

DIGEST

API Documentation

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1 Module DIGEST

Main script for DIGEST workflow CCRT version

Requires:

- python¹ (tested with 2.7.3)
- hashlib²
- BWA³
- RayMeta⁴
- Metagene⁵
- cd-hit⁶ (tested with v4.5.8-2012-03-24)
- DIGEST_functions.py (PYTHONPATH)
- SAMparser.py
- ExtractFastaFromSAM.py
- extendTargets_allPossibility.py
- hashlib⁷fasta-splitter.pl
- extractORFsequences.py
- removeIdenticalSeq.py
- cd-hit-para-CCRT.py
- DIGEST_clear.sh
- DIGEST_check.sh

1.1 Functions

```
get_parser()
```

```
main()
```

1.2 Variables

Name	Description
__doc__	Value: ...
__package__	Value: None
e	Value: 2.71828182846
pi	Value: 3.14159265359

¹<https://www.python.org/downloads/>

²<https://pypi.python.org/pypi/hashlib>

³<http://sourceforge.net/projects/bio-bwa/files/>

⁴<http://sourceforge.net/projects/denovoassembler/files/>

⁵http://metagene.nig.ac.jp/metagene/download_mga.html

⁶<https://code.google.com/p/cdhit/downloads/list>

⁷<http://kirill-kryukov.com/study/tools/fasta-splitter/>

2 Module DIGEST_functions

Class and functions use by the DIGEST workflow

Requires:

- jobArrayLSFlauncher_modif.sh
- mpirun-genoscope-modif.sh

2.1 Functions

<p>exist(<i>fname</i>)</p> <hr/> <p>Check the existence of a file.</p> <p>Parameters</p> <p>fname: file name (<i>type=string</i>)</p> <p>Return Value</p> <p>1 if the file is present, 0 otherwise (<i>type=integer</i>)</p>
--

<p>clstrParser(<i>file</i>)</p> <hr/> <p>parse .clstr file from cd hit</p> <p>Parameters</p> <p>file: file name (<i>type=string</i>)</p> <p>Return Value</p> <p>list of cluster object (<i>type=list</i>)</p>

<p>fastaReader(<i>file</i>)</p> <hr/> <p>Fasta parser</p> <p>Parameters</p> <p>file: file name (<i>type=string</i>)</p> <p>Return Value</p> <p>dictionary of sequence object with sequence ID as key (<i>type=dictionary</i>)</p>

geneExtended (<i>orfSTART</i> , <i>orfEND</i> , <i>alignSTART</i> , <i>alignEND</i> , <i>orfSTATUT</i>)
Check if a gene has been extended
Parameters
<i>orfSTART</i> : ORF start position in sequence extended (<i>type=integer</i>)
<i>orfEND</i> : ORF end position in sequence extended (<i>type=integer</i>)
<i>alignSTART</i> : alignment start position of sequence on contig (<i>type=integer</i>)
<i>alignEND</i> : alignment end position of sequence on contig (<i>type=integer</i>)
<i>orfSTATUT</i> : ORF complete or partial (<i>type=string</i>)
Return Value
True if the gene is completed, False otherwise (<i>type=boolean</i>)

geneSeen (<i>orfSTART</i> , <i>orfEND</i> , <i>alignSTART</i> , <i>alignEND</i>)
Check if a gene has been seen
Parameters
<i>orfSTART</i> : ORF start position in sequence extended (<i>type=integer</i>)
<i>orfEND</i> : ORF end position in sequence extended (<i>type=integer</i>)
<i>alignSTART</i> : alignment start position of sequence on contig (<i>type=integer</i>)
<i>alignEND</i> : alignment end position of sequence on contig (<i>type=integer</i>)
Return Value
True if the gene is seen, False otherwise (<i>type=boolean</i>)

reverseComplement (<i>sequen</i>)
make the reverse complement of a sequence
Parameters
<i>sequen</i> : nucleotide sequence (<i>type=string</i>)
Return Value
reverse complement of sequence (<i>type=string</i>)

metageneParser(*file*)

Sotck ORFs of metagene file

Parameters

file: file name
(*type=string*)

Return Value

a a dictionary with contigs IDs as key and contig object as value
(*type=dictionary*)

subjectStartStop(*alignment, subjectLength*)

From an alignment and a length, compute the start and stop alignment position

Parameters

alignment: alignmentSAM object
(*type=alignmentSAM*)
subjectLength: subject sequence length
(*type=integer*)

Return Value

a list with the position start and stop of the alignment (if start = -1 -> alignment start before the subject sequence ; if stop = -2 -> alignment stop after the subject sequence)
(*type=list*)

fileLineNumber(*file*)

Compute the int number of lines from a file

Parameters

file: file name
(*type=string*)

Return Value

number of lines
(*type=integer*)

nbSequenceFasta(*file*)

Compute the number of sequences in a FASTA file

Parameters

file: file name
(*type=string*)

Return Value

number of sequences
(*type=integer*)

```
writeORF(ORFlist, prefix, ID, sequence, n)
```

write ORFs in PREFIX_complete.fasta file or PREFIX_partial.fasta file

Parameters

ORFlist: list of ORF object
(type=list)

prefix: prefix of output file name
(type=string)

ID: sequence ID
(type=string)

sequence: nucleotide sequence
(type=string)

n: limte length for partial ORF
(type=integer)

2.2 Variables

Name	Description
__doc__	Value: ...
__package__	Value: None

2.3 Class MyDialect

```
csv.Dialect ┌
             │
             └─ DIGEST_functions.MyDialect
```

csv class use to read csv files

2.3.1 Methods

Inherited from csv.Dialect

```
__init__()
```

2.3.2 Class Variables

Name	Description
delimiter	Value: '\t'
quotechar	Value: None
escapechar	Value: '\\'

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Name	Description
doublequote	Value: False
lineterminator	Value: '\n'
quoting	Value: 3
skipinitialspace	Value: False

2.4 Class jobLauncher

object —
DIGEST_functions.jobLauncher

Create class able to launch a list of jobs on SLURM or LSF on a Job Scheduler

2.4.1 Methods

```
__init__(self, queue, nbProcesseur, jobName, mode,
option='\'select[defined(mem64)],span[hosts=1],rh5\'' )
```

Initialize the jobLauncher class

Parameters

queue: queue name to execute jobs
(type=string)

nbProcesseur: number of processor used for each jobs
(type=integer)

jobName: job name
(type=string)

mode: LSF or SLURM
(type=string)

option: resource requirements
(default:'select[defined(mem64)],span[hosts=1]')
(type=string)

Overrides: object.__init__

Name	Description
option	resource requirements (default: 'select[defined(mem64)],span[hosts=1]') (<i>type=string</i>)
queue	queue name to execute jobs (<i>type=string</i>)

2.5 Class sequence

object —
DIGEST_functions.sequence

New sequence object

2.5.1 Methods

__init__ (<i>self, header, nucl</i>)
Initialize the sequence class
Parameters
<i>header</i> : sequence header (<i>type=string</i>)
<i>nucl</i> : nucleotide sequence (<i>type=string</i>)
Overrides: object.__init__

Inherited from object

`__delattr__()`, `__format__()`, `__getattr__()`, `__hash__()`, `__new__()`, `__reduce__()`, `__reduce_ex__()`,
`__repr__()`, `__setattr__()`, `__sizeof__()`, `__str__()`, `__subclasshook__()`

2.5.2 Properties

Name	Description
<i>Inherited from object</i>	
<code>__class__</code>	

2.5.3 Class Variables

Name	Description
ID	sequence ID (<i>type=string</i>)
length	sequence length (<i>type=integer</i>)
seq	nucleotide sequence (<i>type=string</i>)

2.6 Class ORF

object —
DIGEST_functions.ORF

New ORF object from MetaGene output

2.6.1 Methods

__init__ (<i>self, ligne</i>)
Initialize the ORF class
Parameters
<i>ligne</i> : ORF line from a MetaGene output file (<i>type=list</i>)
Overrides: object.__init__

Inherited from object

`__delattr__()`, `__format__()`, `__getattr__()`, `__hash__()`, `__new__()`, `__reduce__()`, `__reduce_ex__()`,
`__repr__()`, `__setattr__()`, `__sizeof__()`, `__str__()`, `__subclasshook__()`

2.6.2 Properties

Name	Description
<i>Inherited from object</i>	
<code>__class__</code>	

2.6.3 Class Variables

Name	Description
frame	frame (1,2 or 3) (<i>type=integer</i>)
posEND	ORF stop position in sequence (<i>type=integer</i>)
posSTART	ORF start position in sequence (<i>type=integer</i>)
score	ORF score (<i>type=float</i>)
statut	statut partial or complete (<i>type=string</i>)
strand	strand (+ or -) (<i>type=character</i>)

2.7 Class ContigORF

object └─ **DIGEST_functions.ContigORF**

New contig ORF object from MetaGene output

2.7.1 Methods

<code>--init__(self, ligne1, ligne2)</code>
Initialize the ContigORF class
Parameters
ligne1 : 1st line of a block in a MetaGene output file (<i>type=list</i>)
ligne2 : 2nd line of a block in a MetaGene output file (<i>type=list</i>)
Overrides: object.__init__

Inherited from object

`--delattr__()`, `--format__()`, `--getattr__()`, `--hash__()`, `--new__()`, `--reduce__()`, `--reduce_ex__()`,
`--repr__()`, `--setattr__()`, `--sizeof__()`, `--str__()`, `--subclasshook__()`

2.7.2 Properties

Name	Description
<i>Inherited from object</i>	
__class__	

2.7.3 Class Variables

Name	Description
GC	GC% in sequence (<i>type=float</i>)
ORFlist	list of ORF objects (<i>type=list</i>)
model	ORF model (bacteria, archaea or eukaryote) (<i>type=string</i>)

2.8 Class Cigar



New alignment CIGAR object

2.8.1 Methods

<code>__init__(self, strcigar)</code>
Initialize Cigar class
Parameters
strcigar: CIGAR from a SAM line (<i>type=string</i>)
Overrides: object.__init__

Inherited from object

`__delattr__()`, `__format__()`, `__getattr__()`, `__hash__()`, `__new__()`, `__reduce__()`, `__reduce_ex__()`,
`__repr__()`, `__setattr__()`, `__sizeof__()`, `__str__()`, `__subclasshook__()`

2.8.2 Properties

Name	Description
<i>Inherited from object</i>	
__class__	

2.8.3 Class Variables

Name	Description
AlignLength	number of match and mismatch (<i>type=integer</i>)
Code	code containing int and char compound the CIGAR (<i>type=list</i>)
SumDeletion	number of deletion (<i>type=integer</i>)
SumInsertion	number of insertion (<i>type=integer</i>)

2.9 Class alignmentSAM

object └─
DIGEST_functions.alignmentSAM

New alignmentSAM object from a line of a SAM file, see SAM format for more informations

2.9.1 Methods

__init__(self, ligne)
Initialize the alignmentSAM class
Parameters
ligne : SAM alignment line (<i>type=list</i>)
Overrides: object.__init__

Inherited from object

__delattr__(), __format__(), __getattr__(), __hash__(), __new__(), __reduce__(), __reduce_ex__(),
__repr__(), __setattr__(), __sizeof__(), __str__(), __subclasshook__()

2.9.2 Properties

Name	Description
<i>Inherited from object</i>	
__class__	

2.9.3 Class Variables

Name	Description
CIGAR	Cigar (<i>type=Cigar</i>)
Flag	SAM flag (<i>type=integer</i>)
Length	alignment length (<i>type=integer</i>)
MAPQ	mapping quality score (<i>type=integer</i>)
PNEXT	Position of the primary alignment of the NEXT read (<i>type=string</i>)
Pos	start alignment position on the subject sequence (<i>type=integer</i>)
Query	query sequence ID (<i>type=string</i>)
QuerySequence	query nucleotide sequence (<i>type=string</i>)
RNEXT	Reference sequence name of the primary alignment of the NEXT read (<i>type=string</i>)
Subject	Subject sequence ID (<i>type=string</i>)

2.10 Class cluster



New cluster object

2.10.1 Methods

__init__(*self*)

Initialize the cluster class

Overrides: object.__init__

computeLen(*self*)

Compute the length of the cluster

addSequence(*self*, *clusterSequence*)

Add a clusterSequence in the list

Parameters**clusterSequence**: a clusterSequence object*(type=clusterSequence)***computeMeanPourc**(*self*)

Compute the pourcent mean of similarity

Inherited from object

__delattr__(), __format__(), __getattr__(), __hash__(), __new__(), __reduce__(), __reduce_ex__(),
 __repr__(), __setattr__(), __sizeof__(), __str__(), __subclasshook__()

2.10.2 Properties

Name	Description
<i>Inherited from object</i>	
__class__	

2.10.3 Class Variables

Name	Description
length	cluster length <i>(type=integer)</i>
listseq	list of clusterSequence object compound the cluster <i>(type=list)</i>
meanPourcSimilarity	pourcent mean of similarity in the cluster <i>(type=float)</i>

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Name	Description
ref	ID of the reference sequence (<i>type=string</i>)

2.11 Class `clusterSequence`

object —
DIGEST_functions.clusterSequence

New sequence in a cluster object

2.11.1 Methods

<code>__init__(self, length, header, pourc)</code>
<code>x.__init__(...)</code> initializes x; see <code>help(type(x))</code> for signature
Parameters
length: sequence length <i>(type=integer)</i>
header: sequence header <i>(type=string)</i>
pourc: percent of similarity of the sequence against the cluster reference sequence <i>(type=float)</i>
Overrides: <code>object.__init__</code>

Inherited from object

`__delattr__()`, `__format__()`, `__getattr__()`, `__hash__()`, `__new__()`, `__reduce__()`, `__reduce_ex__()`, `__repr__()`, `__setattr__()`, `__sizeof__()`, `__str__()`, `__subclasshook__()`

2.11.2 Properties

Name	Description
<i>Inherited from object</i>	
<code>__class__</code>	

2.11.3 Class Variables

Name	Description
header	sequence header (<i>type=string</i>)
length	sequence length (<i>type=integer</i>)
pourcSimilarity	pourcent of similarity of the sequence against the cluster reference sequence (<i>type=float</i>)

3 Module **ExtractFastaFromSAM**

Extract overlapped paired-end reads and unmapped paired-end reads from a SAM file sorted by reads names.

Requires: DIGEST_functions.py (PYTHONPATH)

Input : SAM file sorted by reads names Output : overlapped paired-end reads and unmapped paired-end reads in FASTA format

3.1 Functions

<code>get_parser()</code>

<code>main()</code>

3.2 Variables

Name	Description
<code>__doc__</code>	Value: ...
<code>__package__</code>	Value: None

4 Module SAMparser

Extract mapped or unmapped lines of SAM file with or without header and can sort result by query or subject

Requires: SamTools⁸

4.1 Functions

```
get_parser()
```

```
main()
```

4.2 Variables

Name	Description
<code>--doc--</code>	Value: ...
<code>--package--</code>	Value: None

⁸<http://sourceforge.net/projects/samtools/files/>

5 Module `extendTargets_allPossibility`

Extension of each sequence target with the mapped contig, if a target is mapped on several contigs, each possibility are kept.

Unmapped contig are lost.

Requires: `DIGEST_functions.py` (`PYTHONPATH`)

Input : SAM file without header only with mapped line and sort by query Output : target extended FASTA file

5.1 Functions

<code>get_parser()</code>

<code>main()</code>

5.2 Variables

Name	Description
<code>__doc__</code>	Value: ...
<code>__package__</code>	Value: None

6 Module `extractORFsequences`

Extract ORFs sequences in FASTA format from MetaGene output file and target extended FASTA file

Requires: `DIGEST_functions.py` (`PYTHONPATH`)

Output : `PREFIX_complete.fasta` and `PREFIX_partial.fasta`

6.1 Functions

```
get_parser()
```

```
main()
```

6.2 Variables

Name	Description
<code>__doc__</code>	Value: ...
<code>__package__</code>	Value: None

7 Module `removeIdenticalSeq`

Remove identical sequences from a FASTA file

Requires: `hashlib`⁹ python library

Input : `SEQUENCE.fasta` (1 line sequence) Output : `PREFIX.fasta`

7.1 Functions

```
get_parser()
```

```
main()
```

7.2 Variables

Name	Description
<code>__doc__</code>	Value: ...
<code>__package__</code>	Value: None

⁹<https://docs.python.org/2/library/hashlib.html>

8 Script `script-cd_hit_para_CCRT.py`

Launch `cd-hit` program in a parallel mode compatible with the CCRT architecture.

Requires:

- python¹⁰ (tested with 2.7.5)
 - `cd-hit`¹¹ (tested with v4.5.8-2012-03-24)
- Input : a FASTA file Output : a clustering FASTA

8.1 Functions

<code>get_parser()</code>

<code>launchJobCCRT(filename, jobDependency=None)</code>

launch the `ccc_msub` commande with a bash script as arguments and optionnally a job ID for the job dependency. Then this function recovers and return the job ID generated.

Parameters

- filename:** bash script file name
(*type=string*)
- jobDependency:** put an "after" dependency on the set of jobs defined as the argument. \ The submitted job will only be started when the jobs corresponding to the provided ids are terminated.
(*type=string*)

Return Value

- job ID
(*type=string*)

¹⁰<https://github.com/lh3/seqtk>

¹¹<https://code.google.com/p/cdhit/downloads/list>

writeJobScript(*filename, cores, task, queue, projid*)

Create the job parser script header

Parameters

filename: bash script file name
(type=string)

cores: cores number reserved
(type=integer)

task: max task number
(type=integer)

queue: requested queue
(type=string)

main()

8.2 Variables

Name	Description
__doc__	Value: ...
__package__	Value: None

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