
PyKale

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PyKale Contributors

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INTRODUCTION

PyKale is a **Python** library for **knowledge-aware machine learning** from multiple sources, particularly from multiple modalities for **multimodal learning** and from multiple domains for **transfer learning**. This library was motivated by needs in healthcare applications (hence we choose the acronym *kale*, a healthy vegetable) and aims to enable and accelerate interdisciplinary research.

1.1 Objectives

Our objectives are to build *green* machine learning systems.

- *Reduce repetition and redundancy*: refactor code to standardize workflow and enforce styles, and identify and remove duplicated functionalities
- *Reuse existing resources*: reuse the same machine learning pipeline for different data, and reuse existing libraries for available functionalities
- *Recycle learning models across areas*: identify commonalities between applications, and recycle models for one application to another

1.2 API design

To achieve the above objectives, we

- design our API to be pipeline-based to unify the workflow and increase the flexibility, and
- follow core principles of standardization and minimalism in the development.

This design helps us break barriers between different areas or applications and facilitate the fusion and nurture of ideas across discipline boundaries.

1.3 Development

We have Research Software Engineers (RSEs) on our team to help us adopt the best software engineering practices in a research context. We have modern GitHub setup with project boards, discussion, and GitHub actions/workflows. Our repository has automation and continuous integration to build documentation, do linting of our code, perform pre-commit checks (e.g. maximum file size), use **pytest** for testing and **codecov** for analysis of testing.

INSTALLATION

2.1 Requirements

PyKale requires Python 3.7, 3.8, or 3.9. Before installing pykale, you should

- manually [install PyTorch](#) matching your hardware first,
- if you will use APIs related to graphs, you need to manually install [PyTorch Geometric](#) first following its [official instructions](#) and matching your PyTorch installation, and
- If [RDKit](#) will be used, you need to install it via `conda install -c conda-forge rdkit`.

2.2 Pip install

Install PyKale using pip for the stable version:

```
pip install pykale # for the core API only
```

2.3 Install from source

Install from source for the latest version and/or development:

```
git clone https://github.com/pykale/pykale
cd pykale
pip install . # for the core API only
pip install -e .[dev] # editable install for developers including all dependencies and
↳ examples
```

2.4 Installation options

PyKale provides six installation options for different user needs:

- default: `pip install pykale` for essential functionality
- graph: `pip install pykale[graph]` for graph-related functionality (e.g., [TDC](#))
- image: `pip install pykale[image]` for image-related functionality (e.g., [DICOM](#))
- example: `pip install pykale[example]` for examples and tutorials

- full: `pip install pykale[full]` for all functionality, including examples and tutorials
- dev: `pip install pykale[dev]` for development, including all functionality, examples, and tutorials

Multiple options can be chosen by separating them with commas (without whitespace). See examples below.

```
pip install pykale[graph,example]
pip install pykale[graph,image]
pip install pykale[graph,image,example]
```

2.5 Tests

For local unit tests on all kale API, you need to have PyTorch, PyTorch Geometric, and RDKit installed (see the top) and then run `pytest` at the root directory:

```
pytest
```

You can also run `pytest` on individual module (see [pytest documentation](#)).

For *interactive* tutorials, see *Jupyter Notebook tutorials*.

3.1 Usage of Pipeline-based API in Examples

The `kale` API has a unique pipeline-based API design. Each example typically has three essential modules (`main.py`, `config.py`, `model.py`), one optional directory (`configs`), and possibly other modules (`trainer.py`):

- `main.py` is the main module to be run, showing the main workflow.
- `config.py` is the configuration module that sets up the data, prediction problem, and hyper-parameters, etc. The settings in this module is the default configuration.
 - `configs` is the directory to place *customized* configurations for individual runs. We use `.yaml` files for this purpose.
- `model.py` is the model module to define the machine learning model and configure its training parameters.
 - `trainer.py` is the trainer module to define the training and testing workflow. This module is *only needed when NOT using PyTorch Lightning*.

Next, we explain the usage of the pipeline-based API in the modules above, mainly using the [domain adaptation for digits classification example](#).

- The `kale.pipeline` module provides mature, off-the-shelf machine learning pipelines for plug-in usage, e.g. `import kale.pipeline.domain_adapter as domain_adapter` in `digits_dann`'s `model` module.
- The `kale.utils` module provides common utility functions, such as `from kale.utils.seed import set_seed` in `digits_dann`'s `main` module.
- The `kale.loaddata` module provides the input to the machine learning system, such as `from kale.loaddata.image_access import DigitDatase` in `digits_dann`'s `main` module.
- The `kale.prepdata` module provides pre-processing functions to transform the raw input data into a suitable form for machine learning, such as `import kale.prepdata.image_transform as image_transform` in `kale.loaddata.image_access` used in `digits_dann`'s `main` module for image data augmentation.
- The `kale.embed` module provides *embedding* functions (the *encoder*) to *learn* suitable representations from the (pre-processed) input data, such as `from kale.embed.image_cnn import SmallCNNFeature` in `digits_dann`'s `model` module. This is a machine learning module.
- The `kale.predict` module provides prediction functions (the *decoder*) to *learn* a mapping from the input representation to a target prediction, such as `from kale.predict.class_domain_nets import ClassNetSmallImage` in `digits_dann`'s `model` module. This is also a machine learning module.
- The `kale.evaluate` module implements evaluation metrics not yet available, such as the Concordance Index (CI) for measuring the proportion of [concordant pairs](#).

- The `kale.interpret` module aims to provide functions for interpretation of the learned model or the prediction results, such as visualization. This module has no implementation yet.

3.2 Building New Modules or Projects

New modules/projects can be built following the steps below.

- Step 1 - Examples: Choose one of the [examples](#) of your interest (e.g., most relevant to your project) to
 - browse through the configuration, main, and model modules
 - download the data if needed
 - run the example following instructions in the example's README
- Step 2a - New model: To develop new machine learning models under PyKale,
 - define the blocks in your pipeline to figure out what the methods are for data loading, pre-processing data, embedding (encoder/representation), prediction (decoder), evaluation, and interpretation (if needed)
 - modify existing pipelines with your customized blocks or build a new pipeline with PyKale blocks and blocks from other libraries
- Step 2b - New applications: To develop new applications using PyKale,
 - clarify the input data and the prediction target to find matching functionalities in PyKale (request if not found)
 - tailor data loading, pre-processing, and evaluation (and interpretation if needed) to your application

3.3 The Scope of Support

3.3.1 Data

PyKale currently supports graphs, images, and videos, using PyTorch Dataloaders wherever possible. Audios are not supported yet (welcome your contribution).

3.3.2 Machine learning models

PyKale supports modules from the following areas of machine learning

- Deep learning: convolutional neural networks (CNNs), graph neural networks (GNNs) GNN including graph convolutional networks (GCNs), transformers
- Transfer learning: domain adaptation
- Multimodal learning: integration of heterogeneous data
- Dimensionality reduction: multilinear subspace learning, such as multilinear principal component analysis (MPCA)

3.3.3 Example applications

PyKale includes example application from three areas below

- Image/video recognition: imaging recognition with CIFAR10/100, digits (MNIST, USPS, SVHN), action videos (EPIC Kitchen)
- Bioinformatics/graph analysis: link prediction problems in BindingDB and knowledge graphs
- Medical imaging: cardiac MRI classification

JUPYTER NOTEBOOK TUTORIALS

- **Autism detection:** Domain adaptation on multi-site imaging data for autism detection
- **Cardiovascular disease diagnosis:** Cardiac MRI for MPCA-based diagnosis
- **Drug discovery:** BindingDB drug-target interaction prediction
- **Image classification:** Digits domain adaptation
- **Toy data classification:** Toy data domain adaptation

CONFIGURATION USING YAML

5.1 Why YAML?

PyKale has been designed such that users can configure machine learning models and experiments without writing any new Python code. This is achieved via a human and machine readable language called **YAML**. Well thought out default configuration values are first stored using the **YACS** Python module in a `config.py` file. Several customized configurations can then be created in respective `.yaml` files.

This also enables more advanced users to establish their own default and add new configuration parameters with minimal coding. By separating code and configuration, this approach can lead to better **reproducibility**.

5.2 A simple example

The following example is a simple **YAML** file `tutorial.yaml` used by the **digits tutorial notebook**:

```
DAN:
  METHOD: "CDAN"

DATASET:
  NUM_REPEAT: 1
  SOURCE: "svhn"
  VALID_SPLIT_RATIO: 0.5

SOLVER:
  MIN_EPOCHS: 0
  MAX_EPOCHS: 3

OUTPUT:
  PB_FRESH: None
```

Related configuration settings are grouped together. The group headings and allowed values are stored in a **separate Python file** `config.py` which many users will not need to refer to. The headings and parameters in this example are explained below:

The tutorial **YAML** file `tutorial.yaml` above overrides certain defaults in `config.py` to make the machine learning process faster and clearer for demonstration purposes.

5.3 Customization for your applications

Application of an example to your data can be as simple as creating a new YAML file to (change the defaults to) specify your data location, and other preferred configuration customization, e.g., in the choice of models and/or the number of iterations.

LOAD DATA

6.1 Submodules

6.2 kale.loaddata.dataset_access module

Dataset Access API adapted from https://github.com/criteo-research/pytorch-ada/blob/master/adalib/ada/datasets/dataset_access.py

class kale.loaddata.dataset_access.**DatasetAccess**(*n_classes*)

Bases: object

This class ensures a unique API is used to access training, validation and test splits of any dataset.

Parameters

n_classes (*int*) – the number of classes.

n_classes()

get_train()

Returns: a torch.utils.data.Dataset

Dataset: a torch.utils.data.Dataset

get_train_valid(*valid_ratio*)

Randomly split a dataset into non-overlapping training and validation datasets.

Parameters

valid_ratio (*float*) – the ratio for validation set

Returns

a torch.utils.data.Dataset

Return type

Dataset

get_test()

kale.loaddata.dataset_access.**get_class_subset**(*dataset, class_ids*)

Parameters

- **dataset** – a torch.utils.data.Dataset
- **class_ids** (*list, optional*) – List of chosen subset of class ids.

Returns: a torch.utils.data.Dataset

Dataset: a torch.utils.data.Dataset with only classes in class_ids

`kale.loaddata.dataset_access.split_by_ratios(dataset, split_ratios)`

Randomly split a dataset into non-overlapping new datasets of given ratios.

Parameters

- **dataset** (`torch.utils.data.Dataset`) – Dataset to be split.
- **split_ratios** (`list`) – Ratios of splits to be produced, where $0 < \text{sum}(\text{split_ratios}) \leq 1$.

Returns

A list of subsets.

Return type

[List]

Examples

```
>>> import torch
>>> from kale.loaddata.dataset_access import split_by_ratios
>>> subset1, subset2 = split_by_ratios(range(10), [0.3, 0.7])
>>> len(subset1)
3
>>> len(subset2)
7
>>> subset1, subset2 = split_by_ratios(range(10), [0.3])
>>> len(subset1)
3
>>> len(subset2)
7
>>> subset1, subset2, subset3 = split_by_ratios(range(10), [0.3, 0.3])
>>> len(subset1)
3
>>> len(subset2)
3
>>> len(subset3)
4
```

6.3 kale.loaddata.videos module

class `kale.loaddata.videos.VideoFrameDataset`(*root_path: str, annotationfile_path: str, image_modality: str = 'rgb', num_segments: int = 3, frames_per_segment: int = 1, imagefile_template: str = 'img_{:05d}.jpg', transform=None, random_shift: bool = True, test_mode: bool = False*)

Bases: `Dataset`

A highly efficient and adaptable dataset class for videos. Instead of loading every frame of a video, loads `x` RGB frames of a video (sparse temporal sampling) and evenly chooses those frames from start to end of the video, returning a list of `x` PIL images or `FRAMES x CHANNELS x HEIGHT x WIDTH` tensors where `FRAMES=x` if the `kale.prepdata.video_transform.ImglistToTensor()` transform is used.

More specifically, the frame range `[START_FRAME, END_FRAME]` is divided into `NUM_SEGMENTS` segments and `FRAMES_PER_SEGMENT` consecutive frames are taken from each segment.

Note: A demonstration of using this class can be seen in PyKale/examples/video_loading https://github.com/pykale/pykale/tree/master/examples/video_loading

Note: This dataset broadly corresponds to the frame sampling technique introduced in Temporal Segment Networks at ECCV2016 <https://arxiv.org/abs/1608.00859>.

Note: This class relies on receiving video data in a structure where inside a ROOT_DATA folder, each video lies in its own folder, where each video folder contains the frames of the video as individual files with a naming convention such as img_001.jpg ... img_059.jpg. For enumeration and annotations, this class expects to receive the path to a .txt file where each video sample has a row with four (or more in the case of multi-label, see example README on Github) space separated values: VIDEO_FOLDER_PATH START_FRAME END_FRAME LABEL_INDEX. VIDEO_FOLDER_PATH is expected to be the path of a video folder excluding the ROOT_DATA prefix. For example, ROOT_DATA might be home\data\datasetxyz\videos\, inside of which a VIDEO_FOLDER_PATH might be jumping\0052\ or sample1\ or 00053\.

Parameters

- **root_path** – The root path in which video folders lie. this is ROOT_DATA from the description above.
- **annotationfile_path** – The .txt annotation file containing one row per video sample as described above.
- **image_modality** – Image modality (RGB or Optical Flow).
- **num_segments** – The number of segments the video should be divided into to sample frames from.
- **frames_per_segment** – The number of frames that should be loaded per segment. For each segment's frame-range, a random start index or the center is chosen, from which frames_per_segment consecutive frames are loaded.
- **imagefile_template** – The image filename template that video frame files have inside of their video folders as described above.
- **transform** – Transform pipeline that receives a list of PIL images/frames.
- **random_shift** – Whether the frames from each segment should be taken consecutively starting from the center of the segment, or consecutively starting from a random location inside the segment range.
- **test_mode** – Whether this is a test dataset. If so, chooses frames from segments with random_shift=False.

6.4 kale.loaddata.image_access

6.5 kale.loaddata.mnistm module

Dataset setting and data loader for MNIST-M, from https://github.com/criteo-research/pytorch-ada/blob/master/adalib/ada/datasets/dataset_mnistm.py (based on <https://github.com/pytorch/vision/blob/master/torchvision/datasets/mnist.py>) CREDIT: <https://github.com/corenel>

```
class kale.loaddata.mnistm.MNISTM(root, train=True, transform=None, target_transform=None,
                                  download=False)
```

Bases: Dataset

MNIST-M Dataset. Auto-downloads the dataset and provide the torch Dataset API.

Parameters

- **root** (*str*) – path to directory where the MNISTM folder will be created (or exists.)
- **train** (*bool*, *optional*) – defaults to True. If True, loads the training data. Otherwise, loads the test data.
- **transform** (*callable*, *optional*) – defaults to None. A function/transform that takes in an PIL image and returns a transformed version. E.g., `transforms.RandomCrop` This preprocessing function applied to all images (whether source or target)
- **target_transform** (*callable*, *optional*) – default to None, similar to transform. This preprocessing function applied to all target images, after *transform*
- **download** (*bool optional*) – defaults to False. Whether to allow downloading the data if not found on disk.

```
url = 'https://github.com/VanushVaswani/keras_mnistm/releases/download/1.0/keras_mnistm.pkl.gz'
```

```
raw_folder = 'raw'
```

```
processed_folder = 'processed'
```

```
training_file = 'mnist_m_train.pt'
```

```
test_file = 'mnist_m_test.pt'
```

```
download()
```

Download the MNISTM data.

6.6 kale.loaddata.multi_domain module

Construct a dataset with (multiple) source and target domains, adapted from <https://github.com/criteo-research/pytorch-ada/blob/master/adalib/ada/datasets/multisource.py>

```
class kale.loaddata.multi_domain.WeightingType(value)
```

Bases: Enum

An enumeration.

```
NATURAL = 'natural'
```

```

BALANCED = 'balanced'

PRESET0 = 'preset0'

class kale.loaddata.multi_domain.DatasetSizeType(value)
    Bases: Enum
    An enumeration.
    Max = 'max'
    Source = 'source'
    static get_size(size_type, source_dataset, *other_datasets)

class kale.loaddata.multi_domain.DomainsDatasetBase
    Bases: object
    prepare_data_loaders()
        handles train/validation/test split to have 3 datasets each with data from all domains
    get_domain_loaders(split='train', batch_size=32)
        handles the sampling of a dataset containing multiple domains

        Parameters
        • split (string, optional) – [“train”|“valid”|“test”]. Which dataset to iterate on. Defaults to “train”.
        • batch_size (int, optional) – Defaults to 32.

        Returns
        A dataloader with API similar to the torch.dataloader, but returning batches from several domains at each iteration.

        Return type
        MultiDataLoader

class kale.loaddata.multi_domain.MultiDomainDatasets(source_access: DatasetAccess, target_access:
    DatasetAccess, config_weight_type='natural',
    config_size_type=DatasetSizeType.Max,
    valid_split_ratio=0.1,
    source_sampling_config=None,
    target_sampling_config=None,
    n_fewshot=None, random_state=None,
    class_ids=None)

    Bases: DomainsDatasetBase
    is_semi_supervised()
    prepare_data_loaders()
    get_domain_loaders(split='train', batch_size=32)

```

```

class kale.loaddata.multi_domain.MultiDomainImageFolder(root: str, loader: ~typing.Callable[[str],
~typing.Any] = <function default_loader>,
extensions:
~typing.Optional[~typing.Tuple[str, ...]] =
('.jpg', '.jpeg', '.png', '.ppm', '.bmp', '.pgm',
'.tif', '.tiff', '.webp'), transform:
~typing.Optional[~typing.Callable] =
None, target_transform:
~typing.Optional[~typing.Callable] =
None, sub_domain_set=None,
sub_class_set=None, is_valid_file:
~typing.Optional[~typing.Callable[[str],
bool]] = None, return_domain_label:
~typing.Optional[bool] = False,
split_train_test: ~typing.Optional[bool] =
False, split_ratio: float = 0.8)

```

Bases: VisionDataset

A generic data loader where the samples are arranged in this way:

```

root/domain_a/class_1/xxx.ext
root/domain_a/class_1/xyy.ext
root/domain_a/class_2/xxz.ext

root/domain_b/class_1/efg.ext
root/domain_b/class_2/pqr.ext
root/domain_b/class_2/lmn.ext

root/domain_k/class_2/123.ext
root/domain_k/class_1/abc3.ext
root/domain_k/class_1/asd932_.ext

```

Parameters

- **root** (*string*) – Root directory path.
- **loader** (*callable*) – A function to load a sample given its path.
- **extensions** (*tuple[string]*) – A list of allowed extensions. Either extensions or `is_valid_file` should be passed.
- **transform** (*callable, optional*) – A function/transform that takes in a sample and returns a transformed version. E.g, `transforms.RandomCrop` for images.
- **target_transform** (*callable, optional*) – A function/transform that takes in the target and transforms it.
- **sub_domain_set** (*list*) – A list of domain names, which should be a subset of domains (folders) under the root directory. If `None`, all available domains will be used. Defaults to `None`.
- **sub_class_set** (*list*) – A list of class names, which should be a subset of classes (folders) under each domain's directory. If `None`, all available classes will be used. Defaults to `None`.
- **is_valid_file** – A function that takes path of a file and check if the file is a valid file (to check corrupt files). Either extensions or `is_valid_file` should be passed.

`get_train()`

`get_test()`

```
kale.loaddata.multi_domain.make_multi_domain_set(directory: str, class_to_idx: Dict[str, int],
                                                domain_to_idx: Dict[str, int], extensions:
                                                Optional[Tuple[str, ...]] = None, is_valid_file:
                                                Optional[Callable[[str], bool]] = None) →
                                                List[Tuple[str, int, int]]
```

Generates a list of samples of a form (path_to_sample, class, domain). :param directory: root dataset directory :type directory: str :param class_to_idx: dictionary mapping class name to class index :type class_to_idx: Dict[str, int] :param domain_to_idx: dictionary mapping d name to class index :type domain_to_idx: Dict[str, int] :param extensions: A list of allowed extensions. Either extensions or is_valid_file should be passed.

Defaults to None.

Parameters

is_valid_file (*optional*) – A function that takes path of a file and checks if the file is a valid file (to check corrupt files) both extensions and is_valid_file should not be passed. Defaults to None.

Raises

ValueError – In case extensions and is_valid_file are None or both are not None.

Returns

samples of a form (path_to_sample, class, domain)

Return type

List[Tuple[str, int, int]]

```
class kale.loaddata.multi_domain.ConcatMultiDomainAccess(data_access: dict, domain_to_idx: dict,
                                                         return_domain_label: Optional[bool] =
                                                         False)
```

Bases: Dataset

Concatenate multiple datasets as a single dataset with domain labels

Parameters

- **data_access** (*dict*) – Dictionary of domain datasets, e.g. {"Domain1_name": domain1_set, "Domain2_name": domain2_set}
- **domain_to_idx** (*dict*) – Dictionary of domain name to domain labels, e.g. {"Domain1_name": 0, "Domain2_name": 1}
- **return_domain_label** (*Optional[bool]*, *optional*) – Whether return domain labels in each batch. Defaults to False.

```
class kale.loaddata.multi_domain.MultiDomainAccess(data_access: dict, n_classes: int,
                                                    return_domain_label: Optional[bool] = False)
```

Bases: [DatasetAccess](#)

Convert multiple digits-like data accesses to a single data access. :param data_access: Dictionary of data accesses, e.g. {"Domain1_name": domain1_access, "Domain2_name": domain2_access}

Parameters

- **n_classes** (*int*) – number of classes.

- **return_domain_label** (*Optional[bool]*, *optional*) – Whether return domain labels in each batch. Defaults to False.

get_train()

get_test()

```
class kale.loaddata.multi_domain.MultiDomainAdapDataset(data_access, valid_split_ratio=0.1,  
                                                    test_split_ratio=0.2, random_state: int = 1,  
                                                    test_on_all=False)
```

Bases: *DomainsDatasetBase*

The class controlling how the multiple domains are iterated over.

Parameters

- **data_access** (*MultiDomainImageFolder*, or *MultiDomainAccess*) – Multi-domain data access.
- **valid_split_ratio** (*float*, *optional*) – Split ratio for validation set. Defaults to 0.1.
- **test_split_ratio** (*float*, *optional*) – Split ratio for test set. Defaults to 0.2.
- **random_state** (*int*, *optional*) – Random state for generator. Defaults to 1.
- **test_on_all** (*bool*, *optional*) – Whether test model on all target. Defaults to False.

prepare_data_loaders()

get_domain_loaders(*split='train'*, *batch_size=32*)

6.7 kale.loaddata.sampler module

Various sampling strategies for datasets to construct dataloader, from <https://github.com/criteo-research/pytorch-ada/blob/master/adalib/ada/datasets/sampler.py>

```
class kale.loaddata.sampler.SamplingConfig(balance=False, class_weights=None,  
                                           balance_domain=False)
```

Bases: *object*

create_loader(*dataset*, *batch_size*)

Create the data loader

Reference: <https://pytorch.org/docs/stable/data.html#torch.utils.data.Sampler>

Parameters

- **dataset** (*Dataset*) – dataset from which to load the data.
- **batch_size** (*int*) – how many samples per batch to load

```
class kale.loaddata.sampler.FixedSeedSamplingConfig(seed=1, balance=False, class_weights=None,  
                                                  balance_domain=False)
```

Bases: *SamplingConfig*

create_loader(*dataset*, *batch_size*)

Create the data loader with fixed seed.

class kale.loaddata.sampler.**MultiDataLoader**(*dataloaders, n_batches*)

Bases: object

Batch Sampler for a MultiDataset. Iterates in parallel over different batch samplers for each dataset. Yields batches [(x₁, y₁), ..., (x_s, y_s)] for s datasets.

class kale.loaddata.sampler.**BalancedBatchSampler**(*dataset, batch_size*)

Bases: BatchSampler

BatchSampler - from a MNIST-like dataset, samples *n_samples* for each of the *n_classes*. Returns batches of size *n_classes* * (*batch_size* // *n_classes*) adapted from <https://github.com/adambielski/siamese-triplet/blob/master/datasets.py>

class kale.loaddata.sampler.**RewightedBatchSampler**(*dataset, batch_size, class_weights*)

Bases: BatchSampler

BatchSampler - from a MNIST-like dataset, samples *batch_size* according to given input distribution assuming multi-class labels adapted from <https://github.com/adambielski/siamese-triplet/blob/master/datasets.py>

kale.loaddata.sampler.**get_labels**(*dataset*)

Get class labels for dataset

class kale.loaddata.sampler.**InfiniteSliceIterator**(*array, class_*)

Bases: object

reset()

get(*n*)

class kale.loaddata.sampler.**DomainBalancedBatchSampler**(*dataset, batch_size*)

Bases: *BalancedBatchSampler*

BatchSampler - samples *n_samples* for each of the *n_domains*.

Returns batches of size *n_domains* * (*batch_size* / *n_domains*)

Parameters

- **dataset** (*.multi_domain.MultiDomainImageFolder* or *torch.utils.data.Subset*) – Multi-domain data access.
- **batch_size** (*int*) – Batch size

6.8 kale.loaddata.usps module

Dataset setting and data loader for USPS, from https://github.com/criteo-research/pytorch-ada/blob/master/adalib/ada/datasets/dataset_usps.py (based on https://github.com/mingyuliutw/CoGAN/blob/master/cogan_pytorch/src/dataset_usps.py)

class kale.loaddata.usps.**USPS**(*root, train=True, transform=None, download=False*)

Bases: Dataset

USPS Dataset.

Parameters

- **root** (*string*) – Root directory of dataset where dataset file exist.
- **train** (*bool, optional*) – If True, resample from dataset randomly.

- **download** (*bool*, *optional*) – If true, downloads the dataset from the internet and puts it in root directory. If dataset is already downloaded, it is not downloaded again.
- **transform** (*callable*, *optional*) – A function/transform that takes in an PIL image and returns a transformed version. E.g, `transforms.RandomCrop`

```
url = 'https://raw.githubusercontent.com/mingyuliutw/CoGAN/master/cogan_pytorch/
data/uspssample/uspss_28x28.pkl'
```

```
download()
```

Download dataset.

```
load_samples()
```

Load sample images from dataset.

6.9 kale.loaddata.tdc_datasets module

```
class kale.loaddata.tdc_datasets.BindingDBDataset(name: str, split='train', path='./data',
mode='cnn_cnn', y_log=True,
drug_transform=None, protein_transform=None)
```

Bases: Dataset

A custom dataset for loading and processing original TDC data, which is used as input data in DeepDTA model.

Parameters

- **name** (*str*) – TDC dataset name.
- **split** (*str*) – Data split type (train, valid or test).
- **path** (*str*) – dataset download/local load path (default: “./data”)
- **mode** (*str*) – encoding mode (default: `cnn_cnn`)
- **drug_transform** – Transform operation (default: `None`)
- **protein_transform** – Transform operation (default: `None`)
- **y_log** (*bool*) – Whether convert y values to log space. (default: `True`)

6.10 kale.loaddata.video_access module

Action video dataset loading for EPIC-Kitchen, ADL, GTEA, KITCHEN. The code is based on https://github.com/criteo-research/pytorch-ada/blob/master/adalib/ada/datasets/digits_dataset_access.py

```
kale.loaddata.video_access.get_image_modality(image_modality)
```

Change `image_modality` (string) to `rgb` (bool) and `flow` (bool) for efficiency

```
kale.loaddata.video_access.get_videodata_config(cfg)
```

Get the configure parameters for video data from the `cfg` files

```
kale.loaddata.video_access.generate_list(data_name, data_params_local, domain)
```

Parameters

- **data_name** (*string*) – name of dataset
- **data_params_local** (*dict*) – hyper parameters from configure file

- **domain** (*string*) – domain type (source or target)

Returns

image directory of dataset train_listpath (*string*): training list file directory of dataset test_listpath (*string*): test list file directory of dataset

Return type

data_path (*string*)

class kale.loaddata.video_access.VideoDataset(*value*)

Bases: Enum

An enumeration.

EPIC = 'EPIC'

ADL = 'ADL'

GTEA = 'GTEA'

KITCHEN = 'KITCHEN'

static get_source_target(*source*: VideoDataset, *target*: VideoDataset, *seed*, *params*)

Gets data loaders for source and target datasets Sets channel_number as 3 for RGB, 2 for flow. Sets class_number as 8 for EPIC, 7 for ADL, 6 for both GTEA and KITCHEN.

Parameters

- **source** – (VideoDataset): source dataset name
- **target** – (VideoDataset): target dataset name
- **seed** – (int): seed value set manually.
- **params** – (CfgNode): hyper parameters from configure file

Examples::

```
>>> source, target, num_classes = get_source_target(source, target, seed, ↵
↵params)
```

class kale.loaddata.video_access.VideoDatasetAccess(*data_path*, *train_list*, *test_list*, *image_modality*, *frames_per_segment*, *n_classes*, *transform_kind*, *seed*)

Bases: DatasetAccess

Common API for video dataset access

Parameters

- **data_path** (*string*) – image directory of dataset
- **train_list** (*string*) – training list file directory of dataset
- **test_list** (*string*) – test list file directory of dataset
- **image_modality** (*string*) – image type (RGB or Optical Flow)
- **frames_per_segment** (*int*) – length of each action sample (the unit is number of frame)
- **n_classes** (*int*) – number of class
- **transform_kind** (*string*) – types of video transforms

- **seed** – (int): seed value set manually.

get_train_valid(*valid_ratio*)

Get the train and validation dataset with the fixed random split. This is used for joint input like RGB and optical flow, which will call *get_train_valid* twice. Fixing the random seed here can keep the seeds for twice the same.

```
class kale.loaddata.video_access.EPICDatasetAccess(data_path, train_list, test_list, image_modality,  
frames_per_segment, n_classes, transform_kind,  
seed)
```

Bases: *VideoDatasetAccess*

EPIC data loader

get_train()

get_test()

```
class kale.loaddata.video_access.GTEADatasetAccess(data_path, train_list, test_list, image_modality,  
frames_per_segment, n_classes, transform_kind,  
seed)
```

Bases: *VideoDatasetAccess*

GTEA data loader

get_train()

get_test()

```
class kale.loaddata.video_access.ADLDatasetAccess(data_path, train_list, test_list, image_modality,  
frames_per_segment, n_classes, transform_kind,  
seed)
```

Bases: *VideoDatasetAccess*

ADL data loader

get_train()

get_test()

```
class kale.loaddata.video_access.KITCHENDatasetAccess(data_path, train_list, test_list,  
image_modality, frames_per_segment,  
n_classes, transform_kind, seed)
```

Bases: *VideoDatasetAccess*

KITCHEN data loader

get_train()

get_test()

6.11 kale.loaddata.video_datasets module

```
class kale.loaddata.video_datasets.BasicVideoDataset(root_path: str, annotationfile_path: str,
                                                    dataset_split: str, image_modality: str,
                                                    num_segments: int = 1, frames_per_segment:
                                                    int = 16, imagefile_template: str =
                                                    'img_{:010d}.jpg', transform=None,
                                                    random_shift: bool = True, test_mode: bool =
                                                    False, n_classes: int = 8)
```

Bases: [VideoFrameDataset](#)

Dataset for GTEA, ADL and KITCHEN.

Parameters

- **root_path** (*string*) – The root path in which video folders lie.
- **annotationfile_path** (*string*) – The annotation file containing one row per video sample.
- **dataset_split** (*string*) – Split type (train or test)
- **image_modality** (*string*) – Image modality (RGB or Optical Flow)
- **num_segments** (*int*) – The number of segments the video should be divided into to sample frames from.
- **frames_per_segment** (*int*) – The number of frames that should be loaded per segment.
- **imagefile_template** (*string*) – The image filename template.
- **transform** (*Compose*) – Video transform.
- **random_shift** (*bool*) – Whether the frames from each segment should be taken consecutively starting from the center(False) of the segment, or consecutively starting from a random(True) location inside the segment range.
- **test_mode** (*bool*) – Whether this is a test dataset. If so, chooses frames from segments with random_shift=False.
- **n_classes** (*int*) – The number of classes.

make_dataset()

Load data from the EPIC-Kitchen list file and make them into the united format. Different datasets correspond to a different number of classes.

Returns

list of (video_name, start_frame, end_frame, label)

Return type

data (list)

```
class kale.loaddata.video_datasets.EPIC(root_path: str, annotationfile_path: str, dataset_split: str,
                                         image_modality: str, num_segments: int = 1,
                                         frames_per_segment: int = 16, imagefile_template: str =
                                         'img_{:010d}.jpg', transform=None, random_shift: bool = True,
                                         test_mode: bool = False, n_classes: int = 8)
```

Bases: [VideoFrameDataset](#)

Dataset for EPIC-Kitchen.

make_dataset()

Load data from the EPIC-Kitchen list file and make them into the united format. Because the original list files are not the same, inherit from class BasicVideoDataset and be modified.

6.12 kale.loaddata.video_multi_domain module

Construct a dataset for videos with (multiple) source and target domains

```
class kale.loaddata.video_multi_domain.VideoMultiDomainDatasets(source_access_dict,  
target_access_dict,  
image_modality, seed,  
config_weight_type='natural',  
con-  
fig_size_type=DatasetSizeType.Max,  
valid_split_ratio=0.1,  
source_sampling_config=None,  
target_sampling_config=None,  
n_fewshot=None,  
random_state=None,  
class_ids=None)
```

Bases: *MultiDomainDatasets*

prepare_data_loaders()

get_domain_loaders(*split='train', batch_size=32*)

6.13 Module contents

PREPROCESS DATA

7.1 Submodules

7.2 `kale.prepdata.chem_transform` module

Functions for labeling and encoding chemical characters like Compound SMILES and atom string, refer to <https://github.com/hkmztrk/DeepDTA> and <https://github.com/thinng/GraphDTA>.

`kale.prepdata.chem_transform.integer_label_smiles(smiles, max_length=85, isomeric=False)`

Integer encoding for SMILES string sequence.

Parameters

- **smiles** (*str*) – Simplified molecular-input line-entry system, which is a specification in the form of a line
- **strings.** (*notation for describing the structure of chemical species using short ASCII*) –
- **max_length** (*int*) – Maximum encoding length of input SMILES string. (default: 85)
- **isomeric** (*bool*) – Whether the input SMILES string includes isomeric information (default: False).

`kale.prepdata.chem_transform.integer_label_protein(sequence, max_length=1200)`

Integer encoding for protein string sequence.

Parameters

- **sequence** (*str*) – Protein string sequence.
- **max_length** – Maximum encoding length of input protein string. (default: 1200)

7.3 `kale.prepdata.image_transform` module

7.4 `kale.prepdata.supergraph_construct` module

7.5 `kale.prepdata.tensor_reshape` module

`kale.prepdata.tensor_reshape.spatial_to_seq(image_tensor: Tensor)`

Takes a torch tensor of shape (batch_size, channels, height, width) as used and outputted by CNNs and creates a sequence view of shape (sequence_length, batch_size, channels) as required by torch's transformer module. In other words, unrolls the spatial grid into the sequence length and rearranges the dimension ordering.

Parameters

image_tensor – tensor of shape (batch_size, channels, height, width) (required).

`kale.prepdata.tensor_reshape.seq_to_spatial(sequence_tensor: Tensor, desired_height: int, desired_width: int)`

Takes a torch tensor of shape (sequence_length, batch_size, num_features) as used and outputted by Transformers and creates a view of shape (batch_size, num_features, height, width) as used and outputted by CNNs. In other words, rearranges the dimension ordering and rolls sequence_length into (height,width). height*width must equal the sequence length of the input sequence.

Parameters

- **sequence_tensor** – sequence tensor of shape (sequence_length, batch_size, num_features) (required).
- **desired_height** – the height into which the sequence length should be rolled into (required).
- **desired_width** – the width into which the sequence length should be rolled into (required).

7.6 kale.prepdata.video_transform module

`kale.prepdata.video_transform.get_transform(kind, image_modality)`

Define transforms (for commonly used datasets)

Parameters

- **kind** ([type]) – the dataset (transformation) name
- **image_modality** (string) – image type (RGB or Optical Flow)

`class kale.prepdata.video_transform.ImglistToTensor`

Bases: Module

Converts a list of PIL images in the range [0,255] to a torch.FloatTensor of shape (NUM_IMAGES x CHANNELS x HEIGHT x WIDTH) in the range [0,1]. Can be used as first transform for `kale.loaddata.videos.VideoFrameDataset`.

forward(img_list)

For RGB input, converts each PIL image in a list to a torch Tensor and stacks them into a single tensor. For flow input, converts every two PIL images (x(u)_img, y(v)_img) in a list to a torch Tensor and stacks them. For example, if input list size is 16, the dimension is [16, 1, 224, 224] and the frame order is [frame 1_x, frame 1_y, frame 2_x, frame 2_y, frame 3_x, ..., frame 8_x, frame 8_y]. The output will be [[frame 1_x, frame 1_y], [frame 2_x, frame 2_y], [frame 3_x, ..., [frame 8_x, frame 8_y]] and the dimension is [8, 2, 224, 224].

Parameters

img_list – list of PIL images.

Returns

tensor of size `` NUM_IMAGES x CHANNELS x HEIGHT x WIDTH ``

class kale.prepdata.video_transform.**TensorPermute**

Bases: Module

Convert a torch.FloatTensor of shape (NUM_IMAGES x CHANNELS x HEIGHT x WIDTH) to a torch.FloatTensor of shape (CHANNELS x NUM_IMAGES x HEIGHT x WIDTH).

7.7 Module contents

8.1 Submodules

8.2 kale.embed.attention_cnn module

```
class kale.embed.attention_cnn.ContextCNNGeneric(cnn: Module, cnn_output_shape: Tuple[int, int, int, int], contextualizer: Module, output_type: str)
```

Bases: Module

A template to construct a feature extractor consisting of a CNN followed by a sequence-to-sequence contextualizer like a Transformer-Encoder. Before inputting the CNN output tensor to the contextualizer, the tensor's spatial dimensions are unrolled into a sequence.

Parameters

- **cnn** – any convolutional neural network that takes in batches of images of shape (batch_size, channels, height, width) and outputs tensor representations of shape (batch_size, out_channels, out_height, out_width).
- **cnn_output_shape** – A tuple of shape (batch_size, num_channels, height, width) describing the output shape of the given CNN (required).
- **contextualizer** – A sequence-to-sequence model that takes inputs of shape (num_timesteps, batch_size, num_features) and uses attention to contextualize the sequence and returns a sequence of the exact same shape. This will mainly be a Transformer-Encoder (required).
- **output_type** – One of 'sequence' or 'spatial'. If Spatial then the final output of the model, which is a sequence, will be reshaped to resemble the image-batch shape of the output of the CNN. If Sequence then the output sequence is returned as is (required).

Examples

```
>>> cnn = nn.Sequential(nn.Conv2d(3, 32, kernel_size=3),
>>>                      nn.Conv2d(32, 64, kernel_size=3),
>>>                      nn.MaxPool2d(2))
>>> cnn_output_shape = (-1, 64, 8, 8)
>>> contextualizer = nn.TransformerEncoderLayer(...)
>>> output_type = 'spatial'
>>>
>>> attention_cnn = ContextCNNGeneric(cnn, cnn_output_shape, contextualizer, output_
```

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```

→type)
>>> output = attention_cnn(torch.randn((32, 3, 16, 16)))
>>>
>>> output.size() == cnn_output_shape # True

```

forward(*x*: *Tensor*)

Pass the input through the cnn and then the contextualizer.

Parameters**x** – input image batch exactly as for CNNs (required).**training**: **bool**

```

class kale.embed.attention_cnn.CNNTransformer(cnn: Module, cnn_output_shape: Tuple[int, int, int, int],
                                             num_layers: int, num_heads: int, dim_feedforward: int,
                                             dropout: float, output_type: str, positional_encoder:
                                             Optional[Module] = None)

```

Bases: [ContextCNNGeneric](#)

A feature extractor consisting of a given CNN backbone followed by a standard Transformer-Encoder. See documentation of “ContextCNNGeneric” for more information.

Parameters

- **cnn** – any convolutional neural network that takes in batches of images of shape (batch_size, channels, height, width) and outputs tensor representations of shape (batch_size, out_channels, out_height, out_width) (required).
- **cnn_output_shape** – a tuple of shape (batch_size, num_channels, height, width) describing the output shape of the given CNN (required).
- **num_layers** – number of attention layers in the Transformer-Encoder (required).
- **num_heads** – number of attention heads in each transformer block (required).
- **dim_feedforward** – number of neurons in the intermediate dense layer of each transformer feedforward block (required).
- **dropout** – dropout rate of the transformer layers (required).
- **output_type** – one of ‘sequence’ or ‘spatial’. If Spatial then the final output of the model, which is the sequence output of the Transformer-Encoder, will be reshaped to resemble the image-batch shape of the output of the CNN (required).
- **positional_encoder** – None or a nn.Module that expects inputs of shape (sequence_length, batch_size, embedding_dim) and returns the same input after adding some positional information to the embeddings. If *None*, then the default and fixed sin-cos positional encodings of base transformers are applied (optional).

Examples

See `pykale/examples/cifar_cnnttransformer/model.py`

training: bool

8.3 kale.embed.factorization module

Python implementation of a tensor factorization algorithm Multilinear Principal Component Analysis (MPCA) and a matrix factorization algorithm Maximum Independence Domain Adaptation (MIDA)

class `kale.embed.factorization.MPCA`(*var_ratio=0.97, max_iter=1, vectorize=False, n_components=None*)

Bases: `BaseEstimator, TransformerMixin`

MPCA implementation compatible with sickit-learn

Parameters

- **var_ratio** (*float, optional*) – Percentage of variance explained (between 0 and 1). Defaults to 0.97.
- **max_iter** (*int, optional*) – Maximum number of iteration. Defaults to 1.
- **vectorize** (*bool*) – Whether return the transformed/projected tensor in vector. Defaults to False.
- **n_components** (*int*) – Number of components to keep. Applies only when `vectorize=True`. Defaults to None.

proj_mats

A list of transposed projection matrices, shapes $(P_1, I_1), \dots, (P_N, I_N)$, where P_1, \dots, P_N are output tensor shape for each sample.

Type

list of arrays

idx_order

The ordering index of projected (and vectorized) features in decreasing variance.

Type

array-like

mean_

Per-feature empirical mean, estimated from the training set, shape (I_1, I_2, \dots, I_N) .

Type

array-like

shape_in

Input tensor shapes, i.e. (I_1, I_2, \dots, I_N) .

Type

tuple

shape_out

Output tensor shapes, i.e. (P_1, P_2, \dots, P_N) .

Type

tuple

Reference:

Haiping Lu, K.N. Plataniotis, and A.N. Venetsanopoulos, “MPCA: Multilinear Principal Component Analysis of Tensor Objects”, IEEE Transactions on Neural Networks, Vol. 19, No. 1, Page: 18-39, January 2008. For initial Matlab implementation, please go to <https://uk.mathworks.com/matlabcentral/fileexchange/26168>.

Examples

```
>>> import numpy as np
>>> from kale.embed.mpca import MPCA
>>> x = np.random.random((40, 20, 25, 20))
>>> x.shape
(40, 20, 25, 20)
>>> mpca = MPCA()
>>> x_projected = mpca.fit_transform(x)
>>> x_projected.shape
(40, 18, 23, 18)
>>> x_projected = mpca.transform(x)
>>> x_projected.shape
(40, 7452)
>>> x_projected = mpca.transform(x)
>>> x_projected.shape
(40, 50)
>>> x_rec = mpca.inverse_transform(x_projected)
>>> x_rec.shape
(40, 20, 25, 20)
```

fit(*x*, *y=None*)

Fit the model with input training data *x*.

Args

x (array-like tensor): Input data, shape (*n_samples*, *I_1*, *I_2*, ..., *I_N*), where *n_samples* is the number of samples, *I_1*, *I_2*, ..., *I_N* are the dimensions of corresponding mode (1, 2, ..., *N*), respectively.

y (None): Ignored variable.

Returns

self (object). Returns the instance itself.

transform(*x*)

Perform dimension reduction on *x*

Parameters

x (array-like tensor) – Data to perform dimension reduction, shape (*n_samples*, *I_1*, *I_2*, ..., *I_N*).

Returns

Projected data in lower dimension, shape (*n_samples*, *P_1*, *P_2*, ..., *P_N*) if *self.vectorize==False*. If *self.vectorize==True*, features will be sorted based on their explained variance ratio, shape (*n_samples*, *P_1* * *P_2* * ... * *P_N*) if *self.n_components* is None, and shape (*n_samples*, *n_components*) if *self.n_component* is a valid integer.

Return type

array-like tensor

inverse_transform(*x*)

Reconstruct projected data to the original shape and add the estimated mean back

Parameters

x (*array-like tensor*) – Data to be reconstructed, shape (n_samples, P_1, P_2, ..., P_N), if self.vectorize == False, where P_1, P_2, ..., P_N are the reduced dimensions of corresponding mode (1, 2, ..., N), respectively. If self.vectorize == True, shape (n_samples, self.n_components) or shape (n_samples, P_1 * P_2 * ... * P_N).

Returns

Reconstructed tensor in original shape, shape (n_samples, I_1, I_2, ..., I_N)

Return type

array-like tensor

```
class kale.embed.factorization.MIDA(n_components, kernel='linear', lambda_=1.0, mu=1.0, eta=1.0,
                                     augmentation=False, kernel_params=None)
```

Bases: BaseEstimator, TransformerMixin

Maximum independence domain adaptation :param n_components: Number of components to keep. :type n_components: int :param kernel: “linear”, “rbf”, or “poly”. Kernel to use for MIDA. Defaults to “linear”. :type kernel: str :param mu: Hyperparameter of the l2 penalty. Defaults to 1.0. :type mu: float :param eta: Hyperparameter of the label dependence. Defaults to 1.0. :type eta: float :param augmentation: Whether using covariates as augment features. Defaults to False. :type augmentation: bool :param kernel_params: Parameters for the kernel. Defaults to None. :type kernel_params: dict or None

References

[1] Yan, K., Kou, L. and Zhang, D., 2018. Learning domain-invariant subspace using domain features and independence maximization. IEEE transactions on cybernetics, 48(1), pp.288-299.

```
fit(x, y=None, covariates=None)
```

Parameters

- **x** – array-like. Input data, shape (n_samples, n_features)
- **y** – array-like. Labels, shape (n1_samples,)
- **covariates** – array-like. Domain co-variates, shape (n_samples, n_co-variates)

Note: Unsupervised MIDA is performed if y is None. Semi-supervised MIDA is performed is y is not None.

```
fit_transform(x, y=None, covariates=None)
```

Parameters

- **x** – array-like, shape (n_samples, n_features)
- **y** – array-like, shape (n_samples,)
- **covariates** – array-like, shape (n_samples, n_covariates)

Returns

array-like, shape (n_samples, n_components)

Return type

x_transformed

transform(x, covariates=None)**Parameters**

- **x** – array-like, shape (n_samples, n_features)
- **covariates** – array-like, augmentation features, shape (n_samples, n_covariates)

Returns

array-like, shape (n_samples, n_components)

Return type

x_transformed

8.4 kale.embed.gcn module

class kale.embed.gcn.GCNEncoderLayer(*in_channels, out_channels, improved=False, cached=False, bias=True, **kwargs*)

Bases: MessagePassing

Modification of PyTorch Geometric’s nn.GCNConv, which reduces the computational cost of GCN layer for GripNet model. The graph convolutional operator from the “Semi-supervised Classification with Graph Convolutional Networks” (ICLR 2017) paper.

$$\mathbf{X}' = \hat{\mathbf{D}}^{-1/2} \hat{\mathbf{A}} \hat{\mathbf{D}}^{-1/2} \mathbf{X} \Theta,$$

where $\hat{\mathbf{A}} = \mathbf{A} + \mathbf{I}$ denotes the adjacency matrix with inserted self-loops and $\hat{D}_{ii} = \sum_{j=0} \hat{A}_{ij}$ its diagonal degree matrix.

Note: For more information please see Pytorch Geometric’s nn.GCNConv docs.

Parameters

- **in_channels** (*int*) – Size of each input sample.
- **out_channels** (*int*) – Size of each output sample.
- **improved** (*bool, optional*) – If set to True, the layer computes $\hat{\mathbf{A}}$ as $\mathbf{A} + 2\mathbf{I}$. (default: False)
- **cached** (*bool, optional*) – If set to True, the layer will cache the computation of $\hat{\mathbf{D}}^{-1/2} \hat{\mathbf{A}} \hat{\mathbf{D}}^{-1/2}$ on first execution, and will use the cached version for further executions. This parameter should only be set to True in transductive learning scenarios. (default: False)
- **bias** (*bool, optional*) – If set to False, the layer will not learn an additive bias. (default: True)
- ****kwargs** (*optional*) – Additional arguments of torch_geometric.nn.conv.MessagePassing.

reset_parameters()

static norm(*edge_index, num_nodes, edge_weight, improved=False, dtype=None*)

Add self-loops and apply symmetric normalization

forward(*x*, *edge_index*, *edge_weight=None*)

Parameters

- **x** (*torch.Tensor*) – The input node feature embedding.
- **edge_index** (*torch.Tensor*) – Graph edge index in COO format with shape [2, num_edges].
- **edge_weight** (*torch.Tensor*, *optional*) – The one-dimensional relation weight for each edge in *edge_index* (default: None).

class kale.embed.gcn.RGCNEncoderLayer(*in_channels*, *out_channels*, *num_relations*, *num_bases*, *after_relu*, *bias=False*, ***kwargs*)

Bases: MessagePassing

Modification of PyTorch Geometric’s nn.RGCNConv, which reduces the computational and memory cost of RGCN encoder layer for GripNet model. The relational graph convolutional operator from the “Modeling Relational Data with Graph Convolutional Networks” paper.

$$\mathbf{x}'_i = \Theta_{\text{root}} \cdot \mathbf{x}_i + \sum_{r \in \mathcal{R}} \sum_{j \in \mathcal{N}_r(i)} \frac{1}{|\mathcal{N}_r(i)|} \Theta_r \cdot \mathbf{x}_j,$$

where \mathcal{R} denotes the set of relations, *i.e.* edge types. Edge type needs to be a one-dimensional torch.long tensor which stores a relation identifier $\in \{0, \dots, |\mathcal{R}| - 1\}$ for each edge.

Note: For more information please see Pytorch Geometric’s nn.RGCNConv docs.

Parameters

- **in_channels** (*int*) – Size of each input sample.
- **out_channels** (*int*) – Size of each output sample.
- **num_relations** (*int*) – Number of edge relations.
- **num_bases** (*int*) – Use bases-decomposition regularization scheme and num_bases denotes the number of bases.
- **after_relu** (*bool*) – Whether input embedding is activated by relu function or not.
- **bias** (*bool*) – If set to False, the layer will not learn an additive bias. (default: False)
- ****kwargs** (*optional*) – Additional arguments of torch_geometric.nn.conv.MessagePassing.

reset_parameters()

forward(*x*, *edge_index*, *edge_type*, *range_list*)

Parameters

- **x** (*torch.Tensor*) – The input node feature embedding.
- **edge_index** (*torch.Tensor*) – Graph edge index in COO format with shape [2, num_edges].
- **edge_type** (*torch.Tensor*) – The one-dimensional relation type/index for each edge in *edge_index*.
- **range_list** (*torch.Tensor*) – The index range list of each edge type with shape [num_types, 2].

8.5 kale.embed.gripnet module

8.6 kale.embed.image_cnn module

CNNs for extracting features from small images of size 32x32 (e.g. MNIST) and regular images of size 224x224 (e.g. ImageNet). The code is based on <https://github.com/criteo-research/pytorch-ada/blob/master/adalib/ada/models/modules.py>,

which is for domain adaptation.

```
class kale.embed.image_cnn.SmallCNNFeature(num_channels=3, kernel_size=5)
```

Bases: Module

A feature extractor for small 32x32 images (e.g. CIFAR, MNIST) that outputs a feature vector of length 128.

Parameters

- **num_channels** – the number of input channels (default=3).
- **kernel_size** – the size of the convolution kernel (default=5).

Examples::

```
>>> feature_network = SmallCNNFeature(num_channels)
```

forward(input_)

output_size()

training: bool

```
class kale.embed.image_cnn.ResNet18Feature(pretrained=True)
```

Bases: Module

Modified ResNet18 (without the last layer) feature extractor for regular 224x224 images.

Parameters

pretrained (bool) – If True, returns a model pre-trained on ImageNet

Note: Code adapted by pytorch-ada from <https://github.com/thuml/Xlearn/blob/master/pytorch/src/network.py>

forward(x)

output_size()

training: bool

```
class kale.embed.image_cnn.ResNet34Feature(pretrained=True)
```

Bases: Module

Modified ResNet34 (without the last layer) feature extractor for regular 224x224 images.

Parameters

pretrained (bool) – If True, returns a model pre-trained on ImageNet

Note: Code adapted by pytorch-ada from <https://github.com/thuml/Xlearn/blob/master/pytorch/src/network.py>

forward(*x*)

output_size()

training: bool

class kale.embed.image_cnn.**ResNet50Feature**(*pretrained=True*)

Bases: Module

Modified ResNet50 (without the last layer) feature extractor for regular 224x224 images.

Parameters

pretrained (*bool*) – If True, returns a model pre-trained on ImageNet

Note: Code adapted by pytorch-ada from <https://github.com/thuml/Xlearn/blob/master/pytorch/src/network.py>

forward(*x*)

output_size()

training: bool

class kale.embed.image_cnn.**ResNet101Feature**(*pretrained=True*)

Bases: Module

Modified ResNet101 (without the last layer) feature extractor for regular 224x224 images.

Parameters

pretrained (*bool*) – If True, returns a model pre-trained on ImageNet

Note: Code adapted by pytorch-ada from <https://github.com/thuml/Xlearn/blob/master/pytorch/src/network.py>

forward(*x*)

output_size()

training: bool

class kale.embed.image_cnn.**ResNet152Feature**(*pretrained=True*)

Bases: Module

Modified ResNet152 (without the last layer) feature extractor for regular 224x224 images.

Parameters

pretrained (*bool*) – If True, returns a model pre-trained on ImageNet

Note: Code adapted by pytorch-ada from <https://github.com/thuml/Xlearn/blob/master/pytorch/src/network.py>

forward(*x*)

output_size()

training: bool

8.7 kale.embed.positional_encoding module

class kale.embed.positional_encoding.**PositionalEncoding**(*d_model: int, max_len: int = 5000*)

Bases: Module

Implements the positional encoding as described in the NIPS2017 paper ‘Attention Is All You Need’ about Transformers (<https://arxiv.org/abs/1706.03762>). Essentially, for all timesteps in a given sequence, adds information about the relative temporal location of a timestep directly into the features of that timestep, and then returns this slightly-modified, same-shape sequence.

Parameters

- **d_model** – the number of features that each timestep has (required).
- **max_len** – the maximum sequence length that the positional encodings should support (required).

forward(*x*)

Expects input of shape (sequence_length, batch_size, num_features) and returns output of the same shape. sequence_length is at most allowed to be self.max_len and num_features is expected to be exactly self.d_model

Parameters

x – a sequence input of shape (sequence_length, batch_size, num_features) (required).

training: bool

8.8 kale.embed.seq_nn module

DeepDTA based models for drug-target interaction prediction problem.

class kale.embed.seq_nn.**CNNEncoder**(*num_embeddings, embedding_dim, sequence_length, num_kernels, kernel_length*)

Bases: Module

The DeepDTA’s CNN encoder module, which comprises three 1D-convolutional layers and one max-pooling layer. The module is applied to encoding drug/target sequence information, and the input should be transformed information with integer/label encoding. The original paper is “DeepDTA: deep drug–target binding affinity prediction”.

Parameters

- **num_embeddings** (*int*) – Number of embedding labels/categories, depends on the types of encoding sequence.
- **embedding_dim** (*int*) – Dimension of embedding labels/categories.
- **sequence_length** (*int*) – Max length of input sequence.
- **num_kernels** (*int*) – Number of kernels (filters).
- **kernel_length** (*int*) – Length of kernel (filter).

forward(*x*)

training: bool

```
class kale.embed.seq_nn.GCNEncoder(in_channel=78, out_channel=128, dropout_rate=0.2)
```

Bases: Module

The GraphDTA's GCN encoder module, which comprises three graph convolutional layers and one full connected layer. The model is a variant of DeepDTA and is applied to encoding drug molecule graph information. The original paper is “GraphDTA: Predicting drug–target binding affinity with graph neural networks” .

Parameters

- **in_channel** (*int*) – Dimension of each input node feature.
- **out_channel** (*int*) – Dimension of each output node feature.
- **dropout_rate** (*float*) – dropout rate during training.

forward(*x, edge_index, batch*)

training: bool

8.9 kale.embed.video_feature_extractor module

Define the feature extractor for video including I3D, R3D_18, MC3_18 and R2PLUS1D_18 w/o SELayers.

```
kale.embed.video_feature_extractor.get_video_feat_extractor(model_name, image_modality,  
attention, num_classes)
```

Get the feature extractor w/o the pre-trained model and SELayers. The pre-trained models are saved in the path \$XDG_CACHE_HOME/torch/hub/checkpoints/. For Linux, default path is ~/.cache/torch/hub/checkpoints/. For Windows, default path is C:/Users/\$USER_NAME/.cache/torch/hub/checkpoints/. Provide four pre-trained models: “rgb_imagenet”, “flow_imagenet”, “rgb_charades”, “flow_charades”.

Parameters

- **model_name** (*string*) – The name of the feature extractor. (Choices=[“I3D”, “R3D_18”, “R2PLUS1D_18”, “MC3_18”])
- **image_modality** (*string*) – Image type. (Choices=[“rgb”, “flow”, “joint”])
- **attention** (*string*) – The attention type. (Choices=[“SELayerC”, “SELayerT”, “SELayerCoC”, “SELayerMC”, “SELayerCT”, “SELayerTC”, “SELayerMAC”])
- **num_classes** (*int*) – The class number of specific dataset. (Default: No use)

Returns

The network to extract features. **class_feature_dim** (int): The dimension of the feature network output for ClassNet.

It is a convention when the input dimension and the network is fixed.

domain_feature_dim (int): The dimension of the feature network output for DomainNet.

Return type

feature_network (dictionary)

8.10 kale.embed.video_i3d module

Define Inflated 3D ConvNets(I3D) on Action Recognition from <https://ieeexplore.ieee.org/document/8099985> Created by Xianyuan Liu from modifying https://github.com/piergiaj/pytorch-i3d/blob/master/pytorch_i3d.py and <https://github.com/deepmind/kinetics-i3d/blob/master/i3d.py>

```
class kale.embed.video_i3d.MaxPool3dSamePadding(kernel_size: Union[int, Tuple[int, ...]], stride:
Optional[Union[int, Tuple[int, ...]]] = None,
padding: Union[int, Tuple[int, ...]] = 0, dilation:
Union[int, Tuple[int, ...]] = 1, return_indices: bool =
False, ceil_mode: bool = False)
```

Bases: MaxPool3d

Construct 3d max pool with same padding. PyTorch does not provide same padding. Same padding means the output size matches input size for stride=1.

```
compute_pad(dim, s)
```

Get the zero padding number.

```
forward(x)
```

Compute 'same' padding. Add zero to the back position first.

```
kernel_size: Union[int, Tuple[int, int, int]]
```

```
stride: Union[int, Tuple[int, int, int]]
```

```
padding: Union[int, Tuple[int, int, int]]
```

```
dilation: Union[int, Tuple[int, int, int]]
```

```
class kale.embed.video_i3d.Unit3D(in_channels, output_channels, kernel_shape=(1, 1, 1), stride=(1, 1, 1),
padding=0, activation_fn=<function relu>, use_batch_norm=True,
use_bias=False, name='unit_3d'))
```

Bases: Module

Basic unit containing Conv3D + BatchNorm + non-linearity.

```
compute_pad(dim, s)
```

Get the zero padding number.

```
forward(x)
```

Connects the module to inputs. Dynamically pad based on input size in forward function. :param x: Inputs to the Unit3D component.

Returns

Outputs from the module.

```
training: bool
```

```
class kale.embed.video_i3d.InceptionModule(in_channels, out_channels, name)
```

Bases: Module

Construct Inception module. Concatenation after four branches (1x1x1 conv; 1x1x1 + 3x3x3 convs; 1x1x1 + 3x3x3 convs; 3x3x3 max-pool + 1x1x1 conv). In *forward*, we check if SELayers are used, which are channel-wise (SELayerC), temporal-wise (SELayerT), channel-temporal-wise (SELayerTC & SELayerCT).

```
forward(x)
```

training: bool

```
class kale.embed.video_i3d.InceptionI3d(num_classes=400, spatial_squeeze=True,
                                       final_endpoint='Logits', name='inception_i3d', in_channels=3,
                                       dropout_keep_prob=0.5)
```

Bases: Module

Inception-v1 I3D architecture. The model is introduced in:

Quo Vadis, Action Recognition? A New Model and the Kinetics Dataset Joao Carreira, Andrew Zisserman <https://arxiv.org/pdf/1705.07750v1.pdf>.

See also the Inception architecture, introduced in:

Going deeper with convolutions Christian Szegedy, Wei Liu, Yangqing Jia, Pierre Sermanet, Scott Reed, Dragomir Anguelov, Dumitru Erhan, Vincent Vanhoucke, Andrew Rabinovich. <http://arxiv.org/pdf/1409.4842v1.pdf>.

```
VALID_ENDPOINTS = ('Conv3d_1a_7x7', 'MaxPool3d_2a_3x3', 'Conv3d_2b_1x1',
                  'Conv3d_2c_3x3', 'MaxPool3d_3a_3x3', 'Mixed_3b', 'Mixed_3c', 'MaxPool3d_4a_3x3',
                  'Mixed_4b', 'Mixed_4c', 'Mixed_4d', 'Mixed_4e', 'Mixed_4f', 'MaxPool3d_5a_2x2',
                  'Mixed_5b', 'Mixed_5c', 'Logits', 'Predictions')
```

replace_logits(num_classes)

Update the output size with num_classes according to the specific setting.

build()

forward(x)

The output is the result of the final average pooling layer with 1024 dimensions.

extract_features(x)

training: bool

```
kale.embed.video_i3d.i3d(name, num_channels, num_classes, pretrained=False, progress=True)
```

Get InceptionI3d module w/o pretrained model.

```
kale.embed.video_i3d.i3d_joint(rgb_pt, flow_pt, num_classes, pretrained=False, progress=True)
```

Get I3D models for different inputs.

Parameters

- **rgb_pt** (*string, optional*) – the name of pre-trained model for RGB input.
- **flow_pt** (*string, optional*) – the name of pre-trained model for flow input.
- **num_classes** (*int*) – the class number of dataset.
- **pretrained** (*bool*) – choose if pretrained parameters are used. (Default: False)
- **progress** (*bool, optional*) – whether or not to display a progress bar to stderr. (Default: True)

Returns

A dictionary contains RGB and flow models.

Return type

models (dictionary)

8.11 kale.embed.video_res3d module

Define MC3_18, R3D_18, R2plus1D_18 on Action Recognition from <https://arxiv.org/abs/1711.11248> Created by Xianyuan Liu from modifying <https://github.com/pytorch/vision/blob/master/torchvision/models/video/resnet.py>

```
class kale.embed.video_res3d.Conv3DSimple(in_planes, out_planes, midplanes=None, stride=1,  
                                         padding=1)
```

Bases: Conv3d

3D convolutions for R3D (3x3x3 kernel)

```
static get_downsample_stride(stride)
```

```
bias: Optional[Tensor]
```

```
out_channels: int
```

```
kernel_size: Tuple[int, ...]
```

```
stride: Tuple[int, ...]
```

```
padding: Union[str, Tuple[int, ...]]
```

```
dilation: Tuple[int, ...]
```

```
transposed: bool
```

```
output_padding: Tuple[int, ...]
```

```
groups: int
```

```
padding_mode: str
```

```
weight: Tensor
```

```
class kale.embed.video_res3d.Conv2Plus1D(in_planes, out_planes, midplanes, stride=1, padding=1)
```

Bases: Sequential

(2+1)D convolutions for R2plus1D (1x3x3 kernel + 3x1x1 kernel)

```
static get_downsample_stride(stride)
```

```
training: bool
```

```
class kale.embed.video_res3d.Conv3DNoTemporal(in_planes, out_planes, midplanes=None, stride=1,  
                                              padding=1)
```

Bases: Conv3d

3D convolutions without temporal dimension for MCx (1x3x3 kernel)

```
static get_downsample_stride(stride)
```

```
bias: Optional[Tensor]
```

```
out_channels: int
```

```
kernel_size: Tuple[int, ...]
```

```
stride: Tuple[int, ...]
```



```

padding: Union[str, Tuple[int, ...]]
dilation: Tuple[int, ...]
transposed: bool
output_padding: Tuple[int, ...]
groups: int
padding_mode: str
weight: Tensor

```

```
class kale.embed.video_res3d.BasicBlock(inplanes, planes, conv_builder, stride=1, downsample=None)
```

Bases: Module

Basic ResNet building block. Each block consists of two convolutional layers with a ReLU activation function after each layer and residual connections. In *forward*, we check if SELayers are used, which are channel-wise (SELayerC) and temporal-wise (SELayerT).

```
expansion = 1
```

```
forward(x)
```

```
training: bool
```

```
class kale.embed.video_res3d.Bottleneck(inplanes, planes, conv_builder, stride=1, downsample=None)
```

Bases: Module

BottleNeck building block. Default: No use. Each block consists of two $1*n*n$ and one $n*n*n$ convolutional layers with a ReLU activation function after each layer and residual connections.

```
expansion = 4
```

```
forward(x)
```

```
training: bool
```

```
class kale.embed.video_res3d.BasicStem
```

Bases: Sequential

The default conv-batchnorm-relu stem. The first layer normally. (64 $3x7x7$ kernels)

```
training: bool
```

```
class kale.embed.video_res3d.BasicFlowStem
```

Bases: Sequential

The default stem for optical flow.

```
training: bool
```

```
class kale.embed.video_res3d.R2Plus1dStem
```

Bases: Sequential

R(2+1)D stem is different than the default one as it uses separated 3D convolution. (45 $1x7x7$ kernels + 64 $3x1x1$ kernel)

```
training: bool
```

class kale.embed.video_res3d.R2Plus1dFlowStem

Bases: Sequential

R(2+1)D stem for optical flow.

training: bool

class kale.embed.video_res3d.VideoResNet(*block, conv_makers, layers, stem, num_classes=400, zero_init_residual=False*)

Bases: Module

replace_fc(*num_classes, block=<class 'kale.embed.video_res3d.BasicBlock'>*)

Update the output size with num_classes according to the specific setting.

forward(*x*)

training: bool

kale.embed.video_res3d.r3d_18_rgb(*pretrained=False, progress=True, **kwargs*)

Construct 18 layer Resnet3D model for RGB as in <https://arxiv.org/abs/1711.11248>

Parameters

- **pretrained** (*bool*) – If True, returns a model pre-trained on Kinetics-400
- **progress** (*bool*) – If True, displays a progress bar of the download to stderr

Returns

R3D-18 network

Return type

nn.Module

kale.embed.video_res3d.r3d_18_flow(*pretrained=False, progress=True, **kwargs*)

Construct 18 layer Resnet3D model for optical flow.

kale.embed.video_res3d.mc3_18_rgb(*pretrained=False, progress=True, **kwargs*)

Constructor for 18 layer Mixed Convolution network for RGB as in <https://arxiv.org/abs/1711.11248>

Parameters

- **pretrained** (*bool*) – If True, returns a model pre-trained on Kinetics-400
- **progress** (*bool*) – If True, displays a progress bar of the download to stderr

Returns

MC3 Network definition

Return type

nn.Module

kale.embed.video_res3d.mc3_18_flow(*pretrained=False, progress=True, **kwargs*)

Constructor for 18 layer Mixed Convolution network for optical flow.

kale.embed.video_res3d.r2plus1d_18_rgb(*pretrained=False, progress=True, **kwargs*)

Constructor for the 18 layer deep R(2+1)D network for RGB as in <https://arxiv.org/abs/1711.11248>

Parameters

- **pretrained** (*bool*) – If True, returns a model pre-trained on Kinetics-400
- **progress** (*bool*) – If True, displays a progress bar of the download to stderr

Returns

R(2+1)D-18 network

Return type

nn.Module

`kale.embed.video_res3d.r2plus1d_18_flow(pretrained=False, progress=True, **kwargs)`

Constructor for the 18 layer deep R(2+1)D network for optical flow.

`kale.embed.video_res3d.r3d(rgb=False, flow=False, pretrained=False, progress=True)`

Get R3D_18 models.

`kale.embed.video_res3d.mc3(rgb=False, flow=False, pretrained=False, progress=True)`

Get MC3_18 models.

`kale.embed.video_res3d.r2plus1d(rgb=False, flow=False, pretrained=False, progress=True)`

Get R2PLUS1D_18 models.

8.12 kale.embed.video_selayer module

Python implementation of Squeeze-and-Excitation Layers (SELayer) Initial implementation: channel-wise (SELayerC) Improved implementation: temporal-wise (SELayerT), convolution-based channel-wise (SELayerCoC), max-pooling-based channel-wise (SELayerMC), multi-pooling-based channel-wise (SELayerMAC)

[Redundancy and repeat of code will be reduced in the future.]

References

Hu Jie, Li Shen, and Gang Sun. “Squeeze-and-excitation networks.” In CVPR, pp. 7132-7141. 2018. For initial implementation, please go to <https://github.com/hujie-frank/SENet>

`kale.embed.video_selayer.get_selayer(attention)`

Get SELayers referring to attention.

Parameters

attention (*string*) – the name of the SELayer. (Options: [“SELayerC”, “SELayerT”, “SELayerCoC”, “SELayerMC”, “SELayerMAC”])

Returns

the SELayer.

Return type

se_layer (*SELayer*, optional)

class `kale.embed.video_selayer.SELayer(channel, reduction=16)`

Bases: Module

Helper class for SELayer design.

forward(*x*)

training: bool

class `kale.embed.video_selayer.SELayerC(channel, reduction=16)`

Bases: *SELayer*

Construct channel-wise SELayer.

forward(*x*)

training: bool

class kale.embed.video_selayer.**SELayerT**(*channel, reduction=2*)

Bases: *SELayer*

Construct temporal-wise SELayer.

forward(*x*)

training: bool

class kale.embed.video_selayer.**SELayerCoC**(*channel, reduction=16*)

Bases: *SELayer*

Construct convolution-based channel-wise SELayer.

forward(*x*)

training: bool

class kale.embed.video_selayer.**SELayerMC**(*channel, reduction=16*)

Bases: *SELayer*

Construct channel-wise SELayer with max pooling.

forward(*x*)

training: bool

class kale.embed.video_selayer.**SELayerMAC**(*channel, reduction=16*)

Bases: *SELayer*

Construct channel-wise SELayer with the mix of average pooling and max pooling.

forward(*x*)

training: bool

8.13 kale.embed.video_se_i3d module

Add SELayers to I3D

class kale.embed.video_se_i3d.**SEInceptionI3DRGB**(*num_channels, num_classes, attention*)

Bases: *Module*

Add the several SELayers to I3D for RGB input. :param num_channels: the channel number of the input. :type num_channels: int :param num_classes: the class number of dataset. :type num_classes: int :param attention: the name of the SELayer.

(Options: ["SELayerC", "SELayerT", "SELayerCoC", "SELayerMC", "SELayerMAC", "SELayerCT" and "SELayerTC"])

Returns

I3D model with SELayers.

Return type

model (*VideoResNet*)

forward(*x*)

training: bool

class kale.embed.video_se_i3d.**SEInceptionI3DFlow**(*num_channels, num_classes, attention*)

Bases: Module

Add the several SELayers to I3D for optical flow input.

forward(*x*)

training: bool

kale.embed.video_se_i3d.**se_inception_i3d**(*name, num_channels, num_classes, attention, pretrained=False, progress=True, rgb=True*)

Get InceptionI3d module w/o SELayer and pretrained model.

kale.embed.video_se_i3d.**se_i3d_joint**(*rgb_pt, flow_pt, num_classes, attention, pretrained=False, progress=True*)

Get I3D models with SELayers for different inputs.

Parameters

- **rgb_pt** (*string, optional*) – the name of pre-trained model for RGB input.
- **flow_pt** (*string, optional*) – the name of pre-trained model for optical flow input.
- **num_classes** (*int*) – the class number of dataset.
- **attention** (*string, optional*) – the name of the SELayer.
- **pretrained** (*bool*) – choose if pretrained parameters are used. (Default: False)
- **progress** (*bool, optional*) – whether or not to display a progress bar to stderr. (Default: True)

Returns

A dictionary contains models for RGB and optical flow.

Return type

models (dictionary)

8.14 kale.embed.video_se_res3d module

Add SELayers to MC3_18, R3D_18, R2plus1D_18

kale.embed.video_se_res3d.**se_r3d_18_rgb**(*attention, pretrained=False, progress=True, **kwargs*)

kale.embed.video_se_res3d.**se_r3d_18_flow**(*attention, pretrained=False, progress=True, **kwargs*)

kale.embed.video_se_res3d.**se_mc3_18_rgb**(*attention, pretrained=False, progress=True, **kwargs*)

kale.embed.video_se_res3d.**se_mc3_18_flow**(*attention, pretrained=False, progress=True, **kwargs*)

kale.embed.video_se_res3d.**se_r2plus1d_18_rgb**(*attention, pretrained=False, progress=True, **kwargs*)

kale.embed.video_se_res3d.**se_r2plus1d_18_flow**(*attention, pretrained=False, progress=True, **kwargs*)

`kale.embed.video_se_res3d.se_r3d(attention, rgb=False, flow=False, pretrained=False, progress=True)`

Get R3D_18 models with SELayers for different inputs.

Parameters

- **attention** (*string*) – the name of the SELayer.
- **rgb** (*bool*) – choose if RGB model is needed. (Default: False)
- **flow** (*bool*) – choose if optical flow model is needed. (Default: False)
- **pretrained** (*bool*) – choose if pretrained parameters are used. (Default: False)
- **progress** (*bool, optional*) – whether or not to display a progress bar to stderr. (Default: True)

Returns

A dictionary contains models for RGB and optical flow.

Return type

models (dictionary)

`kale.embed.video_se_res3d.se_mc3(attention, rgb=False, flow=False, pretrained=False, progress=True)`

Get MC3_18 models with SELayers for different inputs.

`kale.embed.video_se_res3d.se_r2plus1d(attention, rgb=False, flow=False, pretrained=False, progress=True)`

Get R2+1D_18 models with SELayers for different inputs.

8.15 Module contents

9.1 Submodules

9.2 `kale.predict.class_domain_nets` module

Classification of data or domain

Modules for typical classification tasks (into class labels) and adversarial discrimination of source vs target domains, from <https://github.com/criteo-research/pytorch-ada/blob/master/adalib/ada/models/modules.py>

```
class kale.predict.class_domain_nets.SoftmaxNet(input_dim=15, n_classes=2, name='c', hidden=(),
                                               activation_fn=<class
                                               'torch.nn.modules.activation.ReLU'>,
                                               **activation_args)
```

Bases: Module

Regular and domain classifier network for regular-size images

Parameters

- **input_dim** (*int*, *optional*) – the dimension of the final feature vector.. Defaults to 15.
- **n_classes** (*int*, *optional*) – the number of classes. Defaults to 2.
- **name** (*str*, *optional*) – the classifier name. Defaults to “c”.
- **hidden** (*tuple*, *optional*) – the hidden layer sizes. Defaults to ().
- **activation_fn** (*[type]*, *optional*) – the activation function. Defaults to nn.ReLU.

forward(*input_data*)

extra_repr()

n_classes()

training: bool

```
class kale.predict.class_domain_nets.ClassNetSmallImage(input_size=128, n_class=10)
```

Bases: Module

Regular classifier network for small-size images

Parameters

- **input_size** (*int*, *optional*) – the dimension of the final feature vector. Defaults to 128.
- **n_class** (*int*, *optional*) – the number of classes. Defaults to 10.

n_classes()

forward(*input*)

training: bool

class kale.predict.class_domain_nets.**DomainNetSmallImage**(*input_size=128, bigger_discrim=False*)

Bases: Module

Domain classifier network for small-size images

Parameters

- **input_size** (*int, optional*) – the dimension of the final feature vector. Defaults to 128.
- **bigger_discrim** (*bool, optional*) – whether to use deeper network. Defaults to False.

forward(*input*)

training: bool

class kale.predict.class_domain_nets.**ClassNetVideo**(*input_size=512, n_channel=100, dropout_keep_prob=0.5, n_class=8*)

Bases: Module

Regular classifier network for video input.

Parameters

- **input_size** (*int, optional*) – the dimension of the final feature vector. Defaults to 512.
- **n_channel** (*int, optional*) – the number of channel for Linear and BN layers.
- **dropout_keep_prob** (*int, optional*) – the dropout probability for keeping the parameters.
- **n_class** (*int, optional*) – the number of classes. Defaults to 8.

n_classes()

forward(*input*)

training: bool

class kale.predict.class_domain_nets.**ClassNetVideoConv**(*input_size=1024, n_class=8*)

Bases: Module

Classifier network for video input refer to MMSADA.

Parameters

- **input_size** (*int, optional*) – the dimension of the final feature vector. Defaults to 1024.
- **n_class** (*int, optional*) – the number of classes. Defaults to 8.

References

Munro Jonathan, and Dima Damen. “Multi-modal domain adaptation for fine-grained action recognition.” In CVPR, pp. 122-132. 2020.

forward(*input*)

training: bool

class kale.predict.class_domain_nets.**DomainNetVideo**(*input_size=128, n_channel=100*)

Bases: Module

Regular domain classifier network for video input.

Parameters

- **input_size** (*int, optional*) – the dimension of the final feature vector. Defaults to 512.
- **n_channel** (*int, optional*) – the number of channel for Linear and BN layers.

forward(*input*)

training: bool

9.3 kale.predict.isonet module

The ISONet module, which is based on the ResNet module, from <https://github.com/HaozhiQi/ISONet/blob/master/isonet/models/isonet.py> (based on <https://github.com/facebookresearch/pycls/blob/master/pycls/models/resnet.py>)

kale.predict.isonet.**get_trans_fun**(*name*)

Retrieves the transformation function by name.

class kale.predict.isonet.**SReLU**(*nc*)

Bases: Module

Shifted ReLU

forward(*x*)

training: bool

class kale.predict.isonet.**ResHead**(*w_in, net_params*)

Bases: Module

ResNet head.

forward(*x*)

training: bool

class kale.predict.isonet.**BasicTransform**(*w_in, w_out, stride, has_bn, use_srelu, w_b=None, num_gs=1*)

Bases: Module

Basic transformation: 3x3, 3x3

forward(*x*)

training: bool

```
class kale.predict.isonet.BottleneckTransform(w_in, w_out, stride, has_bn, use_srelu, w_b, num_gs)
```

Bases: Module

Bottleneck transformation: 1x1, 3x3, 1x1, only for very deep networks

```
forward(x)
```

```
training: bool
```

```
class kale.predict.isonet.ResBlock(w_in, w_out, stride, trans_fun, has_bn, has_st, use_srelu, w_b=None, num_gs=1)
```

Bases: Module

Residual block: $x + F(x)$

```
forward(x)
```

```
training: bool
```

```
class kale.predict.isonet.ResStage(w_in, w_out, stride, net_params, d, w_b=None, num_gs=1)
```

Bases: Module

Stage of ResNet.

```
forward(x)
```

```
training: bool
```

```
class kale.predict.isonet.ResStem(w_in, w_out, net_params, kernelsize=3, stride=1, padding=1, use_maxpool=False, poolsize=3, poolstride=2, poolpadding=1)
```

Bases: Module

Stem of ResNet.

```
forward(x)
```

```
training: bool
```

```
class kale.predict.isonet.ISONet(net_params)
```

Bases: Module

ISONet, a modified ResNet model.

```
forward(x)
```

```
ortho(device)
```

regularizes the convolution kernel to be (near) orthogonal during training. This is called in Trainer.loss of the isonet example.

```
ortho_conv(m, device)
```

regularizes the convolution kernel to be (near) orthogonal during training.

Parameters

m (*nn.Module*) – [description]

```
training: bool
```

9.4 kale.predict.losses module

Commonly used losses, from domain adaptation package <https://github.com/criteo-research/pytorch-ada/blob/master/adalib/ada/models/losses.py>

`kale.predict.losses.cross_entropy_logits(linear_output, label, weights=None)`

Computes cross entropy with logits

Examples

See DANN, WDGRL, and MMD trainers in `kale.pipeline.domain_adapter`

`kale.predict.losses.topk_accuracy(output, target, topk=(1,))`

Computes the top-k accuracy for the specified values of k.

Parameters

- **output** (*Tensor*) – Generated predictions. Shape: (batch_size, class_count).
- **target** (*Tensor*) – Ground truth. Shape: (batch_size)
- **topk** (*tuple(int)*) – Compute accuracy at top-k for the values of k specified in this parameter.

Returns

A list of tensors of the same length as topk. Each tensor consists of boolean variables to show if this prediction ranks top k with each value of k. True means the prediction ranks top k and False means not. The shape of tensor is batch_size, i.e. the number of predictions.

Return type

list(Tensor)

Examples

```
>>> output = torch.tensor([[0.3, 0.2, 0.1], [0.3, 0.2, 0.1]])
>>> target = torch.tensor([0, 1])
>>> top1, top2 = topk_accuracy(output, target, topk=(1, 2)) # get the boolean value
>>> top1_value = top1.double().mean() # get the top 1 accuracy score
>>> top2_value = top2.double().mean() # get the top 2 accuracy score
```

`kale.predict.losses.multitask_topk_accuracy(output, target, topk=(1,))`

Computes the top-k accuracy for the specified values of k for multitask input.

Parameters

- **output** (*tuple(Tensor)*) – A tuple of generated predictions. Each tensor is of shape [batch_size, class_count], class_count can vary per task basis, i.e. outputs[i].shape[1] can differ from outputs[j].shape[1].
- **target** (*tuple(Tensor)*) – A tuple of ground truth. Each tensor is of shape [batch_size]
- **topk** (*tuple(int)*) – Compute accuracy at top-k for the values of k specified in this parameter.

Returns

A list of tensors of the same length as topk. Each tensor consists of boolean variables to show if predictions of multitask ranks top k with each value of k. True means predictions of this output

for all tasks ranks top k and False means not. The shape of tensor is batch_size, i.e. the number of predictions.

Examples

```
>>> first_output = torch.tensor([[0.3, 0.2, 0.1], [0.3, 0.2, 0.1]])
>>> first_target = torch.tensor((0, 2))
>>> second_output = torch.tensor([[0.2, 0.1], [0.2, 0.1]])
>>> second_target = torch.tensor((0, 1))
>>> output = (first_output, second_output)
>>> target = (first_target, second_target)
>>> top1, top2 = multitask_topk_accuracy(output, target, topk=(1, 2)) # ↪
↪ get the boolean value
>>> top1_value = top1.double().mean() # get the top 1 accuracy score
>>> top2_value = top2.double().mean() # get the top 2 accuracy score
```

Return type

list(Tensor)

kale.predict.losses.**entropy_logits**(linear_output)

Computes entropy logits in CDAN with entropy conditioning (CDAN+E)

Examples

See CDANTrainer in kale.pipeline.domain_adapter

kale.predict.losses.**entropy_logits_loss**(linear_output)

Computes entropy logits loss in semi-supervised or few-shot domain adaptation

Examples

See FewShotDANNTrainer in kale.pipeline.domain_adapter

kale.predict.losses.**gradient_penalty**(critic, h_s, h_t)

Computes gradient penalty in Wasserstein distance guided representation learning

Examples

See WDGRLTrainer and WDGRLTrainerMod in kale.pipeline.domain_adapter

kale.predict.losses.**gaussian_kernel**(source, target, kernel_mul=2.0, kernel_num=5, fix_sigma=None)

Code from XLearn: computes the full kernel matrix, which is less than optimal since we don't use all of it with the linear MMD estimate.

Examples

See DANTrainer and JANTrainer in `kale.pipeline.domain_adapter`

`kale.predict.losses.compute_mmd_loss(kernel_values, batch_size)`

Computes the Maximum Mean Discrepancy (MMD) between domains.

Examples

See DANTrainer and JANTrainer in `kale.pipeline.domain_adapter`

`kale.predict.losses.hsic(kx, ky, device)`

Perform independent test with Hilbert-Schmidt Independence Criterion (HSIC) between two sets of variables x and y .

Parameters

- **kx** (*2-D tensor*) – kernel matrix of x , shape (n_samples, n_samples)
- **ky** (*2-D tensor*) – kernel matrix of y , shape (n_samples, n_samples)
- **device** (*torch.device*) – the desired device of returned tensor

Returns

Independent test score ≥ 0

Return type

[tensor]

Reference:

[1] Gretton, Arthur, Bousquet, Olivier, Smola, Alex, and Schölkopf, Bernhard. **Measuring Statistical Dependence** with Hilbert-Schmidt Norms. In *Algorithmic Learning Theory (ALT)*, pp. 63–77. 2005.

[2] Gretton, Arthur, Fukumizu, Kenji, Teo, Choon H., Song, Le, Schölkopf, Bernhard, and Smola, Alex J. **A Kernel Statistical Test of Independence**. In *Advances in Neural Information Processing Systems*, pp. 585–592. 2008.

`kale.predict.losses.euclidean(x1, x2)`

Compute the Euclidean distance

Parameters

- **x1** (*torch.Tensor*) – variables set 1
- **x2** (*torch.Tensor*) – variables set 2

Returns

Euclidean distance

Return type

`torch.Tensor`

9.5 kale.predict.decode module

`class kale.predict.decode.MLPDecoder(in_dim, hidden_dim, out_dim, dropout_rate=0.1)`

Bases: Module

The MLP decoder module, which comprises four fully connected neural networks. It's a common decoder for decoding drug-target encoding information.

Parameters

- **in_dim** (*int*) – Dimension of input feature.
- **hidden_dim** (*int*) – Dimension of hidden layers.
- **out_dim** (*int*) – Dimension of output layer.
- **dropout_rate** (*float*) – dropout rate during training.

`forward(x)`

`training: bool`

9.6 Module contents

EVALUATE

10.1 Submodules

10.2 `kale.evaluate.metrics` module

`kale.evaluate.metrics.concord_index(y, y_pred)`

Calculate the Concordance Index (CI), which is a metric to measure the proportion of [concordant pairs](#) between real and predict values.

Parameters

- `y` (*array*) – real values.
- `y_pred` (*array*) – predicted values.

10.3 Module contents

11.1 Submodules

11.2 `kale.interpret.model_weights` module

`kale.interpret.model_weights.select_top_weight(weights, select_ratio: float = 0.05)`

Select top weights in magnitude, and the rest of weights will be zeros

Parameters

- **weights** (*array-like*) – model weights, can be a vector or a higher order tensor
- **select_ratio** (*float, optional*) – ratio of top weights to be selected. Defaults to 0.05.

Returns

top weights in the same shape with the input model weights

Return type

array-like

11.3 `kale.interpret.visualize` module

`kale.interpret.visualize.plot_weights(weight_img, background_img=None, color_marker_pos='rs', color_marker_neg='gs', im_kwargs=None, marker_kwargs=None)`

Visualize model weights

Parameters

- **weight_img** (*array-like*) – Model weight/coefficients in 2D, could be a 2D slice of a 3D or higher order tensor.
- **background_img** (*array-like, optional*) – 2D background image. Defaults to None.
- **color_marker_pos** (*str, optional*) – Color and marker for weights in positive values. Defaults to red “rs”.
- **color_marker_neg** (*str, optional*) – Color and marker for weights in negative values. Defaults to blue “gs”.
- **im_kwargs** (*dict, optional*) – Keyword arguments for background images. Defaults to None.
- **marker_kwargs** (*dict, optional*) – Keyword arguments for background images. Defaults to None.

Returns

Figure to plot.

Return type

[matplotlib.figure.Figure]

`kale.interpret.visualize.plot_multi_images(images, n_cols=1, n_rows=None, marker_locs=None, image_titles=None, marker_titles=None, marker_cmap=None, figsize=None, im_kwargs=None, marker_kwargs=None, legend_kwargs=None, title_kwargs=None)`

Plot multiple images with markers in one figure.

Parameters

- **images** (*array-like*) – Images to plot, shape(n_samples, dim1, dim2)
- **n_cols** (*int, optional*) – Number of columns for plotting multiple images. Defaults to 1.
- **n_rows** (*int, optional*) – Number of rows for plotting multiple images. If None, n_rows = n_samples / n_cols.
- **marker_locs** (*array-like, optional*) – Locations of markers, shape (n_samples, 2 * n_markers). Defaults to None.
- **marker_titles** (*list, optional*) – Names of the markers, where len(marker_names) == n_markers. Defaults to None.
- **marker_cmap** (*str, optional*) – Name of the color map used for plotting markers. Default to None.
- **image_titles** (*list, optional*) – List of title for each image, where len(image_names) == n_samples. Defaults to None.
- **figsize** (*tuple, optional*) – Figure size. Defaults to None.
- **im_kwargs** (*dict, optional*) – Keyword arguments for plotting images. Defaults to None.
- **marker_kwargs** (*dict, optional*) – Keyword arguments for markers. Defaults to None.
- **legend_kwargs** (*dict, optional*) – Keyword arguments for legend. Defaults to None.
- **title_kwargs** (*dict, optional*) – Keyword arguments for title. Defaults to None.

Returns

Figure to plot.

Return type

[matplotlib.figure.Figure]

`kale.interpret.visualize.distplot_1d(data, labels=None, xlabel=None, ylabel=None, title=None, figsize=None, colors=None, title_kwargs=None, hist_kwargs=None)`

Plot distribution of 1D data.

Parameters

- **data** (*array-like or list*) – Data to plot.
- **labels** (*list, optional*) – List of labels for each data. Defaults to None.
- **xlabel** (*str, optional*) – Label for x-axis. Defaults to None.

- **ylabel** (*str*, *optional*) – Label for y-axis. Defaults to None.
- **title** (*str*, *optional*) – Title of the plot. Defaults to None.
- **figsize** (*tuple*, *optional*) – Figure size. Defaults to None.
- **colors** (*str*, *optional*) – Color of the line. Defaults to None.
- **title_kwargs** (*dict*, *optional*) – Keyword arguments for title. Defaults to None.
- **hist_kwargs** (*dict*, *optional*) – Keyword arguments for histogram. Defaults to None.

Returns

Figure to plot.

Return type

[matplotlib.figure.Figure]

11.4 Module contents

12.1 Submodules

12.2 kale.pipeline.deepdta module

```
class kale.pipeline.deepdta.BaseDTATrainer(drug_encoder, target_encoder, decoder, lr=0.001,  
                                           ci_metric=False, **kwargs)
```

Bases: `LightningModule`

Base class for all drug target encoder-decoder architecture models, which is based on pytorch lightning wrapper, for more details about pytorch lightning, please check <https://github.com/PyTorchLightning/pytorch-lightning>. If you inherit from this class, a forward pass function must be implemented.

Parameters

- **drug_encoder** – drug information encoder.
- **target_encoder** – target information encoder.
- **decoder** – drug-target representations decoder.
- **lr** – learning rate. (default: 0.001)
- **ci_metric** – calculate the Concordance Index (CI) metric, and the operation is time-consuming for large-scale
- **(default (dataset.))** – False)

configure_optimizers()

Config adam as default optimizer.

forward(*x_drug, x_target*)

Same as `torch.nn.Module.forward()`

training_step(*train_batch, batch_idx*)

Compute and return the training loss on one step

validation_step(*valid_batch, batch_idx*)

Compute and return the validation loss on one step

test_step(*test_batch, batch_idx*)

Compute and return the test loss on one step

training: bool

```
class kale.pipeline.deepdta.DeepDTATrainer(drug_encoder, target_encoder, decoder, lr=0.001,
                                           ci_metric=False, **kwargs)
```

Bases: *BaseDTATrainer*

An implementation of DeepDTA model based on BaseDTATrainer. :param drug_encoder: drug CNN encoder. :param target_encoder: target CNN encoder. :param decoder: drug-target MLP decoder. :param lr: learning rate.

```
forward(x_drug, x_target)
```

Forward propagation in DeepDTA architecture.

Parameters

- **x_drug** – drug sequence encoding.
- **x_target** – target protein sequence encoding.

```
validation_step(valid_batch, batch_idx)
```

```
training: bool
```

```
precision: int
```

```
prepare_data_per_node: bool
```

```
allow_zero_length_dataloader_with_multiple_devices: bool
```

12.3 kale.pipeline.domain_adapter module

Domain adaptation systems (pipelines) with three types of architectures

This module takes individual modules as input and organises them into an architecture. This is taken directly from <https://github.com/criteo-research/pytorch-ada/blob/master/adalib/ada/models/architectures.py> with minor changes.

This module uses [PyTorch Lightning](#) to standardize the flow.

```
class kale.pipeline.domain_adapter.GradReverse(*args, **kwargs)
```

Bases: *Function*

The gradient reversal layer (GRL)

This is defined in the DANN paper <http://jmlr.org/papers/volume17/15-239/15-239.pdf>

Forward pass: identity transformation. Backward propagation: flip the sign of the gradient.

From <https://github.com/criteo-research/pytorch-ada/blob/master/adalib/ada/models/layers.py>

```
static forward(ctx, x, alpha)
```

```
static backward(ctx, grad_output)
```

```
kale.pipeline.domain_adapter.set_requires_grad(model, requires_grad=True)
```

Configure whether gradients are required for a model

```
kale.pipeline.domain_adapter.get_aggregated_metrics(metric_name_list, metric_outputs)
```

Get a dictionary of the mean metric values (to log) from metric names and their values

```
kale.pipeline.domain_adapter.get_aggregated_metrics_from_dict(input_metric_dict)
```

Get a dictionary of the mean metric values (to log) from a dictionary of metric values

`kale.pipeline.domain_adapter.get_metrics_from_parameter_dict(parameter_dict, device)`

Get a key-value pair from the hyperparameter dictionary

class `kale.pipeline.domain_adapter.Method(value)`

Bases: Enum

Lists the available methods. Provides a few methods that group the methods by type.

Source = 'Source'

DANN = 'DANN'

CDAN = 'CDAN'

CDAN_E = 'CDAN-E'

FSDANN = 'FSDANN'

MME = 'MME'

WDGRL = 'WDGRL'

WDGRLMod = 'WDGRLMod'

DAN = 'DAN'

JAN = 'JAN'

is_mmd_method()

is_dann_method()

is_cdan_method()

is_fewshot_method()

allow_supervised()

`kale.pipeline.domain_adapter.create_mmd_based(method: Method, dataset, feature_extractor, task_classifier, **train_params)`

MMD-based deep learning methods for domain adaptation: DAN and JAN

`kale.pipeline.domain_adapter.create_dann_like(method: Method, dataset, feature_extractor, task_classifier, critic, **train_params)`

DANN-based deep learning methods for domain adaptation: DANN, CDAN, CDAN+E

`kale.pipeline.domain_adapter.create_fewshot_trainer(method: Method, dataset, feature_extractor, task_classifier, critic, **train_params)`

DANN-based few-shot deep learning methods for domain adaptation: FSDANN, MME

class `kale.pipeline.domain_adapter.BaseAdaptTrainer(dataset, feature_extractor, task_classifier, method: Optional[str] = None, lambda_init: float = 1.0, adapt_lambda: bool = True, adapt_lr: bool = True, nb_init_epochs: int = 10, nb_adapt_epochs: int = 50, batch_size: int = 32, init_lr: float = 0.001, optimizer: Optional[dict] = None)`

Bases: `LightningModule`

Base class for all domain adaptation architectures.

This class implements the classic building blocks used in all the derived architectures for domain adaptation. If you inherit from this class, you will have to implement only:

- a forward pass
- a `compute_loss` function that returns the task loss \mathcal{L}_c and adaptation loss

\mathcal{L}_a , as well as a dictionary for summary statistics and other metrics you may want to have access to.

The default training step uses only the task loss \mathcal{L}_c during warmup, then uses the loss defined as:

$$\mathcal{L} = \mathcal{L}_c + \lambda \mathcal{L}_a,$$

where λ will follow the schedule defined by the DANN paper:

$$\lambda_p = \frac{2}{1 + \exp(-\gamma \cdot p)} - 1 \text{ where } p \text{ the learning progress changes linearly from 0 to 1.}$$

Parameters

- **dataset** (`kale.loaddata.multi_domain`) – the multi-domain datasets to be used for train, validation, and tests.
- **feature_extractor** (`torch.nn.Module`) – the feature extractor network (mapping inputs $x \in \mathcal{X}$ to a latent space \mathcal{Z} .)
- **task_classifier** (`torch.nn.Module`) – the task classifier network that learns to predict labels $y \in \mathcal{Y}$ from latent vectors,
- **method** (`Method`, *optional*) – the method implemented by the class. Defaults to `None`. Mostly useful when several methods may be implemented using the same class.
- **lambda_init** (`float`, *optional*) – Weight attributed to the adaptation part of the loss. Defaults to 1.0.
- **adapt_lambda** (`bool`, *optional*) – Whether to make lambda grow from 0 to 1 following the schedule from the DANN paper. Defaults to `True`.
- **adapt_lr** (`bool`, *optional*) – Whether to use the schedule for the learning rate as defined in the DANN paper. Defaults to `True`.
- **nb_init_epochs** (`int`, *optional*) – Number of warmup epochs (during which $\lambda=0$, training only on the source). Defaults to 10.
- **nb_adapt_epochs** (`int`, *optional*) – Number of training epochs. Defaults to 50.
- **batch_size** (`int`, *optional*) – Defaults to 32.
- **init_lr** (`float`, *optional*) – Initial learning rate. Defaults to 1e-3.
- **optimizer** (`dict`, *optional*) – Optimizer parameters, a dictionary with 2 keys: “type”: a string in (“SGD”, “Adam”, “AdamW”) “optim_params”: kwargs for the above PyTorch optimizer. Defaults to `None`.

property method

`get_parameters_watch_list()`

Update this list for parameters to watch while training (ie log with MLFlow)

`forward(x)`

compute_loss(*batch*, *split_name='valid'*)

Define the loss of the model

Parameters

- **batch** (*tuple*) – batches returned by the MultiDomainLoader.
- **split_name** (*str*, *optional*) – learning stage (one of [“train”, “valid”, “test”]). Defaults to “valid” for validation. “train” is for training and “test” for testing. This is currently used only for naming the metrics used for logging.

Returns

a 3-element tuple with task_loss, adv_loss, log_metrics. log_metrics should be a dictionary.

Raises

NotImplementedError – children of this classes should implement this method.

training_step(*batch*, *batch_nb*)

The most generic of training steps

Parameters

- **batch** (*tuple*) – the batch as returned by the MultiDomainLoader dataloader iterator: 2 tuples: (x_source, y_source), (x_target, y_target) in the unsupervised setting 3 tuples: (x_source, y_source), (x_target_labeled, y_target_labeled), (x_target_unlabeled, y_target_unlabeled) in the semi-supervised setting
- **batch_nb** (*int*) – id of the current batch.

Returns

must contain a “loss” key with the loss to be used for back-propagation.
see pytorch-lightning for more details.

Return type

dict

validation_step(*batch*, *batch_nb*)

validation_epoch_end(*outputs*)

test_step(*batch*, *batch_nb*)

test_epoch_end(*outputs*)

configure_optimizers()

train_dataloader()

val_dataloader()

test_dataloader()

training: bool

class kale.pipeline.domain_adapter.**BaseDANNLike**(*dataset*, *feature_extractor*, *task_classifier*, *critic*,
alpha=1.0, *entropy_reg=0.0*, *adapt_reg=True*,
batch_reweighting=False, ***base_params*)

Bases: [BaseAdaptTrainer](#)

Common API for DANN-based methods: DANN, CDAN, CDAN+E, WDGRL, MME, FSDANN

get_parameters_watch_list()

Update this list for parameters to watch while training (ie log with MLFlow)

compute_loss(*batch*, *split_name='valid'*)

validation_epoch_end(*outputs*)

test_epoch_end(*outputs*)

training: bool

precision: int

prepare_data_per_node: bool

allow_zero_length_dataloader_with_multiple_devices: bool

class kale.pipeline.domain_adapter.**DANNTrainer**(*dataset, feature_extractor, task_classifier, critic,*
*method=None, **base_params*)

Bases: *BaseDANNLike*

This class implements the DANN architecture from Ganin, Yaroslav, et al. “Domain-adversarial training of neural networks.” The Journal of Machine Learning Research (2016) <https://arxiv.org/abs/1505.07818>

forward(*x*)

training: bool

precision: int

prepare_data_per_node: bool

allow_zero_length_dataloader_with_multiple_devices: bool

class kale.pipeline.domain_adapter.**CDANTrainer**(*dataset, feature_extractor, task_classifier, critic,*
use_entropy=False, use_random=False,
*random_dim=1024, **base_params*)

Bases: *BaseDANNLike*

Implements CDAN: Long, Mingsheng, et al. “Conditional adversarial domain adaptation.” Advances in Neural Information Processing Systems. 2018. <https://papers.nips.cc/paper/7436-conditional-adversarial-domain-adaptation.pdf>

forward(*x*)

compute_loss(*batch, split_name='valid'*)

training: bool

precision: int

prepare_data_per_node: bool

allow_zero_length_dataloader_with_multiple_devices: bool

class kale.pipeline.domain_adapter.**WDGRLTrainer**(*dataset, feature_extractor, task_classifier, critic,*
k_critic=5, gamma=10, beta_ratio=0,
***base_params*)

Bases: *BaseDANNLike*

Implements WDGRL as described in Shen, Jian, et al. “Wasserstein distance guided representation learning for domain adaptation.” Thirty-Second AAAI Conference on Artificial Intelligence. 2018. <https://arxiv.org/pdf/1707.01217.pdf>

This class also implements the asymmetric (β) variant described in: Wu, Yifan, et al. “Domain adaptation with asymmetrically-relaxed distribution alignment.” ICML (2019) <https://arxiv.org/pdf/1903.01689.pdf>

forward(*x*)

compute_loss(*batch*, *split_name='valid'*)

critic_update_steps(*batch*)

training_step(*batch*, *batch_id*)

configure_optimizers()

training: bool

precision: int

prepare_data_per_node: bool

allow_zero_length_dataloader_with_multiple_devices: bool

```
class kale.pipeline.domain_adapter.WDGRLTrainerMod(dataset, feature_extractor, task_classifier, critic,
                                                    k_critic=5, gamma=10, beta_ratio=0,
                                                    **base_params)
```

Bases: *WDGRLTrainer*

Implements a modified version WDGRL as described in Shen, Jian, et al. “Wasserstein distance guided representation learning for domain adaptation.” Thirty-Second AAAI Conference on Artificial Intelligence. 2018. <https://arxiv.org/pdf/1707.01217.pdf>

This class also implements the asymmetric (β) variant described in: Wu, Yifan, et al. “Domain adaptation with asymmetrically-relaxed distribution alignment.” ICML (2019) <https://arxiv.org/pdf/1903.01689.pdf>

critic_update_steps(*batch*)

training_step(*batch*, *batch_id*, *optimizer_idx*)

optimizer_step(*current_epoch*, *batch_nb*, *optimizer*, *optimizer_i*, *second_order_closure=None*,
on_tpu=False, *using_native_amp=False*, *using_lbfgs=False*)

configure_optimizers()

training: bool

precision: int

prepare_data_per_node: bool

allow_zero_length_dataloader_with_multiple_devices: bool

```
class kale.pipeline.domain_adapter.FewShotDANNTrainer(dataset, feature_extractor, task_classifier,  
                                                    critic, method, **base_params)
```

Bases: *BaseDANNLike*

Implements adaptations of DANN to the semi-supervised setting

naive: task classifier is trained on labeled target data, in addition to source data. MME: implements Saito, Kuniaki, et al. "Semi-supervised domain adaptation via minimax entropy." Proceedings of the IEEE International Conference on Computer Vision. 2019 <https://arxiv.org/pdf/1904.06487.pdf>

```
forward(x)
```

```
compute_loss(batch, split_name='valid')
```

```
training: bool
```

```
precision: int
```

```
prepare_data_per_node: bool
```

```
allow_zero_length_dataloader_with_multiple_devices: bool
```

```
class kale.pipeline.domain_adapter.BaseMMDLike(dataset, feature_extractor, task_classifier,  
                                              kernel_mul=2.0, kernel_num=5, **base_params)
```

Bases: *BaseAdaptTrainer*

Common API for MME-based deep learning DA methods: DAN, JAN

```
forward(x)
```

```
compute_loss(batch, split_name='valid')
```

```
validation_epoch_end(outputs)
```

```
test_epoch_end(outputs)
```

```
training: bool
```

```
precision: int
```

```
prepare_data_per_node: bool
```

```
allow_zero_length_dataloader_with_multiple_devices: bool
```

```
class kale.pipeline.domain_adapter.DANTrainer(dataset, feature_extractor, task_classifier,  
                                              **base_params)
```

Bases: *BaseMMDLike*

This is an implementation of DAN Long, Mingsheng, et al. "Learning Transferable Features with Deep Adaptation Networks." International Conference on Machine Learning. 2015. <http://proceedings.mlr.press/v37/long15.pdf> code based on <https://github.com/thuml/Xlearn>.

```
training: bool
```

```
precision: int
```

```
prepare_data_per_node: bool
```

```
allow_zero_length_dataloader_with_multiple_devices: bool
```

```
class kale.pipeline.domain_adapter.JANTrainer(dataset, feature_extractor, task_classifier,
                                             kernel_mul=(2.0, 2.0), kernel_num=(5, 1),
                                             **base_params)
```

Bases: *BaseMMDLike*

This is an implementation of JAN Long, Mingsheng, et al. “Deep transfer learning with joint adaptation networks.” International Conference on Machine Learning, 2017. <https://arxiv.org/pdf/1605.06636.pdf> code based on <https://github.com/thuml/Xlearn>.

training: bool

precision: int

prepare_data_per_node: bool

allow_zero_length_dataloader_with_multiple_devices: bool

12.4 kale.pipeline.mpca_trainer module

Implementation of MPCA->Feature Selection->Linear SVM/LogisticRegression Pipeline

References

[1] Swift, A. J., Lu, H., Uthoff, J., Garg, P., Cogliano, M., Taylor, J., ... & Kiely, D. G. (2020). A machine learning cardiac magnetic resonance approach to extract disease features and automate pulmonary arterial hypertension diagnosis. *European Heart Journal-Cardiovascular Imaging*. [2] Song, X., Meng, L., Shi, Q., & Lu, H. (2015, October). Learning tensor-based features for whole-brain fMRI classification. In *International Conference on Medical Image Computing and Computer-Assisted Intervention* (pp. 613-620). Springer, Cham. [3] Lu, H., Plataniotis, K. N., & Venetsanopoulos, A. N. (2008). MPCA: Multilinear principal component analysis of tensor objects. *IEEE Transactions on Neural Networks*, 19(1), 18-39.

```
class kale.pipeline.mpca_trainer.MPCATrainer(classifier='svc', classifier_params='auto',
                                             classifier_param_grid=None, mpca_params=None,
                                             n_features=None, search_params=None)
```

Bases: *BaseEstimator, ClassifierMixin*

Trainer of pipeline: MPCA->Feature selection->Classifier

Parameters

- **classifier** (*str, optional*) – Available classifier options: {"svc", "linear_svc", "lr"}, where "svc" trains a support vector classifier, supports both linear and non-linear kernels, optimizes with library "libsvm"; "linear_svc" trains a support vector classifier with linear kernel only, and optimizes with library "liblinear", which suppose to be faster and better in handling large number of samples; and "lr" trains a classifier with logistic regression. Defaults to "svc".
- **classifier_params** (*dict, optional*) – Parameters of classifier. Defaults to 'auto'.
- **classifier_param_grid** (*dict, optional*) – Grids for searching the optimal hyper-parameters. Works only when classifier_params == "auto". Defaults to None by searching from the following hyper-parameter values: 1. svc, {"kernel": ["linear"], "C": [0.0001, 0.001, 0.01, 0.1, 1, 10, 100], "max_iter": [50000]}, 2. linear_svc, {"C": [0.0001, 0.001, 0.01, 0.1, 1, 10, 100]}, 3. lr, {"C": [0.0001, 0.001, 0.01, 0.1, 1, 10, 100]}

- **mpca_params** (*dict, optional*) – Parameters of MPCA, e.g., {"var_ratio": 0.8}. Defaults to None, i.e., using the default parameters (<https://pykale.readthedocs.io/en/latest/kale.embed.html#module-kale.embed.mpca>).
- **n_features** (*int, optional*) – Number of features for feature selection. Defaults to None, i.e., all features after dimension reduction will be used.
- **search_params** (*dict, optional*) – Parameters of grid search, for more detail please see https://scikit-learn.org/stable/modules/grid_search.html#grid-search . Defaults to None, i.e., using the default params: {"cv": 5}.

fit(*x, y*)

Fit a pipeline with the given data *x* and labels *y*

Parameters

- **x** (*array-like tensor*) – input data, shape (n_samples, I_1, I_2, ..., I_N)
- **y** (*array-like*) – data labels, shape (n_samples,)

Returns

self

predict(*x*)

Predict the labels for the given data *x*

Parameters

x (*array-like tensor*) – input data, shape (n_samples, I_1, I_2, ..., I_N)

Returns

Predicted labels, shape (n_samples,)

Return type

array-like

decision_function(*x*)

Decision scores of each class for the given data *x*

Parameters

x (*array-like tensor*) – input data, shape (n_samples, I_1, I_2, ..., I_N)

Returns

decision scores, shape (n_samples,) for binary case, else (n_samples, n_class)

Return type

array-like

predict_proba(*x*)

Probability of each class for the given data *x*. Not supported by "linear_svc".

Parameters

x (*array-like tensor*) – input data, shape (n_samples, I_1, I_2, ..., I_N)

Returns

probabilities, shape (n_samples, n_class)

Return type

array-like

12.5 kale.pipeline.multi_domain_adapter module

Multi-source domain adaptation pipelines

`kale.pipeline.multi_domain_adapter.create_ms_adapt_trainer`(*method: str, dataset, feature_extractor, task_classifier, **train_params*)

Methods for multi-source domain adaptation

Parameters

- **method** (*str*) – Multi-source domain adaptation method, M3SDA or MFSAN
- **dataset** (`kale.loaddata.multi_domain.MultiDomainAdapDataset`) – the multi-domain datasets to be used for train, validation, and tests.
- **feature_extractor** (`torch.nn.Module`) – feature extractor network
- **task_classifier** (`torch.nn.Module`) – task classifier network

Returns

Multi-source domain adaptation trainer.

Return type

[`pl.LightningModule`]

`class kale.pipeline.multi_domain_adapter.BaseMultiSourceTrainer`(*dataset, feature_extractor, task_classifier, n_classes: int, target_domain: str, **base_params*)

Bases: `BaseAdaptTrainer`

Base class for all domain adaptation architectures

Parameters

- **dataset** (`kale.loaddata.multi_domain`) – the multi-domain datasets to be used for train, validation, and tests.
- **feature_extractor** (`torch.nn.Module`) – the feature extractor network
- **task_classifier** (`torch.nn.Module`) – the task classifier network
- **n_classes** (*int*) – number of classes
- **target_domain** (*str*) – target domain name

`forward`(*x*)

`compute_loss`(*batch, split_name='valid'*)

`validation_epoch_end`(*outputs*)

`test_epoch_end`(*outputs*)

`training: bool`

`precision: int`

`prepare_data_per_node: bool`

`allow_zero_length_dataloader_with_multiple_devices: bool`

```
class kale.pipeline.multi_domain_adapter.M3SDATrainer(dataset, feature_extractor, task_classifier,
                                                    n_classes: int, target_domain: str, k_moment:
                                                    int = 3, **base_params)
```

Bases: *BaseMultiSourceTrainer*

Moment matching for multi-source domain adaptation (M3SDA).

Reference:

Peng, X., Bai, Q., Xia, X., Huang, Z., Saenko, K., & Wang, B. (2019). Moment matching for multi-source domain adaptation. In Proceedings of the IEEE/CVF International Conference on Computer Vision (pp. 1406-1415). https://openaccess.thecvf.com/content_ICCV_2019/html/Peng_Moment_Matching_for_Multi-Source_Domain_Adaptation_ICCV_2019_paper.html

```
compute_loss(batch, split_name='valid')
```

```
training: bool
```

```
precision: int
```

```
prepare_data_per_node: bool
```

```
allow_zero_length_dataloader_with_multiple_devices: bool
```

```
class kale.pipeline.multi_domain_adapter.MFSANTrainer(dataset, feature_extractor, task_classifier,
                                                    n_classes: int, target_domain: str,
                                                    domain_feat_dim: int = 100, kernel_mul:
                                                    float = 2.0, kernel_num: int = 5,
                                                    input_dimension: int = 2, **base_params)
```

Bases: *BaseMultiSourceTrainer*

Multiple Feature Spaces Adaptation Network (MFSAN)

Reference: Zhu, Y., Zhuang, F. and Wang, D., 2019, July. **Aligning domain-specific distribution and classifier**

for cross-domain classification from multiple sources. In AAAI. <https://ojs.aaai.org/index.php/AAAI/article/view/4551>

Original implementation: <https://github.com/easezyc/deep-transfer-learning/tree/master/MUDA/MFSAN>

```
compute_loss(batch, split_name='valid')
```

```
cls_discrepancy(x)
```

Compute discrepancy between all classifiers' probabilistic outputs

```
training: bool
```

```
precision: int
```

```
prepare_data_per_node: bool
```

```
allow_zero_length_dataloader_with_multiple_devices: bool
```

```
class kale.pipeline.multi_domain_adapter.CoIRLS(kernel='linear', kernel_kwargs=None, alpha=1.0,
                                                lambda_=1.0)
```

Bases: *BaseEstimator*, *ClassifierMixin*

Covariate-Independence Regularized Least Squares (CoIRLS)

Parameters

- **kernel** (*str*, *optional*) – {"linear", "rbf", "poly"}. Kernel to use. Defaults to "linear".

- **kernel_kwargs** (*dict or None, optional*) – Hyperparameter for the kernel. Defaults to None.
- **alpha** (*float, optional*) – Hyperparameter of the l2 (Ridge) penalty. Defaults to 1.0.
- **lambda** (*float, optional*) – Hyperparameter of the covariate dependence. Defaults to 1.0.

Reference:

[1] Zhou, S., 2022. **Interpretable Domain-Aware Learning for Neuroimage Classification (Doctoral dissertation,**
University of Sheffield).

[2] Zhou, S., Li, W., Cox, C.R., & Lu, H. (2020). **Side Information Dependence as a Regularizer for Analyzing**
Human Brain Conditions across Cognitive Experiments. AAAI 2020, New York, USA.

fit(*x, y, covariates*)

fit a model with input data, labels and covariates

Parameters

- **x** (*np.ndarray or tensor*) – shape (n_samples, n_features)
- **y** (*np.ndarray or tensor*) – shape (n_samples,)
- **covariates** (*np.ndarray or tensor*) – (n_samples, n_covariates)

predict(*x*)

Predict labels for data x

Parameters

x (*np.ndarray or tensor*) – Samples need prediction, shape (n_samples, n_features)

Returns

Predicted labels, shape (n_samples,)

Return type

y (np.ndarray)

decision_function(*x*)

Compute decision scores for data x

Parameters

x (*np.ndarray or tensor*) – Samples need decision scores, shape (n_samples, n_features)

Returns

Decision scores, shape (n_samples,)

Return type

scores (np.ndarray)

12.6 kale.pipeline.video_domain_adapter module

Domain adaptation systems (pipelines) for video data, e.g., for action recognition. Most are inherited from `kale.pipeline.domain_adapter`.

```
kale.pipeline.video_domain_adapter.create_mmd_based_video(method: Method, dataset,
                                                         image_modality, feature_extractor,
                                                         task_classifier, **train_params)
```

MMD-based deep learning methods for domain adaptation on video data: DAN and JAN

```
kale.pipeline.video_domain_adapter.create_dann_like_video(method: Method, dataset,
                                                         image_modality, feature_extractor,
                                                         task_classifier, critic, **train_params)
```

DANN-based deep learning methods for domain adaptation on video data: DANN, CDAN, CDAN+E

```
class kale.pipeline.video_domain_adapter.BaseMMDLikeVideo(dataset, image_modality,
                                                         feature_extractor, task_classifier,
                                                         kernel_mul=2.0, kernel_num=5,
                                                         **base_params)
```

Bases: `BaseMMDLike`

Common API for MME-based domain adaptation on video data: DAN, JAN

forward(*x*)

compute_loss(*batch, split_name='valid'*)

training: bool

precision: int

prepare_data_per_node: bool

allow_zero_length_dataloader_with_multiple_devices: bool

```
class kale.pipeline.video_domain_adapter.DANTrainerVideo(dataset, image_modality,
                                                         feature_extractor, task_classifier,
                                                         **base_params)
```

Bases: `BaseMMDLikeVideo`

This is an implementation of DAN for video data.

training: bool

precision: int

prepare_data_per_node: bool

allow_zero_length_dataloader_with_multiple_devices: bool

```
class kale.pipeline.video_domain_adapter.JANTrainerVideo(dataset, image_modality,
                                                         feature_extractor, task_classifier,
                                                         kernel_mul=(2.0, 2.0), kernel_num=(5,
                                                         1), **base_params)
```

Bases: `BaseMMDLikeVideo`

This is an implementation of JAN for video data.

training: bool**precision: int****prepare_data_per_node: bool****allow_zero_length_dataloader_with_multiple_devices: bool**

```
class kale.pipeline.video_domain_adapter.DANNTrainerVideo(dataset, image_modality,
                                                         feature_extractor, task_classifier, critic,
                                                         method, **base_params)
```

Bases: *DANNTrainer*

This is an implementation of DANN for video data.

forward(*x*)**compute_loss**(*batch, split_name='valid'*)**training_step**(*batch, batch_nb*)**training: bool****precision: int****prepare_data_per_node: bool****allow_zero_length_dataloader_with_multiple_devices: bool**

```
class kale.pipeline.video_domain_adapter.CDANTrainerVideo(dataset, image_modality,
                                                         feature_extractor, task_classifier, critic,
                                                         use_entropy=False, use_random=False,
                                                         random_dim=1024, **base_params)
```

Bases: *CDANTrainer*

This is an implementation of CDAN for video data.

forward(*x*)**compute_loss**(*batch, split_name='valid'*)**training: bool****precision: int****prepare_data_per_node: bool****allow_zero_length_dataloader_with_multiple_devices: bool**

```
class kale.pipeline.video_domain_adapter.WDGRLTrainerVideo(dataset, image_modality,
                                                           feature_extractor, task_classifier, critic,
                                                           k_critic=5, gamma=10, beta_ratio=0,
                                                           **base_params)
```

Bases: *WDGRLTrainer*

This is an implementation of WDGRL for video data.

forward(*x*)**compute_loss**(*batch, split_name='valid'*)

```
configure_optimizers()  
critic_update_steps(batch)  
training: bool  
precision: int  
prepare_data_per_node: bool  
allow_zero_length_dataloader_with_multiple_devices: bool
```

12.7 Module contents

13.1 Submodules

13.2 kale.utils.download module

Data downloading and compressed data extraction functions, Based on <https://github.com/pytorch/vision/blob/master/torchvision/datasets/utils.py> <https://github.com/pytorch/pytorch/blob/master/torch/hub.py>

`kale.utils.download.download_file_by_url(url, output_directory, output_file_name, file_format=None)`

Download file/compressed file by url.

Parameters

- **url** (*string*) – URL of the object to download
- **output_directory** (*string, optional*) – Full path where object will be saved Absolute path recommended. Relative path also works.
- **output_file_name** (*string, optional*) – File name which object will be saved as
- **file_format** (*string, optional*) – File format For compressed file, support ["tar.xz", "tar", "tar.gz", "tgz", "gz", "zip"]

Example: (Grab the raw link from GitHub. Notice that using “raw” in the URL.)

```
>>> url = "https://github.com/pykale/data/raw/main/videos/video_test_data/ADL/  
↪ annotations/labels_train_test/adl_P_04_train.pkl"  
>>> download_file_by_url(url, "data", "a.pkl", "pkl")
```

```
>>> url = "https://github.com/pykale/data/raw/main/videos/video_test_data.zip"  
>>> download_file_by_url(url, "data", "video_test_data.zip", "zip")
```

`kale.utils.download.download_file_gdrive(id, output_directory, output_file_name, file_format=None)`

Download file/compressed file by Google Drive id.

Parameters

- **id** (*string*) – Google Drive file id of the object to download
- **output_directory** (*string, optional*) – Full path where object will be saved Absolute path recommended. Relative path also works.
- **output_file_name** (*string, optional*) – File name which object will be saved as

- **file_format** (*string, optional*) – File format For compressed file, support ["tar.xz", "tar", "tar.gz", "tgz", "gz", "zip"]

Example

```
>>> gdrive_id = "1U4D23R8u8MJX9KVKb92bZZX-tbpKwtga"  
>>> download_file_gdrive(gdrive_id, "data", "demo_datasets.zip", "zip")
```

```
>>> gdrive_id = "1SV7fmAnWj-6AU9X5BGOrvGMoh2Gu9Nih"  
>>> download_file_gdrive(gdrive_id, "data", "dummy_data.csv", "csv")
```

13.3 kale.utils.logger module

Logging functions, based on <https://github.com/HaozhiQi/ISONet/blob/master/isonet/utils/logger.py>

`kale.utils.logger.out_file_core()`

Creates an output file name concatenating a formatted date and uuid, but without an extension.

Returns

A string to be used in a file name.

Return type

string

`kale.utils.logger.construct_logger(name, save_dir)`

Constructs a logger. Saves the output as a text file at a specified path. Also saves the output of *git diff HEAD* to the same folder.

Reference: <https://docs.python.org/3/library/logging.html>

Parameters

- **name** (*str*) – the logger name, typically the method name
- **save_dir** (*str*) – the path to save the log file (.txt)

13.4 kale.utils.print module

Screen printing functions, from <https://github.com/HaozhiQi/ISONet/blob/master/isonet/utils/misc.py>

`kale.utils.print.tprint(*args)`

Temporarily prints things on the screen so that it won't be flooded

`kale.utils.print.pprint(*args)`

Permanently prints things on the screen to have all info displayed

`kale.utils.print.pprint_without_newline(*args)`

Permanently prints things on the screen, separated by space rather than newline

13.5 kale.utils.seed module

Setting seed for reproducibility

`kale.utils.seed.set_seed(seed=1000)`

Sets the seed for generating random numbers to get (as) reproducible (as possible) results.

The CuDNN options are set according to the official PyTorch guidance on reproducibility: <https://pytorch.org/docs/stable/notes/randomness.html>. Another references are <https://discuss.pytorch.org/t/difference-between-torch-manual-seed-and-torch-cuda-manual-seed/13848/6> https://pytorch.org/docs/stable/cuda.html#torch.cuda.manual_seed <https://github.com/open-mmlab/mmcv/blob/master/mmcv/runner/utils.py#L58>

Parameters

seed (*int*, *optional*) – The desired seed. Defaults to 1000.

13.6 Module contents

Kale APIs above are ordered following the machine learning pipeline, i.e., functionalities, rather than alphabetically.

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