PaddleHelix

Release 1.0.0

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OVERVIEW


飞桨 PaddleHelix

CHAPTER

ONE

INSTALLATION

1.1 OS support

Windows, Linux and OSX

1.2 Python version

Python **3.6, 3.7**

1.3 Dependencies

- PaddlePaddle **>= 2.0.0rc0**
- pgl **>= 2.1**

1.4 Quick Start

- PaddleHelix can be installed directly with `pip`:

```
$ pip install paddlehelix
```

- or install from source:

```
$ pip install --upgrade git+https://github.com/PaddlePaddle/PaddleHelix.git
```

Note: Please check our *Installation guide* part for full installation prerequisites and guide.

CHAPTER

TWO

TUTORIALS

- We provide abundant *Tutorials* to help you navigate the repository and start quickly.
- PaddleHelix is based on PaddlePaddle, a high-performance Parallelized Deep Learning Platform.

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- Compound Representation Learning and Property Prediction
- Protein Representation Learning and Property Prediction
- Drug Target Interaction
- Molecular Generation
- Drug Drug Synergy
- LinearRNA

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GUIDE FOR DEVELOPERS

- If you need help in modifying the source code of **PaddleHelix**, please see our *Guide for developers*.

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CONTRIBUTION

If you would like to develop and maintain PaddleHelix with us, please refer to our GitHub repo.

5.1 Installation guide

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5.1.1 Prerequisites

- OS support: Windows, Linux and OSX
- Python version: **3.6, 3.7**

5.1.2 Dependencies

(- means no specific version requirement for that package)

Name	Version
numpy	-
pandas	-
networkx	-
paddlepaddle	>=2.0.0rc0
pgl	>=2.1
rdkit	-
sklearn	-

5.1.3 Instruction

Since PaddleHelix depends on the `paddlepaddle` of version 2.0.0rc0 or above, and `rdkit` cannot be installed directly using `pip`, we suggest using `conda` to create a new environment for the installation. Detailed instruction is shown below:

- If you do not have `conda` installed, please install it at first:
- Create a new environment with `conda`:

```
$ conda create -n paddlehelix python=3.7
```

- Activate the environment just created:

```
$ conda activate paddlehelix
```

- Install `rdkit` using `conda`:

```
$ conda install -c conda-forge rdkit
```

- Install the right version of `paddlepaddle` according to the device (CPU/GPU) you want to run PaddleHelix on.

1) If you want to use the GPU version of `paddlepaddle`, run this:

```
$ python -m pip install paddlepaddle-gpu -f https://paddlepaddle.org.cn/whl/stable.html
```

2) Or if you want to use the CPU version of `paddlepaddle`, run this:

```
$ python -m pip install paddlepaddle -i https://mirror.baidu.com/pypi/simple
```

Note: The version of `paddlepaddle` should be higher than **2.0**. Check paddlepaddle official document for more installation guide.

- Install **pgl** using `pip`:

```
$ pip install pgl
```

- Install **PaddleHelix** using `pip`:

```
$ pip install paddlehelix
```

- The installation is done!

Note: After playing, if you want to deactivate the `conda` environment, do this:

```
$ conda deactivate
```

5.2 Tutorials

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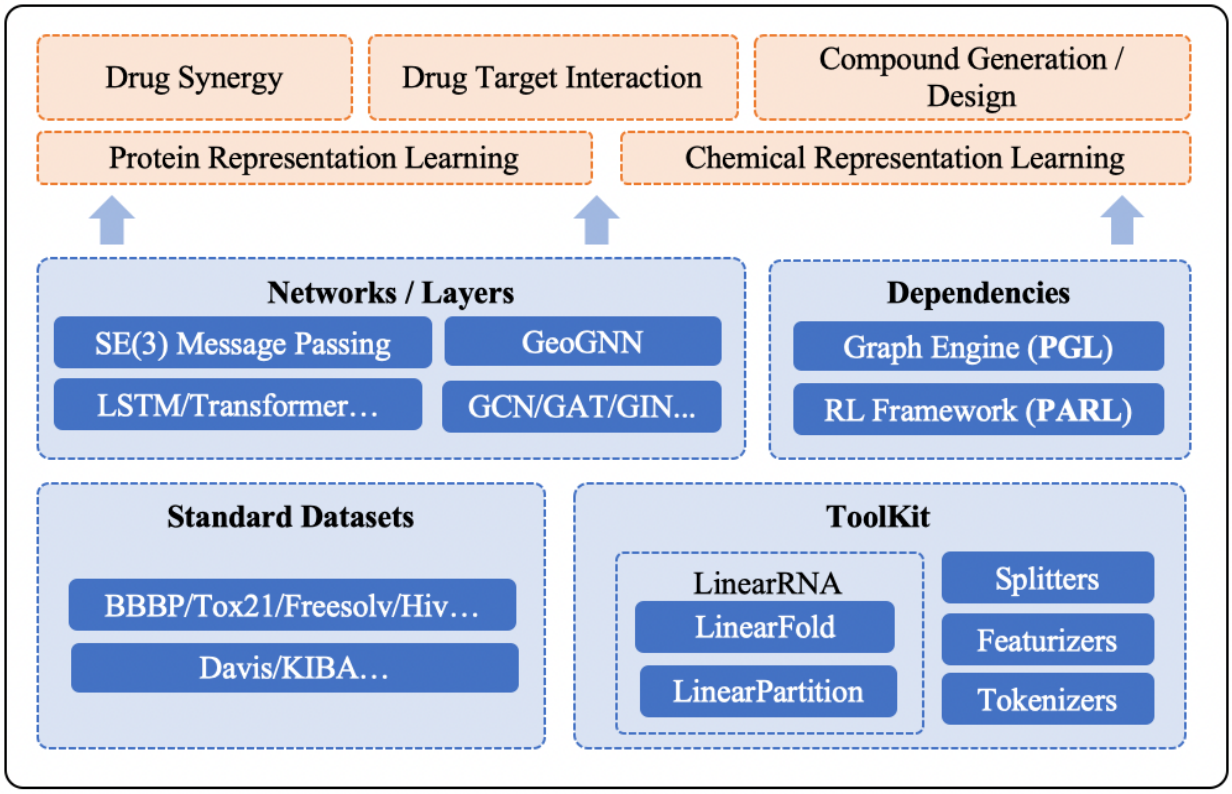
5.2.1 Backgrounds

Machine learning (ML), especially deep learning (DL), is playing an increasingly important role in the pharmaceutical industry and bio-informatics. For instance, the DL-based methodology is found to predict the drug target interaction and molecule properties with reasonable precision and quite low computational cost, while those properties can only be accessed through *in vivo*/ *in vitro* experiments or computationally expensive simulations (molecular dynamics simulation etc.) before. As another example, *in silico* RNA folding and protein folding are becoming more likely to be accomplished with the help of deep neural models. The usage of ML and DL can greatly improve efficiency, and thus reduce the cost of drug discovery, vaccine design, etc.

In contrast to the powerful ability of DL metrics, a key challenge lying in utilizing them in the drug industry is the contradiction between the demand for huge data for training and the limited annotated data. Recently, there is a tremendous success in adopting self-supervised learning in natural language processing and computer vision, showing that a large corpus of unlabeled data can be beneficial to learning universal tasks. In molecule representations, there is a similar situation. We have a large amount of unlabeled data, including protein sequences (over 100 million) and compounds (over 50 million) but relatively small annotated data. It is quite promising to adopt the DL-based pre-training technique in the representation learning of chemical compounds, proteins, RNA, etc.

PaddleHelix is a high-performance ML-based bio-computing framework. It features large-scale representation learning and easy-to-use APIs, providing pharmaceutical and biological researchers and engineers convenient access to the most up-to-date and state-of-the-art AI tools.

5.2.2 Navigating PaddleHelix



5.2.3 Tutorials

- Predicting Drug Target Interaction_GraphDTA, MolTrans
- Compound Representation Learning and Property Prediction
- Protein Representation Learning and Property Prediction
- Molecular Generation
- Predicting RNA Secondary Structure

5.2.4 Run tutorials locally

The tutorials are written as **Jupyter Notebooks** and designed to be smoothly run on you own machine. If you don't have Jupyter installed, please refer to here. And please also install **PaddleHelix** before proceeding (*Installation guide*).

After the installation of **Jypyter**, please go through the following steps:

1. Clone this repository to your own machine
2. Change the working directory of your shell to `path_to_your_repo/PaddleHelix/tutorials/`
3. Open `Jupyter lab` with the command *jupyter-lab*, wait for your web browser being called out
4. All the tutorials should be in the `File Browser` now, click and enjoy!

5.3 Guide for developers

If you need to modify the algorithms/models in **PaddleHelix**, you have to switch to the developer mode. The core algorithms of **PaddleHelix** are mostly implemented in Python, but some also in C++, so you cannot develop **PaddleHelix** simply with `pip install --editable {pahelix_path}`. To develop on your machine, please do the following:

- Please follow the *Installation guide* part to install all dependencies of **PaddleHelix** (`paddlepaddle >= 2.0.0rc0`, `pgl >= 2.1`).
- If you have already installed distributed **PaddleHelix** with `pip install paddlehelix`, please uninstall it with:

```
$ pip uninstall paddlehelix
```

- Clone this repository to your local machine, supposed path at */path_to_your_repo/*:

```
$ git clone https://github.com/PaddlePaddle/PaddleHelix.git /path_to_your_repo/

$ cd /path_to_your_repo/
```

- Depends on which model you'd like to modify, go to **LinearRNA** or **Other algorithms**:

  LinearRNA

  The source code of LinearRNA is at *./c/pahelix/toolkit/linear_rna/linear_rna*. You could modify it for your needs. Then remember to return to the root directory of the repository, run scripts below to re-compile (please ensure there are `cmake >= 3.6` and `g++ >= 4.8` on your machine):

```
$ sh scripts/prepare.sh

$ sh scripts/build.sh
```

- After a successful compilaiton, *import* LinearRNA as following:

```
$ cd build

$ python
>>> import c.pahelix.toolkit.linear_rna.linear_rna as linear_rna
```

- Except LinearRNA, other algorithms in PaddleHelix are all implemented in Python.

  Other algorithms

  If you want to change these algorithms, just find and modify corresponding `.py` files under the path *./pahelix*, then add */path_to_your_repo/* to your Python environment path:

```
import sys
sys.path.append('/path_to_your_repo/')
import pahelix
```

- If you have any question or suggestion, feel free to file on our GitHub issue page. We will response **ASAP**.

5.4 Contact Us

5.4.1 Bug Reports

You can file bug reports on our GitHub issue page, and they will be addressed **ASAP**.

Note: Reporting Issues

When reporting a bug, please include detailed information that will help us solve the issue. See sample format as below:

- Issue name
- URL
- Your contact information
- Expected result
- Actual result
- Action taken

5.4.2 Join Us

If you have any questions and concern, or if you want to contribute together with us, please join QQ group: 699105483

We are available 24/7 and we will get back to you **ASAP**!

5.5 pahelix.datasets

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5.5.1 bace_dataset

Processing of bace dataset.

It contains quantitative IC50 and qualitative (binary label) binding results for a set of inhibitors of human beta-secretase 1 (BACE=1). The data are experimental values collected from the scientific literature which contains 152 compounds and their 2D structures and properties

You can download the dataset from http://moleculenet.ai/datasets-1 and load it into pahelix reader creators

`pahelix.datasets.bace_dataset.`**`get_default_bace_task_names`**`()`

Get that default bace task names.

`pahelix.datasets.bace_dataset.`**`load_bace_dataset`**`(`*data_path*, *task_names=None*`)`

Load bace dataset ,process the classification labels and the input information.

Description:

The data file contains a csv table, in which columns below are used:

mol: The smile representation of the molecular structure;

pIC50: The negative log of the IC50 binding affinity;

class: The binary labels for inhibitor.

Parameters

- **`data_path`** (*`str`*) – the path to the cached npz path.
- **`task_names`** (*`list`*) – a list of header names to specify the columns to fetch from the csv file.

Returns

an InMemoryDataset instance.

Example

```
dataset = load_bace_dataset('./bace')
print(len(dataset))
```

References:

[1]Subramanian, Govindan, et al. "Computational modeling of -secretase 1 (BACE-1) inhibitors using ligand based approaches." Journal of chemical information and modeling 56.10 (2016): 1936-1949.

5.5.2 bbbp_dataset

Processing of Blood-Brain Barrier Penetration dataset

The Blood-brain barrier penetration (BBBP) dataset is extracted from a study on the modeling and prediction of the barrier permeability. As a membrane separating circulating blood and brain extracellular fluid, the blood-brain barrier blocks most drugs, hormones and neurotransmitters. Thus penetration of the barrier forms a long-standing issue in development of drugs targeting central nervous system. This dataset includes binary labels for over 2000 compounds on their permeability properties.

You can download the dataset from http://moleculenet.ai/datasets-1 and load it into pahelix reader creators

pahelix.datasets.bbbp_dataset.**get_default_bbbp_task_names**()

Get that default bbbp task names and return the binary labels

pahelix.datasets.bbbp_dataset.**load_bbbp_dataset**(*data_path*, *task_names=None*)

Load bbbp dataset ,process the classification labels and the input information.

Description:

The data file contains a csv table, in which columns below are used:

Num:number

name:Name of the compound

smiles:SMILES representation of the molecular structure

p_np:Binary labels for penetration/non-penetration

Parameters

- **data_path** (*str*) – the path to the cached npz path.
- **task_names** (*list*) – a list of header names to specify the columns to fetch from the csv file.

Returns

an InMemoryDataset instance.

Example

```
dataset = load_bbbp_dataset('./bbbp')
print(len(dataset))
```

References:

[1] Martins, Ines Filipa, et al. "A Bayesian approach to in silico blood-brain barrier penetration modeling." Journal of chemical information and modeling 52.6 (2012): 1686-1697.

5.5.3 chembl_filtered_dataset

Processing of chembl filtered dataset.

The ChEMBL dataset containing 456K molecules with 1310 kinds of diverse and extensive biochemical assays. The database is unique because of its focus on all aspects of drug discovery and its size, containing information on more than 1.8 million compounds and over 15 million records of their effects on biological systems.

pahelix.datasets.chembl_filtered_dataset.**get_chembl_filtered_task_num**()

Get that default bace task names and return class

pahelix.datasets.chembl_filtered_dataset.**load_chembl_filtered_dataset**(*data_path*)

Load chembl_filtered dataset ,process the classification labels and the input information.

Introduction:

Note that, in order to load this dataset, you should have other datasets (bace, bbbp, clintox, esol, freesolv, hiv, lipophilicity, muv, sider, tox21, toxcast) downloaded. Since the chembl dataset may overlap with the above listed dataset, the overlapped smiles for test will be filtered for a fair evaluation.

Description:

The data file contains a csv table, in which columns below are used:

It contains the ID, SMILES/CTAB, InChI and InChIKey compound information

smiles: SMILES representation of the molecular structure

Parameters

data_path (*str*) – the path to the cached npz path

Returns

an InMemoryDataset instance.

Example

```
dataset = load_bbbp_dataset('./bace')
print(len(dataset))
```

References:

[1] Gaulton, A; et al. (2011). "ChEMBL: a large-scale bioactivity database for drug discovery". Nucleic Acids Research. 40 (Database issue): D1100-7.

5.5.4 clintox_dataset

Processing of clintox dataset

The ClinTox dataset compares drugs approved by the FDA and drugs that have failed clinical trials for toxicity reasons. The dataset includes two classification tasks for 1491 drug compounds with known chemical structures: (1) clinical trial toxicity (or absence of toxicity) and (2) FDA approval status. List of FDA-approved drugs are compiled from the SWEETLEAD database, and list of drugs that failed clinical trials for toxicity reasons are compiled from the Aggregate Analysis of ClinicalTrials.gov(AACT) database.

You can download the dataset from http://moleculenet.ai/datasets-1 and load it into pahelix reader creators

pahelix.datasets.clintox_dataset.**get_default_clintox_task_names**()

Get that default clintox task names and return class

pahelix.datasets.clintox_dataset.**load_clintox_dataset**(*data_path*, *task_names=None*)

Load Clintox dataset ,process the classification labels and the input information.

Description:

The data file contains a csv table, in which columns below are used:

smiles: SMILES representation of the molecular structure

FDA_APPROVED: FDA approval status

CT_TOX: Clinical trial results

Parameters

- **data_path** (*str*) – the path to the cached npz path.
- **task_names** (*list*) – a list of header names to specify the columns to fetch from the csv file.

Returns

an InMemoryDataset instance.

Example

```
dataset = load_clintox_dataset('./clintox')
print(len(dataset))
```

References:

[1] Gayvert, Kaitlyn M., Neel S. Madhukar, and Olivier Elemento. "A data-driven approach to predicting successes and failures of clinical trials." Cell chemical biology 23.10 (2016): 1294-1301.

[2] Artemov, Artem V., et al. "Integrated deep learned transcriptomic and structure-based predictor of clinical trials outcomes." bioRxiv (2016): 095653.

[3] Novick, Paul A., et al. "SWEETLEAD: an in silico database of approved drugs, regulated chemicals, and herbal isolates for computer-aided drug discovery." PloS one 8.11 (2013): e79568.

[4] Aggregate Analysis of ClincalTrials.gov (AACT) Database. https://www.ctti-clinicaltrials.org/aact-database

5.5.5 davis_dataset

Processing of davis dataset

pahelix.datasets.davis_dataset.**load_davis_dataset**(*data_path*, *featurizer*)

tbd

5.5.6 ddi_dataset

Processing of ddi dataset. The DDI dataset includes 23,052 Drug-Drug Synergy pairs from 39 celllines. You can download the dataset from http://www.bioinf.jku.at/software/DeepSynergy/labels.csv and load it into pahelix reader creators

pahelix.datasets.ddi_dataset.**get_default_ddi_task_names**()

Get that default ddi task names and return class label

pahelix.datasets.ddi_dataset.**load_ddi_dataset**(*data_path*, *task_names=None*, *cellline=None*)

Load ddi dataset,process the input information.

Description:

The data file contains a csv table, in which columns below are used:

drug_a_name: drug name

drug_b_name: drug name

cell_line: cell line which the drug pairs were tested on

synergy: continuous values represent the synergy effect, we use 30 as threshold to binarize the data into binary labels. 1 as positive and 0 as negative

Parameters

- **data_path** (*str*) – the path to the cached npz path.
- **task_names** (*list*) – a list of header names to specify the columns to fetch from the csv file.
- **cellline** – the exact cellline model you want to test on.

Returns

an InMemoryDataset instance.

Example

```
dataset = load_hddi_dataset('./ddi/raw')
print(len(dataset))
```

References:

[1] Drug-Drug Dynergy Data. https://academic.oup.com/bioinformatics/advance-article/doi/10.1093/bioinformatics/btx806/4747884

5.5.7 dti_dataset

Processing of DTi dataset. The DTI dataset were extracted from the DrugCombDB. You can download the dataset from http://drugcombdb.denglab.org/download/drug_protein_links.rar and load it into pahelix reader creators

pahelix.datasets.dti_dataset.**get_default_dti_task_names**()

Get that default dti task names

pahelix.datasets.dti_dataset.**load_dti_dataset**(*data_path*, *task_names=None*, *featurizer=None*)

Load dti dataset,process the input information and the featurizer.

Description:

The data file contains a tsv table, in which columns below are used:

chemical: drug name

protein: targeted protein name

Parameters

- **data_path** (*str*) – the path to the cached npz path.
- **task_names** (*list*) – a list of header names to specify the columns to fetch from the csv file.

Returns

an InMemoryDataset instance.

Example

```
dataset = load_hddi_dataset('./dti/raw')
print(len(dataset))
```

5.5.8 esol_dataset

Processing of esol dataset.

ESOL (delaney) is a standard regression data set,which is also called delaney dataset. In the dataset, you can find the structure and water solubility data of 1128 compounds. It's a good choice to validate machine learning models and to estimate solubility directly based on molecular structure which was encoded in SMILES string.

You can download the dataset from http://moleculenet.ai/datasets-1 and load it into pahelix reader creators.

pahelix.datasets.esol_dataset.**get_default_esol_task_names**()

Get that default esol task names and return measured values

pahelix.datasets.esol_dataset.**get_esol_stat**(*data_path*, *task_names*)

Return mean and std of labels

pahelix.datasets.esol_dataset.**load_esol_dataset**(*data_path*, *task_names=None*)

Load esol dataset ,process the classification labels and the input information.

Description:

The data file contains a csv table, in which columns below are used:

smiles: SMILES representation of the molecular structure

Compound ID: Name of the compound

measured log solubility in mols per litre: Log-scale water solubility of the compound, used as label

Parameters

- **data_path** (*str*) – the path to the cached npz path.
- **task_names** (*list*) – a list of header names to specify the columns to fetch from the csv file.

Returns

an InMemoryDataset instance.

Example

```
dataset = load_esol_dataset('./esol')
print(len(dataset))
```

References:

[1] Delaney, John S. "ESOL: estimating aqueous solubility directly from molecular structure." Journal of chemical information and computer sciences 44.3 (2004): 1000-1005.

5.5.9 freesolv_dataset

Processing of freesolv dataset.

The Free Solvation Dataset provides rich information. It contains calculated values and experimental values about hydration free energy of small molecules in water.You can get the calculated values by molecular dynamics simulations,which are derived from alchemical free energy calculations. However,the experimental values are included in the benchmark collection.

You can download the dataset from http://moleculenet.ai/datasets-1 and load it into pahelix reader creators.

pahelix.datasets.freesolv_dataset.**get_default_freesolv_task_names**()

Get that default freesolv task names and return measured expt

pahelix.datasets.freesolv_dataset.**get_freesolv_stat**(*data_path*, *task_names*)

Return mean and std of labels

pahelix.datasets.freesolv_dataset.**load_freesolv_dataset**(*data_path*, *task_names=None*)

Load freesolv dataset,process the input information and the featurizer.

Description:

The data file contains a csv table, in which columns below are used:

smiles: SMILES representation of the molecular structure

Compound ID: Name of the compound

measured log solubility in mols per litre: Log-scale water solubility of the compound, used as label.

Parameters

- **data_path** (*str*) – the path to the cached npz path.
- **task_names** (*list*) – a list of header names to specify the columns to fetch from the csv file.

Returns
an InMemoryDataset instance.

Example

```
dataset = load_freesolv_dataset('./freesolv')
print(len(dataset))
```

References:

[1] Mobley, David L., and J. Peter Guthrie. "FreeSolv: a database of experimental and calculated hydration free energies, with input files." Journal of computer-aided molecular design 28.7 (2014): 711-720.

[2] https://github.com/MobleyLab/FreeSolv

5.5.10 hiv_dataset

Processing of hiv dataset.

The HIV dataset was introduced by the Drug Therapeutics Program (DTP) AIDS Antiviral Screen, which tested the ability to inhibit HIV replication for over 40,000 compounds. Screening results were evaluated and placed into three categories: confirmed inactive (CI),confirmed active (CA) and confirmed moderately active (CM). We further combine the latter two labels, making it a classification task between inactive (CI) and active (CA and CM).

You can download the dataset from http://moleculenet.ai/datasets-1 and load it into pahelix reader creators

pahelix.datasets.hiv_dataset.**get_default_hiv_task_names**()

Get that default hiv task names and return class label

pahelix.datasets.hiv_dataset.**load_hiv_dataset**(*data_path*, *task_names=None*)

Load hiv dataset,process the input information.

Description:

The data file contains a csv table, in which columns below are used:

smiles: SMILES representation of the molecular structure

activity: Three-class labels for screening results: CI/CM/CA.

HIV_active: Binary labels for screening results: 1 (CA/CM) and 0 (CI)

Parameters

- **data_path** (*str*) – the path to the cached npz path
- **task_names** (*list*) – a list of header names to specify the columns to fetch from the csv file.

Returns
an InMemoryDataset instance.

Example

```
dataset = load_hiv_dataset('./hiv')
print(len(dataset))
```

References:

[1] AIDS Antiviral Screen Data. https://wiki.nci.nih.gov/display/NCIDTPdata/AIDS+Antiviral+Screen+Data

5.5.11 inmemory_dataset

In-memory dataset.

class pahelix.datasets.inmemory_dataset.**InMemoryDataset**(*data_list=None*, *npz_data_path=None*, *npz_data_files=None*)

Description:

The InMemoryDataset manages `data_list` which is a list of *data* and the *data* is a dict of numpy ndarray. And each dict has the same keys.

It works like a list: you can call *dataset[i] to get the i-th element of the ``data_list`* and call *len(dataset)* to get the length of `data_list`.

The `data_list` can be cached in npz files by calling *dataset.save_data(data_path)* and after that, call *InMemoryDataset(data_path)* to reload.

data_list

a list of dict of numpy ndarray.

Type

list

Example

```
data_list = [{'a': np.zeros([4, 5])}, {'a': np.zeros([7, 5])}]
dataset = InMemoryDataset(data_list=data_list)
print(len(dataset))
dataset.save_data('./cached_npz')   # save data_list to ./cached_npz

dataset2 = InMemoryDataset(npz_data_path='./cached_npz')    # will load the saved␣
↪`data_list`
print(len(dataset))
```

get_data_loader(*batch_size*, *num_workers=4*, *shuffle=False*, *collate_fn=None*)

It returns an batch iterator which yields a batch of data. Firstly, a sub-list of *data* of size `batch_size` will be draw from the `data_list`, then the function `collate_fn` will be applied to the sub-list to create a batch and yield back. This process is accelerated by multiprocess.

Parameters

- **batch_size** (*int*) – the batch_size of the batch data of each yield.
- **num_workers** (*int*) – the number of workers used to generate batch data. Required by multiprocess.
- **shuffle** (*bool*) – whether to shuffle the order of the `data_list`.

- **collate_fn** (*function*) – used to convert the sub-list of `data_list` to the aggregated batch data.

Yields
the batch data processed by `collate_fn`.

save_data(*data_path*)

Save the `data_list` to the disk specified by `data_path` with npz format. After that, call *InMemoryDataset(data_path)* to reload the `data_list`.

Parameters
data_path (*str*) – the path to the cached npz path.

transform(*transform_fn*, *num_workers=4*, *drop_none=False*)

Inplace apply *transform_fn* on the *data_list* with multiprocess.

5.5.12 kiba_dataset

Processing of kiba dataset

pahelix.datasets.kiba_dataset.**load_kiba_dataset**(*data_path*, *featurizer*)

tbd

5.5.13 lipophilicity_dataset

Processing of lipohilicity dataset.

Lipophilicity is a dataset curated from ChEMBL database containing experimental results on octanol/water distribution coefficient (logD at pH=7.4).As the Lipophilicity plays an important role in membrane permeability and solubility. Related work deserves more attention.

You can download the dataset from http://moleculenet.ai/datasets-1 and load it into pahelix reader creators.

pahelix.datasets.lipophilicity_dataset.**get_default_lipophilicity_task_names**()

Get that default lipophilicity task names and return measured expt

pahelix.datasets.lipophilicity_dataset.**get_lipophilicity_stat**(*data_path*, *task_names*)

Return mean and std of labels

pahelix.datasets.lipophilicity_dataset.**load_lipophilicity_dataset**(*data_path*, *task_names=None*)

Load lipophilicity dataset,process the input information.

Description:

The data file contains a csv table, in which columns below are used:

smiles: SMILES representation of the molecular structure

exp: Measured octanol/water distribution coefficient (logD) of the compound, used as label

Parameters

- **data_path** (*str*) – the path to the cached npz path.
- **task_names** (*list*) – a list of header names to specify the columns to fetch from the csv file.

Returns
an InMemoryDataset instance.

Example

```
dataset = load_lipophilicity_dataset('./lipophilicity')
print(len(dataset))
```

References:

[1]Hersey, A. ChEMBL Deposited Data Set - AZ dataset; 2015. https://doi.org/10.6019/chembl3301361

5.5.14 muv_dataset

Processing of muv dataset.

The Maximum Unbiased Validation (MUV) group is a benchmark dataset selected from PubChem BioAssay by applying a refined nearest neighbor analysis. The MUV dataset contains 17 challenging tasks for around 90,000 compounds and is specifically designed for validation of virtual screening techniques.

You can download the dataset from http://moleculenet.ai/datasets-1 and load it into pahelix reader creators.

pahelix.datasets.muv_dataset.**get_default_muv_task_names**()

Get that default hiv task names and return the measured results for bioassays

pahelix.datasets.muv_dataset.**load_muv_dataset**(*data_path*, *task_names=None*)

Load muv dataset,process the input information.

Description:

The data file contains a csv table, in which columns below are used:

smiles: SMILES representation of the molecular structure.

mol_id: PubChem CID of the compound.

MUV-XXX: Measured results (Active/Inactive) for bioassays.

Parameters

- **data_path** (*str*) – the path to the cached npz path.
- **task_names** (*list*) – a list of header names to specify the columns to fetch from the csv file.

Returns

an InMemoryDataset instance.

Example

```
dataset = load_muv_dataset('./muv')
print(len(dataset))
```

References:

[1]Rohrer, Sebastian G., and Knut Baumann. “Maximum unbiased validation (MUV) data sets for virtual screening based on PubChem bioactivity data.” Journal of chemical information and modeling 49.2 (2009): 169-184.

5.5.15 ppi_dataset

Processing of PPI dataset. The DDI dataset were extracted from DrugCombDB. You can download the dataset from http://drugcombdb.denglab.org/download/protein_protein_links.rar and load it into pahelix reader creators

pahelix.datasets.ppi_dataset.**get_default_ppi_task_names**()

Get that default ppi task names

pahelix.datasets.ppi_dataset.**load_ppi_dataset**(*data_path*, *task_names=None*, *featurizer=None*)

Load ppi dataset,process the input information and the featurizer.

Description:

The data file contains a txt file, in which columns below are used:

protein1: protein1 name

protein2: protein2 name

Parameters

- **data_path** (*str*) – the path to the cached npz path.
- **task_names** (*list*) – a list of header names to specify the columns to fetch from the txt file.

Returns

an InMemoryDataset instance.

Example

```
dataset = load_ppi_dataset('./ppi/raw')
print(len(dataset))
```

5.5.16 sider_dataset

Processing of sider dataset.

The Side Effect Resource (SIDER) is a database of marketed drugs and adverse drug reactions (ADR). The version of the SIDER dataset in DeepChem has grouped drug side effects into 27 system organ classes following MedDRA classifications measured for 1427 approved drugs.

You can download the dataset from http://moleculenet.ai/datasets-1 and load it into pahelix reader creators.

pahelix.datasets.sider_dataset.**get_default_sider_task_names**()

Get that default sider task names and return the side results for the drug

pahelix.datasets.sider_dataset.**load_sider_dataset**(*data_path*, *task_names=None*)

Load sider dataset,process the input information.

Description:

The data file contains a csv table, in which columns below are used:

smiles: SMILES representation of the molecular structure.

Hepatobiliary disorders: Injury, poisoning and procedural complications, recorded side effects for the drug

Parameters

- **data_path** (*str*) – the path to the cached npz path.
- **task_names** (*list*) – a list of header names to specify the columns to fetch from the csv file.

Returns
an InMemoryDataset instance.

Example

```
dataset = load_sider_dataset('./sider')
print(len(dataset))
```

References:

[1]Kuhn, Michael, et al. "The SIDER database of drugs and side effects." Nucleic acids research 44.D1 (2015): D1075-D1079.

[2]Altae-Tran, Han, et al. "Low data drug discovery with one-shot learning." ACS central science 3.4 (2017): 283-293.

[3]Medical Dictionary for Regulatory Activities. http://www.meddra.org/

[4]Please refer to http://sideeffects.embl.de/se/?page=98 for details on ADRs.

5.5.17 tox21_dataset

Processing of tox21 dataset.

The "Toxicology in the 21st Century" (Tox21) initiative created a public database measuring toxicity of compounds, which has been used in the 2014 Tox21 Data Challenge. This dataset contains qualitative toxicity measurements for 8k compounds on 12 different targets, including nuclear receptors and stress response pathways.

You can download the dataset from http://moleculenet.ai/datasets-1 and load it into pahelix reader creators.

pahelix.datasets.tox21_dataset.**get_default_tox21_task_names**()

Get that default tox21 task names and return the bioassays results

pahelix.datasets.tox21_dataset.**load_tox21_dataset**(*data_path*, *task_names=None*)

Load tox21 dataset,process the input information.

Description:

The data file contains a csv table, in which columns below are used:

smiles: SMILES representation of the molecular structure.

NR-XXX: Nuclear receptor signaling bioassays results.

SR-XXX: Stress response bioassays results

Parameters

- **data_path** (*str*) – the path to the cached npz path.
- **task_names** (*list*) – a list of header names to specify the columns to fetch from the csv file.

Returns
an InMemoryDataset instance.

Example

```
dataset = load_tox21_dataset('./tox21')
print(len(dataset))
```

References:

[1]Tox21 Challenge. https://tripod.nih.gov/tox21/challenge/

[2]please refer to the links at https://tripod.nih.gov/tox21/challenge/data.jsp for details.

5.5.18 toxcast_dataset

Processing of toxcast dataset.

ToxCast is an extended data collection from the same initiative as Tox21, providing toxicology data for a large library of compounds based on in vitro high-throughput screening. The processed collection includes qualitative results of over 600 experiments on 8k compounds.

You can download the dataset from http://moleculenet.ai/datasets-1 and load it into pahelix reader creators.

pahelix.datasets.toxcast_dataset.**get_default_toxcast_task_names**(*data_path*)

Get that default toxcast task names and return the list of the input information

pahelix.datasets.toxcast_dataset.**load_toxcast_dataset**(*data_path*, *task_names=None*)

Load toxcast dataset,process the input information.

Description:

The data file contains a csv table, in which columns below are used:

smiles: SMILES representation of the molecular structure.

ACEA_T47D_80hr_Negative: "Tanguay_ZF_120hpf_YSE_up" - Bioassays results

SR-XXX: Stress response bioassays results

Parameters

- **data_path** (*str*) – the path to the cached npz path.
- **task_names** (*list*) – a list of header names to specify the columns to fetch from the csv file.

Returns

an InMemoryDataset instance.

Example

```
dataset = load_toxcast_dataset('./toxcast')
print(len(dataset))
```

References:

[1]Richard, Ann M., et al. "ToxCast chemical landscape: paving the road to 21st century toxicology." Chemical research in toxicology 29.8 (2016): 1225-1251.

[2]please refer to the section "high-throughput assay information" at https://www.epa.gov/chemical-research/toxicity-forecaster-toxcasttm-data for details.

5.5.19 zinc_dataset

Processing of ZINC dataset.

The ZINC database is a curated collection of commercially available chemical compounds prepared especially for virtual screening. ZINC15 is designed to bring together biology and chemoinformatics with a tool that is easy to use for nonexperts, while remaining fully programmable for chemoinformaticians and computational biologists.

pahelix.datasets.zinc_dataset.**load_zinc_dataset**(*data_path*)

Load ZINC dataset,process the input information.

Description:

The data file contains a csv table, in which columns below are used:

smiles: SMILES representation of the molecular structure.

zinc_id: the id of the compound

Parameters
data_path (*str*) – the path to the cached npz path.

Returns
an InMemoryDataset instance.

Example

```
dataset = load_zinc_dataset('./zinc')
print(len(dataset))
```

References:

[1]Teague Sterling and John J. Irwin. Zinc 15 – ligand discovery for everyone. Journal of Chemical Information and Modeling, 55(11):2324–2337, 2015. doi: 10.1021/acs.jcim.5b00559. PMID: 26479676.

5.5.20 Helpful Link

Please refer to our GitHub repo to see the whole module.

5.6 pahelix.featurizers

Table of Contents

5.6.1 het_gnn_featurizer

Featurizers for DDI Heterogenous graph.

class pahelix.featurizers.het_gnn_featurizer.**DDiFeaturizer**

Featurizer for drugs

collate_fn(*ddi_data*, *dti_data*, *ppi_data*, *features*)

Aggregate all needed nodes into a Hetrogenous graph

pahelix.featurizers.het_gnn_featurizer.**num_nodes_stat**(*data*)

count the number of nodes from data

Examples

data: {'pair': (a, b)}

pahelix.featurizers.het_gnn_featurizer.**nx_graph_build**(*hg*, *nodes_dict*, *label*)

Build Heterogenous graph with node name not idx.

5.6.2 pretrain_gnn_featurizer

Featurizers for pretrain-gnn.

Adapted from https://github.com/snap-stanford/pretrain-gnns/tree/master/chem/utils.py

class pahelix.featurizers.pretrain_gnn_featurizer.**AttrmaskTransformFn**

Gen features for attribute mask model of pretrain gnns

class pahelix.featurizers.pretrain_gnn_featurizer.**AttrmaskCollateFn**(*atom_names*, *bond_names*, *mask_ratio=0.15*)

CollateFn for attribute mask model of pretrain gnns

class pahelix.featurizers.pretrain_gnn_featurizer.**SupervisedTransformFn**

Gen features for supervised model of pretrain gnns

class pahelix.featurizers.pretrain_gnn_featurizer.**SupervisedCollateFn**(*atom_names*, *bond_names*)

CollateFn for supervised model of pretrain gnns

5.6.3 Helpful Link

Please refer to our GitHub repo to see the whole module.

5.7 pahelix.model_zoo

Table of Contents

5.7.1 pretrain_gnns_model

This is an implementation of pretrain gnns: https://arxiv.org/abs/1905.12265

class pahelix.model_zoo.pretrain_gnns_model.**AttrmaskModel**(**args: Any*, ***kwargs: Any*)

This is a pretraning model used by pretrain gnns for attribute mask training.

Returns
the loss variance of the model.

Return type
loss

forward(*graphs*, *masked_node_indice*, *masked_node_labels*)

Build the network.

class pahelix.model_zoo.pretrain_gnns_model.**PretrainGNNModel**(**args: Any*, ***kwargs: Any*)

The basic GNN Model used in pretrain gnns.

Parameters
model_config (*dict*) – a dict of model configurations.

forward(*graph*)

Build the network.

property graph_dim

the out dim of graph_repr

property node_dim

the out dim of graph_repr

class pahelix.model_zoo.pretrain_gnns_model.**SupervisedModel**(**args: Any*, ***kwargs: Any*)

This is a pretraning model used by pretrain gnns for supervised training.

Returns
the loss variance of the model.

Return type
self.loss

forward(*graphs*, *labels*, *valids*)

Build the network.

5.7.2 protein_sequence_model

Sequence-based models for protein.

class pahelix.model_zoo.protein_sequence_model.**LstmEncoderModel**(*vocab_size*, *emb_dim=128*, *hidden_size=1024*, *n_layers=3*, *padding_idx=0*, *epsilon=1e-05*, *dropout_rate=0.1*)

forward(*input*, *pos*)

class pahelix.model_zoo.protein_sequence_model.**ResnetEncoderModel**(*vocab_size*, *emb_dim=128*, *hidden_size=256*, *kernel_size=9*, *n_layers=35*, *padding_idx=0*, *dropout_rate=0.1*, *epsilon=1e-06*)

forward(*input*, *pos*)

init_weights(*layer*)

Initialization hook

class pahelix.model_zoo.protein_sequence_model.**TransformerEncoderModel**(*vocab_size*, *emb_dim=512*, *hidden_size=512*, *n_layers=8*, *n_heads=8*, *padding_idx=0*, *dropout_rate=0.1*)

forward(*input*, *pos*)

init_weights(*layer*)

Initialization hook

class pahelix.model_zoo.protein_sequence_model.**PretrainTaskModel**(*class_num*, *model_config*, *encoder_model*)

forward(*input*, *pos*)

class pahelix.model_zoo.protein_sequence_model.**SeqClassificationTaskModel**(*class_num*, *model_config*, *encoder_model*)

forward(*input*, *pos*)

class pahelix.model_zoo.protein_sequence_model.**ClassificationTaskModel**(*class_num*, *model_config*, *encoder_model*)

forward(*input*, *pos*)

class pahelix.model_zoo.protein_sequence_model.**RegressionTaskModel**(*model_config*, *encoder_model*)

forward(*input*, *pos*)

class pahelix.model_zoo.protein_sequence_model.**ProteinEncoderModel**(*model_config*, *name=''*)

ProteinSequenceModel

forward(*input*, *pos*)

class pahelix.model_zoo.protein_sequence_model.**ProteinModel**(*encoder_model*, *model_config*)

forward(*input*, *pos*)

class pahelix.model_zoo.protein_sequence_model.**ProteinCriterion**(*model_config*)

cal_loss(*pred*, *label*)

5.7.3 seq_vae_model

class pahelix.model_zoo.seq_vae_model.**VAE**(*vocab*, *model_config*)

The sequence VAE model

Parameters

- **vocab** – the vocab object.
- **model_config** – the json files of model parameters.

forward(*x*)

Model forward

forward_decoder(*x*, *z*)

decoder

forward_encoder(*x*)

encoder

sample(*n_batch*, *max_len=100*, *z=None*, *temp=1.0*)

Generating n_batch samples in eval mode (z could be not on same device)

Parameters

- **n_batch** – number of sentences to generate
- **max_len** – max len of samples
- **z** – (n_batch, d_z) of floats, latent vector z or None
- **temp** – temperature of softmax

Returns

list of tensors of strings, samples sequence x

sample_z_prior(*n_batch*)

Sampling z ~ p(z) = N(0, I)

Parameters

n_batch – number of batches

Returns

(n_batch, d_z) of floats, sample of latent z

tensor2string(*tensor*)

convert tensor values to sequence string

5.7.4 Helpful Link

Please refer to our GitHub repo to see the whole module.

5.8 pahelix.networks

Table of Contents

5.8.1 basic_block

Some frequently used basic blocks

class pahelix.networks.basic_block.**Activation**(**args: Any*, ***kwargs: Any*)

forward(*x*)

tbd

class pahelix.networks.basic_block.**MLP**(**args: Any*, ***kwargs: Any*)

forward(*x*)

Parameters

x (*tensor*) – (-1, dim).

5.8.2 compound_encoder

Basic Encoder for compound atom/bond features.

class pahelix.networks.compound_encoder.**AtomEmbedding**(**args: Any*, ***kwargs: Any*)

Atom Encoder

forward(*node_features*)

Parameters
node_features (*dict of tensor*) – node features.

class pahelix.networks.compound_encoder.**AtomFloatEmbedding**(**args: Any*, ***kwargs: Any*)

Atom Float Encoder

forward(*feats*)

Parameters
feats (*dict of tensor*) – node float features.

class pahelix.networks.compound_encoder.**BondAngleFloatRBF**(**args: Any*, ***kwargs: Any*)

Bond Angle Float Encoder using Radial Basis Functions

forward(*bond_angle_float_features*)

Parameters
bond_angle_float_features (*dict of tensor*) – bond angle float features.

class pahelix.networks.compound_encoder.**BondEmbedding**(**args: Any*, ***kwargs: Any*)

Bond Encoder

forward(*edge_features*)

Parameters
edge_features (*dict of tensor*) – edge features.

class pahelix.networks.compound_encoder.**BondFloatRBF**(**args: Any*, ***kwargs: Any*)

Bond Float Encoder using Radial Basis Functions

forward(*bond_float_features*)

Parameters
bond_float_features (*dict of tensor*) – bond float features.

5.8.3 gnn_block

Blocks for Graph Neural Network (GNN)
Adapted from https://github.com/snap-stanford/pretrain-gnns/blob/master/chem/model.py

class pahelix.networks.gnn_block.**GIN**(**args: Any*, ***kwargs: Any*)

Implementation of Graph Isomorphism Network (GIN) layer with edge features

forward(*graph*, *node_feat*, *edge_feat*)

Parameters

- **node_feat** (*tensor*) – node features with shape (num_nodes, feature_size).
- **edge_feat** (*tensor*) – edges features with shape (num_edges, feature_size).

class pahelix.networks.gnn_block.**GraphNorm**(**args: Any*, ***kwargs: Any*)

Implementation of graph normalization. Each node features is divied by sqrt(num_nodes) per graphs.

Parameters

- **graph** – the graph object from (Graph)
- **feature** – A tensor with shape (num_nodes, feature_size).

Returns
A tensor with shape (num_nodes, hidden_size)

References:

[1] BENCHMARKING GRAPH NEURAL NETWORKS. https://arxiv.org/abs/2003.00982

forward(*graph*, *feature*)

graph norm

class pahelix.networks.gnn_block.**MeanPool**(**args: Any*, ***kwargs: Any*)

TODO: temporary class due to pgl mean pooling

forward(*graph*, *node_feat*)

mean pooling

5.8.4 involution_block

class pahelix.networks.involution_block.**Involution2D**(*in_channel*, *out_channel*, *sigma_mapping=None*, *kernel_size=7*, *stride=1*, *groups=1*, *reduce_ratio=1*, *dilation=1*, *padding=3*)

Involution module.

Parameters

- **in_channel** – The channel size of input.
- **out_channel** – The channel size of output.
- **sigma_mapping** – Sigma mapping.
- **kernel_size** – Kernel size.
- **stride** – Stride size.
- **groups** – Group size.
- **reduce_ratio** – The ratio of reduce.
- **dilation** – The dilation size.
- **padding** – The padding size.

Returns
Tbe output of Involution2D block.

Return type
output

References:

[1] Involution: Inverting the Inherence of Convolution for Visual Recognition. https://arxiv.org/abs/2103.06255

forward(*x*)

Involution block

5.8.5 lstm_block

Lstm block.

pahelix.networks.lstm_block.**lstm_encoder**(*input*, *hidden_size*, *n_layer=1*, *is_bidirectory=True*, *param_initializer=None*, *name='lstm'*)

The encoder is composed of a stack of lstm layers.

Parameters

- **input** – The input of lstm encoder.
- **hidden_size** – The hidden size of lstm.
- **n_layer** – The number of lstm layers.
- **is_bidirectory** – True if the lstm is bidirectory.
- **param_initializer** – The parameter initializer for lstm encoder.
- **name** – The prefix of the parameters' name in lstm encoder.

Returns

The hidden units of lstm encoder. checkpoints: The checkpoints for recompute mechanism.

Return type

hidden

5.8.6 optimizer

class pahelix.networks.optimizer.**AdamW**(**args*, ***kwargs*)

AdamW object for dygraph.

apply_optimize(*loss*, *startup_program*, *params_grads*)

Update params with weight decay.

5.8.7 pre_post_process

pahelix.networks.pre_post_process.**pre_post_process_layer**(*prev_out*, *out*, *process_cmd*, *dropout_rate=0.0*, *epsilon=1e-05*, *name=''*, *is_test=False*)

Add residual connection, layer normalization and droput to the out tensor optionally according to the value of process_cmd.

This will be used before or after multi-head attention and position-wise feed-forward networks.

5.8.8 resnet_block

Resnet block.

pahelix.networks.resnet_block.**resnet_encoder**(*input*, *hidden_size*, *n_layer=1*, *filter_size=3*, *act='gelu'*, *epsilon=1e-06*, *param_initializer=None*, *name='resnet'*)

The encoder is composed of a stack of resnet layers.

Parameters

- **input** – The input of resnet encoder.
- **hidden_size** – The hidden size of resnet.
- **n_layer** – The number of resnet layers.
- **act** – The activation function.
- **param_initializer** – The parameter initializer for resnet encoder.
- **name** – The prefix of the parameters' name in resnet encoder.

Returns
The hidden units of resnet encoder. checkpoints: The checkpoints for recompute mechanism.

Return type
hidden

5.8.9 transformer_block

Transformer block.

pahelix.networks.transformer_block.**multi_head_attention**(*queries*, *keys*, *values*, *attn_bias*, *d_key*, *d_value*, *d_model*, *n_head=1*, *dropout_rate=0.0*, *cache=None*, *gather_idx=None*, *store=False*, *param_initializer=None*, *lr=1.0*, *name='multi_head_att'*, *is_test=False*)

Multi-Head Attention.

Note that attn_bias is added to the logit before computing softmax activiation to mask certain selected positions so that they will not considered in attention weights.

pahelix.networks.transformer_block.**positionwise_feed_forward**(*x*, *d_inner_hid*, *d_hid*, *dropout_rate*, *hidden_act*, *num_flatten_dims=2*, *param_initializer=None*, *name='ffn'*, *is_test=False*)

Position-wise Feed-Forward Networks.

This module consists of two linear transformations with a ReLU activation in between, which is applied to each position separately and identically.

pahelix.networks.transformer_block.**transformer_encoder**(*enc_input*, *attn_bias*, *n_layer*, *n_head*, *d_key*, *d_value*, *d_model*, *d_inner_hid*, *prepostprocess_dropout*, *attention_dropout*, *act_dropout*, *hidden_act*, *preprocess_cmd='n'*, *postprocess_cmd='da'*, *param_initializer=None*, *name=''*, *epsilon=1e-05*, *n_layer_per_block=1*, *param_share='normal'*, *caches=None*, *gather_idx=None*, *store=False*, *is_test=False*)

The encoder is composed of a stack of identical layers returned by calling transformer_encoder_layer.

pahelix.networks.transformer_block.**transformer_encoder_layer**(*input*, *attn_bias*, *n_head*, *d_key*, *d_value*, *d_model*, *d_inner_hid*, *prepostprocess_dropout*, *attention_dropout*, *act_dropout*, *hidden_act*, *preprocess_cmd='n'*, *postprocess_cmd='da'*, *param_initializer=None*, *name=''*, *epsilon=1e-05*, *cache=None*, *gather_idx=None*, *store=False*, *is_test=False*)

The encoder layers that can be stacked to form a deep encoder.

This module consits of a multi-head (self) attention followed by position-wise feed-forward networks and both the two components companied with the pre_process_layer / post_process_layer to add residual connection, layer normalization and droput.

5.8.10 Helpful Link

Please refer to our GitHub repo to see the whole module.

5.9 pahelix.utils

Table of Contents

5.9.1 basic_utils

Basic utils

pahelix.utils.basic_utils.**load_json_config**(*path*)

tbd

pahelix.utils.basic_utils.**mp_pool_map**(*list_input*, *func*, *num_workers*)

list_output = [func(input) for input in list_input]

5.9.2 compound_tools

Tools for compound features.
Adapted from https://github.com/snap-stanford/pretrain-gnns/blob/master/chem/loader.py

class pahelix.utils.compound_tools.**Compound3DKit**

the 3Dkit of Compound

static get_2d_atom_poses(*mol*)

get 2d atom poses

static get_MMFF_atom_poses(*mol*, *numConfs=None*, *return_energy=False*)

the atoms of mol will be changed in some cases.

static get_atom_poses(*mol*, *conf*)

tbd

static get_bond_lengths(*edges*, *atom_poses*)

get bond lengths

static get_superedge_angles(*edges*, *atom_poses*, *dir_type='HT'*)

get superedge angles

class pahelix.utils.compound_tools.**CompoundKit**

static atom_to_feat_vector(*atom*)

tbd

static check_partial_charge(*atom*)

tbd

static get_atom_feature_id(*atom*, *name*)

get atom features id

static get_atom_feature_size(*name*)

get atom features size

static get_atom_names(*mol*)

get atom name list TODO: to be remove in the future

static get_atom_value(*atom*, *name*)

get atom values

static get_bond_feature_id(*bond*, *name*)

get bond features id

static get_bond_feature_size(*name*)

get bond features size

static get_bond_value(*bond*, *name*)

get bond values

static get_daylight_functional_group_counts(*mol*)

get daylight functional group counts

static get_maccs_fingerprint(*mol*)

get maccs fingerprint

static get_morgan2048_fingerprint(*mol*, *radius=2*)

get morgan2048 fingerprint

static get_morgan_fingerprint(*mol*, *radius=2*)

get morgan fingerprint

static get_ring_size(*mol*)

return (N,6) list

pahelix.utils.compound_tools.**check_smiles_validity**(*smiles*)

Check whether the smile can't be converted to rdkit mol object.

pahelix.utils.compound_tools.**create_standardized_mol_id**(*smiles*)

Parameters

smiles – smiles sequence.

Returns

inchi.

pahelix.utils.compound_tools.**get_atom_feature_dims**(*list_acquired_feature_names*)

tbd

pahelix.utils.compound_tools.**get_bond_feature_dims**(*list_acquired_feature_names*)

tbd

pahelix.utils.compound_tools.**get_gasteiger_partial_charges**(*mol*, *n_iter=12*)

Calculates list of gasteiger partial charges for each atom in mol object.

Parameters

- **mol** – rdkit mol object.
- **n_iter** (*int*) – number of iterations. Default 12.

Returns

list of computed partial charges for each atom.

pahelix.utils.compound_tools.**get_largest_mol**(*mol_list*)

Given a list of rdkit mol objects, returns mol object containing the largest num of atoms. If multiple containing largest num of atoms, picks the first one.

Parameters

mol_list (*list*) – a list of rdkit mol object.

Returns
the largest mol.

pahelix.utils.compound_tools.**mol_to_geognn_graph_data**(*mol*, *atom_poses*, *dir_type*)

mol: rdkit molecule dir_type: direction type for bond_angle grpah

pahelix.utils.compound_tools.**mol_to_geognn_graph_data_MMFF3d**(*mol*)

tbd

pahelix.utils.compound_tools.**mol_to_geognn_graph_data_raw3d**(*mol*)

tbd

pahelix.utils.compound_tools.**mol_to_graph_data**(*mol*)

Parameters

- **atom_features** – Atom features.
- **edge_features** – Edge features.
- **morgan_fingerprint** – Morgan fingerprint.
- **functional_groups** – Functional groups.

pahelix.utils.compound_tools.**new_mol_to_graph_data**(*mol*)

mol_to_graph_data

Parameters

- **atom_features** – Atom features.
- **edge_features** – Edge features.
- **morgan_fingerprint** – Morgan fingerprint.
- **functional_groups** – Functional groups.

pahelix.utils.compound_tools.**new_smiles_to_graph_data**(*smiles*, ***kwargs*)

Convert smiles to graph data.

pahelix.utils.compound_tools.**rdchem_enum_to_list**(*values*)

values = {0: rdkit.Chem.rdchem.ChiralType.CHI_UNSPECIFIED, 1: rdkit.Chem.rdchem.ChiralType.CHI_TETRAHEDRAL_CW, 2: rdkit.Chem.rdchem.ChiralType.CHI_TETRAHEDRAL_CCW, 3: rdkit.Chem.rdchem.ChiralType.CHI_OTHER}

pahelix.utils.compound_tools.**safe_index**(*alist*, *elem*)

Return index of element e in list l. If e is not present, return the last index

pahelix.utils.compound_tools.**split_rdkit_mol_obj**(*mol*)

Split rdkit mol object containing multiple species or one species into a list of mol objects or a list containing a single object respectively.

Parameters
mol – rdkit mol object.

5.9.3 data_utils

Tools for data.

pahelix.utils.data_utils.**get_part_files**(*data_path*, *trainer_id*, *trainer_num*)

Split the files in data_path so that each trainer can train from different examples.

pahelix.utils.data_utils.**load_npz_to_data_list**(*npz_file*)

Reload the data list save by `save_data_list_to_npz`.

Parameters
npz_file (*str*) – the npz file location.

Returns
a list of data where each data is a dict of numpy ndarray.

pahelix.utils.data_utils.**save_data_list_to_npz**(*data_list*, *npz_file*)

Save a list of data to the npz file. Each data is a dict of numpy ndarray.

Parameters

- **data_list** (*list*) – a list of data.
- **npz_file** (*str*) – the npz file location.

5.9.4 language_model_tools

Tools for language models.

pahelix.utils.language_model_tools.**apply_bert_mask**(*inputs*, *pad_mask*, *tokenizer*)

Apply BERT mask to the token_ids.

Parameters
token_ids – The list of token ids.

Returns
The list of masked token ids. labels: The labels for traininig BERT.

Return type
masked_token_ids

5.9.5 protein_tools

class pahelix.utils.protein_tools.**ProteinTokenizer**

Protein Tokenizer.

convert_token_to_id(*token*)

Converts a token to an id.

Parameters
token – Token.

Returns
The id of the input token.

Return type
id

`convert_tokens_to_ids`(*tokens*)

Convert multiple tokens to ids.

Parameters
tokens – The list of tokens.

Returns
The id list of the input tokens.

Return type
ids

`gen_token_ids`(*sequence*)

Generate the list of token ids according the input sequence.

Parameters
sequence – Sequence to be tokenized.

Returns
The list of token ids.

Return type
token_ids

`tokenize`(*sequence*)

Split the sequence into token list.

Parameters
sequence – The sequence to be tokenized.

Returns
The token lists.

Return type
tokens

5.9.6 splitters

Splitters

`class` pahelix.utils.splitters.**RandomSplitter**

Random splitter.

`split`(*dataset*, *frac_train=None*, *frac_valid=None*, *frac_test=None*, *seed=None*)

Parameters

- **dataset** (InMemoryDataset) – the dataset to split.
- **frac_train** (*float*) – the fraction of data to be used for the train split.
- **frac_valid** (*float*) – the fraction of data to be used for the valid split.
- **frac_test** (*float*) – the fraction of data to be used for the test split.
- **seed** (*int* | *None*) – the random seed.

class pahelix.utils.splitters.**IndexSplitter**

Split daatasets that has already been orderd. The first *frac_train* proportion is used for train set, the next *frac_valid* for valid set and the final *frac_test* for test set.

split(*dataset*, *frac_train=None*, *frac_valid=None*, *frac_test=None*)

Parameters

- **dataset** (InMemoryDataset) – the dataset to split.
- **frac_train** (*float*) – the fraction of data to be used for the train split.
- **frac_valid** (*float*) – the fraction of data to be used for the valid split.
- **frac_test** (*float*) – the fraction of data to be used for the test split.

class pahelix.utils.splitters.**ScaffoldSplitter**

Adapted from https://github.com/deepchem/deepchem/blob/master/deepchem/splits/splitters.py

Split dataset by Bemis-Murcko scaffolds

split(*dataset*, *frac_train=None*, *frac_valid=None*, *frac_test=None*)

Parameters

- **dataset** (InMemoryDataset) – the dataset to split. Make sure each element in the dataset has key "smiles" which will be used to calculate the scaffold.
- **frac_train** (*float*) – the fraction of data to be used for the train split.
- **frac_valid** (*float*) – the fraction of data to be used for the valid split.
- **frac_test** (*float*) – the fraction of data to be used for the test split.

class pahelix.utils.splitters.**RandomScaffoldSplitter**

Adapted from https://github.com/pfnet-research/chainer-chemistry/blob/master/chainer_chemistry/dataset/splitters/scaffold_splitter.py

Split dataset by Bemis-Murcko scaffolds

split(*dataset*, *frac_train=None*, *frac_valid=None*, *frac_test=None*, *seed=None*)

Parameters

- **dataset** (InMemoryDataset) – the dataset to split. Make sure each element in the dataset has key "smiles" which will be used to calculate the scaffold.
- **frac_train** (*float*) – the fraction of data to be used for the train split.
- **frac_valid** (*float*) – the fraction of data to be used for the valid split.
- **frac_test** (*float*) – the fraction of data to be used for the test split.
- **seed** (*int*|*None*) – the random seed.

pahelix.utils.splitters.**generate_scaffold**(*smiles*, *include_chirality=False*)

Obtain Bemis-Murcko scaffold from smiles

Parameters

- **smiles** – smiles sequence
- **include_chirality** – Default=False

Returns

the scaffold of the given smiles.

5.9.7 Helpful Link

Please refer to our GitHub repo to see the whole module.

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