UNIVERSITÄT BONN

@PuckerLab

Prof. Dr. Boas Pucker

Python - Application examples

Availability of slides

- All materials are freely available (CC BY) - after the lectures:
  - GitHub: https://github.com/bpucker/teaching/tree/master/WBIO-A-07

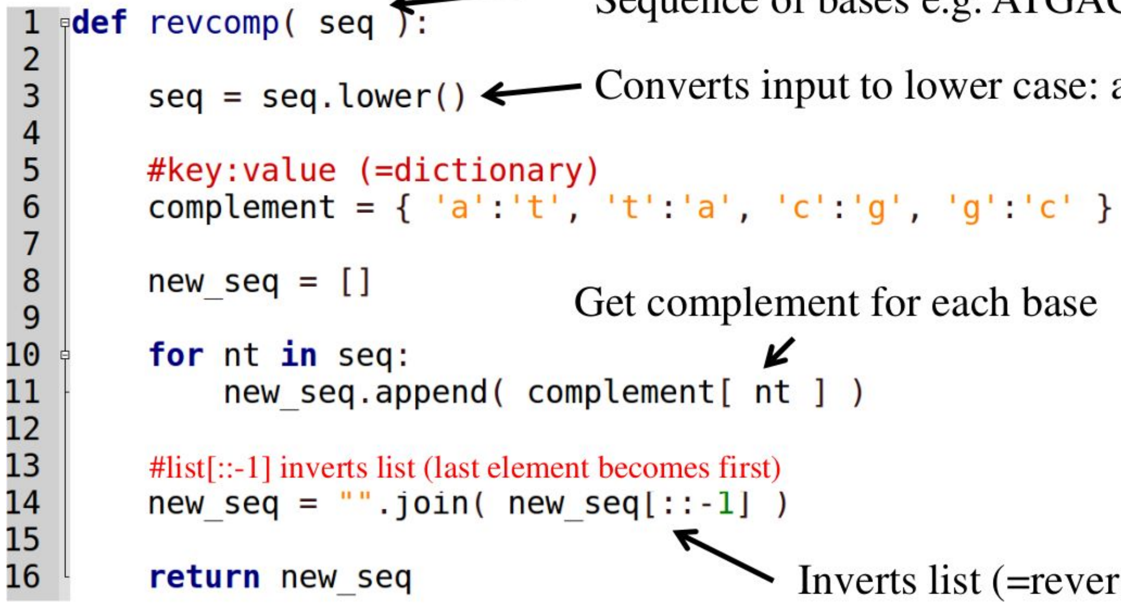
- Questions: Feel free to ask at any time

- Feedback, comments, or questions: pucker[a]uni-bonn.de

UNIVERSITÄT BONN

Reverse complement of nucleotide sequence

What happens here?



```
def revcomp( seq ):

    seq = seq.lower()

    #key:value (=dictionary)
    complement = { 'a':'t', 't':'a', 'c':'g', 'g':'c' }

    new_seq = []

    for nt in seq:
        new_seq.append( complement[ nt ] )

    #list[::-1] inverts list (last element becomes first)
    new_seq = "".join( new_seq[::-1] )

    return new_seq
```

Sequence of bases e.g. ATGACATGA

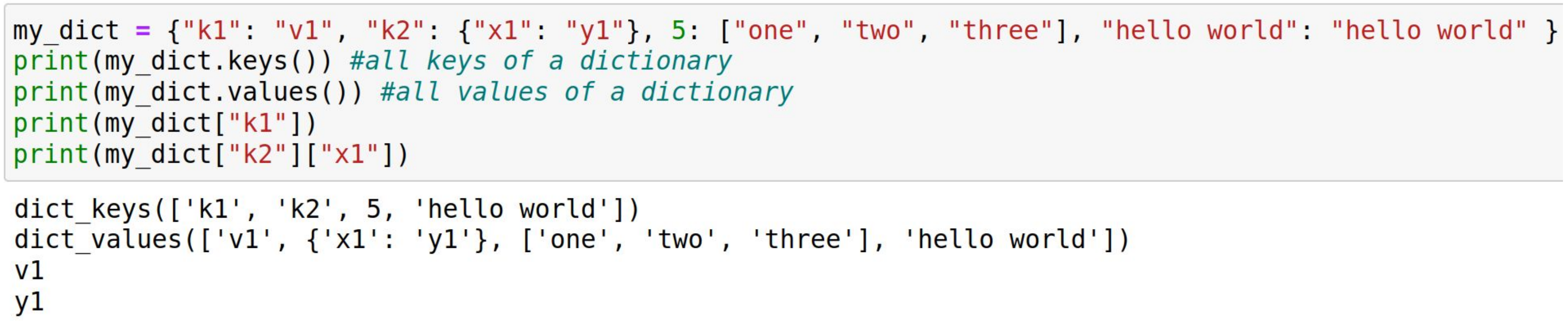
Converts input to lower case: atgacatga

Get complement for each base

Inverts list (=reverse)

How to use dictionaries

- Values are accessible via keys
- Keys need to be unique
- Quick access to data based on key
- Higher memory occupation than lists/strings



```python
my_dict = {"k1": "v1", "k2": {"x1": "y1"}, 5: ["one", "two", "three"], "hello world": "hello world" }
print(my_dict.keys()) #all keys of a dictionary
print(my_dict.values()) #all values of a dictionary
print(my_dict["k1"])
print(my_dict["k2"]["x1"])
```

```
dict_keys(['k1', 'k2', 5, 'hello world'])
dict_values(['v1', {'x1': 'y1'}, ['one', 'two', 'three'], 'hello world'])
v1
y1
```

Exercises - Part 6a

- 6.1) Write a function to get the reverse complement (upper case letters) of a DNA sequence given in upper case letters!
- 6.2) Write a function to translate a DNA sequence into amino acids (first frame only)!

- 6.X1) Write a function to translate DNA sequences in all 6 frames into peptide sequences! The longest peptide sequence per DNA sequence should be returned!
- 6.X2) Write a function to grep a sequence from a FASTA file based on the name of this sequence!

UNIVERSITÄT BONN

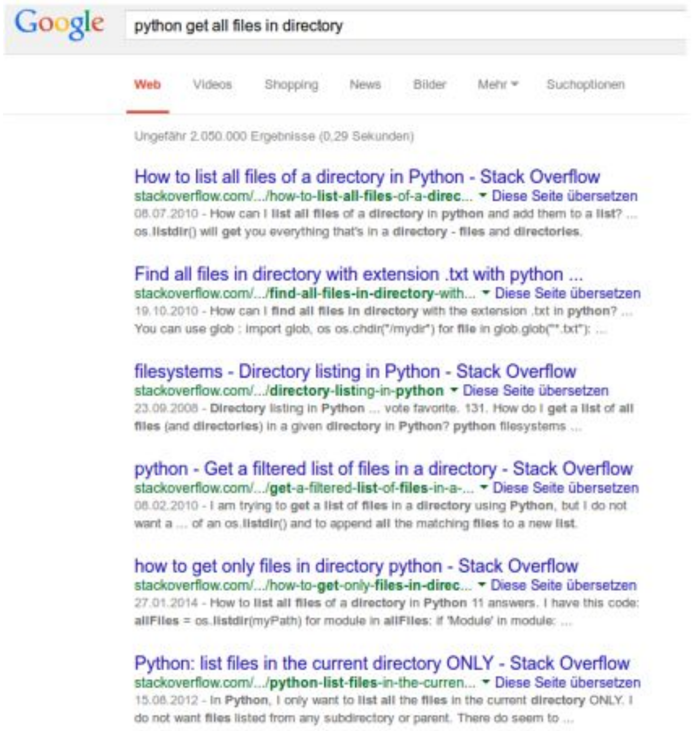
How to approach a bioinfo challenge?

- Identify the problem that needs to be solved
- Split the problem into smallest possible parts
- Solutions for small parts of the problem might be available already
- Precise description of the problem is required for online search
- Best hit often leads to stack overflow:
  - Problem is described by the asking person
  - Multiple solutions are suggested by the community
  - Community votes to identify the best solution
  - Green marking highlights the answer that solved the problem

Example

- Problem: get paths of all files in a certain directory

- Search expression: ‘python get all files in directory’



python get all files in directory

Ungefähr 2.050.000 Ergebnisse (0,29 Sekunden)

How to list all files of a directory in Python - Stack Overflow
stackoverflow.com/.../how-to-list-all-files-of-a-direc... ▾ Diese Seite übersetzen
08.07.2010 - How can I list all files of a directory in python and add them to a list? ... os.listdir() will get you everything that's in a directory - files and directories.

Find all files in directory with extension .txt with python ...
stackoverflow.com/.../find-all-files-in-directory-with... ▾ Diese Seite übersetzen
19.10.2010 - How can I find all files in directory with the extension .txt in python? ... You can use glob : import glob, os os.chdir("/mydir") for file in glob.glob("*.txt"): ...

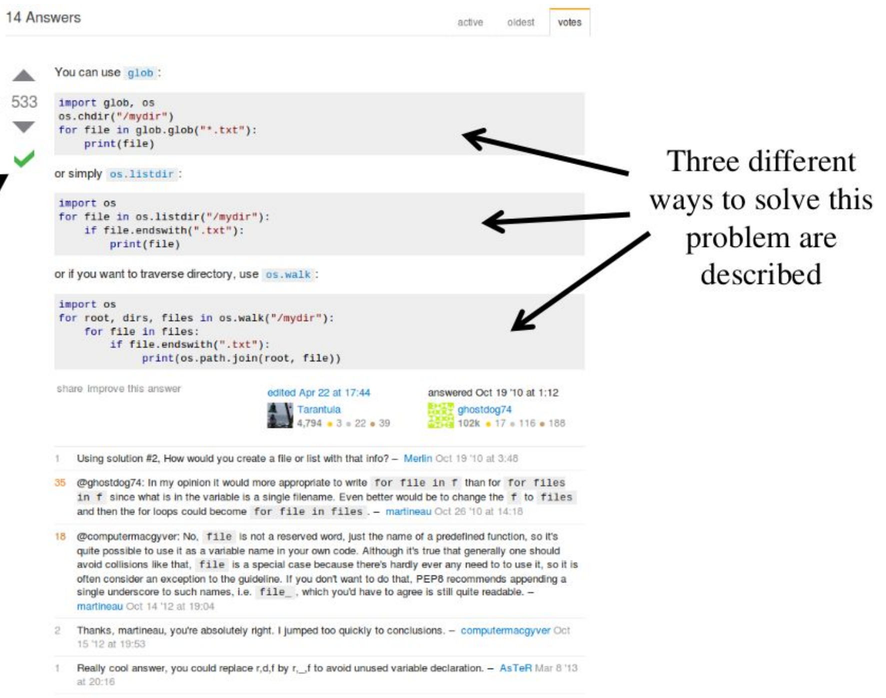
filesystems - Directory listing in Python - Stack Overflow
stackoverflow.com/.../directory-listing-in-python ▾ Diese Seite übersetzen
23.09.2008 - Directory listing in Python ... vote favorite. 131. How do I get a list of all files (and directories) in a given directory in Python? python filesystems ...

python - Get a filtered list of files in a directory - Stack Overflow
stackoverflow.com/.../get-a-filtered-list-of-files-in-a-... ▾ Diese Seite übersetzen
08.02.2010 - I am trying to get a list of files in a directory using Python, but I do not want a ... of an os.listdir() and to append all the matching files to a new list.

how to get only files in directory python - Stack Overflow
stackoverflow.com/.../how-to-get-only-files-in-direc... ▾ Diese Seite übersetzen
27.01.2014 - How to list all files of a directory in Python 11 answers. I have this code: allFiles = os.listdir(myPath) for module in allFiles: if 'Module' in module: ...

Python: list files in the current directory ONLY - Stack Overflow
stackoverflow.com/.../python-list-files-in-the-curren... ▾ Diese Seite übersetzen
15.08.2012 - In Python, I only want to list all the files in the current directory ONLY. I do not want files listed from any subdirectory or parent. There do seem to ...

Best hit on stackoverflow


533 user like this answer
This answers solved the question
Three different ways to solve this problem are described

14 Answers

active oldest votes

533

You can use `glob`:

```
import glob, os
os.chdir("/mydir")
for file in glob.glob("*.txt"):
    print(file)
```

or simply `os.listdir`:

```
import os
for file in os.listdir("/mydir"):
    if file.endswith(".txt"):
        print(file)
```

or if you want to traverse directory, use `os.walk`:

```
import os
for root, dirs, files in os.walk("/mydir"):
    for file in files:
        if file.endswith(".txt"):
             print(os.path.join(root, file))
```

share improve this answer

edited Apr 22 at 17:44
Tarantula
4,794 ● 3 ● 22 ● 39

answered Oct 19 '10 at 1:12
ghostdog74
102k ● 17 ● 116 ● 188

1 Using solution #2, How would you create a file or list with that info? – Merlin Oct 19 '10 at 3:48

35 @ghostdog74: In my opinion it would more appropriate to write `for file in f` than for `for files in f` since what is in the variable is a single filename. Even better would be to change the `f` to `files` and then the for loops could become `for file in files`. – martineau Oct 26 '10 at 14:18

18 @computermacgyver: No, `file` is not a reserved word, just the name of a predefined function, so it's quite possible to use it as a variable name in your own code. Although it's true that generally one should avoid collisions like that, `file` is a special case because there's hardly ever any need to to use it, so it is often consider an exception to the guideline. If you don't want to do that, PEP8 recommends appending a single underscore to such names, i.e. `file_`, which you'd have to agree is still quite readable. – martineau Oct 14 '12 at 19:04

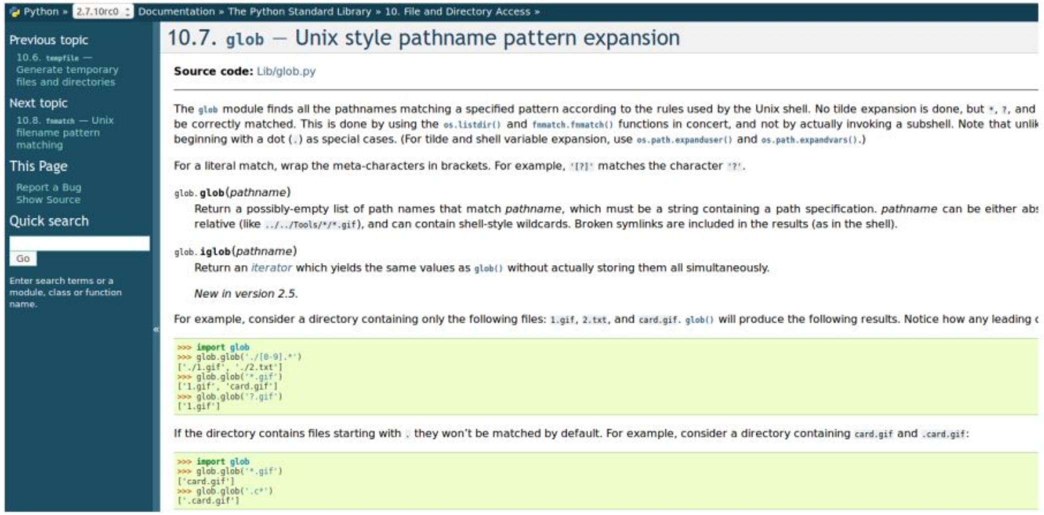
2 Thanks, martineau, you're absolutely right. I jumped too quickly to conclusions. – computermacgyver Oct 15 '12 at 19:53

1 Really cool answer, you could replace r,d,f by r,_,f to avoid unused variable declaration. – AsTeR Mar 8 '13 at 20:16

Official Python documentation

- Systematic documentation of all functions in a module with all possible arguments

- Sometimes examples are given



Python » 2.7.10rc0 Documentation » The Python Standard Library » 10. File and Directory Access »

Previous topic

10.6. `tempfile` — Generate temporary files and directories

Next topic

10.8. `fnmatch` — Unix filename pattern matching

This Page

Report a Bug
Show Source

Quick search

Go

Enter search terms or a module, class or function name.

10.7. `glob` — Unix style pathname pattern expansion

Source code: Lib/glob.py

The `glob` module finds all the pathnames matching a specified pattern according to the rules used by the Unix shell. No tilde expansion is done, but `*`, `?`, and
be correctly matched. This is done by using the `os.listdir()` and `fnmatch.fnmatch()` functions in concert, and not by actually invoking a subshell. Note that unlik
beginning with a dot (`.`) as special cases. (For tilde and shell variable expansion, use `os.path.expanduser()` and `os.path.expandvars()`.)

For a literal match, wrap the meta-characters in brackets. For example, `'[?]'` matches the character `'?'`.

`glob.`**`glob`**(*pathname*)

Return a possibly-empty list of path names that match *pathname*, which must be a string containing a path specification. *pathname* can be either abs
relative (like `../../Tools/*/*.gif`), and can contain shell-style wildcards. Broken symlinks are included in the results (as in the shell).

`glob.`**`iglob`**(*pathname*)

Return an *iterator* which yields the same values as `glob()` without actually storing them all simultaneously.

New in version 2.5.

For example, consider a directory containing only the following files: `1.gif`, `2.txt`, and `card.gif`. `glob()` will produce the following results. Notice how any leading

```
>>> import glob
>>> glob.glob('./[0-9].*')
['./1.gif', './2.txt']
>>> glob.glob('*.gif')
['1.gif', 'card.gif']
>>> glob.glob('?.gif')
['1.gif']
```

If the directory contains files starting with `.` they won't be matched by default. For example, consider a directory containing `card.gif` and `.card.gif`:

```
>>> import glob
>>> glob.glob('*.gif')
['card.gif']
>>> glob.glob('.c*')
['.card.gif']
```

UNIVERSITÄT BONN

Linux (Ubuntu)

- Ubuntu is an operating system with a graphical user interface
- Excellent environment to perform bioinformatics
- Offers a powerful terminal and comes with comprehensive support
- Processing of large data sets is more efficient via command line tools
- Dual boot system with Windows is possible
- Configuration of USB stick for Ubuntu is possible to explore opportunities

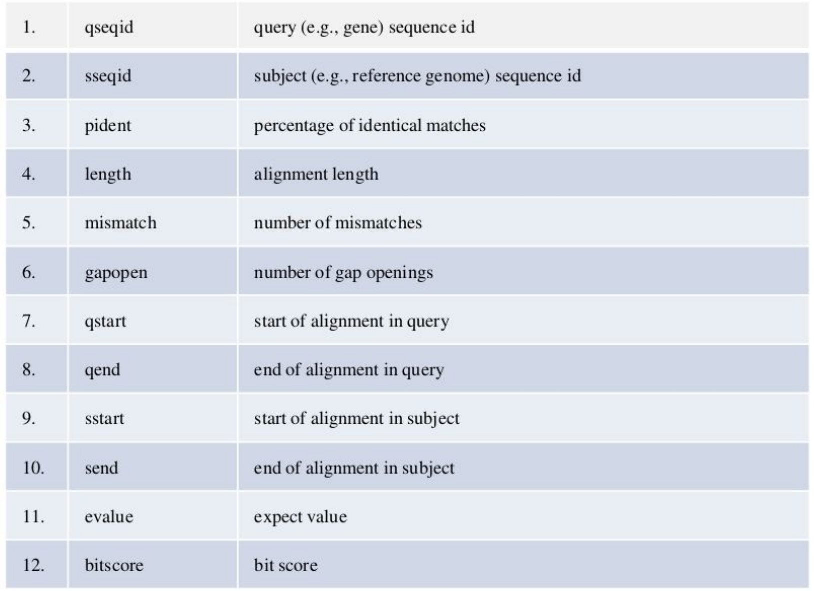
https://ubuntu.com/tutorials/create-a-usb-stick-on-ubuntu#1-overview

UNIVERSITÄT BONN

How to run BLAST?

- Running at the NCBI website does not give you full control over all parameters
- Python can be used to run a local search:

```
blastn \
-query <query_file> \
-subject <subject_file> \
-out <output_file> \
-outfmt 6 \
-evalue 0.01 \
-word_size 4
```



1.	qseqid	query (e.g., gene) sequence id
2.	sseqid	subject (e.g., reference genome) sequence id
3.	pident	percentage of identical matches
4.	length	alignment length
5.	mismatch	number of mismatches
6.	gapopen	number of gap openings
7.	qstart	start of alignment in query
8.	qend	end of alignment in query
9.	sstart	start of alignment in subject
10.	send	end of alignment in subject
11.	evalue	expect value
12.	bitscore	bit score

https://www.metagenomics.wiki/tools/blast/blastn-output-format-6

How to execute processes via shell?

- Running shell commands through the subprocess module:

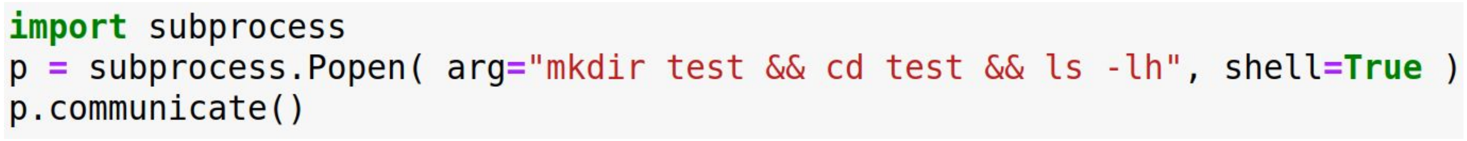
  p = subprocess.Popen(arg='ls -lh', shell=True)

  p.communicate()

- Can be used to run everything via Python

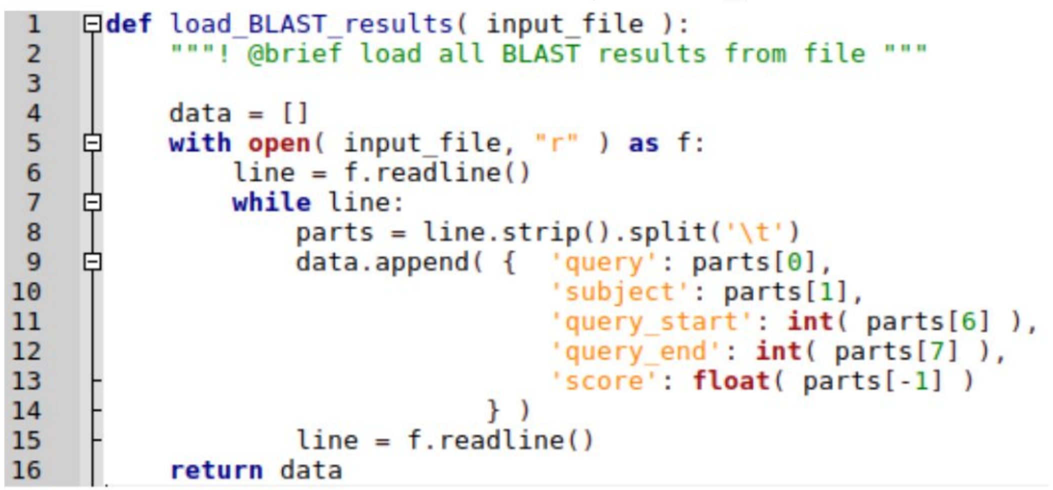
- Python waits until the command is completed

- Example:

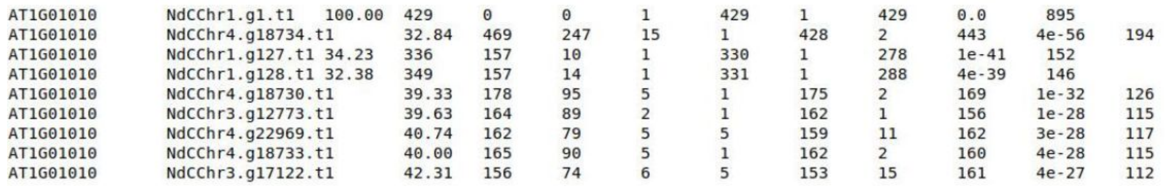


```
import subprocess
p = subprocess.Popen( arg="mkdir test && cd test && ls -lh", shell=True )
p.communicate()
```

How to process BLAST results?



```python
def load_BLAST_results( input_file ):
	"""! @brief load all BLAST results from file """
	
	data = []
	with open( input_file, "r" ) as f:
		line = f.readline()
		while line:
			parts = line.strip().split('\t')
			data.append( {	'query': parts[0],
							'subject': parts[1],
							'query_start': int( parts[6] ),
							'query_end': int( parts[7] ),
							'score': float( parts[-1] )
						} )
			line = f.readline()
	return data
```



```
AT1G01010       NdCChr1.g1.t1   100.00  429     0       0       1       429     1       429     0.0      895
AT1G01010       NdCChr4.g18734.t1       32.84   469     247     15      1       428     2       443     4e-56   194
AT1G01010       NdCChr1.g127.t1 34.23   336     157     10      1       330     1       278     1e-41    152
AT1G01010       NdCChr1.g128.t1 32.38   349     157     14      1       331     1       288     4e-39    146
AT1G01010       NdCChr4.g18730.t1       39.33   178     95      5       1       175     2       169     1e-32   126
AT1G01010       NdCChr3.g12773.t1       39.63   164     89      2       1       162     1       156     1e-28   115
AT1G01010       NdCChr4.g22969.t1       40.74   162     79      5       5       159     11      162     3e-28   117
AT1G01010       NdCChr4.g18733.t1       40.00   165     90      5       1       162     2       160     4e-28   115
AT1G01010       NdCChr3.g17122.t1       42.31   156     74      6       5       153     15      161     4e-27   112
```

Exercises - Part6b

- 6.6) Collect the best CHS BLAST result per contig from the CHS_vs_Digitalis.txt file.

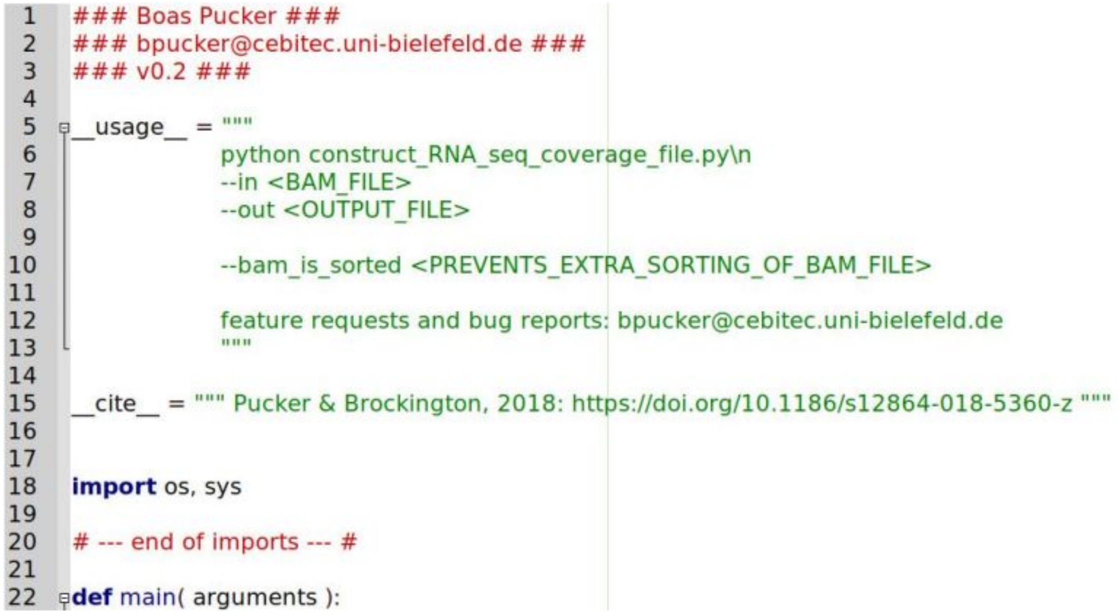
- 6.7) Count the number of BLAST hits that show a similarity >80%, an alignment length >200, and an e-value<10^{-10}.

How to organize a Python script

- Make a script recognize that it needs to run with Python:

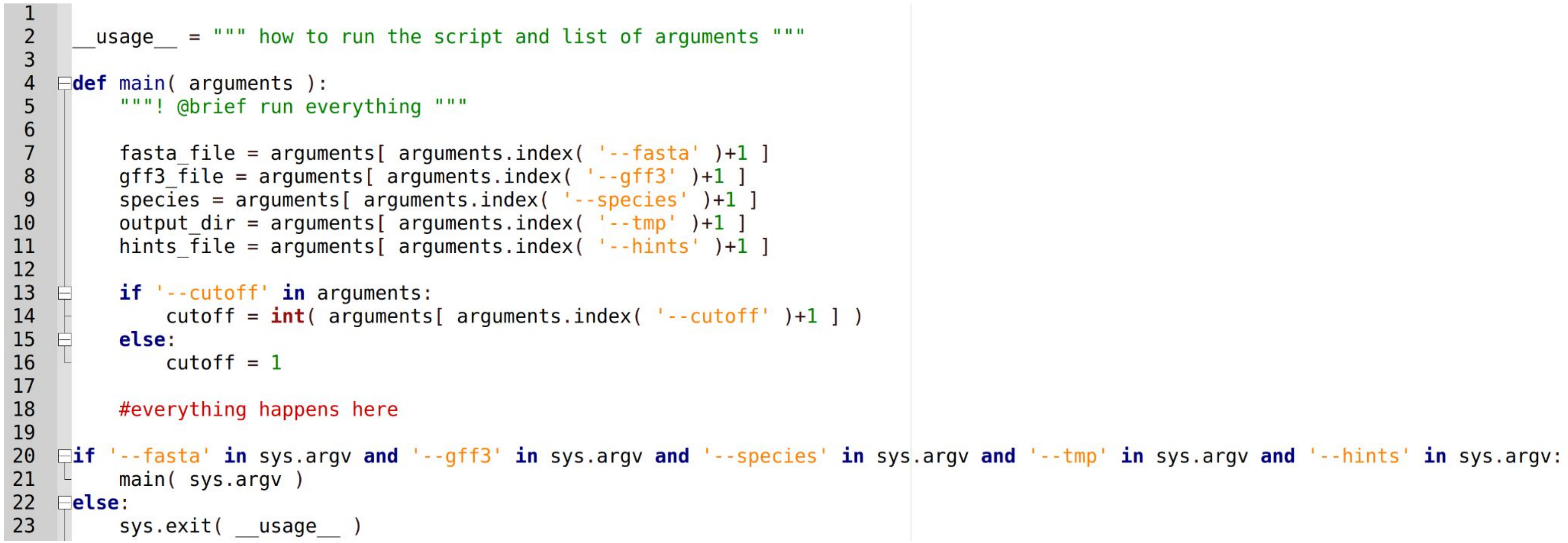
  #!/usr/bin/env python3

- Other information to include:
  - Author
  - Version
  - Usage
  - Imports



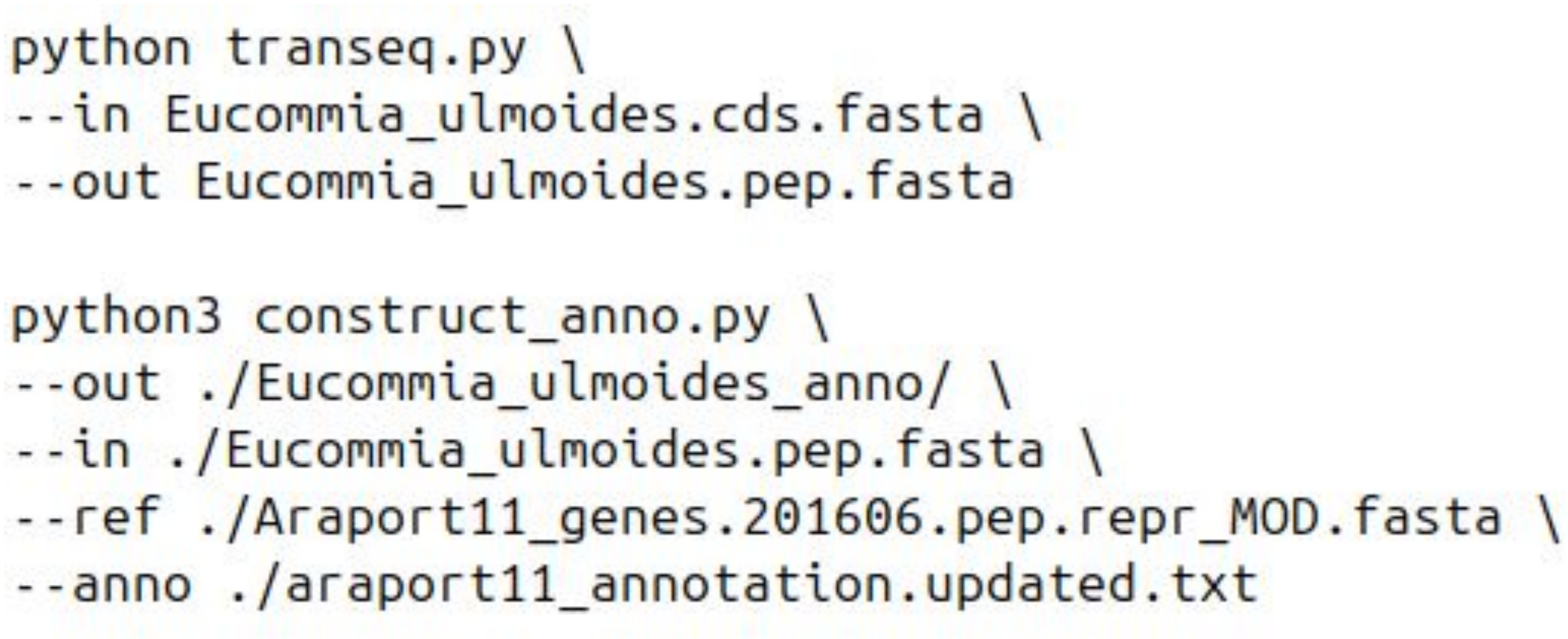
```
### Boas Pucker ###
### bpucker@cebitec.uni-bielefeld.de ###
### v0.2 ###

__usage__ = """
					python construct_RNA_seq_coverage_file.py\n
					--in <BAM_FILE>
					--out <OUTPUT_FILE>

					--bam_is_sorted <PREVENTS_EXTRA_SORTING_OF_BAM_FILE>

					feature requests and bug reports: bpucker@cebitec.uni-bielefeld.de
					"""

__cite__ = """ Pucker & Brockington, 2018: https://doi.org/10.1186/s12864-018-5360-z """


import os, sys

# --- end of imports --- #

def main( arguments ):
```

How to pass arguments to a Python script?



```

__usage__ = """ how to run the script and list of arguments """

def main( arguments ):
    """! @brief run everything """

    fasta_file = arguments[ arguments.index( '--fasta' )+1 ]
    gff3_file = arguments[ arguments.index( '--gff3' )+1 ]
    species = arguments[ arguments.index( '--species' )+1 ]
    output_dir = arguments[ arguments.index( '--tmp' )+1 ]
    hints_file = arguments[ arguments.index( '--hints' )+1 ]

    if '--cutoff' in arguments:
        cutoff = int( arguments[ arguments.index( '--cutoff' )+1 ] )
    else:
        cutoff = 1

    #everything happens here

if '--fasta' in sys.argv and '--gff3' in sys.argv and '--species' in sys.argv and '--tmp' in sys.argv and '--hints' in sys.argv:
    main( sys.argv )
else:
    sys.exit( __usage__ )
```

Command line examples



```
python transeq.py \
--in Eucommia_ulmoides.cds.fasta \
--out Eucommia_ulmoides.pep.fasta

python3 construct_anno.py \
--out ./Eucommia_ulmoides_anno/ \
--in ./Eucommia_ulmoides.pep.fasta \
--ref ./Araport11_genes.201606.pep.repr_MOD.fasta \
--anno ./araport11_annotation.updated.txt
```

UNIVERSITÄT BONN

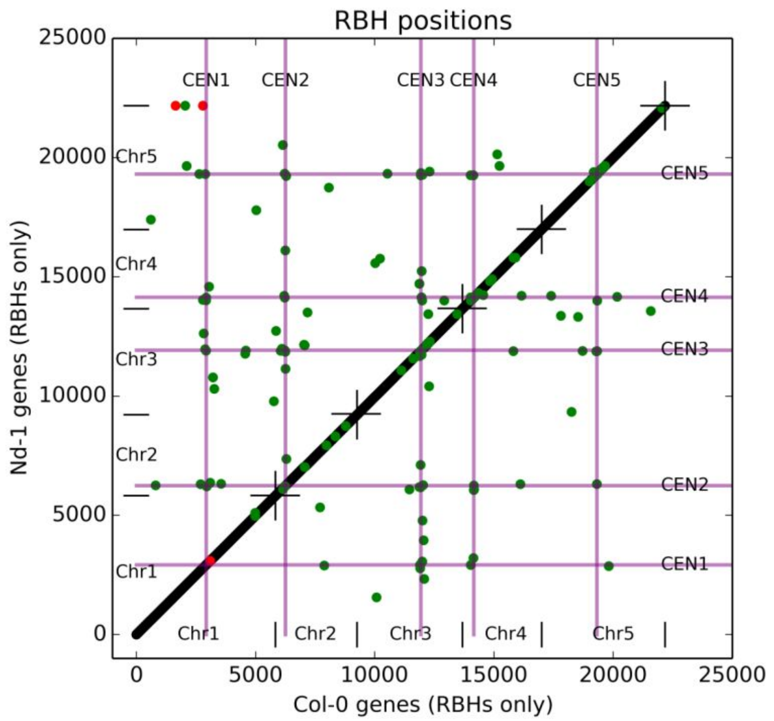
matplotlib

- Importing matplotlib:
  import matplotlib.pyplot as plt

- Visualization of complex data

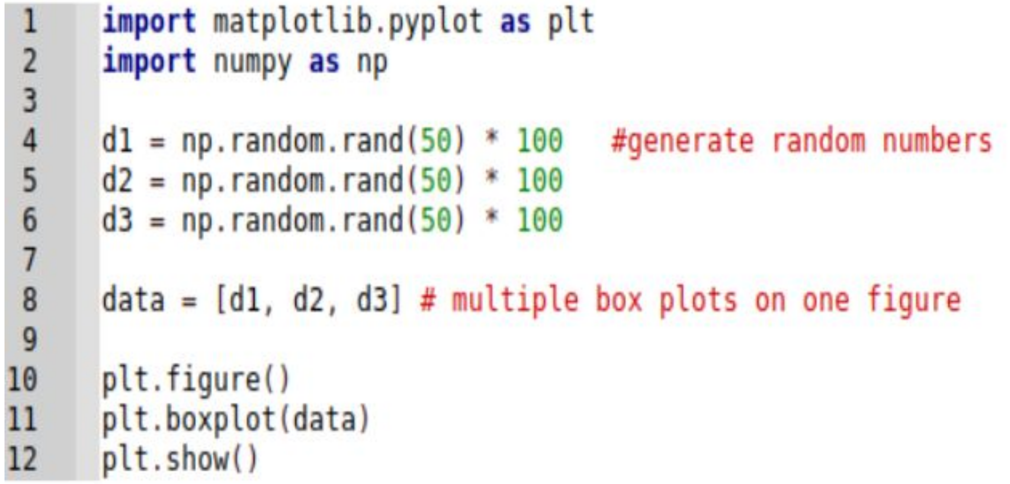
- Automatic generation of plots

- Unlimited customization options

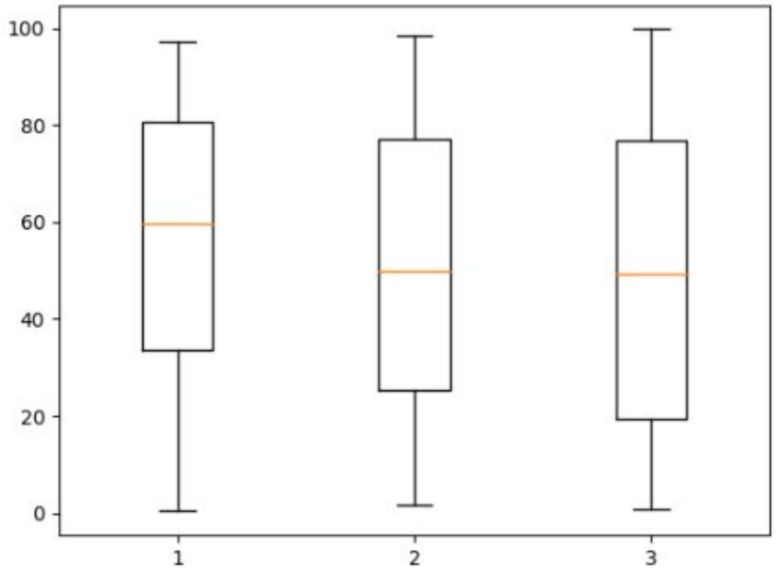


Pucker et al., 2016: 10.1371/journal.pone.0164321

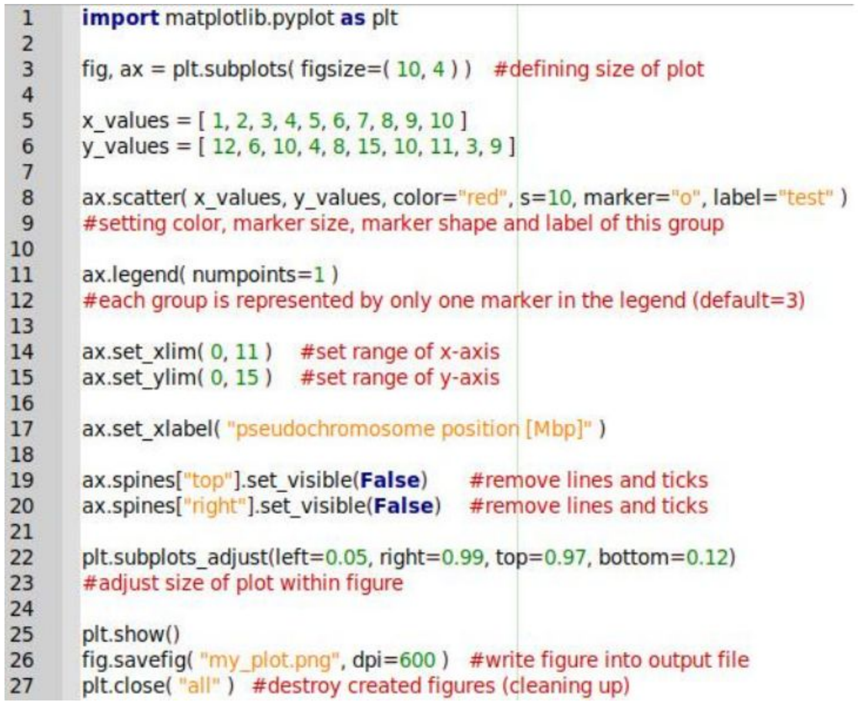
Box plot



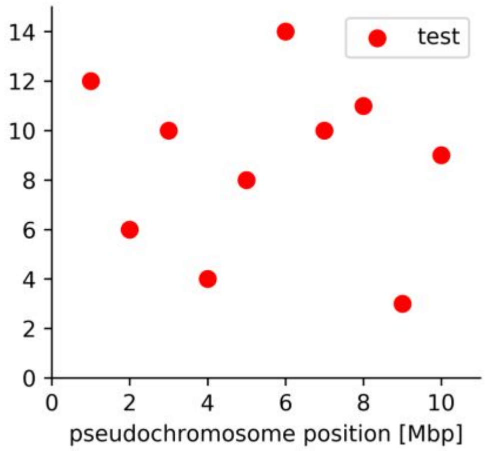
```python
import matplotlib.pyplot as plt
import numpy as np

d1 = np.random.rand(50) * 100   #generate random numbers
d2 = np.random.rand(50) * 100
d3 = np.random.rand(50) * 100

data = [d1, d2, d3] # multiple box plots on one figure

plt.figure()
plt.boxplot(data)
plt.show()
```



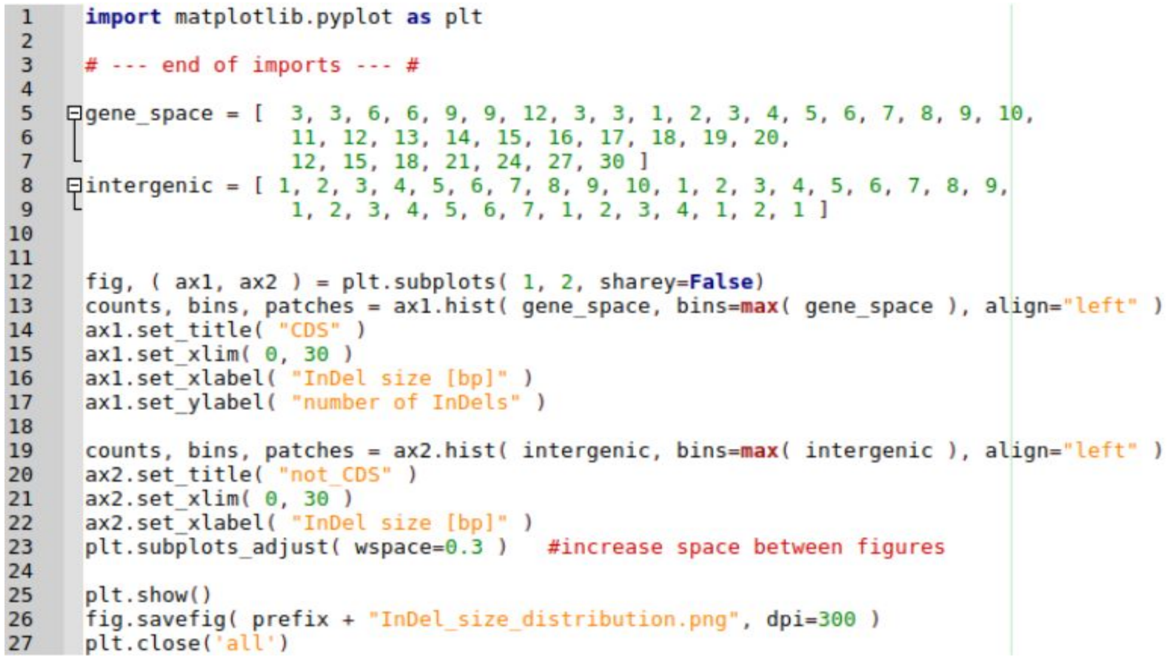
Scatter plot



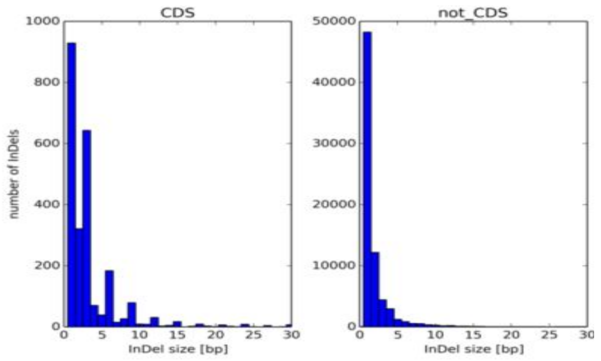
```python
import matplotlib.pyplot as plt

fig, ax = plt.subplots( figsize=( 10, 4 ) )   #defining size of plot

x_values = [ 1, 2, 3, 4, 5, 6, 7, 8, 9, 10 ]
y_values = [ 12, 6, 10, 4, 8, 15, 10, 11, 3, 9 ]

ax.scatter( x_values, y_values, color="red", s=10, marker="o", label="test" )
#setting color, marker size, marker shape and label of this group

ax.legend( numpoints=1 )
#each group is represented by only one marker in the legend (default=3)

ax.set_xlim( 0, 11 )    #set range of x-axis
ax.set_ylim( 0, 15 )    #set range of y-axis

ax.set_xlabel( "pseudochromosome position [Mbp]" )

ax.spines["top"].set_visible(False)      #remove lines and ticks
ax.spines["right"].set_visible(False)    #remove lines and ticks

plt.subplots_adjust(left=0.05, right=0.99, top=0.97, bottom=0.12)
#adjust size of plot within figure

plt.show()
fig.savefig( "my_plot.png", dpi=600 )   #write figure into output file
plt.close( "all" )   #destroy created figures (cleaning up)
```



Histogram

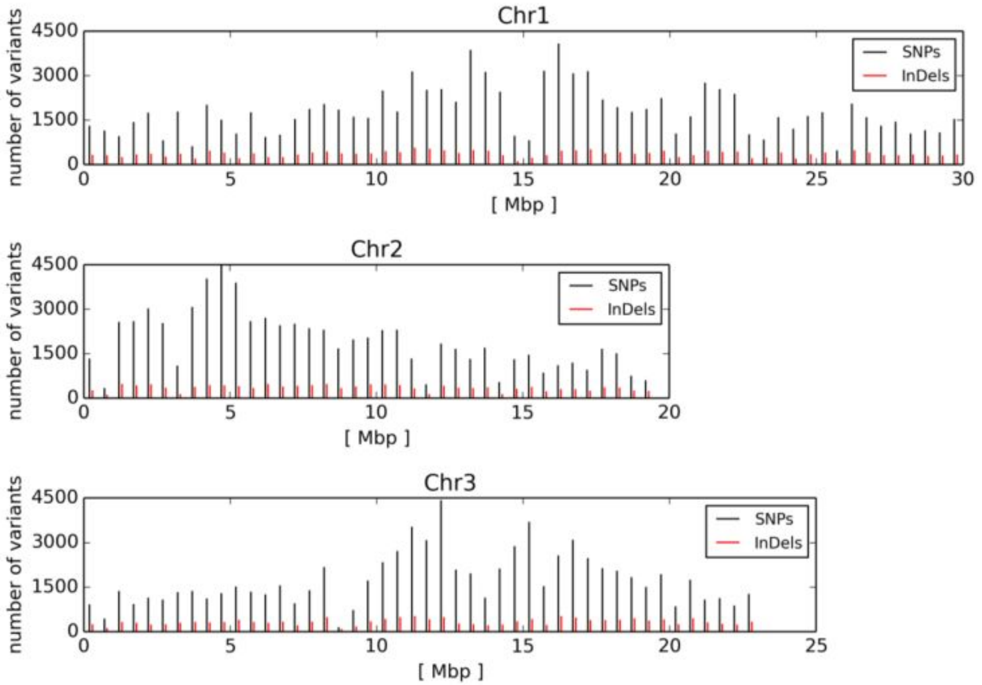


```
import matplotlib.pyplot as plt

# --- end of imports --- #

gene_space = [  3, 3, 6, 6, 9, 9, 12, 3, 3, 1, 2, 3, 4, 5, 6, 7, 8, 9, 10,
                11, 12, 13, 14, 15, 16, 17, 18, 19, 20,
                12, 15, 18, 21, 24, 27, 30 ]
intergenic = [ 1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 1, 2, 3, 4, 5, 6, 7, 8, 9,
                1, 2, 3, 4, 5, 6, 7, 1, 2, 3, 4, 1, 2, 1 ]


fig, ( ax1, ax2 ) = plt.subplots( 1, 2, sharey=False)
counts, bins, patches = ax1.hist( gene_space, bins=max( gene_space ), align="left" )
ax1.set_title( "CDS" )
ax1.set_xlim( 0, 30 )
ax1.set_xlabel( "InDel size [bp]" )
ax1.set_ylabel( "number of InDels" )

counts, bins, patches = ax2.hist( intergenic, bins=max( intergenic ), align="left" )
ax2.set_title( "not_CDS" )
ax2.set_xlim( 0, 30 )
ax2.set_xlabel( "InDel size [bp]" )
plt.subplots_adjust( wspace=0.3 )   #increase space between figures

plt.show()
fig.savefig( prefix + "InDel_size_distribution.png", dpi=300 )
plt.close('all')
```



Pucker et al., 2016: 10.1371/journal.pone.0164321

Barplot figure



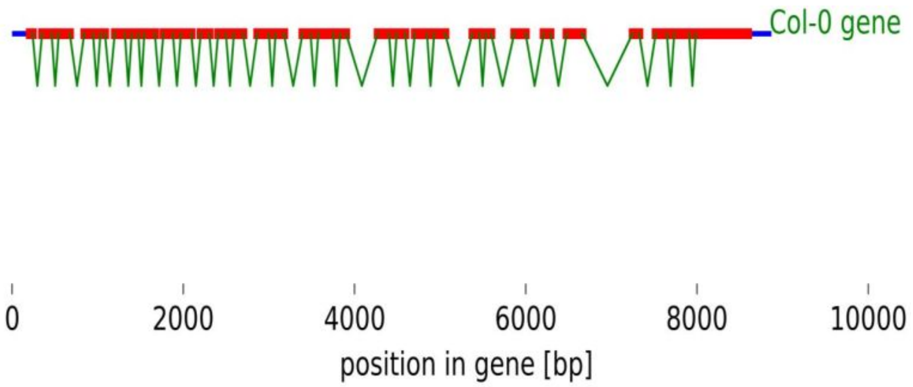
barplots.py generates barplots at specific positions by drawing a normal line

(script is available in course repository)

Pucker et al., 2016: 10.1371/journal.pone.0164321

Gene structure plot

- gene_structure_plot.py generates visualizations of gene/transcript structures based on GFF annotations



Pucker et al., 2017: 10.1186/s13104-017-2985-y

Exercises - Part6c

- 6.8) Construct a figure to illustrate the order and orientation of genes in the gum gene cluster of *Xanthomonas campestris* pv. campestris!

- 6.9) Save this figure in different file formats (png, jpg, pdf, svg)!

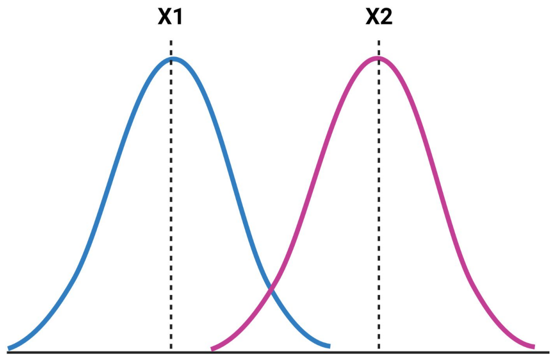
Statistics

- Compare observed sample against the expected distribution
- Check if two samples are derived from same distribution

- H0 = samples were taken from same distribution

- H0 can only be rejected or kept due to insufficient evidence against it

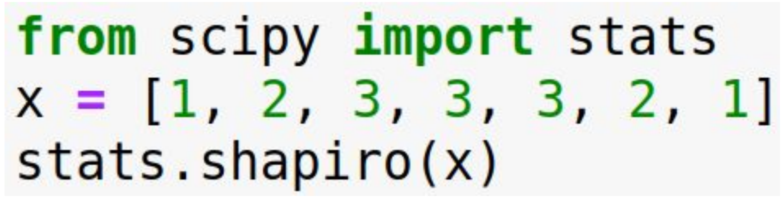
- H0 can NEVER be confirmed



Shapiro-Wilk test

- Testing data set for normal distribution

- Important for decision about potential tests



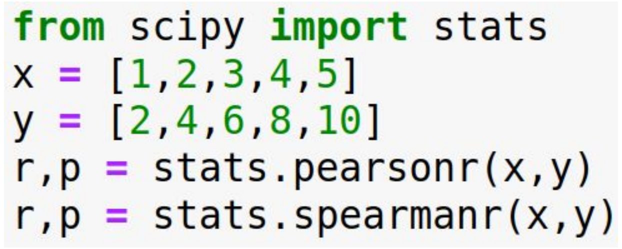
```
from scipy import stats
x = [1, 2, 3, 3, 3, 2, 1]
stats.shapiro(x)
```

UNIVERSITÄT BONN

Correlation

- Pearson correlation coefficient is suitable for data following a normal distribution

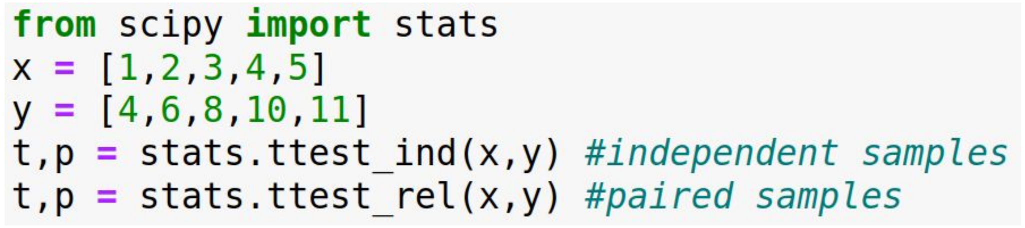
- Spearman correlation coefficient is better if data distribution is unknown



```python
from scipy import stats
x = [1,2,3,4,5]
y = [2,4,6,8,10]
r,p = stats.pearsonr(x,y)
r,p = stats.spearmanr(x,y)
```

t-test

- Samples need to show normal distribution
- Comparison of one sample against a reference value
- Comparison of two samples:
  - Paired samples (ttest_rel)
  - Unpaired samples (ttest_ind)

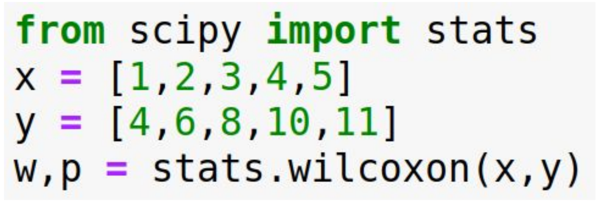


```python
from scipy import stats
x = [1,2,3,4,5]
y = [4,6,8,10,11]
t,p = stats.ttest_ind(x,y) #independent samples
t,p = stats.ttest_rel(x,y) #paired samples
```

W-test

- Wilcoxon (W) test compares two paired samples

- Normal distribution is not required

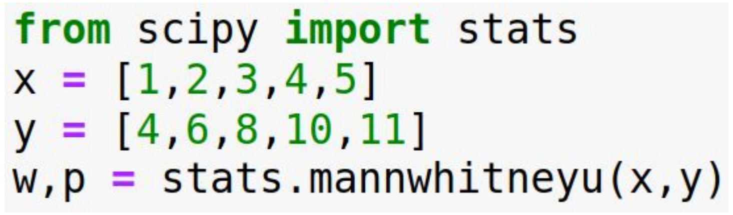


```
from scipy import stats
x = [1,2,3,4,5]
y = [4,6,8,10,11]
w,p = stats.wilcoxon(x,y)
```

U-test

- Comparison of unpaired samples

- Normal distribution is not required

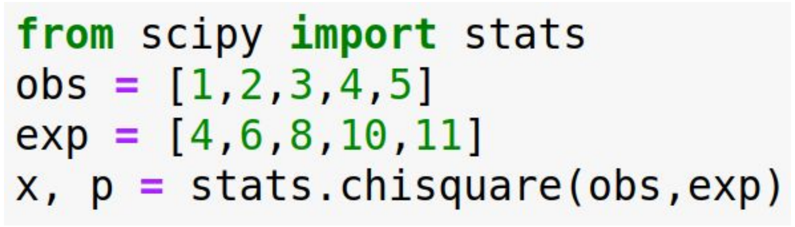


```
from scipy import stats
x = [1,2,3,4,5]
y = [4,6,8,10,11]
w,p = stats.mannwhitneyu(x,y)
```

Chi square test

- Comparison of an observation against an expectation

- Comparisons of two observations



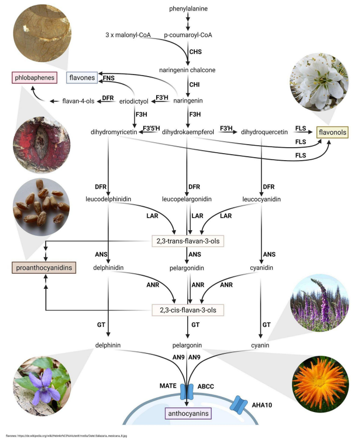
```python
from scipy import stats
obs = [1,2,3,4,5]
exp = [4,6,8,10,11]
x, p = stats.chisquare(obs,exp)
```

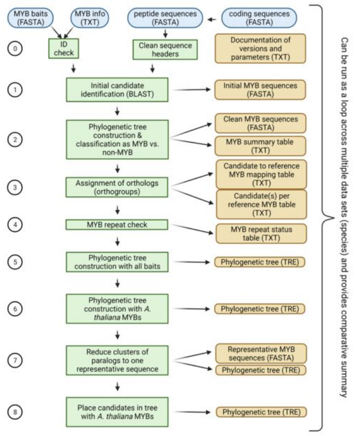
Exercises - Part6c (UNKNOWN_DATA.ods)

- 6.10) Construct a suitable visualization!
- 6.11) Analyze distribution and trends!
- 6.12) Apply statistical test to investigate difference!

Looking for more Python opportunities?

- Molecular Plant Sciences group is working on:
  - Plant genomics
  - Plant transcriptomics (RNA-seq)
  - Specialized plant metabolites
  - Synthetic biology
  - Big data comparative studies
  - Tool development
  - Data reuse




MYB baits (FASTA)
MYB info (TXT)
peptide sequences (FASTA)
coding sequences (FASTA)
0
ID check
Clean sequence headers
Documentation of versions and parameters (TXT)
1
Initial candidate identification (BLAST)
Initial MYB sequences (FASTA)
2
Phylogenetic tree construction & classification as MYB vs. non-MYB
Clean MYB sequences (FASTA)
MYB summary table (TXT)
3
Assignment of orthologs (orthogroups)
Candidate to reference MYB mapping table (TXT)
Candidate(s) per reference MYB table (TXT)
4
MYB repeat check
MYB repeat status table (TXT)
5
Phylogenetic tree construction with all baits
Phylogenetic tree (TRE)
6
Phylogenetic tree construction with A. thaliana MYBs
Phylogenetic tree (TRE)
7
Reduce clusters of paralogs to one representative sequence
Representative MYB sequences (FASTA)
Phylogenetic tree (TRE)
8
Place candidates in tree with A. thaliana MYBs
Phylogenetic tree (TRE)
Can be run as a loop across multiple data sets (species) and provides comparative summary

- Details: https://www.mps.uni-bonn.de/
- Web server: https://pbb-tools.de/

Time for questions!

References

- Nd-1 genome assembly (Pucker *et al.*, 2016)
  - https://doi.org/10.1371/journal.pone.0164321
- Non-canonical splice sites (Pucker *et al.*, 2017)
  - https://doi.org/10.1186/s13104-017-2985-y
- *Croton tiglium* transcriptome assembly (Haak *et al.*, 2018)
  - https://doi.org/10.3389/fmolb.2018.00062
- Genome-wide non-canonical splice sites in plants (Pucker & Brockington, 2018)
  - https://doi.org/10.1186/s12864-018-5360-z
- Chromosome-level Nd-1 genome assembly (Pucker *et al.*, 2019)
  - https://doi.org/10.1371/journal.pone.0216233
- NAVIP (Baasner *et al.*, 2025)
  - https://doi.org/10.1371/journal.pcbi.1012732