DataPipeline

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Chapter 1

Usage:

merger.py automatically attempts to read **'new_pubchem.csv'** and **'new_swiss.csv'** from **./data** and then outputs **./merger/merge.csv**

Altnernatively, use **merger.py -h** to show arguments that allow passing of specific files on input.
populate_chem.py attempts to read data from **./merger/merge.csv** then output it to **./chem/new_attrib.csv**

Chapter 2

Namespace Index

2.1 Packages

Here are the packages with brief descriptions (if available):

Chapter 3

Hierarchical Index

3.1 Class Hierarchy

This inheritance list is sorted roughly, but not completely, alphabetically:

Chapter 4

Class Index

4.1 Class List

Here are the classes, structs, unions and interfaces with brief descriptions:

Chapter 5

File Index

5.1 File List

Here is a list of all files with brief descriptions:

Chapter 6

Namespace Documentation

6.1 cleaner Namespace Reference

Functions

- def load_data (csv_file_name)
- def set_proper_data_type (df)
- def unique_count (column)
- def remove_useless_columns (df)
- list get_duplicit_correlated_descriptors (graphs, descriptors)
- def get_correlated_descriptors (df, threshold, fig_location)
- def create_correlation_graphs (correlations, fig_location, threshold)
- def save_mask (df, mask_name, [None, list] columns=None, [None, list] rows=None)
- pd.DataFrame check_correlated_column (df, threshold=0.9, remove=False, preserve_columns=[], graph_location='./plot/correlations_grapgs_{}.jpeg', heatmap_location='./plot/correlations_heatmap_{}.jpeg')
- def remove_duplicits (pd.DataFrame df, subset, keep='first')
- def check_outliers (df, threshold=4.2, remove=False)
- def main (input_file, output_file, correlation_threshold=0.95, outliers_threshold=4.2, preserve_columns=None, remove=False)
- dict process_config (config_file='conf/cleaner.ini')

Variables

- dict args = process_config('conf/cleaner.ini')

6.1.1 Function Documentation

6.1.1.1 check_correlated_column()

```
pd.DataFrame cleaner.check_correlated_column (
              df,
              threshold = 0.9,
              remove = False,
              preserve_columns = [],
              graph_location = './plot/correlations_grapgs_{}.jpeg',
              heatmap_location = './plot/correlations_heatmap_{}.jpeg' )
```

6.1.1.2 check_outliers()

```
def cleaner.check_outliers (
              df,
              threshold = 4.2,
              remove = False )
```

6.1.1.3 create_correlation_graphs()

```
def cleaner.create_correlation_graphs (
              correlations,
              fig_location,
              threshold )
```

6.1.1.4 get_correlated_descriptors()

```
def cleaner.get_correlated_descriptors (
              df,
              threshold,
              fig_location )
```

6.1.1.5 get_duplicit_correlated_descriptors()

```
list cleaner.get_duplicit_correlated_descriptors (
              graphs,
              descriptors )
```

6.1.1.6 load_data()

```
def cleaner.load_data (
              csv_file_name )
```

6.1.1.7 main()

```
def cleaner.main (
              input_file,
              output_file,
              correlation_threshold = 0.95,
              outliers_threshold = 4.2,
              preserve_columns = None,
              remove = False )
```

6.1.1.8 process_config()

```
dict cleaner.process_config (
              config_file = 'conf/cleaner.ini' )
```

```
Process input config and extract
:param config_file: config file name location
:return: confuguration
```

6.1.1.9 remove_duplicits()

```
def cleaner.remove_duplicits (
             pd.DataFrame df,
              subset,
              keep = 'first' )
```

6.1.1.10 remove_useless_columns()

```
def cleaner.remove_useless_columns (
              df )
```

6.1.1.11 save_mask()

```
def cleaner.save_mask (
              df,
              mask_name,
             [None, list]  columns = None,
             [None, list]  rows = None )
```

6.1.1.12 set_proper_data_type()

```
def cleaner.set_proper_data_type (
              df )
```

6.1.1.13 unique_count()

```
def cleaner.unique_count (
              column )
```

6.1.2 Variable Documentation

6.1.2.1 args

```
dict cleaner.args = process_config('conf/cleaner.ini')
```

6.2 crawler_orchestrator Namespace Reference

Functions

- def main (file)

6.2.1 Function Documentation

6.2.1.1 main()

```
def crawler_orchestrator.main (
              file )
```

6.3 dependencies Namespace Reference

Namespaces

- pubchem
- swissadme
- swisstarget

6.4 dependencies.pubchem Namespace Reference

Functions

- def crawl (prefs)

6.4.1 Function Documentation

6.4.1.1 crawl()

```
def dependencies.pubchem.crawl (
              prefs )
```

6.5 dependencies.swissadme Namespace Reference

Functions

- def is_file_downloaded (filename, timeout=5)
- def crawl (prefs)

6.5.1 Function Documentation

6.5.1.1 crawl()

```
def dependencies.swissadme.crawl (
              prefs )
```

6.5.1.2 is_file_downloaded()

```
def dependencies.swissadme.is_file_downloaded (
              filename,
              timeout = 5 )
```

6.6 dependencies.swisstarget Namespace Reference

Functions

- def is_file_downloaded (filename, timeout=5)
- def crawl (prefs)

6.6.1 Function Documentation

6.6.1.1 crawl()

```
def dependencies.swisstarget.crawl (
              prefs )
```

6.6.1.2 is_file_downloaded()

```
def dependencies.swisstarget.is_file_downloaded (
              filename,
              timeout = 5 )
```

6.7 merger Namespace Reference

Functions

- def merge ()

6.7.1 Function Documentation

6.7.1.1 merge()

```
def merger.merge ( )
```

6.8 pipe_handler Namespace Reference

Classes

- class IgnoreBrokenPipe

6.9 populate_chem Namespace Reference

Functions

- def populate ()

6.9.1 Function Documentation

6.9.1.1 populate()

```
def populate_chem.populate ( )
```

6.10 run_pipeline Namespace Reference

Variables

- parser = argparse.ArgumentParser()
- type
- str
- help
- args = parser.parse_args()

6.10.1 Variable Documentation

6.10.1.1 args

```
run_pipeline.args = parser.parse_args()
```

6.10.1.2 help

```
run_pipeline.help
```

6.10.1.3 parser

```
run_pipeline.parser = argparse.ArgumentParser()
```

6.10.1.4 str

```
run_pipeline.str
```

6.10.1.5 type

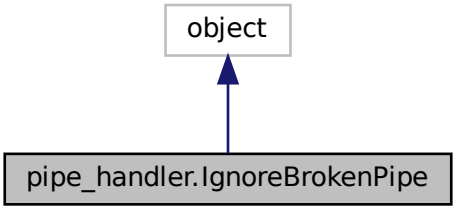
```
run_pipeline.type
```

Chapter 7

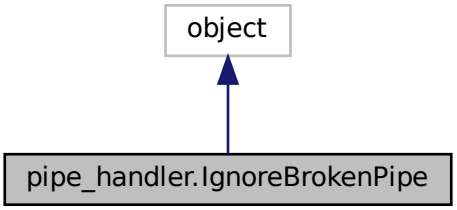
Class Documentation

7.1 pipe_handler.IgnoreBrokenPipe Class Reference

Inheritance diagram for pipe_handler.IgnoreBrokenPipe:



Collaboration diagram for pipe_handler.IgnoreBrokenPipe:



Public Member Functions

- def __init__ (self, stream)

Public Attributes

- stream

- write
- flush

7.1.1 Constructor & Destructor Documentation

7.1.1.1 __init__()

```
def pipe_handler.IgnoreBrokenPipe.__init__ (
              self,
              stream )
```

7.1.2 Member Data Documentation

7.1.2.1 flush

```
pipe_handler.IgnoreBrokenPipe.flush
```

7.1.2.2 stream

```
pipe_handler.IgnoreBrokenPipe.stream
```

7.1.2.3 write

```
pipe_handler.IgnoreBrokenPipe.write
```

The documentation for this class was generated from the following file:

- pipe_handler.py

Chapter 8

File Documentation

8.1 cleaner.py File Reference

Namespaces

- cleaner

Functions

- def cleaner.load_data (csv_file_name)
- def cleaner.set_proper_data_type (df)
- def cleaner.unique_count (column)
- def cleaner.remove_useless_columns (df)
- list cleaner.get_duplicit_correlated_descriptors (graphs, descriptors)
- def cleaner.get_correlated_descriptors (df, threshold, fig_location)
- def cleaner.create_correlation_graphs (correlations, fig_location, threshold)
- def cleaner.save_mask (df, mask_name, [None, list] columns=None, [None, list] rows=None)
- pd.DataFrame cleaner.check_correlated_column (df, threshold=0.9, remove=False, preserve_columns=[ ], graph_location='./plot/correlations_grapgs_{}.jpeg', heatmap_location='./plot/correlations_heatmap_{}.jpeg')
- def cleaner.remove_duplicits (pd.DataFrame df, subset, keep='first')
- def cleaner.check_outliers (df, threshold=4.2, remove=False)
- def cleaner.main (input_file, output_file, correlation_threshold=0.95, outliers_threshold=4.2, preserve_↩ columns=None, remove=False)
- dict cleaner.process_config (config_file='conf/cleaner.ini')

Variables

- dict cleaner.args = process_config('conf/cleaner.ini')

8.2 crawlers/crawler_orchestrator.py File Reference

Namespaces

- crawler_orchestrator

Functions

- def crawler_orchestrator.main (file)

8.3 crawlers/dependencies/__init__.py File Reference

Namespaces

- dependencies

8.4 crawlers/dependencies/pubchem.py File Reference

Namespaces

- dependencies.pubchem

Functions

- def dependencies.pubchem.crawl (prefs)

8.5 crawlers/dependencies/swissadme.py File Reference

Namespaces

- dependencies.swissadme

Functions

- def dependencies.swissadme.is_file_downloaded (filename, timeout=5)
- def dependencies.swissadme.crawl (prefs)

8.6 crawlers/dependencies/swisstarget.py File Reference

Namespaces

- dependencies.swisstarget

Functions

- def dependencies.swisstarget.is_file_downloaded (filename, timeout=5)
- def dependencies.swisstarget.crawl (prefs)

8.7 merger.py File Reference

Namespaces

- merger

Functions

- def merger.merge ()

8.8 pipe_handler.py File Reference

Classes

- class pipe_handler.IgnoreBrokenPipe

Namespaces

- pipe_handler

8.9 populate_chem.py File Reference

Namespaces

- populate_chem

Functions

- def populate_chem.populate ()

8.10 README.md File Reference

8.11 run_pipeline.py File Reference

Namespaces

- run_pipeline

Variables

- run_pipeline.parser = argparse.ArgumentParser()
- run_pipeline.type
- run_pipeline.str
- run_pipeline.help
- run_pipeline.args = parser.parse_args()

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