



# Wrap up

02.12.2023



# Course program

## Basic python



## Scientific data analysis



### 1. Intro. Git, GitHub

2. Python recap, data types
3. Functions
4. Modules and libraries
5. Files
6. IDEs
7. Virtual environments
8. Regular expressions
9. Numpy
10. Pandas
11. Visualisation
12. Statistics
13. Discussion

*next semester...*



## Advanced python

- OOP, classes
- Decorators
- Iterators & generators
- Web scraping

## Tools development

- Parallel programming
- Profiling, performance
- Open source
- SQL

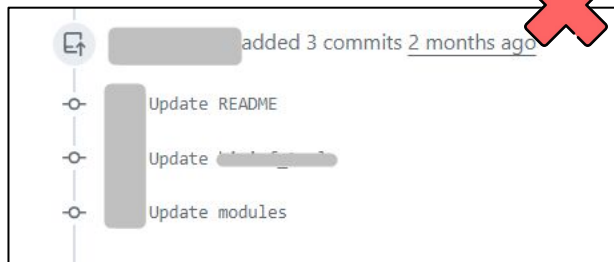


**ДЗ 2 - 6**



# КОММИТЫ:

- Use **imperative** mood
- Start with **Capital** letter
- Line size < **50** symbols
- Be **informative**
- Do not end with a period
- Use the body if you need





# README



Описание репо

Public

Watch 1

Fork 0

Star 0

3 branches

0 tags

Go to file

Add file

<> Code

About

This branch is 25 commits ahead of main.

#1

This is the repo for the homework of the BI Python 2023 course



# README



Описание репо



Небольшое  
красочное интро

☰ README.md



Determine the characteristics of amino acid sequences, Obtain processed DNA or RNA, Delete low-quality fastq sequences

The idea of this program is to make life easier for experimenters and bioinformatics working with nucleic acids, amino acid sequences (both long and short), as well as fastq sequences. This tool is designed to work with nucleotide, amino acid sequences and fastq sequences. The tool includes **3 modules**:

- `run_dna_rna_tools` — this module is designed to work with sequences of nucleic acids (DNA and RNA)
- `run_aminoacid_seq` — this module is designed to work with amino acid sequences
- `filter_read` - this module is designed to filter a dictionary with fastq sequences by specified parameters





# README



Описание репо



Небольшое  
красочное интро



Содержание

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- [Fastq tool](#)
- [RNA DNA tool](#)
- [Protein tool](#)
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## Table of Contents

- [Installation](#)
- [Functions](#)
  - [protein\\_tool](#)
  - [dna\\_rna\\_tools](#)
  - [fastqc\\_filter](#)



# README

- ✓ Описание репо
- ✓ Небольшое красочное интро
- ✓ Содержание
- ✓ Установка

## Installation

To use this toolbox one need to clone repository

```
git clone https://github.com/[redacted]/pybioseq-utils/  
cd pybioseq-utils
```



## System requirements:

Key packages and programs:

- [Python](#) (version >= 3.9)

## System requirements

- OS
- Python/R/... version

## Installation

- `git clone <URL>`
- `cd <dir>`





# README



Описание репо



Небольшое  
красочное интро



Содержание



Установка



Использование и  
описание

## Usage

```
# import main functions
from biopyseq_utils import run_nucleic_seq_processing, run_protein_seq_processing, run_fastaq_filtering
```

### filter\_fastaq

`filter_fastaq` is a function for filtering fasta-sequences. It is possible to filter sequences by GC-content, length and quality.

#### Inputs

- `seqs` - dictionary of fasta sequences. The key is a string, the name of the sequence. The value is a tuple of two strings: sequence and quality.
- `gc_bounds` - GC-content interval (in percent) for filtering (*default* `gc_bounds = (0, 100)`). If only one value is entered, the interval from 0 to the entered value is considered. Both borders are included.
- `length_bounds` - length interval for filtering (*default* `length_bounds = (0, 2**32)`). If only one value is entered, the interval from 0 to the entered value is considered. Both borders are included.
- `quality_threshold` - threshold value (phred33 scale) of the average quality of the read for filtering (*default* `quality_threshold = 0`). Reads with average quality for all nucleotides below the threshold are discarded.

#### Outputs

A dictionary with the original structure, but with sequences that satisfy the filtering conditions.

#### Usage example

```
filter_fastaq(fasta_dict, gc_bounds = (35, 80), length_bounds = (70, 88), quality_threshold = 32)
```





# README



Описание репо



Небольшое  
красочное интро



Содержание



Установка



Использование и  
описание



Траблшутинг

## Troubleshooting

It might be arised errors in the next cases:

- If you are not entering DNA or RNA sequences in `run_dna_rna_tools`
- If you are trying to transcribe a non-DNA sequence in `run_dna_rna_tools`
- If you enter neither a one-letter nor a three-letter protein sequence in `run_protein_tools`

## Troubleshooting

`run_protein_analyzer_tool` raises errors in two cases:

- Operation is not one from list: "content\_check", "seq\_length", "protein\_formula", "protein\_mass", "charge". If you are sure that input is correct, perform spell check.
- Argument for `abbreviation` parameter is not integer from 1 or 3.

In other cases `run_protein_analyzer_tool` will not halt the execution. In other scenarios troubleshooting can be performed using second element in tuple returned by `run_protein_analyzer_tool`, `corrupt_seqs` list. This list contains sequences recognized as non-valid together with their indices in original sequence. in form of tuple (`<sequence_index>`, `<sequence>`). Sequence is suggested to be non-valid in these cases:

- If sequence is not type `str`. Other iterable objects are not supported by the time.
- Sequence is empty string.



# README

- ✓ Описание репо
- ✓ Небольшое красочное интро
- ✓ Содержание
- ✓ Установка
- ✓ Использование и описание
- ✓ Траблшутинг
- ✓ Контакты, ссылки

## Contacts

We hope our module provides useful tool for your work. If you encounter any errors, please mail one from our team:

[Oskilova Angelina](#) - [\[redacted\]@gmail.com](#) Implemented: `protein_formula`, `protein_mass`, `seq_length`.

[Argamant'yakov](#) - [\[redacted\]@mail.ru](#) Implemented: `aa_content_check`, `aa_chain_charge`.

[Orelov Denis](#) - [\[redacted\]@gmail.com](#) Teamlead. Implemented: `dna_rna_tools` module and `Mann_Whitney_U`, `decomposition`, `seq_transform`, `check_and_procees_seq`, `print_result`, `run_protein_analyzer_tool` from ``module.

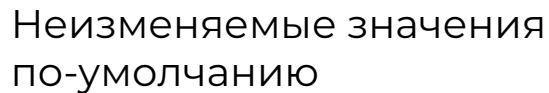
## Contributions and contacts

Feel free to report any bugs and problems encountered. Any bug reported is appreciated. Email:

[\[redacted\]@gmail.com](#)

## References

1. T.F. Smith, M.S. Waterman, (1981). [Identification of common molecular subsequences](#). Journal of Molecular Biology. [\[redacted\]](#)

[illegible]





# Немного о коде

Шебанг

Докстринга модуля

Импорты

Функции

Code

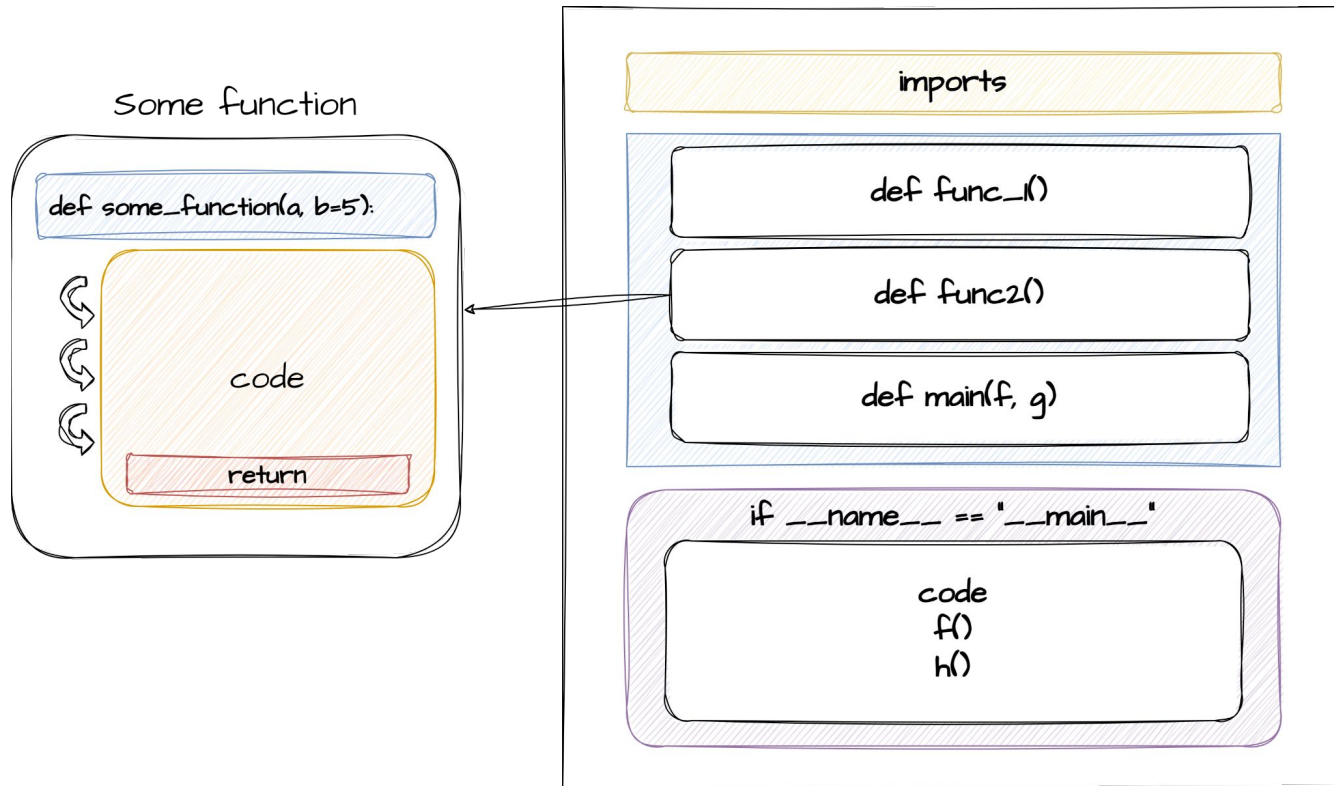
Blame

96 lines (72 loc) · 2.8 KB

```
1  #!/usr/bin/env python3
2  """
3  FASTQ_TOOL
4  """
5
6  from typing import Union
7
8
9  def calc_gc(seq: str) -> float:
10     """
11     calculates GC ratio of a given sequence
12
13     Args:
14     seq - a sequence to use
15
16     Returns:
17     gc_ratio - a GC-content of a given sequence
18     """
19
20     gc_ratio = round(((seq.count('G') + seq.count('C'))/len(seq)) * 100, 2)
21     return gc_ratio
22
```



# Немного о коде



Автопроверка импортов: [isort](#)

- Разделяются на 3 группы:
  1. Стандартная библиотека
  2. Сторонние библиотеки
  3. Локальные модули
- Сперва `import`, потом `from import`
- В алфавитном порядке







# ДЗ 7



# Запуск pain.py

Характеристики ОС  
Ссылка на conda/mamba

```
wget <URL> && cd <dir>
```

```
conda env create -f environment.yaml
```

```
conda activate env
```

Редактирование pandas

```
python pain.py
```





# Редактирование pandas

Путь до файла

```
/<env_path>/lib/python3.12/site-packages/pandas/core/frame.py
```

"Comment two following lines"

```
if isinstance(index, set):  
    raise ValueError("index cannot be a set")
```

nano / vim

```
nano +699 <file>
```



# Редактирование pandas

Путь до файла

```
<env_path>/lib/python3.12/site-packages/pandas/core/frame.py
```

"Comment two following lines"


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if isinstance(index, set):  
    raise ValueError("index cannot be a set")
```

nano / vim

```
nano +699 <file>
```

Патч

 .github

 README.md

 frame.py

Then, please, **copy file** `frame.py`, which where in the repository using:

```
cp /home/hw7_final/frame.py /home/hw7_final/hw7_final_venv/lib/python3.12/site-packages/pandas/core
```



# Редактирование pandas

Путь до файла

```
<env_path>/lib/python3.12/site-packages/pandas/core/frame.py
```

"Comment two following lines"

```
if isinstance(index, set):  
    raise ValueError("index cannot be a set")
```

nano / vim

```
nano +699 <file>
```

Патч

📁 .github

📄 README.md

📄 frame.py

Then, please, copy file `frame.py`, which where in the repository using:

```
cp /home/hw7_final/frame.py /home/hw7_final/hw7_final_venv/lib/python3.12/site-packages/pandas/core
```

```
sed -i "/# GH47215/,/^$/ {/^$\|!# GH47215/! s/^/#/g}" <file>
```



**ДЗ 8**



# Перевод на соленый язык

```
def salt_vowel(vowel):  
    return vowel.group() + 'c' + vowel.group().lower()  
  
def salt_text(text):  
    vowels = re.compile(r'([ауоиэыяюеёАУОИЭЫЯЮЕЁ])')  
    return re.sub(pattern=pattern, repl=salt_vowel, string=text)
```



# Перевод на соленый язык

```
def salt_vowel(vowel):  
    return vowel.group() + 'c' + vowel.group().lower()  
  
def salt_text(text):  
    vowels = re.compile(r'([ауоиэыяюеёАУОИЭЫЯЮЕЁ])')  
    return re.sub(pattern=pattern, repl=salt_vowel, string=text)
```





# Аккорды

```
def get_chords(input_path: str) -> set:
    """
    Get chords from a song in russian

    Argument:
    -input_path(str): input path to the file
    with lyrics and chords of the song

    Returns:
    -chords(set): a set with chords
    """
    pattern = r'[a-zA-Z]+\b'
    chords = set()
    with open('data/song.txt') as f:
        for line in f:
            chords = chords.union(re.findall(pattern, line))
    return chords
```



# Аккорды

```
def get_chords(input_path: str) -> set:
    """
    Get chords from a song in russian

    Argument:
    -input_path(str): input path to the file
    with lyrics and chords of the song

    Returns:
    -chords(set): a set with chords
    """
    pattern = r'[a-zA-Z]+\b'
    chords = set()
    with open('data/song.txt') as f:
        for line in f:
            chords = chords.union(re.findall(pattern, line))
    return chords
```

`r'[A-Z][m]?'`

`r"[A-Z][a-z]?\\b"`

`r'[CDEFGAB][m7]?'`

`r"[AC-H]+#?m?7?"`

`r'\\b[A-H]m?[1-7]?\\b'`



# Аккорды

```
def get_chords(input_path: str) -> set:
    """
    Get chords from a song in russian

    Argument:
    -input_path(str): input path to the file
    with lyrics and chords of the song

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    -chords(set): a set with chords
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    pattern = r'[a-zA-Z]+\b'
    chords = set()
    with open('data/song.txt') as f:
        for line in f:
            chords = chords.union(re.findall(pattern, line))
    return chords
```

`r'[A-Z][m]?'`

`r"[A-Z][a-z]?\\b"`

`r'[CDEFGAB][m7]?'`

`r"[AC-H]+#?m?7?"`

`r'\\b[A-H]m?[1-7]?\\b'`

`r'\\b[A-G](?:#|b)?(?:maj|m|min|sus|dim|aug)?(?:[0-9]?(?:#|b)?(?:\\/[A-G](?:#|b)?)?\\b'`

`r'(?:[ABCDEFGH]|[ABCDEFGH][abdfegh])(?:\\#|)(?:[abdfegh]|)(?:dim|aug|sus|maj|)(?:\\d|)(?:\\#\\d|)(?:\\s|\\n|\\t|\\S)'`



# Переименовалка

```
def rename_files(dir: str, pattern: str, new_pattern: str = None, sample_names: dict = None, to_replace = False):
    """
    Rename files by a chosen pattern and/or by a dictionary of sample names

    Arguments:
    - dir (str): the name of the directory with files
    - pattern (str): the pattern for files selection
    - new_pattern (str): the pattern by which the files are renamed
    - sample_names (dict): the dictionary that sets the rules for renaming
      samples (applied after renaming by the pattern)
    - to_replace (bool, default = False): rename files with the deletion of
      the original ones (True), or with copying (False)
    """
    files = os.listdir(dir)
    for file in files:
        if re.match(pattern, file):
            if new_pattern:
                new_file = re.sub(pattern, new_pattern, file)
            if sample_names:
                for pattern in sample_names:
                    new_file = re.sub(pattern, sample_names[pattern], new_file)
            old_path = os.path.join(dir, file)
            new_path = os.path.join(dir, new_file)
            if to_replace:
                os.rename(old_path, new_path)
            else:
                shutil.copy2(old_path, new_path)
```



# Квиз!

Я вам показываю регулярку



Вы угадываете что это было  
за задание





# Квиз!

г'Ваш текст'





# Квиз!

`r'Ваш текст'`

## Задание 1

*это пример*

Получите фразу `['Ваш текст']`





# Квиз!

`r'\d'`







# Квиз!

```
r'\d'
```

## Задание 2

Получите все цифры в строке (в чем разница между цифрами и числами?).

Ответ: `['2', '5', '1', '2']`





# Квиз!

`r'[0-9]'`





# Квиз!

```
r'[0-9]'
```

## Задание 2

Получите все цифры в строке (в чем разница между цифрами и числами?).

Ответ: `['2', '5', '1', '2']`



# Квиз!

`r'^[а-яА-ЯёЁ]+'`



# Квиз!

```
r'^[а-яА-ЯёЁ]+'
```

## Задание 6

Получите слово которое находится в начале строки

Ответ: `['Путь']`





# Квиз!

`r'^w+'`





# Квиз!

```
r'^\w+'
```

## Задание 6

Получите слово которое находится в начале строки

Ответ: `['Путь']`





# Квиз!

`r"[А-Я][а-я]*"`







# Квиз!

```
r"[А-Я][а-я]*"
```

## Задание 6

Получите слово которое находится в начале строки

Ответ: `['Путь']`

```
pattern = r"[А-Я][а-я]*"
```





# Квиз!

`r"D"`





# Квиз!

```
r"D"
```

## Задание 3

Получите все буквы в строке.

Ответ: `['О', 'л', 'ь', 'г', 'а']`

```
pattern = r"D"
```





# Квиз!

`r'.{1}'`



# Квиз!

`r'.{1}'`

## Задание 3

Получите все буквы в строке.

Ответ: `['0', 'л', 'ь', 'г', 'а']`

```
pattern = '.{1}'
```





# Квиз!

`r'^{^s}+'`



# Квиз!

`r'^[^\s]+'`

## Задание 6

Получите слово которое находится в начале строки

Ответ: `['Путь']`

```
: pattern = r'^[^\s]+'
```





# Квиз!

`r'\S{1,}'`





# Квиз!

`r'\S{1,}'`

## Задание 4

Получите все слова в строке.

Ответ: `['Подходит', 'желтый', 'гладкий', 'горошек']`

```
pattern = r'\S{1,}'
```





# Квиз!

`r'\S+'`





# Квиз!

`r'\S+'`

## Задание 14

Получите как можно больше чисел из этого набора.

Ответ: `['4', '8.0', '+16', '-16', '-23.42', '3.14e15']`

```
pattern = r"\S+"
```





# Еще пара слов

## Задание 14

Получите как можно больше чисел из этого набора.

Ответ: ['4', '8.0', '+16', '-16', '-23.42', '3.14e15', '23e-42', '100.000.000', '-3.099e-734.149']

```
number = r'(?:\d+)' + r'(?:\.\d+)*'
number = r'[+-]?' + number
exponential_part = fr'(?:[eE]{number})?'
number = number + exponential_part
```

[illegible]



# Еще пара слов

## Задание 15

Получите все валидные номера телефона из 'data/phones.txt'.

Ответ: `['"7(911) 345-34-56"', '"7(923)355-56-53"', '"+7(923)355-56-53"', '"8(988)245 45 32"', '"88005553535"', '"+7 921 445 43 22"']`



[illegible]



# ДЗ 10





# NA, NaN, None, NULL, ...

Объект	Класс	Если обернуть в bool()  <i>Пример: bool(float('nan'))</i>	Равен сам себе через ==?  <i>Пример: float('nan') == float('nan')</i>	Равен сам себе через is?  <i>Пример: float('nan') is float('nan')</i>
None	<class 'NoneType'>	False	True	True
float('nan')	<class 'float'>	True	False	True
math.nan	<class 'float'>	True	False	True
numpy.nan	<class 'float'>	True	False	True
pandas.NA	<class 'pandas._libs.missing.NAType'>	Ошибка	<NA>	True

# NA, NaN, None, NULL, ...

positive value



1



0



negative value



Infinity



NaN



null



undefined





# NA, NaN, None, NULL, ...

---

Анекдот: заходят в бар NA, None, NAN и NULL и пзаказали по пинте пива: NA ничего не получил, потому что для него нет пива, None принесли пустую кружку, потому что пиво кончилось, NAN принесли кружку, но там было вино, а NULL ничего не получил, потому что его не поняли.



# EDA-модуль



Аннотация типов



Краткое описание



Содержание анализа



Упомянуто про печать в stdout

```
def run_eda(df: pd.DataFrame) -> None:
    """
    Makes exploratory data analysis and prints results to the stdout

    Analysis includes:
    1. Showing shape of the dataframe
    2. Defining columns data type
    3. Defining counts and frequencies for dataframe categorical data
    4. Defining min, max, mean, std, q0.25, q0.75 for numerical data
    5. Defining number of outliers
    6. Defining number of NA values
    7. Defining number of duplicated rows
    8. Showing correlation matrix
    9. Showing head of the dataframe

    Parameters
    -----
    df: pandas.DataFrame
        Dataframe for EDA

    Returns
    -----
    None
    """
```



# EDA-модуль

- ✓ Разбиение на блоки пустой строкой
- ✓ Результаты в виде списков и табличек
- ✓ Нету лишней информации
- ➡ Округлить числа

Praise the Ommissiah! Welcome to the Sanctum of Exploratory Data Analysis.

Number of Observations (Rows): 418

Number of Parameters (Columns): 11

Data Types of Each Column:

PassengerId	int64
Pclass	category
Name	object
Sex	category
Age	float64
SibSp	int64
Parch	int64
Ticket	object
Fare	float64
Cabin	object
Embarked	category

Numerical features: PassengerId, Age, SibSp, Parch, Fare

String features: Name, Ticket, Cabin

Categorical features: Pclass, Sex, Embarked

Counts and Frequencies for Categorical Features:

	count	Frequency
Pclass		
1	107	0.255981
2	93	0.222488
3	218	0.521531
Sex		
female	152	0.363636
male	266	0.636364
Embarked		
C	102	0.244019
Q	46	0.110048
S	270	0.645933



# EDA-модуль

- ✓ Разбиение на блоки пустой строкой
- ✓ Результаты в виде списков и табличек
- ✓ Нету лишней информации
- ➡ Округлить числа
- ✓ Оформление жирным и цветом

```
Number of observations (rows):
418
Number of parameters (columns):
11

=====

Data types of each column:
PassengerId      int64
Pclass           int64
Name             object
Sex              object
Age             float64
SibSp            int64
Parch            int64
Ticket           object
Fare            float64
Cabin            object
Embarked         object

=====

Numerical features:
['PassengerId', 'Age', 'SibSp', 'Parch', 'Fare']

String features:
['Name', 'Ticket', 'Cabin']

Categorical features:
['Pclass', 'Sex', 'Embarked']
```



# EDA-модуль

- ✓ Разбиение на блоки пустой строкой
- ✓ Результаты в виде списков и табличек
- ✓ Нету лишней информации
- ➡ Округлить числа
- ✓ Оформление жирным и цветом
- ✓ Оформление табличек

Hello, I'm an assistant, my name is Rex 🐙. Today I will be your guide to the world of your dataframe.

1) **Number of columns:** 11,  
**Number of rows:** 418

2) **Numerical columns:** ['PassengerId', 'Age', 'Fare'],  
**String columns:** ['Name', 'Ticket', 'Cabin'],  
**Categorical columns:** ['Pclass', 'Sex', 'SibSp', 'Parch', 'Embarked']

3) **Number of values and their frequencies:**

**Pclass**

Name	Count	Frequencies
3	218	0.522
1	107	0.256
2	93	0.222

**Sex**

Name	Count	Frequencies
male	266	0.636
female	152	0.364



# Домашка на каникулы

---





# Домашка на каникулы

---

- Отдых



# Домашка на каникулы

- Отдых

## ОСНОВЫ **Git**

- [LearningGitBranching](#)
- [Hexlet Git course](#)

## ОСНОВЫ **python**

- [Stepik python course](#) (BI)
- [Stepik python course](#) (BEEGEEK)

## YouTube

- [Хитрый питон](#)
- [Moscow Python](#) (конференции и подкаст)
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- [Python Russian](#)
- [Python Clinic](#)
- [Все доклады Григория Петрова на MoscowPython](#)
- [Т. Хирьянов, Алгоритмы и структуры данных на Python 3](#)

[Сохранение cluster map в виде sub-plot.](#)