TreSucMs

Release 1.0

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"TreSucMs" a tool to choose, harvest and analyse expression and methylation data of the TCGA-projects for revealing Biomarkers which indicate treatment success.

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ONE

INSTALLING FROM GITHUB.COM:

```
$ git clone https://github.com/dendemayer/TreSucMs-TCGA.git
$ cd TreSucMs-TCGA
$ pip install .
```

To start the analysis with help of the interactive mode, call the pipeline without any argument:

\$ TreSucMs

Calling the help or the manual page:

- \$ TreSucMs --help
- \$ man TreSucMs

HELP PAGE OF THE PIPELINE:

2.1 TreSucMs

"TreSucMs2" a tool to choose, harvest and analyse expression and methylation data of the TCGA-projects for revealing Biomarkers which indicate threapy specific treatment success predictions.

Calling the pipeline without any argument starts the interactive mode to help setting all needed parameters for the analysis.

TreSucMs [OPTIONS]

Options

-o, --out_path <out_path>

path to save the result files

Default

/homes/biertruck/gabor/TreSucMs2

-p, --project

TCGA project(s) to be applied. Any TCGA project can be chosen, like: -p TCGA-CESC -p TCGA-HNSC ...

-d, --drugs <drugs>

drug(s), like: -d drug1 -d drug2 or drugcombination(s), like: -d drug1,drug2

-c, --cores <cores>

number of cores provided to snakemake

Default

1

-C, --cutoff <cutoff>

Cut-off parameter

Default

0

-t, --threshold <threshold>

threshold parameter

Default

0

-e, --execute <execute>

choose which pipeline shall be executed

Default

DESeq2, metilene

-N, --dryrun

snakemake dryrun

Default

False

-D, --download

if set, just download raw and meta data for given projects and analysis types, revise them, link them, but do not run any analysis

Default

False

-u, --unlock

in case the analysis crashs, snakemake locks the output directory, run with -u to unlock, then repeat the analysis

Default

False

-v, --version

printing out version information: Version 2.0.0

SHORT TUTORIAL:

3.1 Usage of the interactive mode:

The following example composition of projects, drugs and parameters creates the example configuration given in TODO.

The same configuration can be applied by issuing the following command (the number of cores hereby can be adjusted and would also give the same results):

```
$ TreSucMs -p TCGA-CESC -p TCGA-HNSC -p TCGA-LUSC -d cisplatin -d carboplatin,paclitaxel...

-d carboplatin -o /scr/TreSucMs_out -c 40 -t 5 -t 10 -t 20 -C 5 -C 8
```

Calling the pipeline without any argument starts the interactive mode:

```
$ TreSucMs
OUTPUT_PATH:
                          /homes/biertruck/gabor/TreSucMs
SCRIPT_PATH:
                          /homes/biertruck/gabor/phd/test_git_doc/TreSucMs/src/shared/
→modules
PIPELINES executed:
                          ['DESeq2', 'metilene']
which projects do you want to include in your analysis:
 0:
         TCGA-CESC
                             Cervical Squamous Cell Carcinoma and Endocervical
→Adenocarcinoma
 1:
         TCGA-HNSC
                             Head and Neck Squamous Cell Carcinoma
 2:
         TCGA-LUSC
                             Lung Squamous Cell Carcinoma
         TCGA-ESCA
                             Esophageal Carcinoma
 3:
 4:
         TCGA-BRCA
                             Breast Invasive Carcinoma
         TCGA-GBM
 5:
                             Glioblastoma Multiforme
 6:
         TCGA-OV
                             Ovarian Serous Cystadenocarcinaoma
 7:
         TCGA-LUAD
                             Lung Adenocarcinoma
         TCGA-UCEC
                             Uterine Corpus Endometrial Carinoma
 8:
                             kindney renal clear cell carcinoma
 9:
         TCGA-KIRC
                             brain lower grade glioma
 10:
         TCGA-LGG
11:
         TCGA-THCA
                             thyroid carcinoma
12:
         TCGA-PRAD
                             prostate adenocarcinoma
                             skin cutaneous melanoma
13:
         TCGA-SKCM
 14:
         TCGA-COAD
                             colon adenocarcinoma
                             stomach adenocarcinoma
 15:
         TCGA-STAD
```

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```
16:
        TCGA-BLCA
                             bladder urothelial carcinoma
17:
        TCGA-LIHC
                             liver hepatocellular carcinoma
18:
        TCGA-KIRP
                             kidney renal papillary cell carcinoma
19:
        TCGA-SARC
                             sarcoma
20:
        TCGA-PAAD
                             pancreatic adenocarcinoma
21:
        TCGA-PCPG
                            pheochromocytoma and paraganglioma
                             rectum adenocarcinoma
22:
        TCGA-READ
23:
                             testicular germcelltumors
        TCGA-TGCT
24:
        TCGA-THYM
                             thymoma
                             kidney chromophobe
25:
        TCGA-KICH
                             adrenochordical carcinoma
26:
        TCGA-ACC
27:
        TCGA-MESO
                             mesothelioma
28:
        TCGA-UVM
                             uveal melanoma
29:
                             lymphoid neoplasm diffuse large b-cell lymphoma
        TCGA-DLBC
30:
        TCGA-UCS
                             uterine carcinoma
31:
        TCGA-CHOL
                             cholangiocarcinoma
enter your choices one by one, when you are done, simply press "Enter":
```

As suggested, you can now, one by one include the projects you are interested in. A default OUTPUT_PATH is also already given together with the default analysis types "DESeq" and "metilene". Those defaults can also be adjusted in next steps with help of the interactive mode.

To recreate the example set, the first three projects have to be selected, afterwards the following prompt is given:

```
vou choose:
PROJECTS:
                 ['TCGA-CESC', 'TCGA-HNSC', 'TCGA-LUSC']
which therapy approach do you want to include in your analysis:
0: cisplatin
                                              TCGA-CESC: 103 TCGA-HNSC: 64 TCGA-LUSC: 1
1: carboplatin, paclitaxel
                                              TCGA-CESC: 5 TCGA-HNSC: 26 TCGA-LUSC: 14
2: 5-fluorouracil, cisplatin
                                              TCGA-CESC: 5 TCGA-HNSC: 2 TCGA-LUSC: 0
3: carboplatin
                                              TCGA-CESC: 3 TCGA-HNSC: 6 TCGA-LUSC: 3
4: carboplatin, cisplatin, paclitaxel
                                              TCGA-CESC: 3 TCGA-HNSC: 0 TCGA-LUSC: 1
                                              TCGA-CESC: 3 TCGA-HNSC: 0 TCGA-LUSC: 9
 5: cisplatin, gemcitabine
 6: paclitaxel
                                              TCGA-CESC: 2 TCGA-HNSC: 1 TCGA-LUSC: 0
7: erbitux
                                              TCGA-CESC: 1 TCGA-HNSC: 9 TCGA-LUSC: 0
8: cisplatin, vectibix
                                              TCGA-CESC: 0 TCGA-HNSC: 5 TCGA-LUSC: 0
9: carboplatin, erbitux, paclitaxel
                                              TCGA-CESC: 0 TCGA-HNSC: 4 TCGA-LUSC: 0
10: cisplatin,erbitux
                                              TCGA-CESC: 0 TCGA-HNSC: 3 TCGA-LUSC: 0
11: carboplatin,cisplatin,erbitux,paclitaxel TCGA-CESC: 0 TCGA-HNSC: 3 TCGA-LUSC: 0
12: carboplatin, cisplatin
                                              TCGA-CESC: 0 TCGA-HNSC: 2 TCGA-LUSC: 0
13: docetaxel, erbitux
                                              TCGA-CESC: 0 TCGA-HNSC: 2 TCGA-LUSC: 0
14: cisplatin, docetaxel
                                              TCGA-CESC: 0 TCGA-HNSC: 1 TCGA-LUSC: 10
15: carboplatin, docetaxel
                                              TCGA-CESC: 0 TCGA-HNSC: 1 TCGA-LUSC: 3
16: cisplatin, vinorelbine
                                              TCGA-CESC: 0 TCGA-HNSC: 0 TCGA-LUSC: 21
17: carboplatin, vinorelbine
                                              TCGA-CESC: 0 TCGA-HNSC: 0 TCGA-LUSC: 8
                                              TCGA-CESC: 0 TCGA-HNSC: 0 TCGA-LUSC: 7
18: cisplatin, etoposide
19: carboplatin, gemcitabine
                                              TCGA-CESC: 0 TCGA-HNSC: 0 TCGA-LUSC: 5
                                              TCGA-CESC: 0 TCGA-HNSC: 0 TCGA-LUSC: 3
20: cisplatin, pemetrexed
21: cisplatin, docetaxel, gemcitabine
                                              TCGA-CESC: 0 TCGA-HNSC: 0 TCGA-LUSC: 2
22: carboplatin,gemcitabine,paclitaxel
                                              TCGA-CESC: 0 TCGA-HNSC: 0 TCGA-LUSC: 2
23: carboplatin, cisplatin, vinorelbine
                                              TCGA-CESC: 0 TCGA-HNSC: 0 TCGA-LUSC: 2
```

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```
24: carboplatin,docetaxel,gemcitabine
TCGA-CESC: 0 TCGA-HNSC: 0 TCGA-LUSC: 2
```

Here are therapies listed where the maximum of a row is greater than 1. We apply row 0, 1 and 3 to include cisplatin, the combination of carboplatin and paclitaxel and cases which got solely treated with carboplatin. In the following, every other parameter is requested. With the next prompt, the default OUTPUT_PATH can be confirmed or replaced:

```
do you want to keep the default OUTPUT_PATH of:
/homes/biertruck/gabor/TreSucMs
if so, press ENTER, if not, enter your custom output path:
```

In this example, we confirm the suggested OUTPUT_PATH and are asked to confirm

or set the number of cores which shall be invoked into the analyses:

```
do you want to keep the default number of cores invoked of 1? if so, press ENTER, if not, enter the number of cores:
```

We set the cores to 40 and then can decide which analysis approaches shall be triggered, per default, DESeq2 and metilene based biomarker predictions are produced:

```
which pipeline do you want to include into your analysis press ENTER if DESeq2 and metilene (default) or 1 for DESeq2 or 2 for metilene
```

We confirm the default of those two analyses and can set the cutoff values, if we want to add those at all:

```
do you want to add one or multiple cutoffs?
it is recommend to choose cutoff values between 5 and 10 years
if not, just press ENTER, if so enter the coutoffs one by one:
5
```

Like the example set, we add here a cutoff of 5 and 8. Then the thresholds are requested:

```
do you want to add one or multiple thresholds?
it is recommend to choose threshold values which do not exceed a value of 50
if not, just press ENTER, if so enter the thresholds one by one:
5
10
20
```

We apply thresholds of 5, 10 and 20. All mandatory and optional parameters are set with that and are finally listed before the whole approach is started:

```
OUTPUT_PATH: /homes/biertruck/gabor/TreSucMs
PROJECT: ['TCGA-CESC', 'TCGA-HNSC', 'TCGA-LUSC']
DRUGS: ['carboplatin', 'carboplatin,paclitaxel', 'cisplatin']
pipelines executed: ['DESeq2', 'metilene']
```

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cores: 40
cutoff: [0, 5, 8]
threshold: [0, 5, 10, 20]
press ENTER to start or q to quit:

If something went wrong, you can quit now and start over, or of course start the analysis.

..Documentation of modules, classes and functions: ..-

.... automodule:: shared.modules.choose_therapy ..:members:

 $.... automodule:: shared.modules.download_with_api$

..:members:

 $.... automodule:: tcga_metilene.modules.main_metilene\\$

..:members:

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