Introduction to



with Application to Bioinformatics

- Day 4

- Why does it matter what type a variable has?
 - What is the difference between '1'*2 and 1*2?
 - Is '2' < '12'?
- How (and when) can you change the type of those? When does it not work?
 - How do you make the string '0.29' into a number?
- You have worked with a number of data containers; lists, sets, dictionaries. What is the difference between them and when should you use which?
- What is a function?
 - Write a function that multiplies the input argument by 2.

• Why does it matter what type a variable has?

• Why does it matter what type a variable has?

Values of different types stores different types of information.

Different types can be used with different operations, functions and methods.

1+2

In []: "1"+"2"

In []: "1"+2

In []: "1"*2





• How can you change (convert) the type of a value? When does it not work?

• How can you change (convert) the type of a value? When does it not work?

```
In [ ]: float("1")
In [ ]: int("1")
In [ ]: str(1)
```

• How can you change (convert) the type of a value? When does it not work?

```
In [ ]: float("1")
In [ ]: int("1")
In [ ]: str(1)
In [ ]: int("2.2")
```



In []: list("hello")

Converting between strings and lists

```
In [ ]: list("hello")
In [ ]: str(['h', 'e', 'l', 'o'])
```

Converting between strings and lists

```
In [ ]: list("hello")
In [ ]: str(['h', 'e', 'l', 'l', 'o'])
In [ ]: ''.join(['h', 'e', 'l', 'l', 'o'])
```

• You have worked with a number of data containers; lists, sets, dictionaries. What is the difference between them and when should you use which?

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- **lists**: when order is important
- dictionaries: to keep track of the relation between keys and values
- sets: to check for membership. No order, no duplicates.

- You have worked with a number of data containers; lists, sets, dictionaries. What is the difference between them and when should you use which?
- **lists**: when order is important
- dictionaries: to keep track of the relation between keys and values
- **sets**: to check for membership. No order, no duplicates.

```
In [ ]: mylist = ["comedy", "drama", "sci-fi"]
myset = set(mylist)
print('All genres', myset)
mydict = {"genre": "drama", "title": "Toy Story"}
```

• What is a function?

• What is a function?

A named piece of code that performs a specific task.

A relation between input data (arguments) and a result (output data).

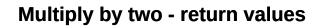
• The def keyword

- The def keyword
- Arguments

- The def keyword
- Arguments
- Indentation!

- The def keyword
- Arguments
- Indentation!
- return

Multiply by two



Multiply by two - return values

```
In [ ]: def multiply_by_two(x):
    return x*2

result = multiply_by_two(2)
print('Result', result)
```

Multiply by two - return values

Multiply by two - return values

```
In [ ]: def multiply_by_two(x):
    result = multiply_by_two(2)
    print('Result', result)

In [ ]: def multiply_by_two(x):
    result = multiply_by_two(2)
    print('Result', result)

In [ ]: def multiply_by_two(x):
    x*2
    res = multiply_by_two(2)
    print('Result', result)
```

TODAY

- Loops and functions, code structure
- Pandas explore your data!

Common concepts

In []: a

```
In [ ]: a
In [ ]: def myfunc(a, b):
    print(a)
    a
```

```
In []: a
In []: def myfunc(a, b):
    print(a)
    a

In []: a = 5
    def myfunc(a):
        a += 2
        return a
        b = myfunc(8)
        a, b
```

```
In []: a
In []: def myfunc(a, b):
    print(a)
    a

In []: a = 5
    def myfunc(a):
        a += 2
        return a
        b = myfunc(8)
        a, b
```

The local a in my func shadows the global a.

```
In []: a
In []: def myfunc(a, b):
    print(a)
    a

In []: a = 5
    def myfunc(a):
        a += 2
        return a
    b = myfunc(8)
    a, b
```

The local a in my func shadows the global a.

The variables inside functions are *local*. To avoid confusion, use different variable names.

```
In [ ]: global_a = 5

def myfunc(value):
    value += 2
    return value

result = myfunc(8)

global_a, result
```

No confusion!

myfunc has unique variable names.

Return values

What is None? Why? When is it used?

What is None? Why? When is it used?

- What is it?
 - A keyword with a constant value (like True, False)
 - Null

What is None? Why? When is it used?

- What is it?
 - A keyword with a constant value (like True, False)
 - Null
- Why and when?
 - To signal "emtpy values"
 - Variables with no values yet
 - Functions that don't return anything meaningful

```
In []: value = None
if value is not None:
    print('value is something')
else:
    print('no value!')

In []: None == True

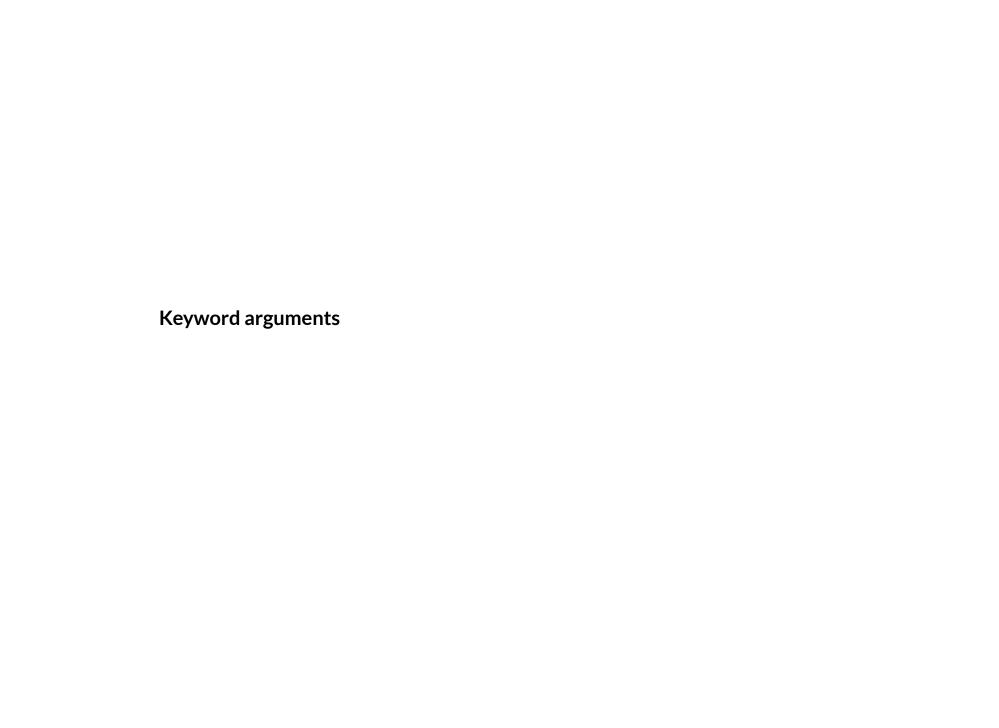
In []: None == False
```

```
In [ ]: myvalue = None
   if myvalue > 10:
        print('Big value')
```

Exercise A

Write a function that takes one argument called value.

- If value is not None and if it is greater to or equal to 10, the function should print "big number".
- If it is not None, and if it is between 0 and 10, the function should print "small number".
- Otherwise, the function should print "No number".



Keyword arguments

```
open('../files/250.imdb', 'r', encoding='utf-8')
```

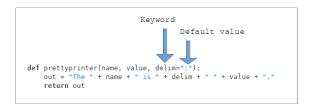
```
In [ ]: def prettyprinter(name, value, delim=":"):
    out = "The " + name + " is " + delim + " " + value + "."
    return out
```

```
In [ ]: def prettyprinter(name, value, delim=":"):
    out = "The " + name + " is " + delim + " " + value + "."
    return out
```

• Programmer can set default values

```
In [ ]: def prettyprinter(name, value, delim=":"):
    out = "The " + name + " is " + delim + " " + value + "."
    return out
```

• Programmer can set default values



```
In [ ]: def prettyprinter(name, value, delim=":"):
    out = "The " + name + " is " + delim + " " + value + "."
    return out
```

• Programmer can set default values

```
def prettyprinter(name, value, delim=":"):
   out = "The " + name + " is " + delim + " " + value + "."
   return out
```

```
In [ ]: prettyprinter("title", "Movie")
```

• User can ignore the arguments (default value is used)

```
def prettyprinter(name, value, delim=":"):
   out = "The " + name + " is " + delim + " " + value + "."
   return out
```

```
In [ ]: prettyprinter("genre", "Drama", delim="=")
```

def prettyprinter(name, value, delim=":"):

return out

out = "The " + name + " is " + delim + " " + value + "."

```
In [ ]: prettyprinter("genre", "Drama", delim="=")
```

def prettyprinter(name, value, delim=":"):

return out

In []: prettyprinter("genre", "Drama", "=")

out = "The " + name + " is " + delim + " " + value + "."

```
In [ ]: def prettyprinter(name, value, delim=":", end=None):
    out = "The " + name + " is " + delim + " " + value
    if end:
        out += end
    return out

my_str = prettyprinter("title", "Movie")
print(my_str)
```

```
In [ ]: def prettyprinter(name, value, delim=":", end=None):
    out = "The " + name + " is " + delim + " " + value
    if end:
        out += end
    return out

my_str = prettyprinter("title", "Movie")
print(my_str)
In [ ]: prettyprinter("genre", "Drama", "=", ".")
```

```
In [ ]: def prettyprinter(name, value, delim=":", end=None):
    out = "The " + name + " is " + delim + " " + value
    if end:
        out += end
        return out

my_str = prettyprinter("title", "Movie")
print(my_str)

In [ ]: prettyprinter("genre", "Drama", "=", ".")
In [ ]: prettyprinter("genre", "Drama", end="!", delim="=")
```

```
open(file, mode='r', buffering=-1, encoding=None, errors=None,
    newline=None, closefd=True, opener=None)
```

```
open(file, mode='r', buffering=-1, encoding=None, errors=None,
    newline=None, closefd=True, opener=None)
```

```
open('../files/250.imdb', 'r', encoding='utf-8')
```

```
open(file, mode='r', buffering=-1, encoding=None, errors=None,
    newline=None, closefd=True, opener=None)
```

```
open('../files/250.imdb', 'r', encoding='utf-8')
open('../files/250.imdb', mode='r', encoding='utf-8')
```

```
open(file, mode='r', buffering=-1, encoding=None, errors=None,
    newline=None, closefd=True, opener=None)
```

```
open('../files/250.imdb', 'r', encoding='utf-8')

open('../files/250.imdb', mode='r', encoding='utf-8')

open('../files/250.imdb', encoding='utf-8', mode='r')
```

Keyword arguments

- programmer: set default values
- user: ignore arguments
- better overview

Exercise B

Rewrite the function from previous exercise, so that it takes one **keyword argument**, value. The default value of this argument is **None**.

- If value is not None and if it is greater to or equal to 10, the function should print "big number".
- If it is not None, and if it is between 0 and 10, the function should print "small number".
- Otherwise, the function should print "No number".

```
In [ ]:     def tester(value=None):
        if value is not None and value >= 10:
            print("big number")
        elif value is not None and 0 < value < 10:
            print("small number")
        else:
            print("No number")</pre>
In [ ]:     tester(11)

In [ ]:     tester(3)
```

```
for x in lines_in_a_big_file:
    if x.startswith('>'): # this is the only line I want!
        do_something(x)
```

```
for x in lines_in_a_big_file:
    if x.startswith('>'): # this is the only line I want!
        do_something(x)
```

...waste of time!

```
for x in lines_in_a_big_file:
    if x.startswith('>'): # this is the only line I want!
        do_something(x)
```

...waste of time!

```
for x in lines_in_a_big_file:
   if x.startswith('>'): # this is the only line I want!
        do_something(x)
        break # break the loop
```

break

```
for line in file:
    if line.startswith('#'):
        break
    do_something(line)

print("I am done")
```

```
for x in lines_in_a_big_file:
    if x.startswith('>'): # this is a comment
        # just skip this! don't do anything
    do_something(x)

for x in lines_in_a_big_file:
    if x.startswith('>'): # this is a comment
        continue # go on to the next iteration
    do something(x)
```

```
for x in lines_in_a_big_file:
    if x.startswith('>'): # this is a comment
        # just skip this! don't do anything
    do_something(x)

for x in lines_in_a_big_file:
    if x.startswith('>'): # this is a comment
        continue # go on to the next iteration
    do_something(x)

for x in lines_in_a_big_file:
    if not x.startswith('>'): # this is *not* a comment
        do_something(x)
```

continue

```
for line in file:
    if line.startswith('#'):
        continue
    do_something(line)

print("I am done")
```

Exercise 1

```
pick_movie(year=1996, rating_min=8.5)
The Bandit
pick_movie(rating_max=8.0, genre="Mystery")
Twelve Monkeys
```

→ Notebook Day_4_Exercise_1

A short note on code structure

- functions
- modules (files)
- documentation

Remember?

Why functions?

- Cleaner code
- Better defined tasks in code
- Re-usability
- Better structure

Why modules?

- Cleaner code
- Better defined tasks in code
- Re-usability
- Better structure

Why modules?

- Cleaner code
- Better defined tasks in code
- Re-usability
- Better structure
- Collect all related functions in one file / module
- Import a module to use its functions
- Only need to understand what the functions do, not how

Example: sys

import sys

sys.argv[1]

or

import imbd_parser as imdb
imdb.parse('250.imdb')

Python standard modules

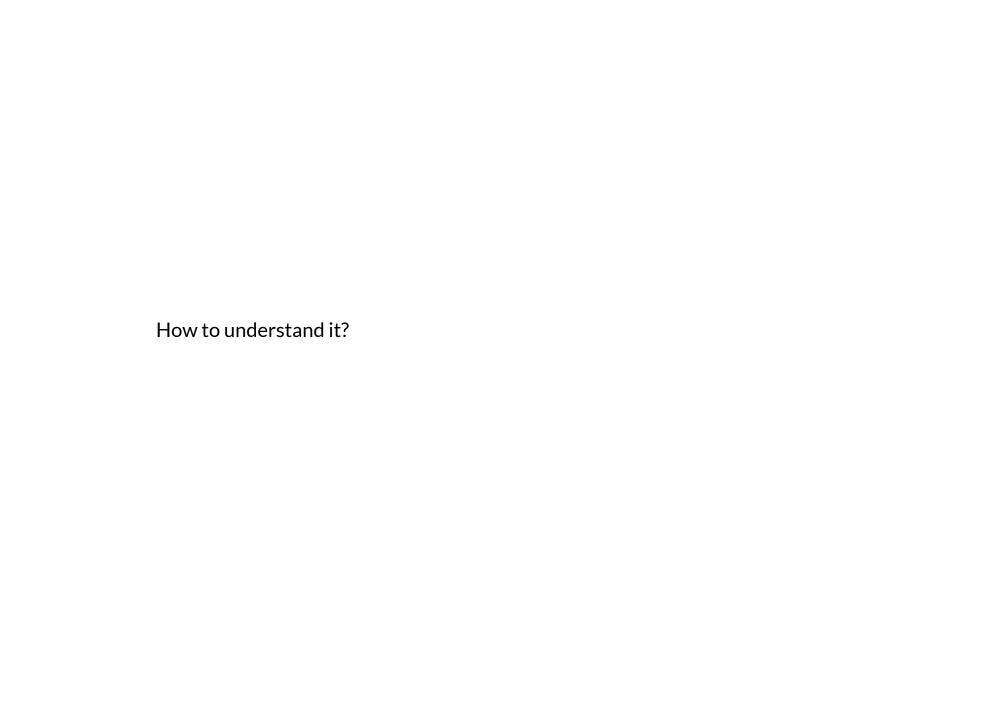
Check out the module index (https://docs.python.org/3.6/py-modindex.html)

How to find the right module?

How to understand it?

How to find the right module?

- look at the module index
- search PyPI (http://pypi.org)
- ask your colleagues
- search the web!



How to understand it?

In []: import math
 help(math)

In []: help(math.sqrt)

In []: math.sqrt(3)

Importing

In []: import math
 math.sqrt(3)

Importing

In []:	import math
	math.sqrt(3)
In []:	<pre>import math as m m.sqrt(3)</pre>

Importing

In	[]:		<pre>import math math.sqrt(3)</pre>
In	[]:	:	<pre>import math as m m.sqrt(3)</pre>
In	[]:	:	<pre>from math import sqrt sqrt(3)</pre>

Documentation and commenting your code

Remember help()?

Works because somebody else has documented their code!

?

:

In []:

In []: help(process_file)

def process file(filename, chrom, pos):

if col[0] == chrom and col[1] == pos:

print(col[9:])

Your code may have two types of users:

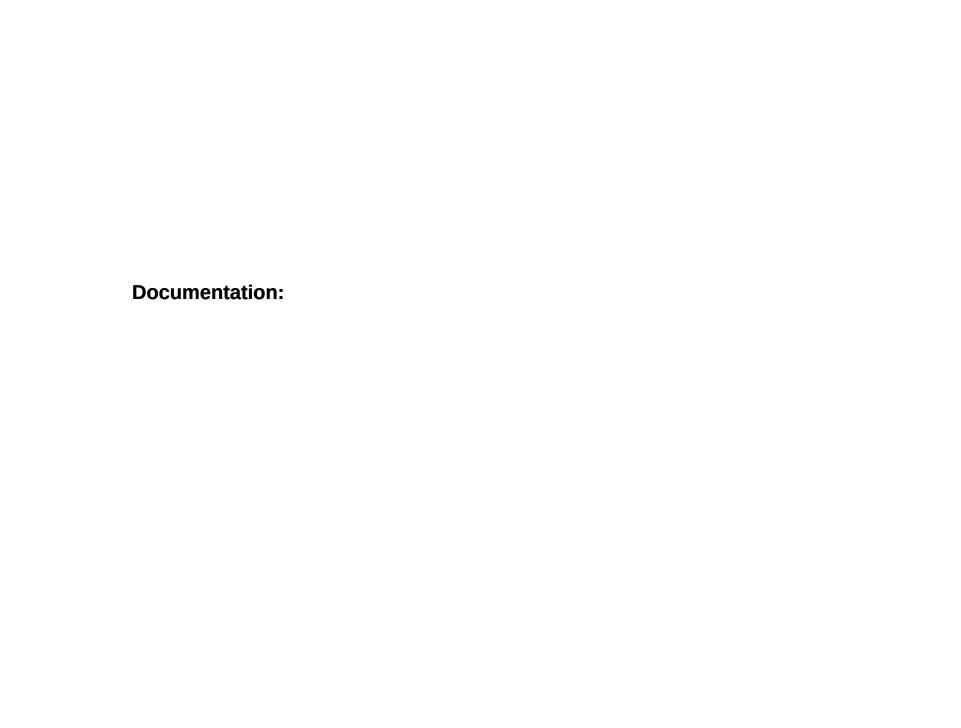
- library users
- maintainers (maybe yourself!)

Your code may have two types of users:

- library users
- maintainers (maybe yourself!)

Write documentation for both of them!

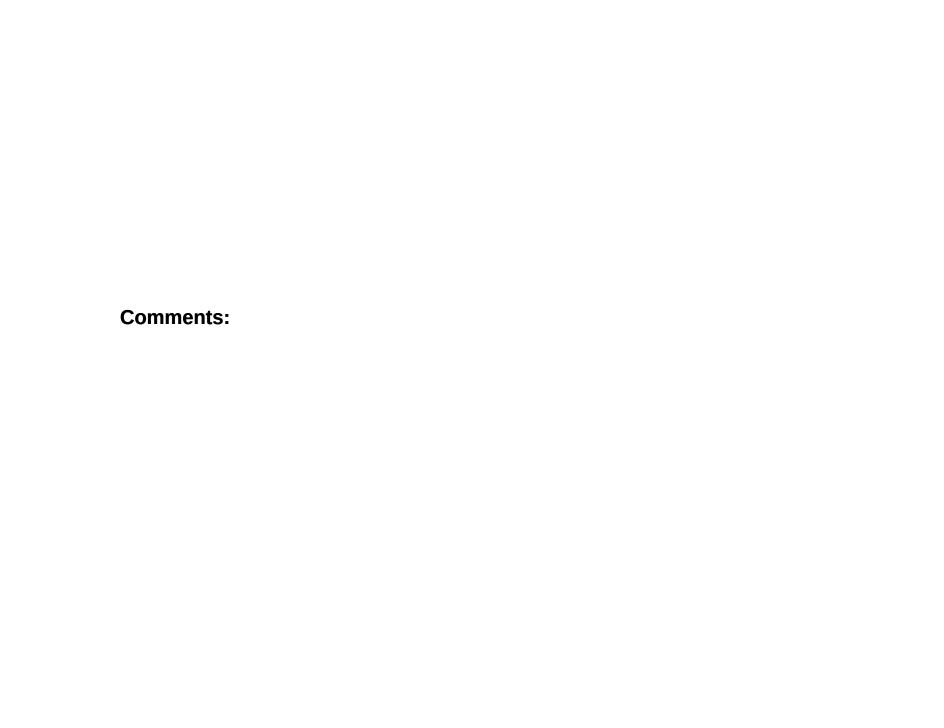
- library users: """What does this function do? """ (doc strings)
- maintainers: # implementation details (comments)



Documentation:

• At the beginning of the file

"""This module provides functions for..."""



Comments:

my_list[5] += other_list[3] # explain why you do this!

Read more:

https://realpython.com/documenting-python-code/ (https://realpython.com/documenting-python-code/)

https://www.python.org/dev/peps/pep-0008/?#comments (https://www.python.org/dev/peps/pep-0008/?#comments)

Formatting

Formatting

```
In [ ]:
    title = 'Great movie'
    rating = 10
    print('The result is: '+ title + 'with rating: ' + rating)
```

Formatting

```
In [ ]:
    title = 'Great movie'
    rating = 10
    print('The result is: '+ title + 'with rating: ' + rating)
```

Formatting!

```
In [ ]: print('The result is: {} with rating {}'.format(title, rating))
```

Formatting

```
In [ ]: title = 'Great movie'
rating = 10
print('The result is: '+ title + 'with rating: ' + rating)
```

Formatting!

```
In [ ]: print('The result is: {} with rating {}'.format(title, rating))
```

Formatting - f-strings

```
In [ ]: print(f'The result is: {title} with rating {rating}') # python version >= 3.6
```

Formatting

```
In [ ]: title = 'Great movie'
rating = 10
print('The result is: '+ title + 'with rating: ' + rating)
```

Formatting!

```
In [ ]: print('The result is: {} with rating {}'.format(title, rating))
```

Formatting - f-strings

```
In [ ]: print(f'The result is: {title} with rating {rating}') # python version >= 3.6
```

Formatting - the old way

```
In [ ]: print('The result is: %s with rating %s' % (title, rating)) # python2
```

Formatting

```
f'some text {variable:^50} text' # center in a 50 character wide column f'some text {variable:<50} text' # left align in 50 character wide column f'some text {variable:.2f} text' # round a float to 2 digits
```

Learn more from the Python docs: https://docs.python.org/3.4/library/string.html#format-string-syntax)

Exercise 2

 \rightarrow Notebook Day_4_Exercise_2

Pandas

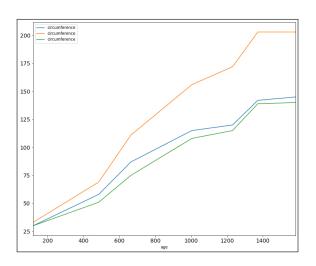
Library for working with tabular data

- comma separated (csv)
- tab separated (tsv)
- ..

Data analysis, graph plotting...

Pandas

	circumference	height
age		
1	2	30
2	3	35
3	5	40
4	10	50



Pandas - a short overview

In]:	import pandas as pd
In]:	help(pd)

Orange tree data

0range_1.tsv:

age	circumference	height
1	2	30
2	3	35
3	5	40
4	10	50

Orange tree data

0range_1.tsv:

```
age circumference height
1 2 30
2 3 35
3 5 40
4 10 50
```

```
In [ ]: tree_growth = pd.read_table('../downloads/Orange_1.tsv', index_col=0)
```

Dataframes

```
In [ ]: tree_growth
```

- One index (in this case age)
- A bunch of colums (in this case circumference and height)
- A bunch of rows (identified by their index)

Dataframes

```
In [ ]: tree_growth
```

- One index (in this case age)
- A bunch of colums (in this case circumference and height)
- A bunch of rows (identified by their index)

```
In [ ]: tree_growth.columns
```

Dataframes

```
In [ ]: tree_growth
```

- One index (in this case age)
- A bunch of colums (in this case circumference and height)
- A bunch of rows (identified by their index)

```
In [ ]: tree_growth.columns
In [ ]: tree_growth.index
```

In []: tree_growth.circumference

dataframe.columnname

dataframe['columnname']

In []	 : [tree_growth.circumference
			dataframe.columnname
			dataframe['columnname']
In []	:[tree_growth.height

In	[]:	tree_growth.circumference
			dataframe.columnname
			dataframe['columnname']
In	[]:	tree_growth.height
In	[]:	tree_growth.circumference.max()

In []: tree_growth.loc[4]

dataframe.loc[row_name]

Reading data

```
dataframe = pandas.read_table(filepath, index_col=N)
dataframe.columnname
dataframe.loc[row_name]
```

Exercise 3

- Read the Orange_1.tsv
- Print the height column
- Print the data for the tree at age 2

```
In [ ]: tree_growth = pd.read_table('../downloads/Orange_1.tsv', index_col=0)
    tree_growth
```

```
In [ ]: tree_growth = pd.read_table('../downloads/Orange_1.tsv', index_col=0)
In [ ]: tree_growth.height
In [ ]: tree_growth.loc[2]
```

Many trees!

0range.tsv

Tree	age	circumference
1	118	30
1	484	58
1	664	87
1	1004	115
2	118	33
2	484	69

```
In [ ]: tree_growth = pd.read_table('../downloads/Orange.tsv', index_col=0)
    tree_growth
```

In []:	tree_growth.index
In []:	tree_growth.columns

In []: tree_growth.age

In []:	tree_growth.age
In []:	tree_growth.age.values

In []: tree_growth.age.unique()

```
In [ ]: tree_growth.age.unique()
```

Works like a normal list:

In []: tree_growth.age.unique()

Works like a normal list:

In []: tree_growth.age.unique()[0]

```
In [ ]: tree_growth.age.unique()
```

Works like a normal list:

```
In [ ]: tree_growth.age.unique()[0]
In [ ]: len(tree_growth.age.unique())
```

Columns

dataframe.columnname

Methods:

```
.max(),.min(),unique(),.values,.mean(),.sum()...
```

```
In [ ]: tree_growth.circumference # selecting a column
```

```
In [ ]: tree_growth.circumference # selecting a column
In [ ]: tree_growth.loc[2] # selecting rows with index 2
```

```
In [ ]: tree_growth.circumference # selecting a column
In [ ]: tree_growth.loc[2] # selecting rows with index 2
```

tree_growth.loc[criteria] # select all rows that fullfills this criteria

Selecting parts of the table

Find the data points where the tree is younger than 200 years!

- Find rows => use tree_growth.loc[]
- Select these based on the value of column age => tree_growth.age

```
In [ ]: # The answer...
```

Selecting parts of the table

Find the data points where the tree is younger than 200 years!

- Find rows => use tree_growth.loc[]
- Select these based on the value of column age => tree_growth.age

```
In [ ]: # The answer...
In [ ]: young = tree_growth.loc[tree_growth.age < 200]
young</pre>
```

Exercise 4

- Read the data Orange.tsv
- Find the maximum circumference
- What tree reached that circumference, and how old was it at that time?

tree_growth.loc[tree_growth.age < 200]</pre>

In []: import pandas as pd
tree_growth = pd.read_table('../downloads/Orange.tsv',index_col=0)

df.columnname.plot()

```
df.columnname.plot()
```

or

What if no plot shows up?

```
%pylab inline # jupyter notebooks
import matplotlib.pyplot as plt
plt.show()
```

Plotting - many trees

Plotting - many trees

• Plot a bar chart

Plotting - many trees

• Plot a bar chart

```
In [ ]: tree_growth.plot(kind='bar')
```

In []: tree_growth.plot(kind='bar', figsize=(12, 12), fontsize=12)

• Plot a line graph

• Plot a line graph

```
In [ ]: # Starting with tree number 1
treel = tree_growth.loc[1]
In [ ]: treel
```

• Plotagraph: dataframe.plot(kind="line", x=..., y=...)

```
In [ ]: tree1.plot(x='age', y='circumference', fontsize=14, figsize=(12,10))
```

• Plotagraph: dataframe.plot(kind="line", x="..", y="...")

• Plotagraph: dataframe.plot(kind="line", x="..", y="...")

Let's plot all the trees!

```
In [ ]: tree_growth.plot(kind='line', x='age', y='circumference', figsize=(12, 10), fontsize=14)
```

```
In [ ]: tree_growth.plot(kind='line', x='age', y='circumference', figsize=(12, 10), fontsize=14)
:(
```

• Plotagraph: dataframe.plot(kind="scatter", x="..", y="...")

```
In [ ]: tree_growth.plot(kind='scatter', x='age', y='circumference', figsize=(12, 10), fontsize=14)
```

What about the lines?

What about the lines?

- Group the table by the index (make subtrees / subdataframes)
- Get one board to plot all the lines
- Draw them one by one

What about the lines?

- Group the table by the index (make subtrees / subdataframes)
- Get one board to plot all the lines
- Draw them one by one

dataframe.groupby([what])

What about the lines?

- Group the table by the index (make subtrees / subdataframes)
- Get one board to plot all the lines
- Draw them one by one

```
import matplotlib.pyplot as plt
fig, ax = plt.subplots()
```

Exercise 5

- Use Pandas to read IMDB
- Explore it by making graphs