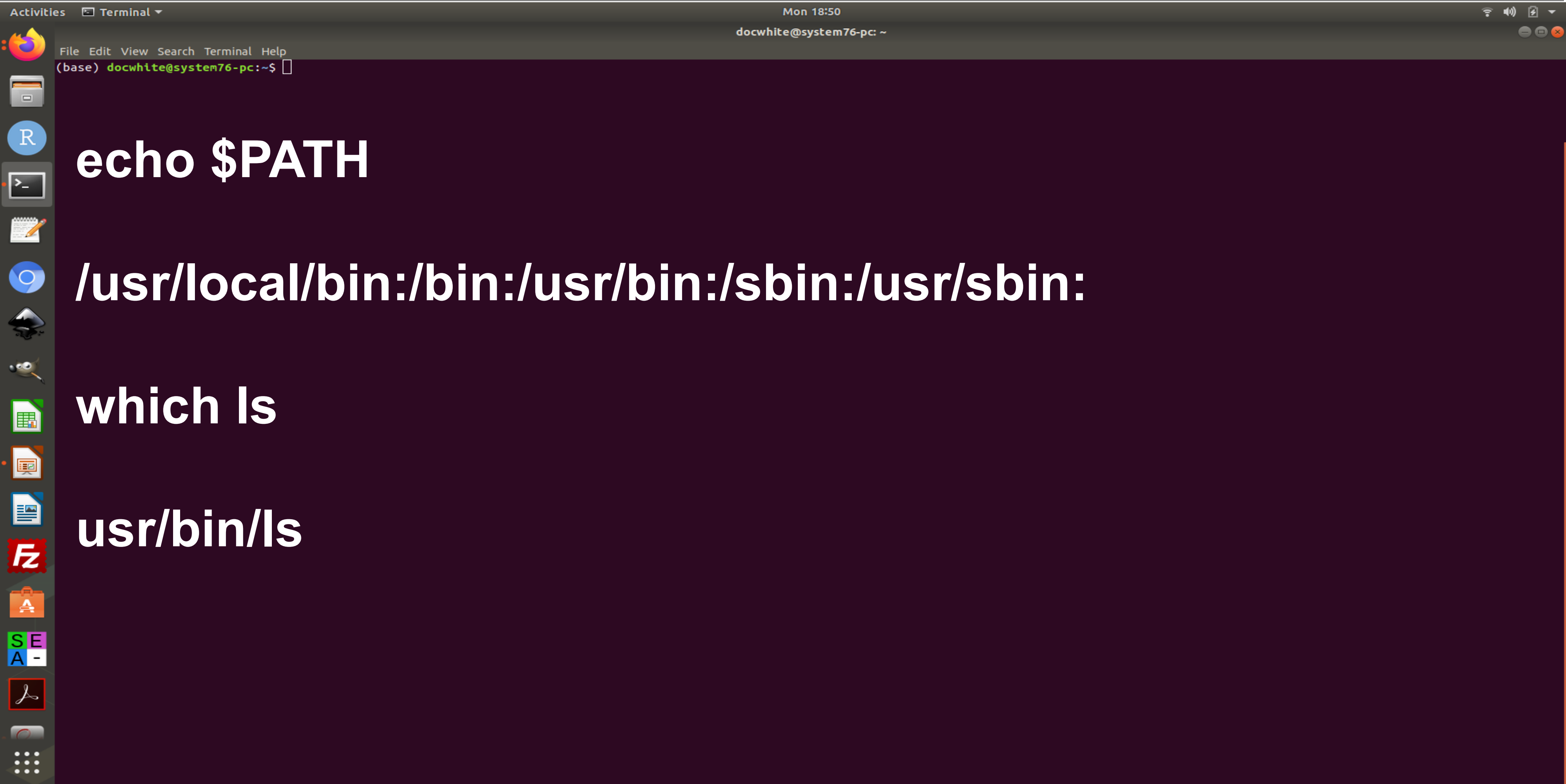
**B) expression 1 acts on line 2, expression 2 acts on line 1.**

C) expression 1 acts on line 1, expression 2 acts on line 2.

# PATHS



# PATHS



```
(base) docwhite@system76-pc:~$
```

```
echo $PATH

/usr/local/bin:/bin:/usr/bin:/sbin:/usr/sbin:

which ls

usr/bin/ls
```

## PATHS

```
echo $PATH
```

Finds which directories your shell is set to check for executable files.

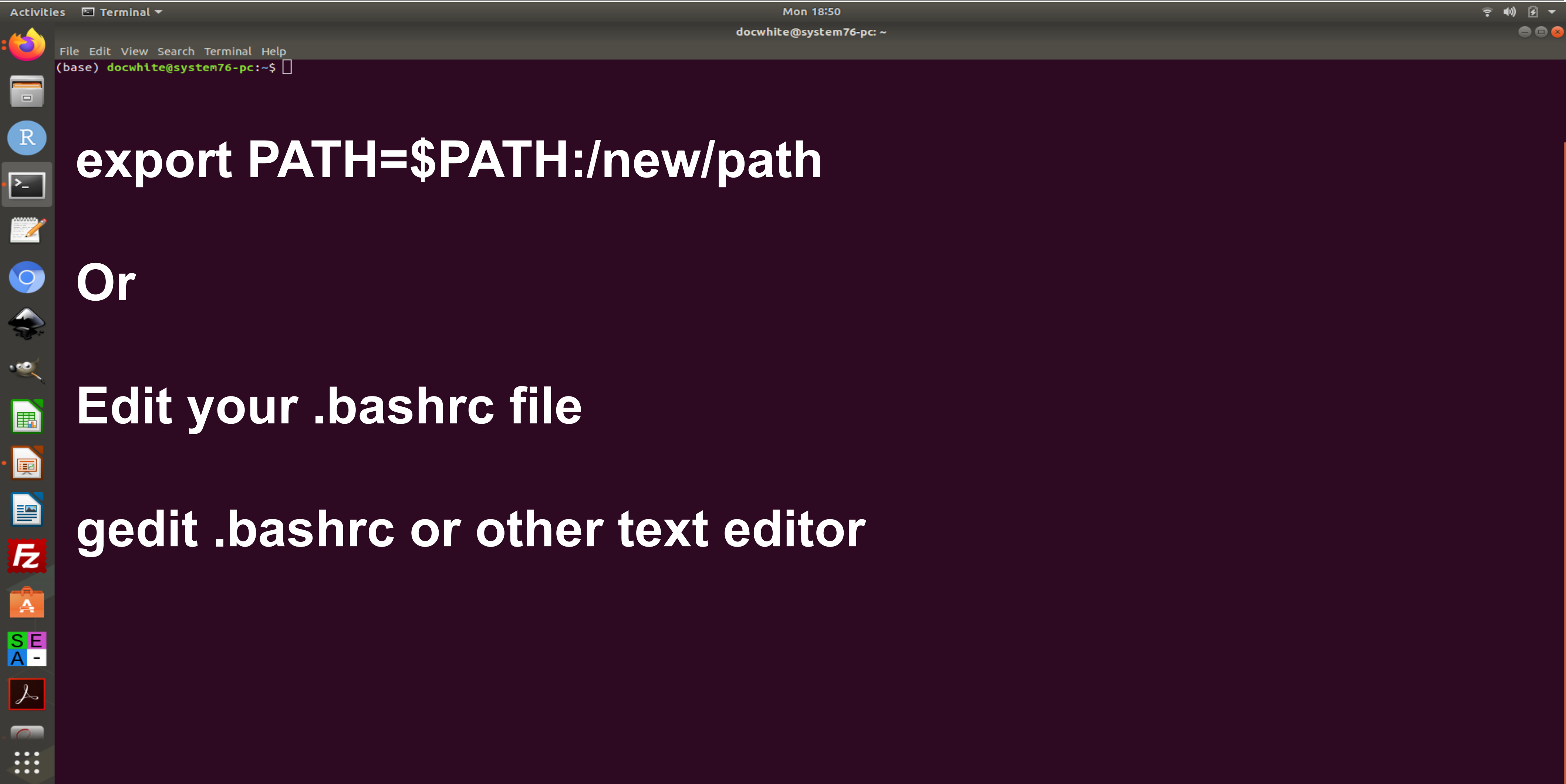
This output is a list of directories where executable files are stored.

This allows you to check which programs are executable from anywhere in the shell terminal. It allows for custom directory to be executed anywhere

If your installing programs this is very helpful to know.

As some have to be in your path in order to run

# PATHS



```
(base) docwhite@system76-pc:~$
```

export PATH=$PATH:/new/path

Or

Edit your .bashrc file

gedit .bashrc or other text editor

## General comments - data

**UNDERSTAND YOUR DATA**

Expectations - Format, Types, Domains, Uniqueness, etc.

Assumptions - Does it make sense to use data from X in a new context Y?

Restrictions - Licenses, Embargos, etc.

**STANDARDIZE YOUR DATA**

Values - ID mapping, Unit conversion, Adding/Removing Prefixes/Suffixes, etc.

Columns - Adding, Removing, Rearranging, Merging, Splitting, etc.

Rows - Filtering data (duplicates, missing data, not relevant to task, etc)

**RECORD YOUR ANALYSIS PROCESS**

Your computer is a lab - Keep a lab notebook!

Use Version Control like GitHub or BitBucket.

# General comments - data formats

**Column-oriented data**

Spreadsheets, CSV, Tabular, delimited

Fixed position

One line per record, fixed set of fields (columns)

**Key-Value data**

Multiple lines per record

Variable number of fields/values

**Hierarchical data (XML, JSON, Ontologies, etc)**

Nested - usually requires a more complex parser

Usually follow a well-defined schema.

**Web-based API resources**

Issue specific commands to get different types of data

**Infinite proprietary formats**

Usually harder to parse but generally act like other types

# General comments: Column-Oriented

**Easy to browse/explore**
- MOST files are this type

**Best for databases**
- Delimiters are tabs or commas between fields
- 1 line = 1 record
- Each record has fixed set of fields

**Complex code not needed:**
- Excel can handle small datasets (<1 million rows)
- UNIX can handle the rest

**CSV**

```
david,abdul,xi,bill
mary,david,bill,abdul
wang,abdul,xi,david
```

**TSV**

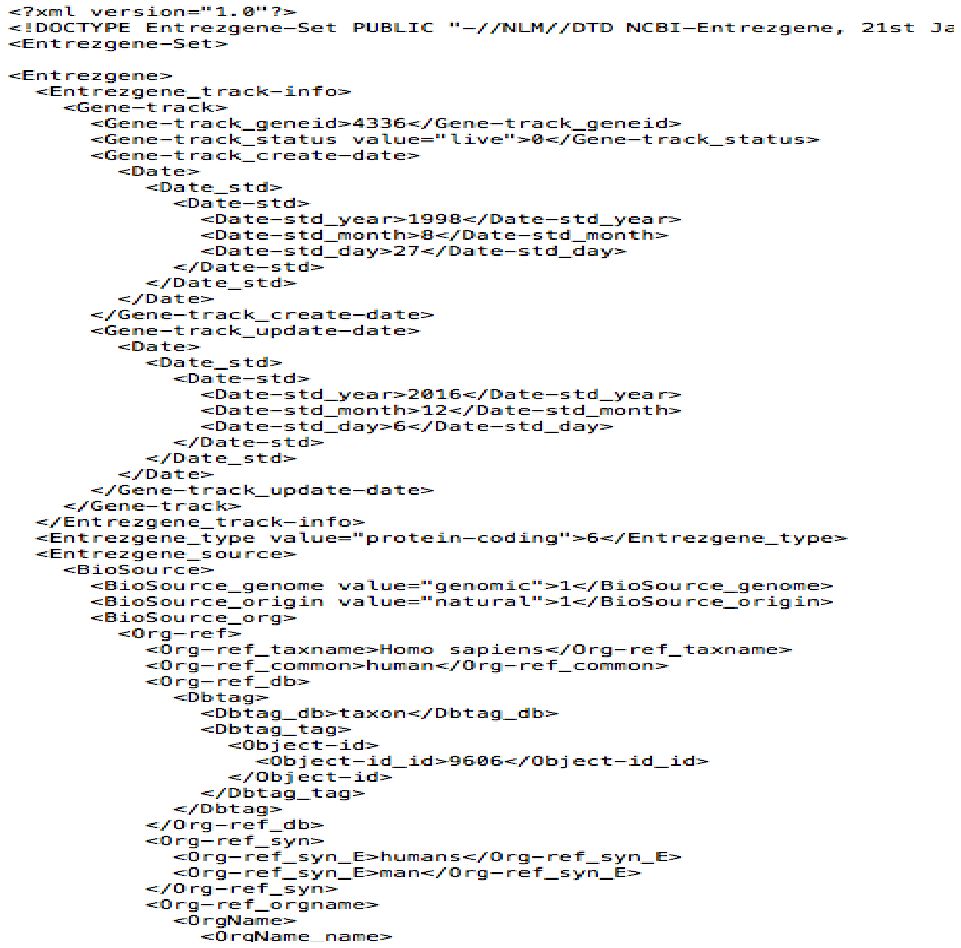
```
David  abdul  xi        bill
Mary   david  bill
abdul
Wang  abdul  xi
david
```

## General comments - XML formats

**Machine-readable**
 - Many tools and libraries available to parse it

**Can represent complex structures**
- multiple values
- nested structures

**Not trivial for non-coders**



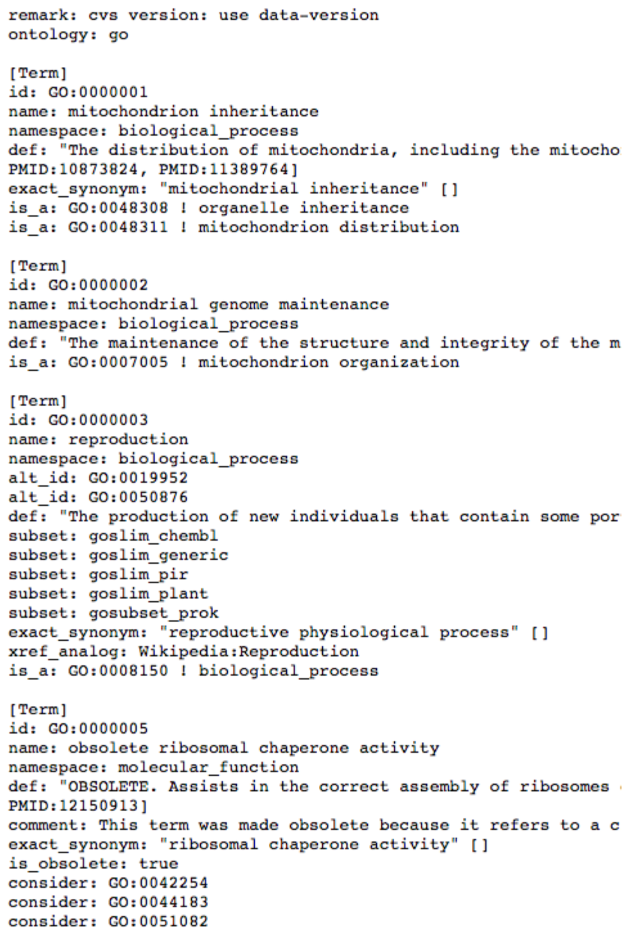
```
<?xml version="1.0"?>
<!DOCTYPE Entrezgene-Set PUBLIC "-//NLM//DTD NCBI-Entrezgene, 21st Ja
<Entrezgene-Set>

<Entrezgene>
  <Entrezgene_track-info>
    <Gene-track>
      <Gene-track_geneid>4336</Gene-track_geneid>
      <Gene-track_status value="live">0</Gene-track_status>
      <Gene-track_create-date>
        <Date>
          <Date_std>
            <Date-std>
              <Date-std_year>1998</Date-std_year>
              <Date-std_month>8</Date-std_month>
              <Date-std_day>27</Date-std_day>
            </Date-std>
          </Date_std>
        </Date>
      </Gene-track_create-date>
      <Gene-track_update-date>
        <Date>
          <Date_std>
            <Date-std>
              <Date-std_year>2016</Date-std_year>
              <Date-std_month>12</Date-std_month>
              <Date-std_day>6</Date-std_day>
            </Date-std>
          </Date_std>
        </Date>
      </Gene-track_update-date>
    </Gene-track>
  </Entrezgene_track-info>
  <Entrezgene_type value="protein-coding">6</Entrezgene_type>
  <Entrezgene_source>
    <BioSource>
      <BioSource_genome value="genomic">1</BioSource_genome>
      <BioSource_origin value="natural">1</BioSource_origin>
      <BioSource_org>
        <Org-ref>
          <Org-ref_taxname>Homo sapiens</Org-ref_taxname>
          <Org-ref_common>human</Org-ref_common>
          <Org-ref_db>
            <Dbtag>
              <Dbtag_db>taxon</Dbtag_db>
              <Dbtag_tag>
                <Object-id>
                  <Object-id_id>9606</Object-id_id>
                </Object-id>
              </Dbtag_tag>
            </Dbtag>
          </Org-ref_db>
          <Org-ref_syn>
            <Org-ref_syn_E>humans</Org-ref_syn_E>
            <Org-ref_syn_E>man</Org-ref_syn_E>
          </Org-ref_syn>
          <Org-ref_orgname>
            <OrgName>
              <OrgName_name>
```

# General comments: Key-value formats

**Easy to read**

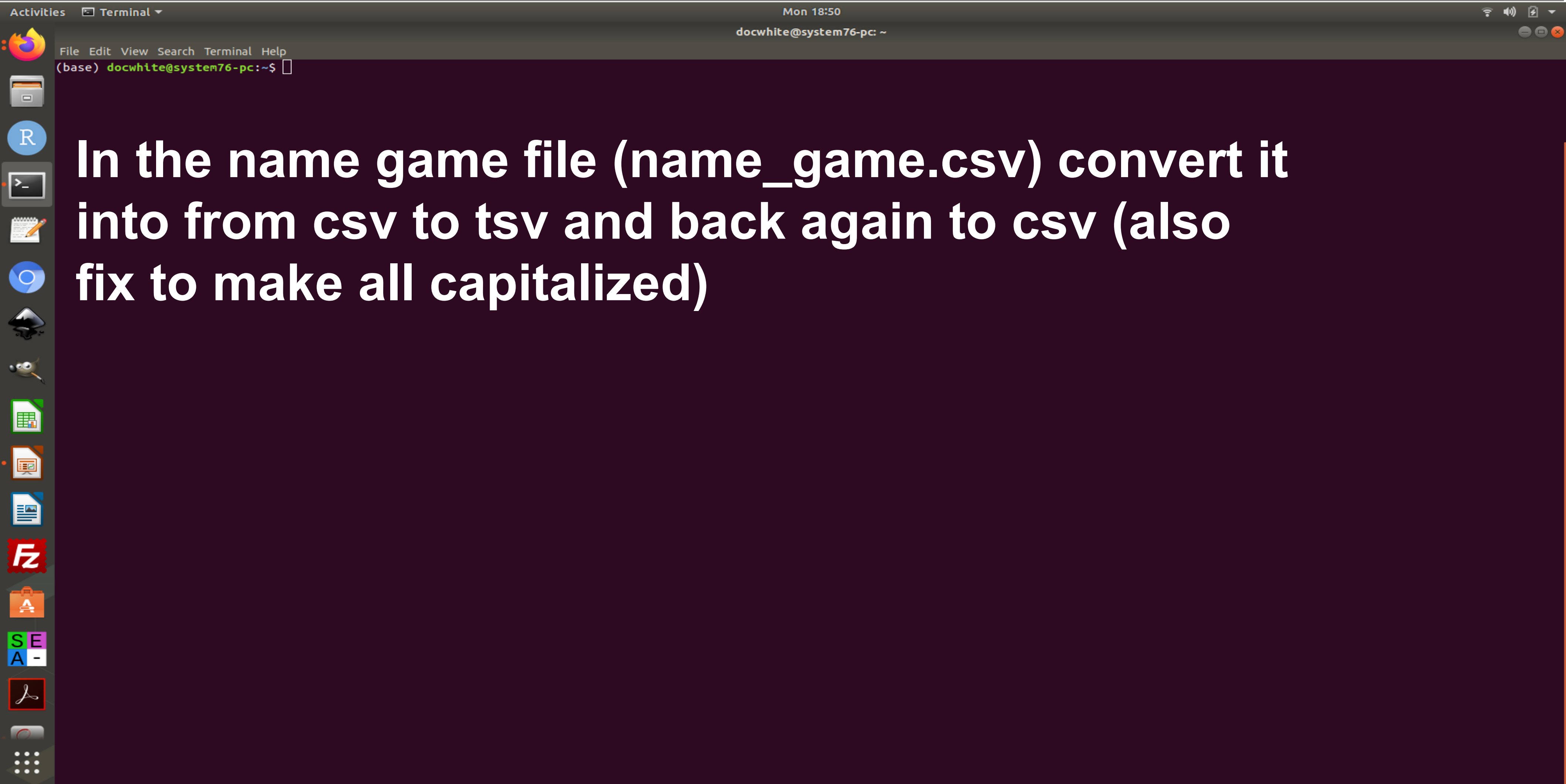
**Straightforward to parse**
- Delimiter for each Record
- One key-value pair per line
- Supports multiple values

**Novice coders can handle it!**



```
remark: cvs version: use data-version
ontology: go

[Term]
id: GO:0000001
name: mitochondrion inheritance
namespace: biological_process
def: "The distribution of mitochondria, including the mitocho
PMID:10873824, PMID:11389764]
exact_synonym: "mitochondrial inheritance" []
is_a: GO:0048308 ! organelle inheritance
is_a: GO:0048311 ! mitochondrion distribution

[Term]
id: GO:0000002
name: mitochondrial genome maintenance
namespace: biological_process
def: "The maintenance of the structure and integrity of the m
is_a: GO:0007005 ! mitochondrion organization

[Term]
id: GO:0000003
name: reproduction
namespace: biological_process
alt_id: GO:0019952
alt_id: GO:0050876
def: "The production of new individuals that contain some por
subset: goslim_chembl
subset: goslim_generic
subset: goslim_pir
subset: goslim_plant
subset: gosubset_prok
exact_synonym: "reproductive physiological process" []
xref_analog: Wikipedia:Reproduction
is_a: GO:0008150 ! biological_process

[Term]
id: GO:0000005
name: obsolete ribosomal chaperone activity
namespace: molecular_function
def: "OBSOLETE. Assists in the correct assembly of ribosomes
PMID:12150913]
comment: This term was made obsolete because it refers to a c
exact_synonym: "ribosomal chaperone activity" []
is_obsolete: true
consider: GO:0042254
consider: GO:0044183
consider: GO:0051082
```

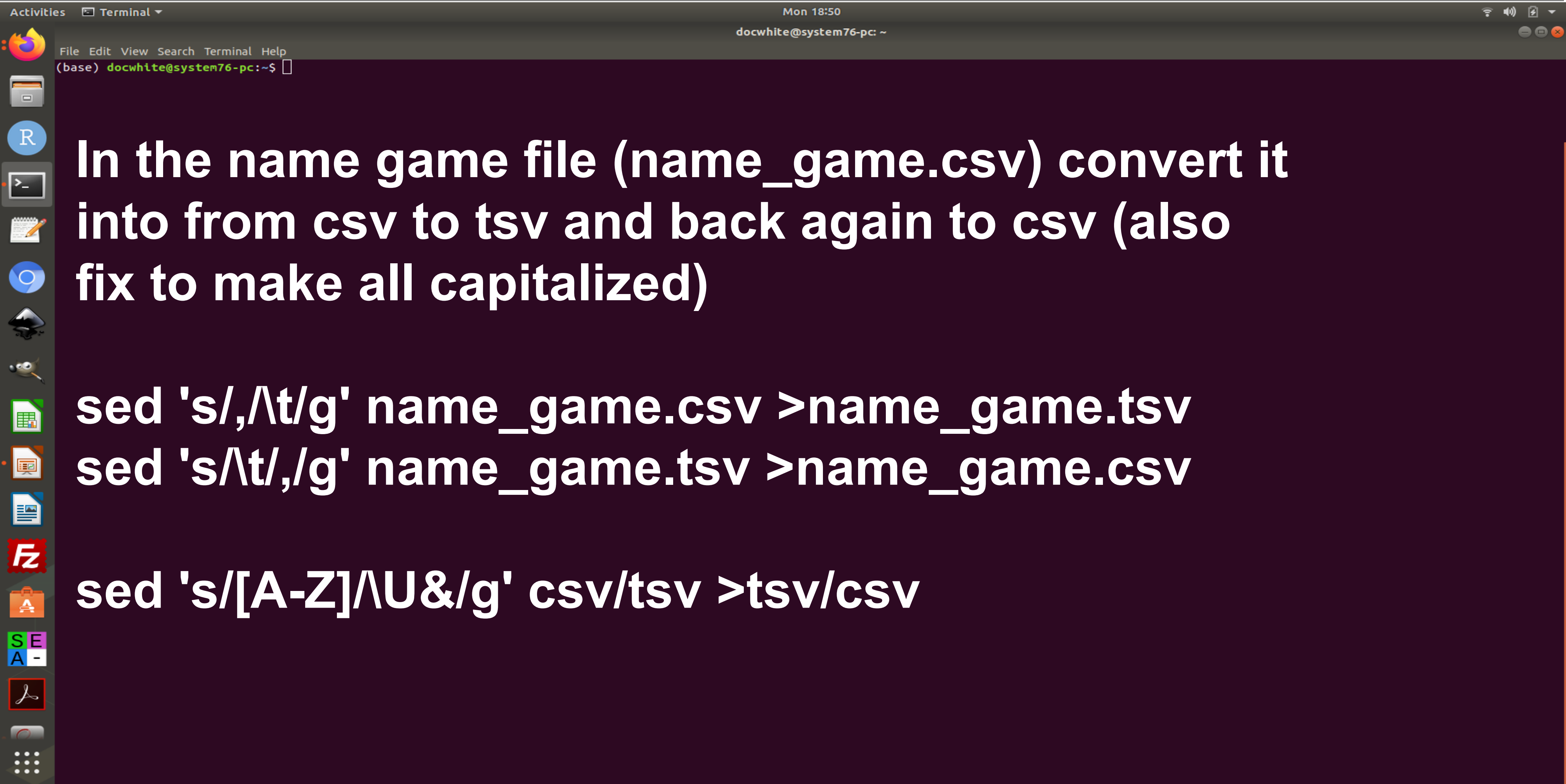
## Column-oriented fixes examples



```
(base) docwhite@system76-pc:~$
```

In the name game file (name_game.csv) convert it into from csv to tsv and back again to csv (also fix to make all capitalized)

# Column-oriented fixes examples



```
(base) docwhite@system76-pc:~$ 
```

In the name game file (name_game.csv) convert it into from csv to tsv and back again to csv (also fix to make all capitalized)

```
sed 's/,/\t/g' name_game.csv >name_game.tsv
sed 's/\t/,/g' name_game.tsv >name_game.csv
```

```
sed 's/[A-Z]/\U&/g' csv/tsv >tsv/csv
```

## cut – syntax anatomy UNIX's scissors

# cut [options] file.txt

-d (--delimiter) "," set field delimiter (default tab)

-f (--fields=LIST) Select by specifying a field

    -f 2 select a field to cut (left is 1)

    -f 2-8,12 select multiple fields to cut

-b (--bytes=LIST) Select by specifying a byte

-c (--characters=LIST) Select by specifying a character

--complement - Complement the selection.

-s (--only-delimited) suppress non-matches

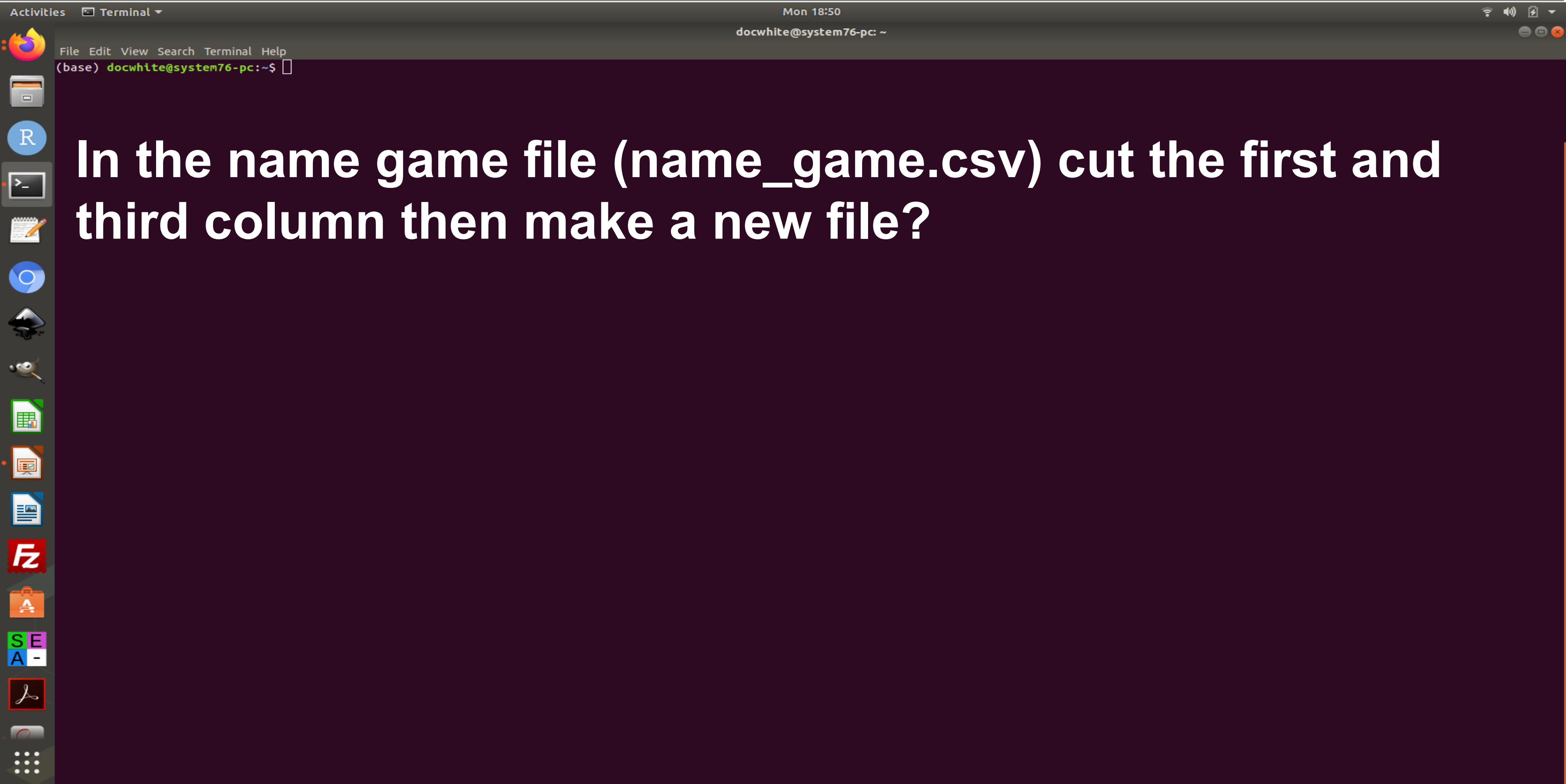
## cut – syntax anatomy UNIX’s scissors

**gcut [options] file.txt**

**Install coreutils**

**brew install coreutils**

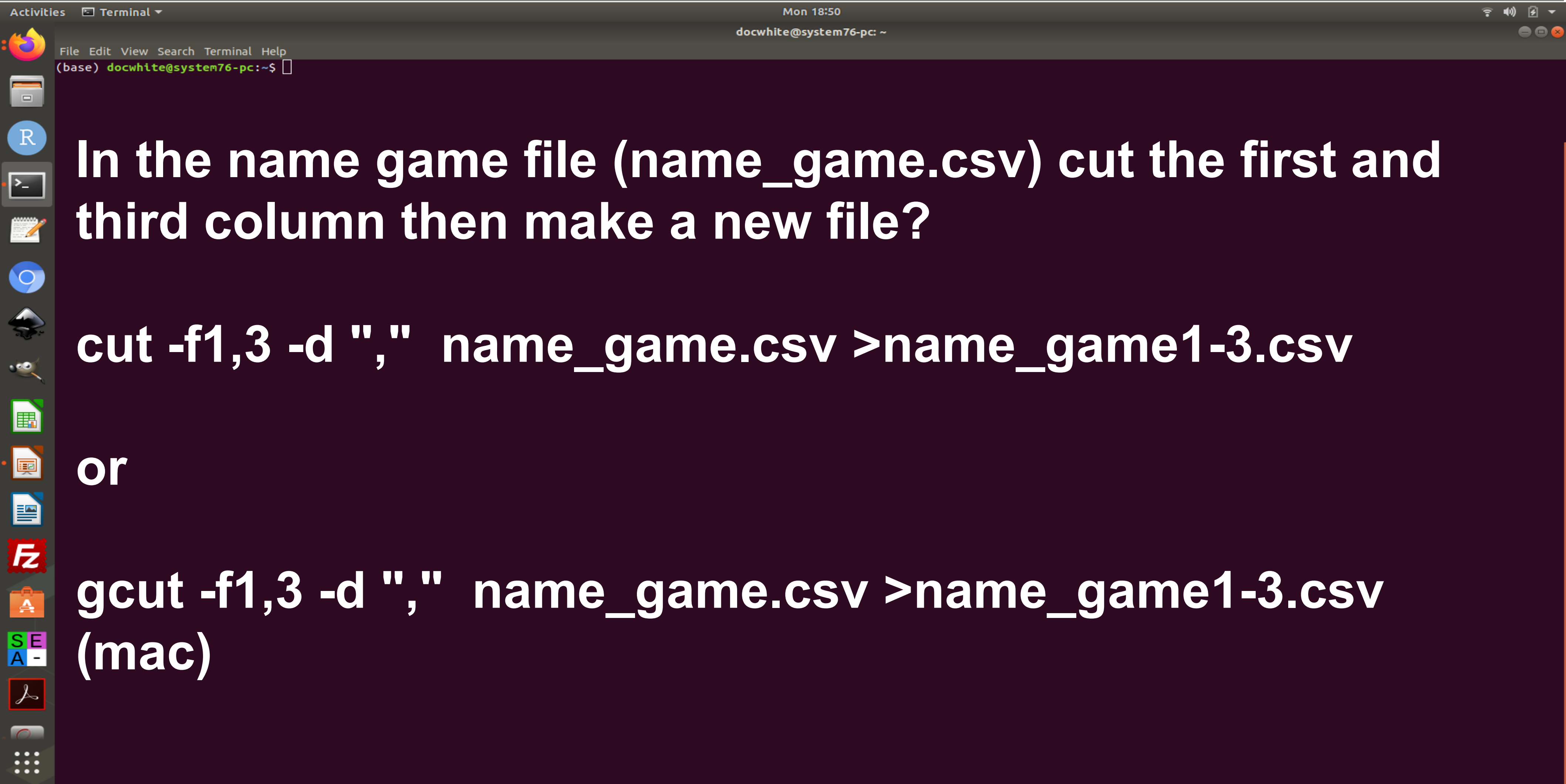
# Cut examples



```
(base) docwhite@system76-pc:~$ 
```

**In the name game file (name_game.csv) cut the first and third column then make a new file?**

# Cut examples



```
(base) docwhite@system76-pc:~$
```

In the name game file (name_game.csv) cut the first and third column then make a new file?

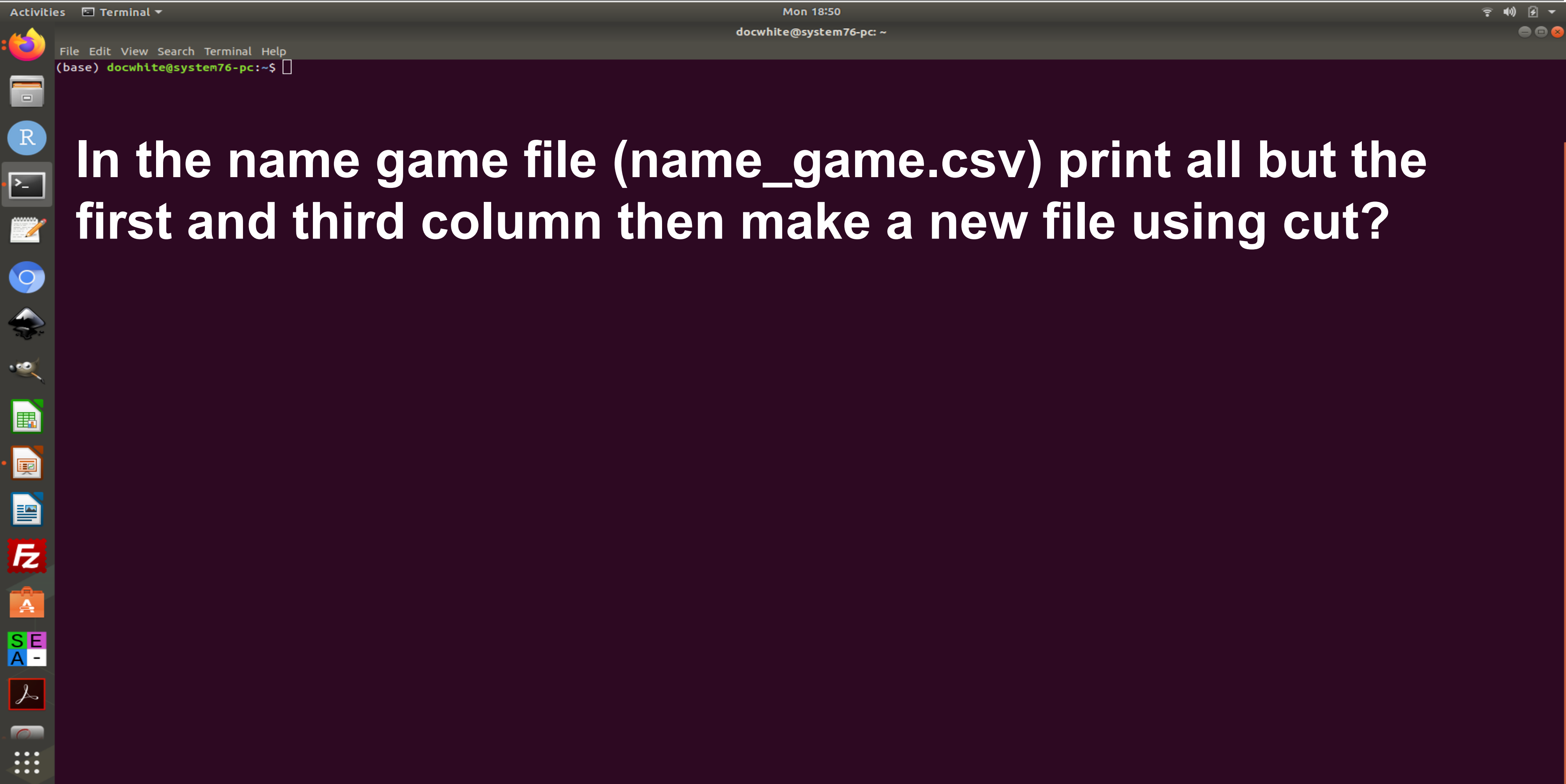
```
cut -f1,3 -d ","  name_game.csv >name_game1-3.csv
```

or

```
gcut -f1,3 -d ","  name_game.csv >name_game1-3.csv
```

(mac)

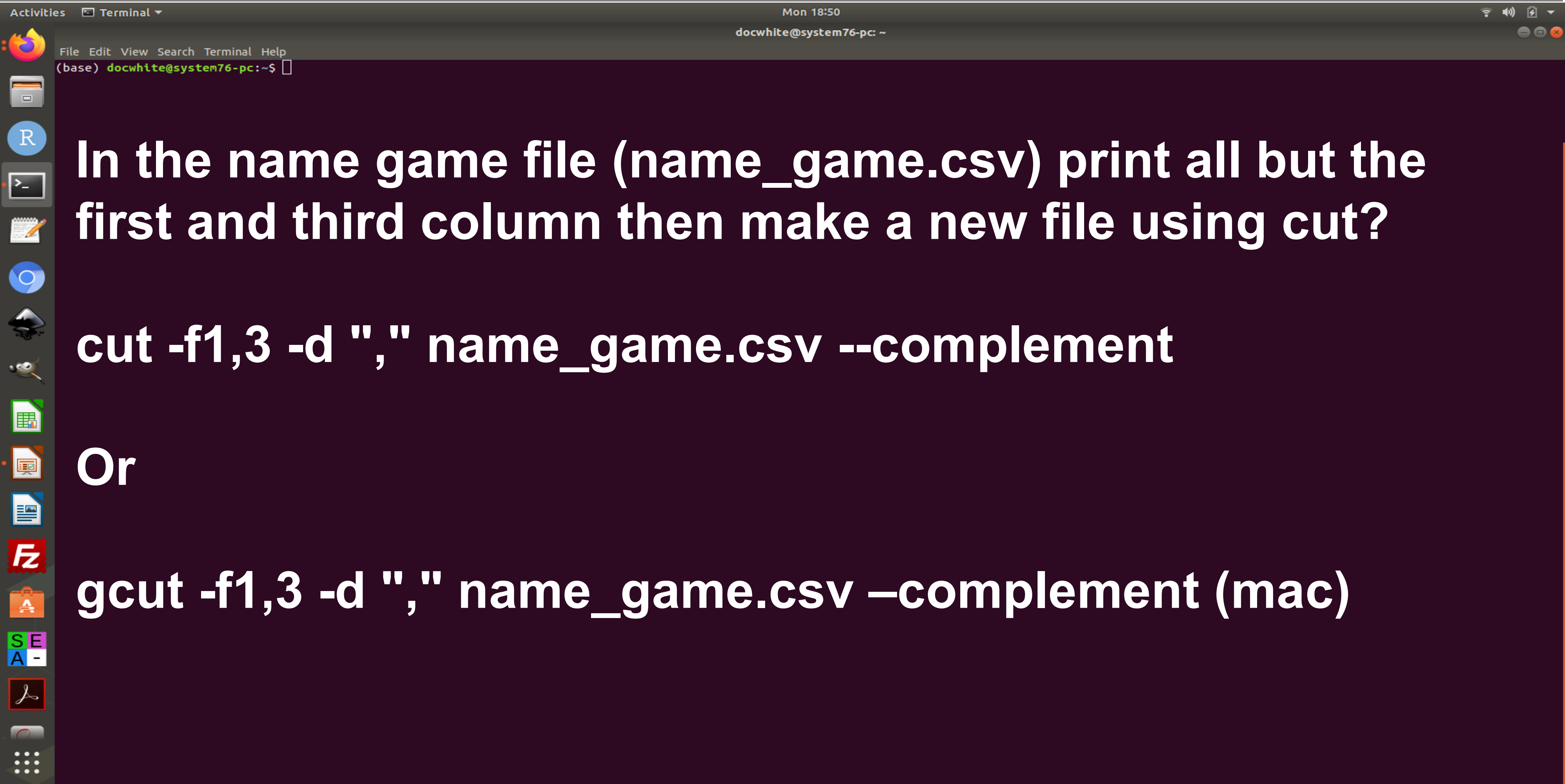
# Cut examples



```
(base) docwhite@system76-pc:~$
```

**In the name game file (name_game.csv) print all but the first and third column then make a new file using cut?**

# Cut examples



```
(base) docwhite@system76-pc:~$
```

In the name game file (name_game.csv) print all but the first and third column then make a new file using cut?

cut -f1,3 -d "," name_game.csv --complement

Or

gcut -f1,3 -d "," name_game.csv –complement (mac)

# sort – syntax anatomy of sort

## sort [options] file.txt

-t “t”  set the delimiter when using -k

default is non-blank to blank transition

-k 3   sort column #3 (left is 1)

-k 2,3  sort multiple columns

-n  sort numerically

-r  reverse sort order

-u  drop duplicates from the result

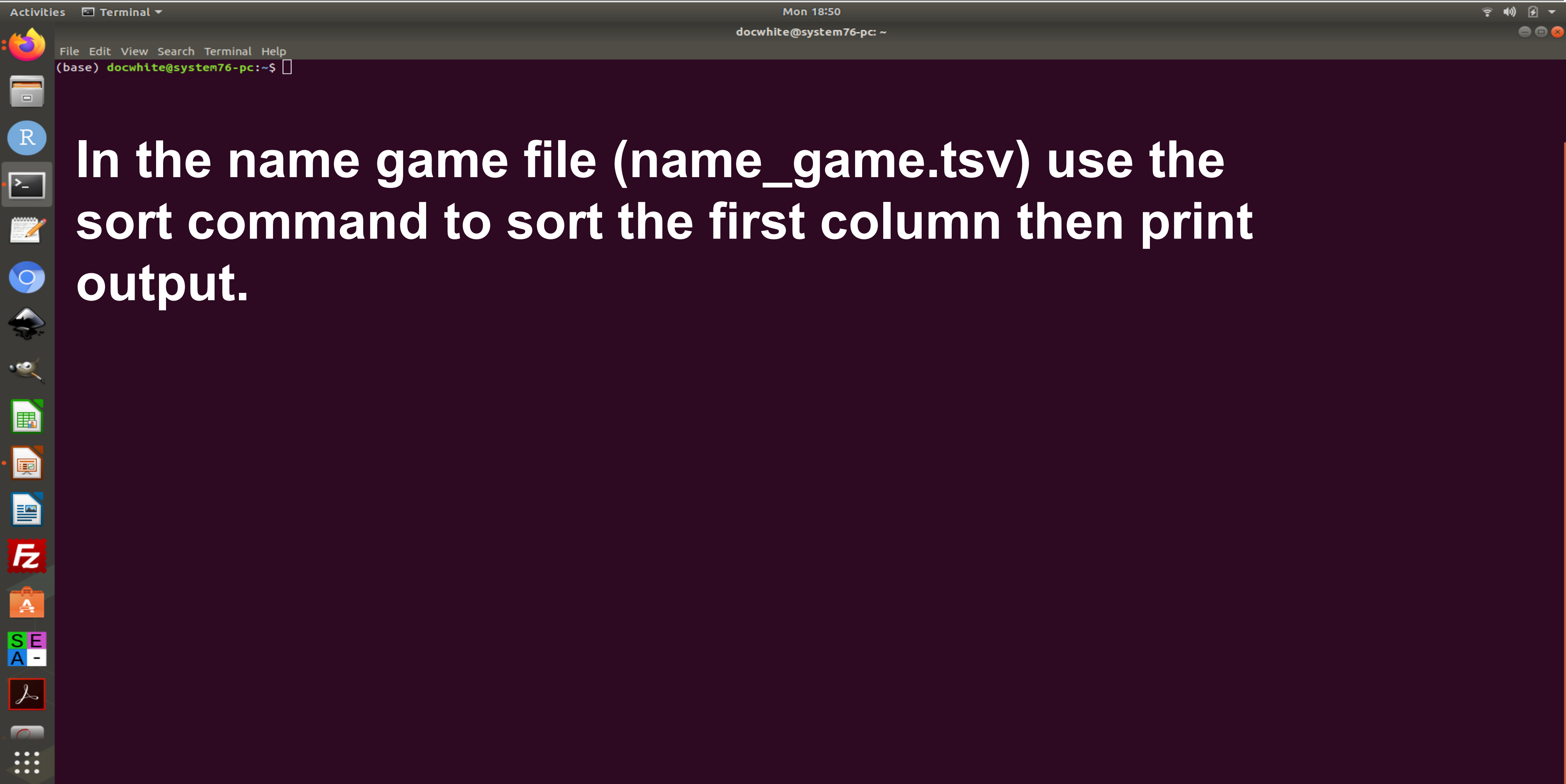
-b, --ignore-leading-blanks, ignore leading blanks

-d, --dictionary-order consider only blanks and alphanumeric characters

-f, --ignore-case fold lower case to upper case characters

No options: sort alphabetically from leftmost character.

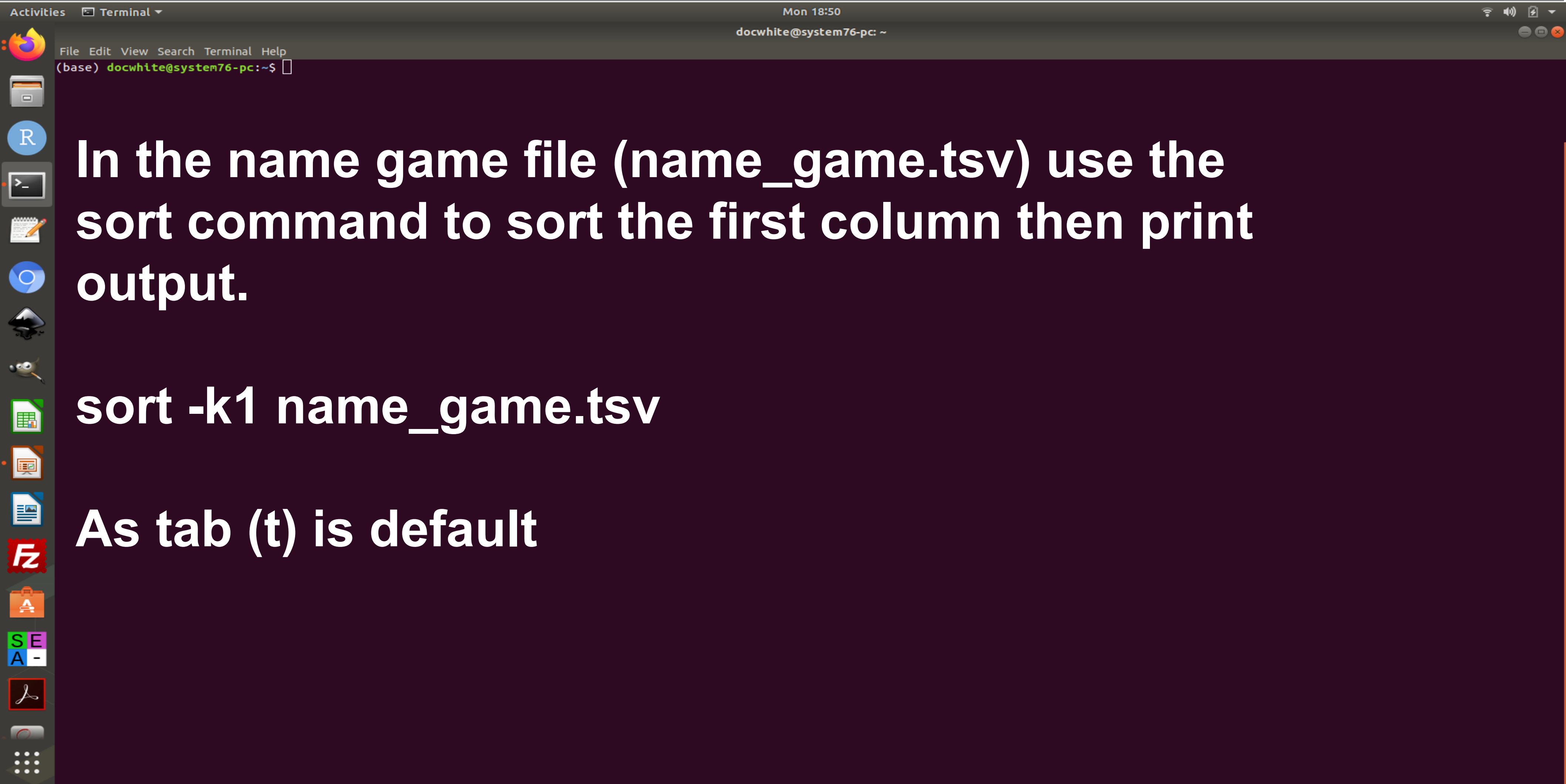
## Sort examples



```
(base) docwhite@system76-pc:~$ 
```

In the name game file (name_game.tsv) use the sort command to sort the first column then print output.

# Sort examples



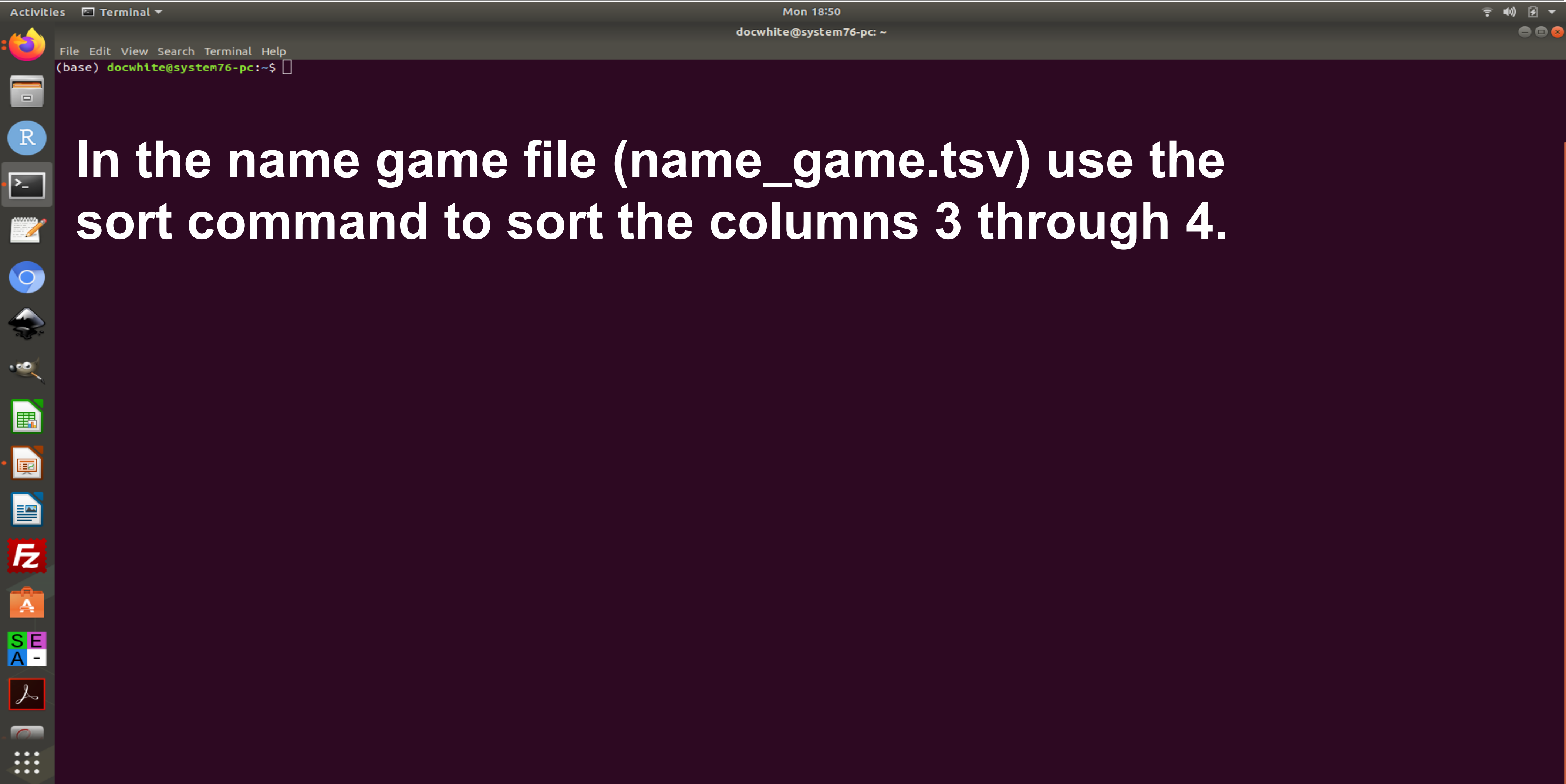
```
(base) docwhite@system76-pc:~$
```

In the name game file (name_game.tsv) use the sort command to sort the first column then print output.

sort -k1 name_game.tsv

As tab (t) is default

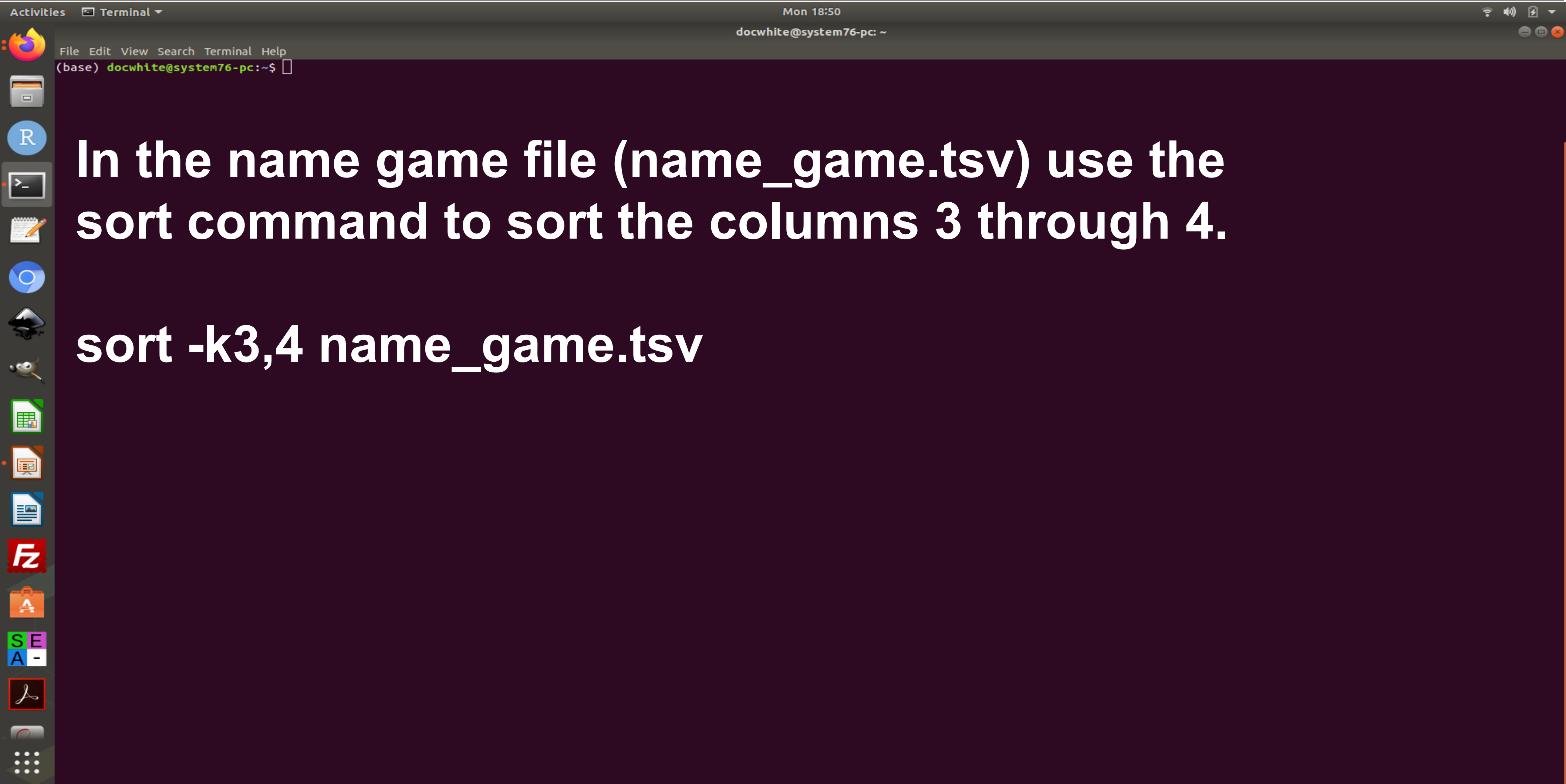
# Sort examples



```
(base) docwhite@system76-pc:~$ 
```

In the name game file (name_game.tsv) use the sort command to sort the columns 3 through 4.

## Sort examples

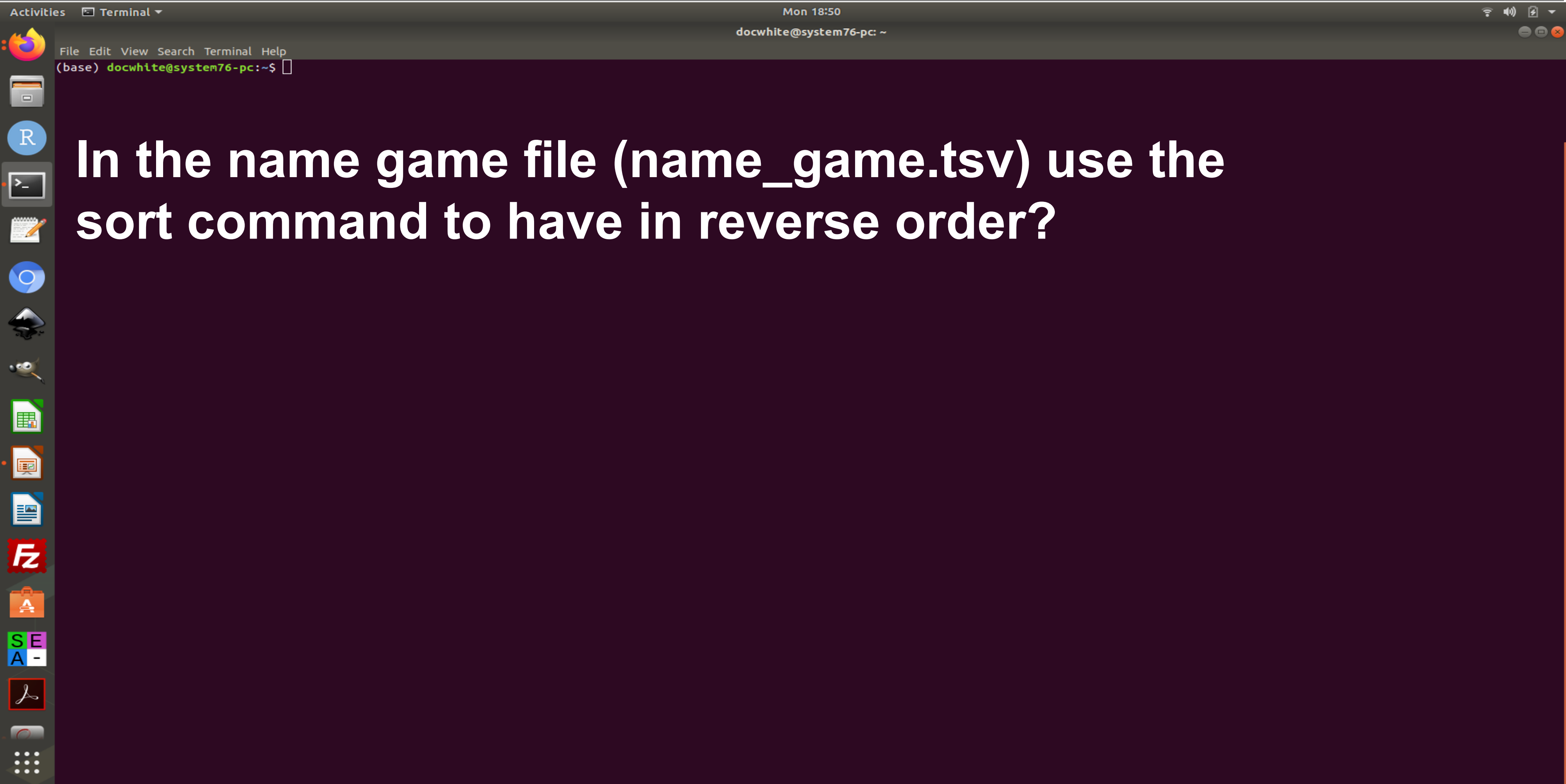


```
(base) docwhite@system76-pc:~$ 
```

In the name game file (name_game.tsv) use the sort command to sort the columns 3 through 4.

```
sort -k3,4 name_game.tsv
```

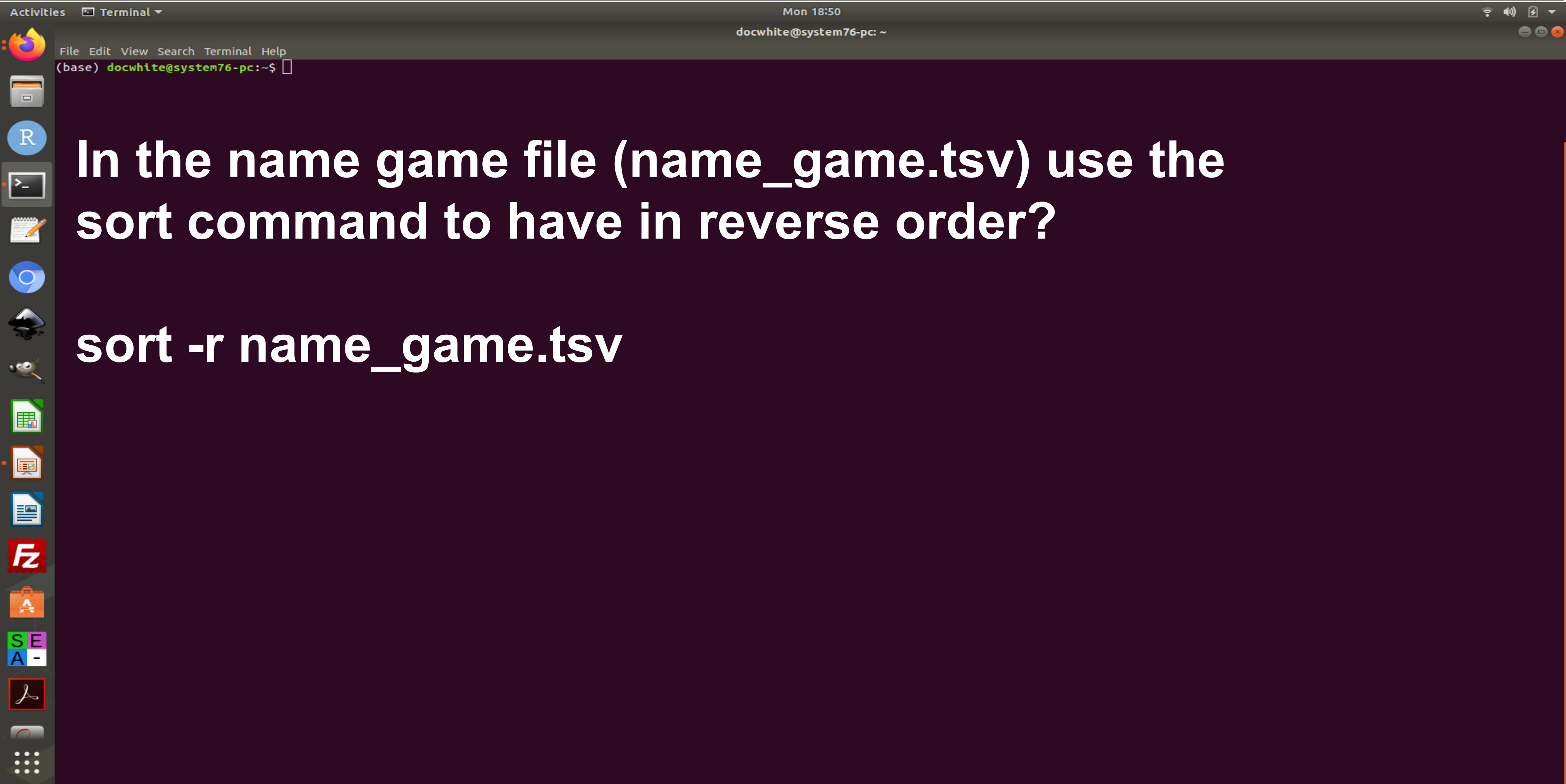
# Sort examples



```
(base) docwhite@system76-pc:~$ 
```

In the name game file (name_game.tsv) use the sort command to have in reverse order?

# Sort examples

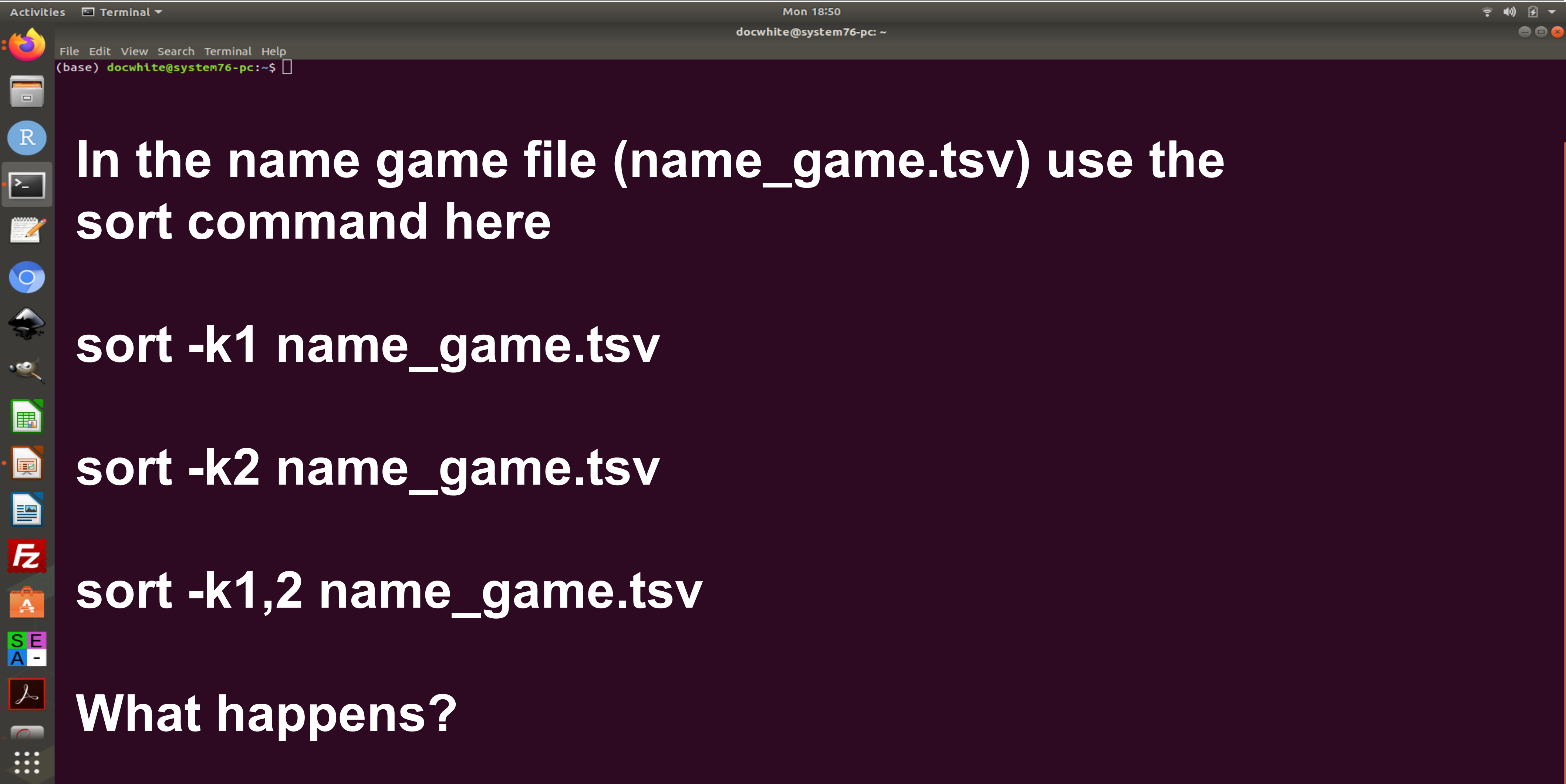


```
(base) docwhite@system76-pc:~$
```

**In the name game file (name_game.tsv) use the sort command to have in reverse order?**

```
sort -r name_game.tsv
```

# Sort examples



```
(base) docwhite@system76-pc:~$ 
```

In the name game file (name_game.tsv) use the sort command here

```
sort -k1 name_game.tsv

sort -k2 name_game.tsv

sort -k1,2 name_game.tsv
```

What happens?

## uniq – syntax anatomy of uniq

**uniq [options] file.txt**

Only works on sorted files and adjacent lines!

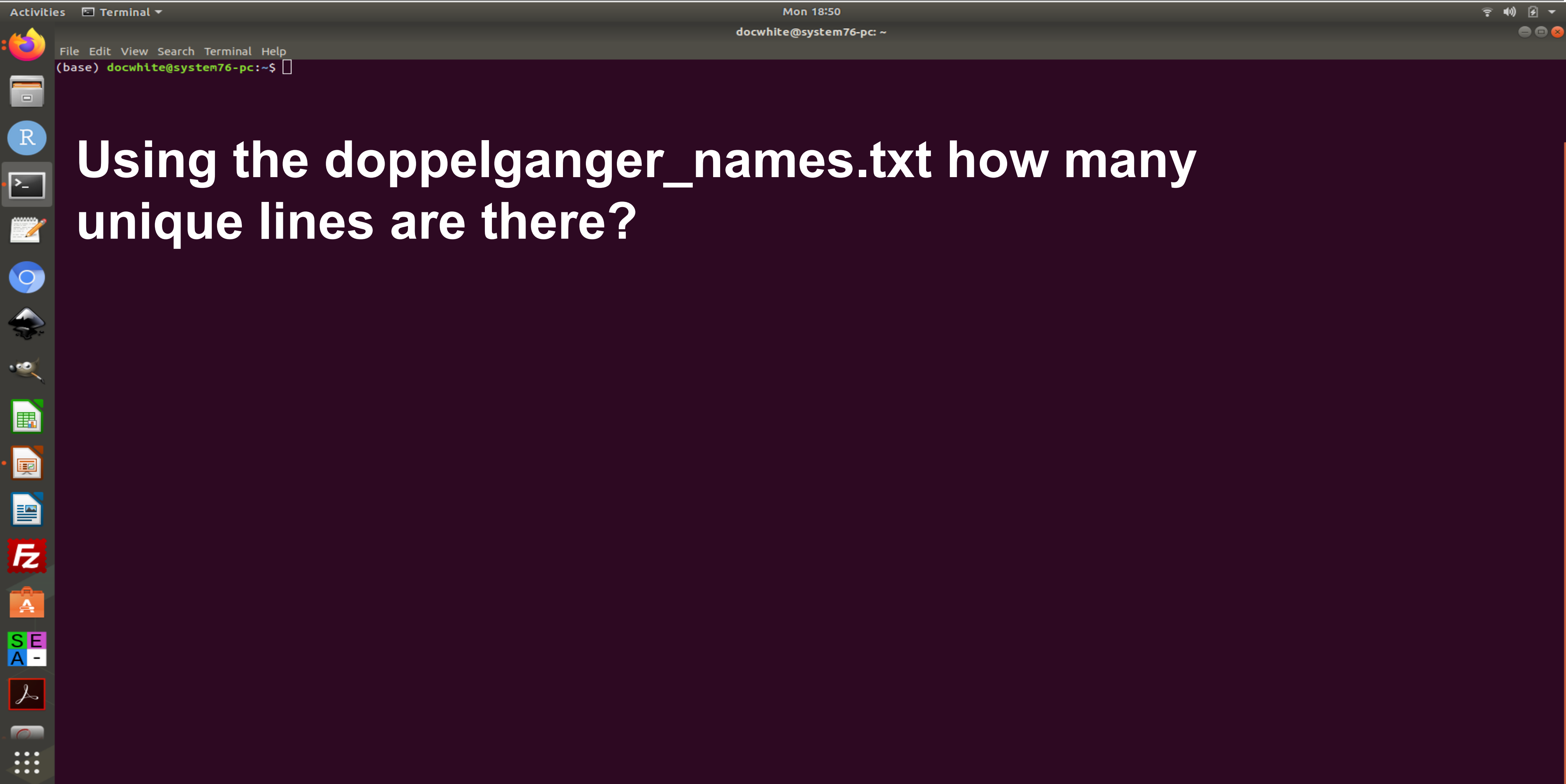
-c count lines for each unique value

-d only report duplicated lines

-u  only report non-duplicated lines

No options: drop all duplicated lines (keeps 1 copy)

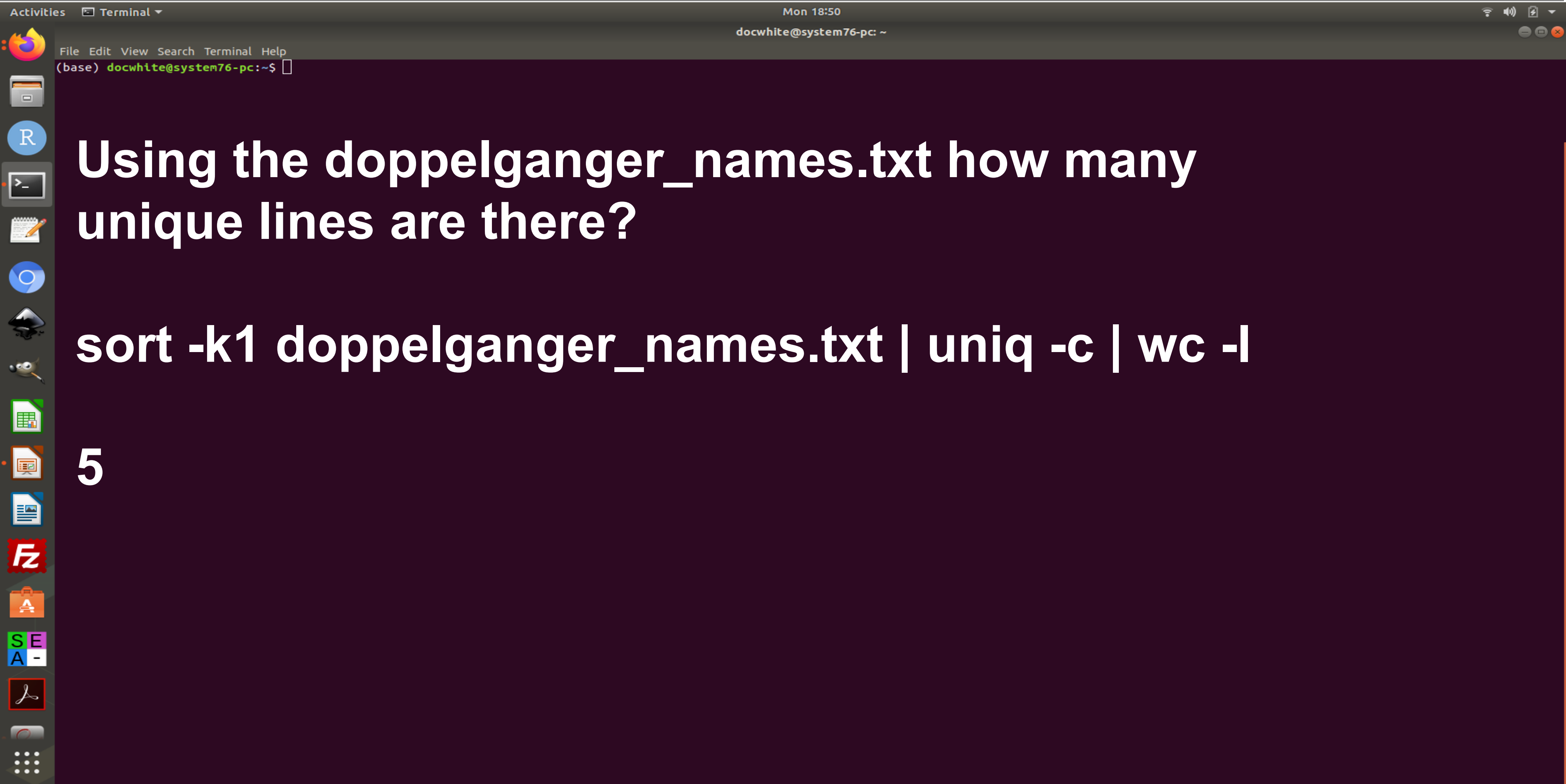
# uniq examples



```
(base) docwhite@system76-pc:~$ 
```

Using the doppelganger_names.txt how many unique lines are there?

# uniq examples



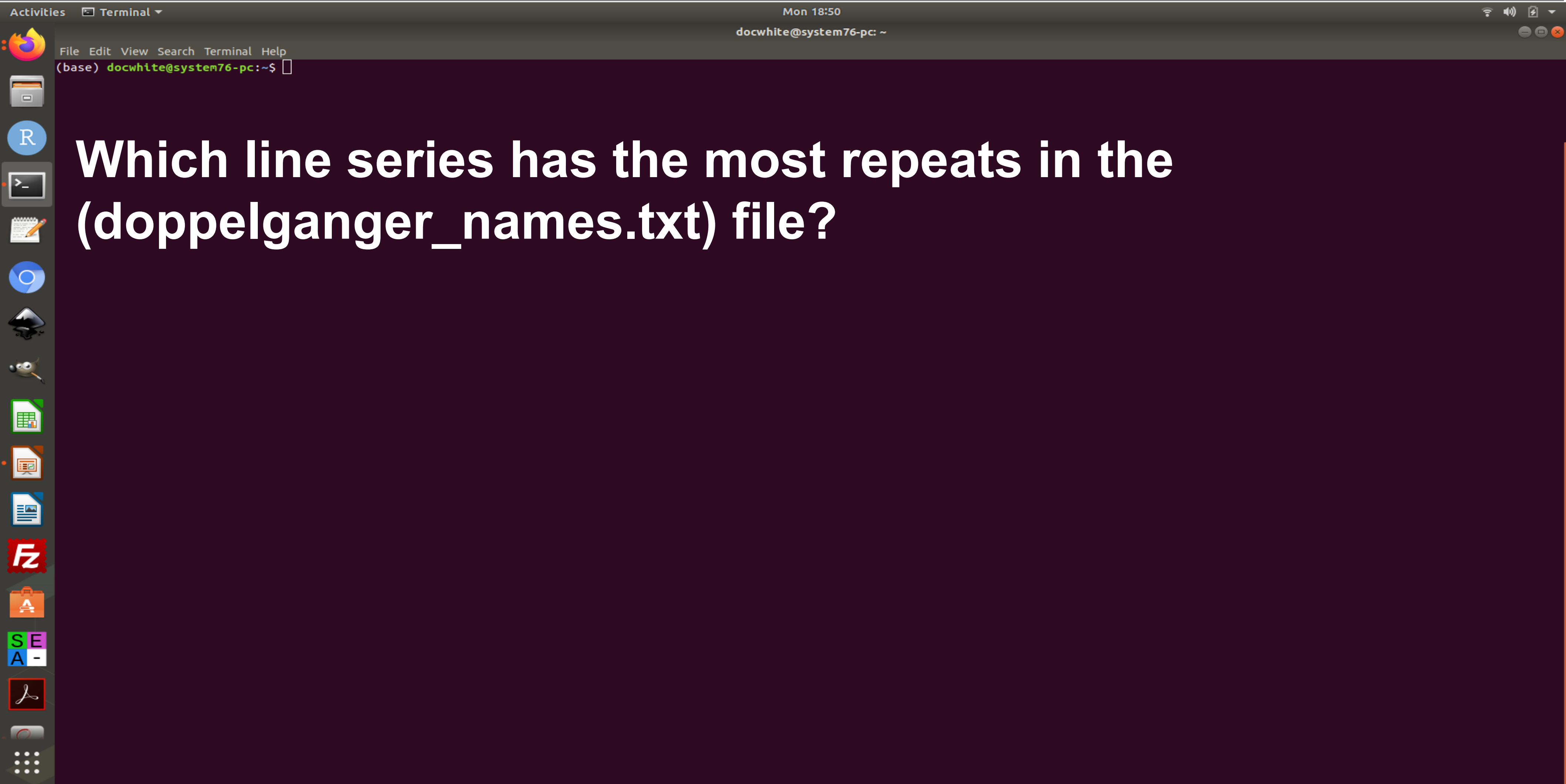
```
(base) docwhite@system76-pc:~$
```

Using the doppelganger_names.txt how many unique lines are there?

```
sort -k1 doppelganger_names.txt | uniq -c | wc -l
```

5

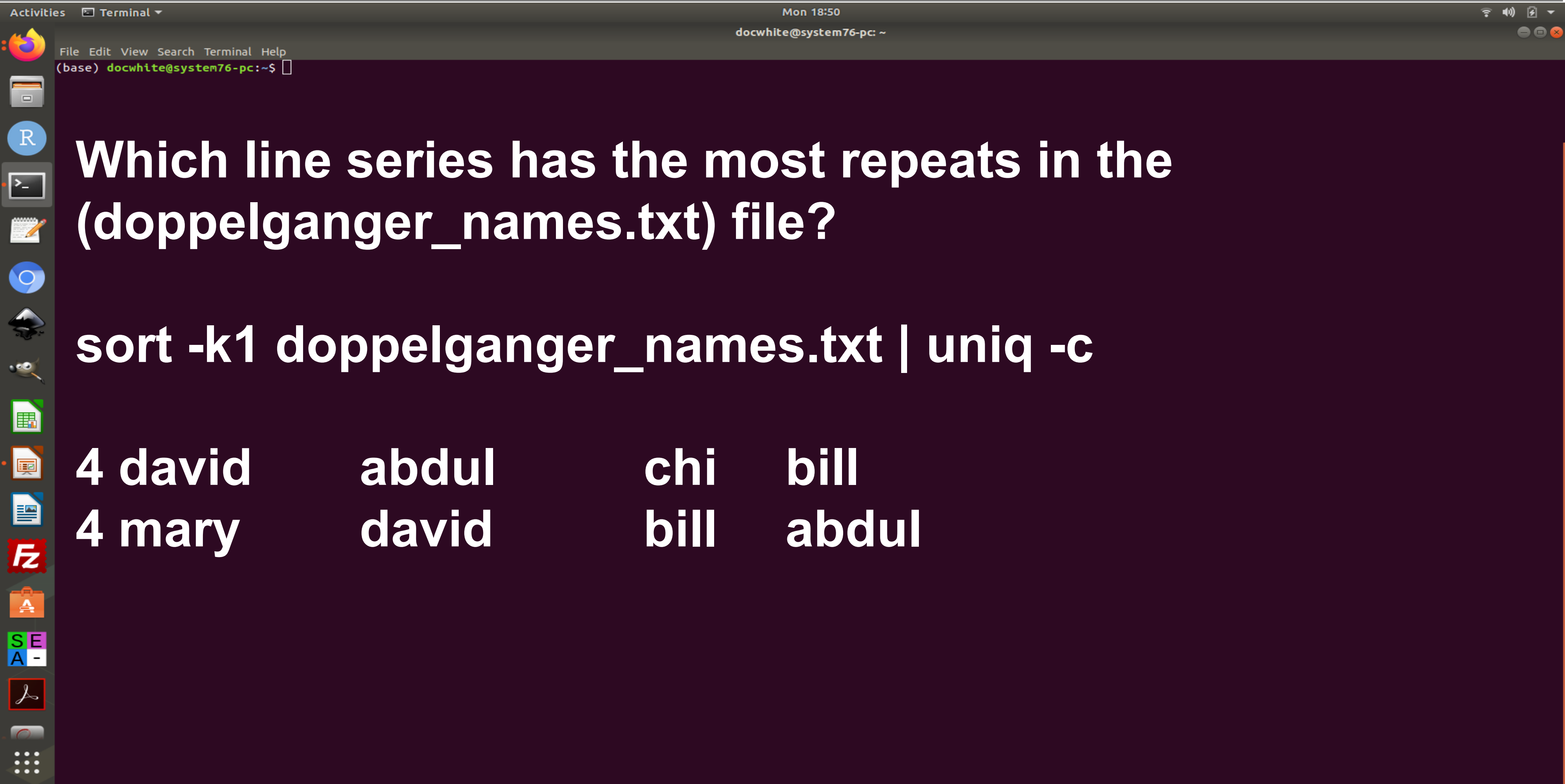
# uniq examples



```
(base) docwhite@system76-pc:~$ 
```

**Which line series has the most repeats in the (doppelganger_names.txt) file?**

# uniq examples



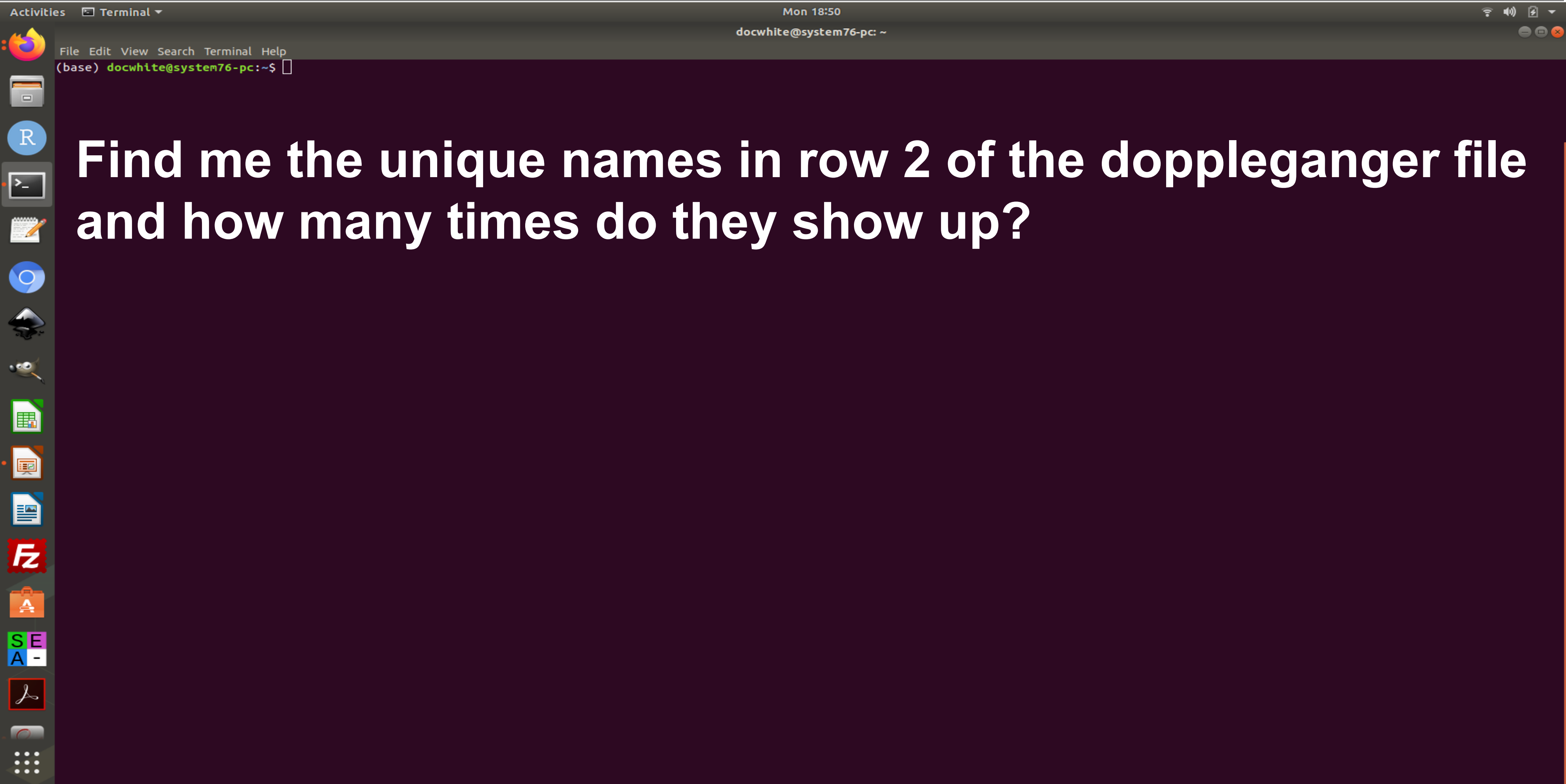
```
(base) docwhite@system76-pc:~$
```

Which line series has the most repeats in the (doppelganger_names.txt) file?

```
sort -k1 doppelganger_names.txt | uniq -c
```

| | | | |
|---|---|---|---|
| 4 david | abdul | chi | bill |
| 4 mary | david | bill | abdul |

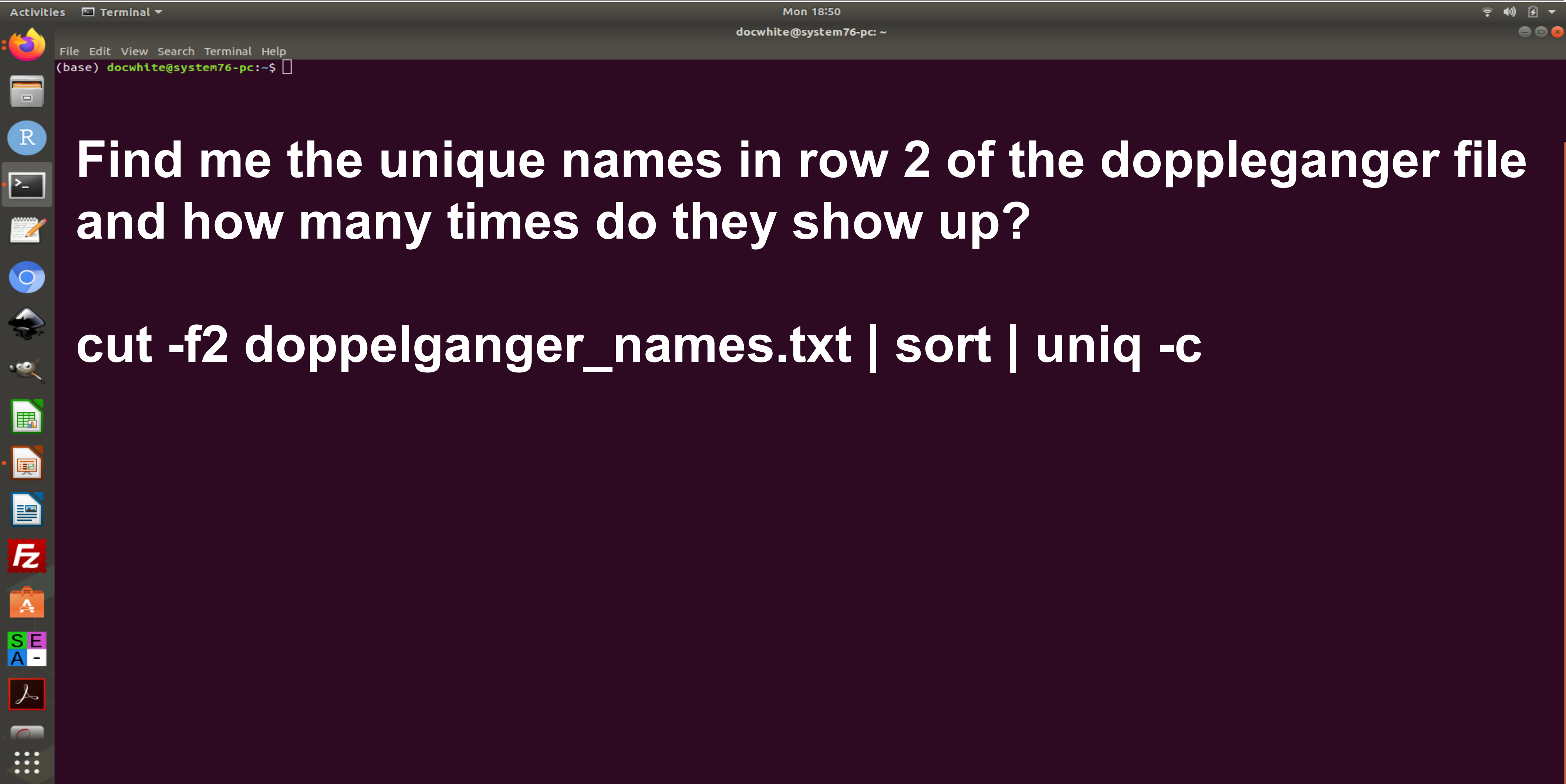
# All together now examples



```
(base) docwhite@system76-pc:~$ 
```

**Find me the unique names in row 2 of the doppleganger file and how many times do they show up?**

# All together now examples



```
(base) docwhite@system76-pc:~$
```

**Find me the unique names in row 2 of the doppleganger file and how many times do they show up?**

```
cut -f2 doppelganger_names.txt | sort | uniq -c
```

## Bonus 5

- Convert name game file (name_game.csv) to tsv with:

→ tr

→ awk

## Quiz 5

- On canvas now