DICE Embeddings

Release 0.1.3.2

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DICE Embeddings[1]: Hardware-agnostic Framework for Large-scale Knowledge Graph Embeddings:

1 Dicee Manual

Version: dicee 0.1.3.2

GitHub repository: https://github.com/dice-group/dice-embeddings

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Dicee is a hardware-agnostic framework for large-scale knowledge graph embeddings.

Knowledge graph embedding research has mainly focused on learning continuous representations of knowledge graphs towards the link prediction problem. Recently developed frameworks can be effectively applied in a wide range of research-related applications. Yet, using these frameworks in real-world applications becomes more challenging as the size of the knowledge graph grows

We developed the DICE Embeddings framework (dicee) to compute embeddings for large-scale knowledge graphs in a hardware-agnostic manner. To achieve this goal, we rely on

1. **Pandas**[3] **& Co.** to use parallelism at preprocessing a large knowledge graph,
2. **PyTorch**[4] **& Co.** to learn knowledge graph embeddings via multi-CPUs, GPUs, TPUs or computing cluster, and
3. **Huggingface**[5] to ease the deployment of pre-trained models.

Why Pandas[6] **& Co. ?** A large knowledge graph can be read and preprocessed (e.g. removing literals) by pandas, modin, or polars in parallel. Through polars, a knowledge graph having more than 1 billion triples can be read in parallel fashion. Importantly, using these frameworks allow us to perform all necessary computations on a single CPU as well as a cluster of computers.

Why PyTorch[7] **& Co. ?** PyTorch is one of the most popular machine learning frameworks available at the time of writing. PytorchLightning facilitates scaling the training procedure of PyTorch without boilerplate. In our framework, we combine PyTorch[8] & PytorchLightning[9]. Users can choose the trainer class (e.g., DDP by Pytorch) to train large knowledge graph embedding models with billions of parameters. PytorchLightning allows us to use state-of-the-art model parallelism techniques (e.g. Fully Sharded Training, FairScale, or DeepSpeed) without extra effort. With our framework, practitioners can directly use PytorchLightning for model parallelism to train gigantic embedding models.

Why Hugging-face Gradio[10]**?** Deploy a pre-trained embedding model without writing a single line of code.

[1] https://github.com/dice-group/dice-embeddings
[2] https://github.com/Demirrr
[3] https://pandas.pydata.org/
[4] https://pytorch.org/
[5] https://huggingface.co/
[6] https://pandas.pydata.org/
[7] https://pytorch.org/
[8] https://pytorch.org/
[9] https://www.pytorchlightning.ai/
[10] https://huggingface.co/gradio

2 Installation

2.1 Installation from Source

```
git clone https://github.com/dice-group/dice-embeddings.git
conda create -n dice python=3.10.13 --no-default-packages && conda activate dice &&
↪cd dice-embeddings &&
pip3 install -e .
```

or

```
pip install dicee
```

3 Download Knowledge Graphs

```
wget https://files.dice-research.org/datasets/dice-embeddings/KGs.zip --no-check-
↪certificate && unzip KGs.zip
```

To test the Installation

```
python -m pytest -p no:warnings -x # Runs >114 tests leading to > 15 mins
python -m pytest -p no:warnings --lf # run only the last failed test
python -m pytest -p no:warnings --ff # to run the failures first and then the rest of
↪the tests.
```

4 Knowledge Graph Embedding Models

1. TransE, DistMult, ComplEx, ConEx, QMult, OMult, ConvO, ConvQ, Keci
2. All 44 models available in https://github.com/pykeen/pykeen#models

   For more, please refer to `examples`.

5 How to Train

To Train a KGE model (KECI) and evaluate it on the train, validation, and test sets of the UMLS benchmark dataset.

```
from dicee.executer import Execute
from dicee.config import Namespace
args = Namespace()
args.model = 'Keci'
args.scoring_technique = "KvsAll"  # 1vsAll, or AllvsAll, or NegSample
args.dataset_dir = "KGs/UMLS"
args.path_to_store_single_run = "Keci_UMLS"
args.num_epochs = 100
args.embedding_dim = 32
args.batch_size = 1024
reports = Execute(args).start()
print(reports["Train"]["MRR"]) # => 0.9912
```

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```
print(reports["Test"]["MRR"]) # => 0.8155
# See the Keci_UMLS folder embeddings and all other files
```

where the data is in the following form

```
$ head -3 KGs/UMLS/train.txt
acquired_abnormality    location_of     experimental_model_of_disease
anatomical_abnormality  manifestation_of        physiologic_function
alga    isa     entity
```

A KGE model can also be trained from the command line

```
dicee --dataset_dir "KGs/UMLS" --model Keci --eval_model "train_val_test"
```

dicee automaticaly detects available GPUs and trains a model with distributed data parallels technique. Under the hood, dicee uses lighning as a default trainer.

```
# Train a model by only using the GPU-0
CUDA_VISIBLE_DEVICES=0 dicee --dataset_dir "KGs/UMLS" --model Keci --eval_model
↪"train_val_test"
# Train a model by only using GPU-1
CUDA_VISIBLE_DEVICES=1 dicee --dataset_dir "KGs/UMLS" --model Keci --eval_model
↪"train_val_test"
NCCL_P2P_DISABLE=1 CUDA_VISIBLE_DEVICES=0,1 python dicee/scripts/run.py --trainer PL -
↪-dataset_dir "KGs/UMLS" --model Keci --eval_model "train_val_test"
```

Under the hood, dicee executes run.py script and uses lighning as a default trainer

```
# Two equivalent executions
# (1)
dicee --dataset_dir "KGs/UMLS" --model Keci --eval_model "train_val_test"
# Evaluate Keci on Train set: Evaluate Keci on Train set
# {'H@1': 0.9518788343558282, 'H@3': 0.9988496932515337, 'H@10': 1.0, 'MRR': 0.
↪9753123402351737}
# Evaluate Keci on Validation set: Evaluate Keci on Validation set
# {'H@1': 0.6932515337423313, 'H@3': 0.9041411042944786, 'H@10': 0.9754601226993865,
↪'MRR': 0.8072362996241839}
# Evaluate Keci on Test set: Evaluate Keci on Test set
# {'H@1': 0.6951588502269289, 'H@3': 0.9039334341906202, 'H@10': 0.9750378214826021,
↪'MRR': 0.8064032293278861}

# (2)
CUDA_VISIBLE_DEVICES=0,1 python dicee/scripts/run.py --trainer PL --dataset_dir "KGs/
↪UMLS" --model Keci --eval_model "train_val_test"
# Evaluate Keci on Train set: Evaluate Keci on Train set
# {'H@1': 0.9518788343558282, 'H@3': 0.9988496932515337, 'H@10': 1.0, 'MRR': 0.
↪9753123402351737}
# Evaluate Keci on Train set: Evaluate Keci on Train set
# Evaluate Keci on Validation set: Evaluate Keci on Validation set
# {'H@1': 0.6932515337423313, 'H@3': 0.9041411042944786, 'H@10': 0.9754601226993865,
↪'MRR': 0.8072362996241839}
# Evaluate Keci on Test set: Evaluate Keci on Test set
# {'H@1': 0.6951588502269289, 'H@3': 0.9039334341906202, 'H@10': 0.9750378214826021,
↪'MRR': 0.8064032293278861}
```

Similarly, models can be easily trained with torchrun

```
torchrun --standalone --nnodes=1 --nproc_per_node=gpu dicee/scripts/run.py --trainer torchDDP --dataset_dir "KGs/UMLS" --model Keci --eval_model "train_val_test"
# Evaluate Keci on Train set: Evaluate Keci on Train set: Evaluate Keci on Train set
# {'H@1': 0.9518788343558282, 'H@3': 0.9988496932515337, 'H@10': 1.0, 'MRR': 0.9753123402351737}
# Evaluate Keci on Validation set: Evaluate Keci on Validation set
# {'H@1': 0.6932515337423313, 'H@3': 0.9041411042944786, 'H@10': 0.9754601226993865, 'MRR': 0.8072499937521418}
# Evaluate Keci on Test set: Evaluate Keci on Test set
{'H@1': 0.6951588502269289, 'H@3': 0.9039334341906202, 'H@10': 0.9750378214826021, 'MRR': 0.8064032293278861}
```

You can also train a model in multi-node multi-gpu setting.

```
torchrun --nnodes 2 --nproc_per_node=gpu  --node_rank 0 --rdzv_id 455 --rdzv_backend c10d --rdzv_endpoint=nebula  dicee/scripts/run.py --trainer torchDDP --dataset_dir KGs/UMLS
torchrun --nnodes 2 --nproc_per_node=gpu  --node_rank 1 --rdzv_id 455 --rdzv_backend c10d --rdzv_endpoint=nebula dicee/scripts/run.py --trainer torchDDP --dataset_dir KGs/UMLS
```

Train a KGE model by providing the path of a single file and store all parameters under newly created directory called `KeciFamilyRun`.

```
dicee --path_single_kg "KGs/Family/family-benchmark_rich_background.owl" --model Keci --path_to_store_single_run KeciFamilyRun --backend rdflib
```

where the data is in the following form

```
$ head -3 KGs/Family/train.txt
_:1 <http://www.w3.org/1999/02/22-rdf-syntax-ns#type> <http://www.w3.org/2002/07/owl#Ontology> .
<http://www.benchmark.org/family#hasChild> <http://www.w3.org/1999/02/22-rdf-syntax-ns#type> <http://www.w3.org/2002/07/owl#ObjectProperty> .
<http://www.benchmark.org/family#hasParent> <http://www.w3.org/1999/02/22-rdf-syntax-ns#type> <http://www.w3.org/2002/07/owl#ObjectProperty> .
```

Apart from n-triples or standard link prediction dataset formats, we support ["owl", "nt", "turtle", "rdf/xml", "n3"]*. Moreover, a KGE model can be also trained by providing **an endpoint of a triple store**.

```
dicee --sparql_endpoint "http://localhost:3030/mutagenesis/" --model Keci
```

For more, please refer to `examples`.

6 Creating an Embedding Vector Database

6.1 Learning Embeddings

```
# Train an embedding model
dicee --dataset_dir KGs/Countries-S1 --path_to_store_single_run CountryEmbeddings --model Keci --p 0 --q 1 --embedding_dim 32 --adaptive_swa
```

6.2 Loading Embeddings into Qdrant Vector Database

```
# Ensure that Qdrant available
# docker pull qdrant/qdrant && docker run -p 6333:6333 -p 6334:6334      -v $(pwd)/
↪qdrant_storage:/qdrant/storage:z      qdrant/qdrant
diceeindex --path_model "CountryEmbeddings" --collection_name "dummy" --location
↪"localhost"
```

6.3 Launching Webservice

```
diceeserve --path_model "CountryEmbeddings" --collection_name "dummy" --collection_
↪location "localhost"
```

Retrieve and Search

Get embedding of germany

```
curl -X 'GET' 'http://0.0.0.0:8000/api/get?q=germany' -H 'accept: application/json'
```

Get most similar things to europe

```
curl -X 'GET' 'http://0.0.0.0:8000/api/search?q=europe' -H 'accept: application/json'
{"result":[{"hit":"europe","score":1.0},
{"hit":"northern_europe","score":0.67126536},
{"hit":"western_europe","score":0.6010134},
{"hit":"puerto_rico","score":0.5051694},
{"hit":"southern_europe","score":0.4829831}]}
```

7 Answering Complex Queries

```
# pip install dicee
# wget https://files.dice-research.org/datasets/dice-embeddings/KGs.zip --no-check-
↪certificate & unzip KGs.zip
from dicee.executer import Execute
from dicee.config import Namespace
from dicee.knowledge_graph_embeddings import KGE
# (1) Train a KGE model
args = Namespace()
args.model = 'Keci'
args.p=0
args.q=1
args.optim = 'Adam'
args.scoring_technique = "AllvsAll"
args.path_single_kg = "KGs/Family/family-benchmark_rich_background.owl"
args.backend = "rdflib"
args.num_epochs = 200
args.batch_size = 1024
args.lr = 0.1
args.embedding_dim = 512
result = Execute(args).start()
# (2) Load the pre-trained model
```

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```
pre_trained_kge = KGE(path=result['path_experiment_folder'])
# (3) Single-hop query answering
# Query: ?E : \exist E.hasSibling(E, F9M167)
# Question: Who are the siblings of F9M167?
# Answer: [F9M157, F9F141], as (F9M167, hasSibling, F9M157) and (F9M167, hasSibling,␣
↪F9F141)
predictions = pre_trained_kge.answer_multi_hop_query(query_type="1p",
                                                     query=('http://www.benchmark.org/
↪family#F9M167',
                                                            ('http://www.benchmark.
↪org/family#hasSibling',)),
                                                     tnorm="min", k=3)
top_entities = [topk_entity for topk_entity, query_score in predictions]
assert "http://www.benchmark.org/family#F9F141" in top_entities
assert "http://www.benchmark.org/family#F9M157" in top_entities
# (2) Two-hop query answering
# Query: ?D : \exist E.Married(D, E) \land hasSibling(E, F9M167)
# Question: To whom a sibling of F9M167 is married to?
# Answer: [F9F158, F9M142] as (F9M157 #married F9F158) and (F9F141 #married F9M142)
predictions = pre_trained_kge.answer_multi_hop_query(query_type="2p",
                                                     query=("http://www.benchmark.org/
↪family#F9M167",
                                                            ("http://www.benchmark.
↪org/family#hasSibling",
                                                             "http://www.benchmark.
↪org/family#married")),
                                                     tnorm="min", k=3)
top_entities = [topk_entity for topk_entity, query_score in predictions]
assert "http://www.benchmark.org/family#F9M142" in top_entities
assert "http://www.benchmark.org/family#F9F158" in top_entities
# (3) Three-hop query answering
# Query: ?T : \exist D.type(D,T) \land Married(D,E) \land hasSibling(E, F9M167)
# Question: What are the type of people who are married to a sibling of F9M167?
# (3) Answer: [Person, Male, Father] since  F9M157 is [Brother Father Grandfather␣
↪Male] and F9M142 is [Male Grandfather Father]

predictions = pre_trained_kge.answer_multi_hop_query(query_type="3p", query=("http://
↪www.benchmark.org/family#F9M167",
                                                                             ("http://
↪www.benchmark.org/family#hasSibling",
                                                                             "http://
↪www.benchmark.org/family#married",
                                                                             "http://
↪www.w3.org/1999/02/22-rdf-syntax-ns#type")),
                                                     tnorm="min", k=5)
top_entities = [topk_entity for topk_entity, query_score in predictions]
print(top_entities)
assert "http://www.benchmark.org/family#Person" in top_entities
assert "http://www.benchmark.org/family#Father" in top_entities
assert "http://www.benchmark.org/family#Male" in top_entities
```

For more, please refer to `examples/multi_hop_query_answering`.

8 Predicting Missing Links

```
from dicee import KGE
# (1) Train a knowledge graph embedding model..
# (2) Load a pretrained model
pre_trained_kge = KGE(path='..')
# (3) Predict missing links through head entity rankings
pre_trained_kge.predict_topk(h=[".."],r=[".."],topk=10)
# (4) Predict missing links through relation rankings
pre_trained_kge.predict_topk(h=[".."],t=[".."],topk=10)
# (5) Predict missing links through tail entity rankings
pre_trained_kge.predict_topk(r=[".."],t=[".."],topk=10)
```

9 Downloading Pretrained Models

```
from dicee import KGE
# (1) Load a pretrained ConEx on DBpedia
model = KGE(url="https://files.dice-research.org/projects/DiceEmbeddings/KINSHIP-Keci-
↪dim128-epoch256-KvsAll")
```

- For more please look at dice-research.org/projects/DiceEmbeddings/[11]

10 How to Deploy

```
from dicee import KGE
KGE(path='...').deploy(share=True,top_k=10)
```

11 Docker

To build the Docker image:

```
docker build -t dice-embeddings .
```

To test the Docker image:

```
docker run --rm -v ~/.local/share/dicee/KGs:/dicee/KGs dice-embeddings ./main.py --
↪model AConEx --embedding_dim 16
```

[11] https://files.dice-research.org/projects/DiceEmbeddings/

12 How to cite

Currently, we are working on our manuscript describing our framework. If you really like our work and want to cite it now, feel free to chose one :)

```
# Keci
@inproceedings{demir2023clifford,
  title={Clifford Embeddings--A Generalized Approach for Embedding in Normed Algebras}
↪,
  author={Demir, Caglar and Ngonga Ngomo, Axel-Cyrille},
  booktitle={Joint European Conference on Machine Learning and Knowledge Discovery in␣
↪Databases},
  pages={567--582},
  year={2023},
  organization={Springer}
}
# LitCQD
@inproceedings{demir2023litcqd,
  title={LitCQD: Multi-Hop Reasoning in Incomplete Knowledge Graphs with Numeric␣
↪Literals},
  author={Demir, Caglar and Wiebesiek, Michel and Lu, Renzhong and Ngonga Ngomo, Axel-
↪Cyrille and Heindorf, Stefan},
  booktitle={Joint European Conference on Machine Learning and Knowledge Discovery in␣
↪Databases},
  pages={617--633},
  year={2023},
  organization={Springer}
}
# DICE Embedding Framework
@article{demir2022hardware,
  title={Hardware-agnostic computation for large-scale knowledge graph embeddings},
  author={Demir, Caglar and Ngomo, Axel-Cyrille Ngonga},
  journal={Software Impacts},
  year={2022},
  publisher={Elsevier}
}
# KronE
@inproceedings{demir2022kronecker,
  title={Kronecker decomposition for knowledge graph embeddings},
  author={Demir, Caglar and Lienen, Julian and Ngonga Ngomo, Axel-Cyrille},
  booktitle={Proceedings of the 33rd ACM Conference on Hypertext and Social Media},
  pages={1--10},
  year={2022}
}
# QMult, OMult, ConvQ, ConvO
@InProceedings{pmlr-v157-demir21a,
  title =          {Convolutional Hypercomplex Embeddings for Link Prediction},
  author =       {Demir, Caglar and Moussallem, Diego and Heindorf, Stefan and Ngonga␣
↪Ngomo, Axel-Cyrille},
  booktitle =          {Proceedings of The 13th Asian Conference on Machine Learning},
  pages =          {656--671},
  year =          {2021},
  editor =          {Balasubramanian, Vineeth N. and Tsang, Ivor},
  volume =          {157},
  series =          {Proceedings of Machine Learning Research},
  month =          {17--19 Nov},
  publisher =    {PMLR},
```

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```
  pdf =           {https://proceedings.mlr.press/v157/demir21a/demir21a.pdf},
  url =           {https://proceedings.mlr.press/v157/demir21a.html},
}
# ConEx
@inproceedings{demir2021convolutional,
title={Convolutional Complex Knowledge Graph Embeddings},
author={Caglar Demir and Axel-Cyrille Ngonga Ngomo},
booktitle={Eighteenth Extended Semantic Web Conference - Research Track},
year={2021},
url={https://openreview.net/forum?id=6T45-4TFqaX}}
# Shallom
@inproceedings{demir2021shallow,
  title={A shallow neural model for relation prediction},
  author={Demir, Caglar and Moussallem, Diego and Ngomo, Axel-Cyrille Ngonga},
  booktitle={2021 IEEE 15th International Conference on Semantic Computing (ICSC)},
  pages={179--182},
  year={2021},
  organization={IEEE}
```

For any questions or wishes, please contact: `caglar.demir@upb.de`

13 dicee

13.1 Subpackages

dicee.models

Submodules

dicee.models.base_model

Module Contents

Classes

BaseKGELightning	Base class for all neural network modules.
BaseKGE	Base class for all neural network modules.
IdentityClass	Base class for all neural network modules.

class dicee.models.base_model.**BaseKGELightning**(**args*, ***kwargs*)

Bases: `lightning.LightningModule`

Base class for all neural network modules.

Your models should also subclass this class.

Modules can also contain other Modules, allowing to nest them in a tree structure. You can assign the submodules as regular attributes:

```python
import torch.nn as nn
import torch.nn.functional as F

class Model(nn.Module):
    def __init__(self):
        super().__init__()
        self.conv1 = nn.Conv2d(1, 20, 5)
        self.conv2 = nn.Conv2d(20, 20, 5)

    def forward(self, x):
        x = F.relu(self.conv1(x))
        return F.relu(self.conv2(x))
```

Submodules assigned in this way will be registered, and will have their parameters converted too when you call `to()`, etc.

Note: As per the example above, an `__init__()` call to the parent class must be made before assignment on the child.

Variables

training (*bool*) – Boolean represents whether this module is in training or evaluation mode.

mem_of_model() → Dict

Size of model in MB and number of params

training_step(*batch*, *batch_idx=None*)

Here you compute and return the training loss and some additional metrics for e.g. the progress bar or logger.

Parameters

- **batch** – The output of your data iterable, normally a `DataLoader`.
- **batch_idx** – The index of this batch.
- **dataloader_idx** – The index of the dataloader that produced this batch. (only if multiple dataloaders used)

Returns

- `Tensor` - The loss tensor
- `dict` - A dictionary which can include any keys, but must include the key `'loss'` in the case of automatic optimization.
- `None` - In automatic optimization, this will skip to the next batch (but is not supported for multi-GPU, TPU, or DeepSpeed). For manual optimization, this has no special meaning, as returning the loss is not required.

In this step you'd normally do the forward pass and calculate the loss for a batch. You can also do fancier things like multiple forward passes or something model specific.

Example:

```python
def training_step(self, batch, batch_idx):
    x, y, z = batch
    out = self.encoder(x)
    loss = self.loss(out, x)
    return loss
```

To use multiple optimizers, you can switch to 'manual optimization' and control their stepping:

```
def __init__(self):
    super().__init__()
    self.automatic_optimization = False


# Multiple optimizers (e.g.: GANs)
def training_step(self, batch, batch_idx):
    opt1, opt2 = self.optimizers()

    # do training_step with encoder
    ...
    opt1.step()
    # do training_step with decoder
    ...
    opt2.step()
```

Note: When `accumulate_grad_batches` > 1, the loss returned here will be automatically normalized by `accumulate_grad_batches` internally.

loss_function(*yhat_batch: torch.FloatTensor*, *y_batch: torch.FloatTensor*)

Parameters

- **yhat_batch** –
- **y_batch** –

on_train_epoch_end(**args*, ***kwargs*)

Called in the training loop at the very end of the epoch.

To access all batch outputs at the end of the epoch, you can cache step outputs as an attribute of the `LightningModule` and access them in this hook:

```
class MyLightningModule(L.LightningModule):
    def __init__(self):
        super().__init__()
        self.training_step_outputs = []

    def training_step(self):
        loss = ...
        self.training_step_outputs.append(loss)
        return loss

    def on_train_epoch_end(self):
        # do something with all training_step outputs, for example:
        epoch_mean = torch.stack(self.training_step_outputs).mean()
        self.log("training_epoch_mean", epoch_mean)
        # free up the memory
        self.training_step_outputs.clear()
```

test_epoch_end(*outputs: List[Any]*)

test_dataloader() → None

An iterable or collection of iterables specifying test samples.

For more information about multiple dataloaders, see this section.

For data processing use the following pattern:

- download in `prepare_data()`
- process and split in `setup()`

However, the above are only necessary for distributed processing.

> **Warning:** do not assign state in prepare_data

- `test()`
- `prepare_data()`
- `setup()`

Note: Lightning tries to add the correct sampler for distributed and arbitrary hardware. There is no need to set it yourself.

Note: If you don't need a test dataset and a `test_step()`, you don't need to implement this method.

val_dataloader`()` → None

An iterable or collection of iterables specifying validation samples.

For more information about multiple dataloaders, see this section.

The dataloader you return will not be reloaded unless you set **:paramref:`~lightning.pytorch.trainer.trainer.Trainer.reload_dataloaders_every_n_epochs`** to a positive integer.

It's recommended that all data downloads and preparation happen in `prepare_data()`.

- `fit()`
- `validate()`
- `prepare_data()`
- `setup()`

Note: Lightning tries to add the correct sampler for distributed and arbitrary hardware There is no need to set it yourself.

Note: If you don't need a validation dataset and a `validation_step()`, you don't need to implement this method.

predict_dataloader`()` → None

An iterable or collection of iterables specifying prediction samples.

For more information about multiple dataloaders, see this section.

It's recommended that all data downloads and preparation happen in `prepare_data()`.

- `predict()`

- `prepare_data()`
- `setup()`

Note: Lightning tries to add the correct sampler for distributed and arbitrary hardware There is no need to set it yourself.

Returns
A `torch.utils.data.DataLoader` or a sequence of them specifying prediction samples.

train_dataloader() → None
An iterable or collection of iterables specifying training samples.

For more information about multiple dataloaders, see this section.

The dataloader you return will not be reloaded unless you set **:paramref:`~lightning.pytorch.trainer.trainer.Trainer.reload_dataloaders_every_n_epochs`** to a positive integer.

For data processing use the following pattern:

- download in `prepare_data()`
- process and split in `setup()`

However, the above are only necessary for distributed processing.

Warning: do not assign state in prepare_data

- `fit()`
- `prepare_data()`
- `setup()`

Note: Lightning tries to add the correct sampler for distributed and arbitrary hardware. There is no need to set it yourself.

configure_optimizers(*parameters=None*)
Choose what optimizers and learning-rate schedulers to use in your optimization. Normally you'd need one. But in the case of GANs or similar you might have multiple. Optimization with multiple optimizers only works in the manual optimization mode.

Returns

Any of these 6 options.

- **Single optimizer**.
- **List or Tuple** of optimizers.
- **Two lists** - The first list has multiple optimizers, and the second has multiple LR schedulers (or multiple `lr_scheduler_config`).
- **Dictionary**, with an `"optimizer"` key, and (optionally) a `"lr_scheduler"` key whose value is a single LR scheduler or `lr_scheduler_config`.

- **None** - Fit will run without any optimizer.

The `lr_scheduler_config` is a dictionary which contains the scheduler and its associated configuration. The default configuration is shown below.

```
lr_scheduler_config = {
    # REQUIRED: The scheduler instance
    "scheduler": lr_scheduler,
    # The unit of the scheduler's step size, could also be 'step'.
    # 'epoch' updates the scheduler on epoch end whereas 'step'
    # updates it after a optimizer update.
    "interval": "epoch",
    # How many epochs/steps should pass between calls to
    # `scheduler.step()`. 1 corresponds to updating the learning
    # rate after every epoch/step.
    "frequency": 1,
    # Metric to to monitor for schedulers like `ReduceLROnPlateau`
    "monitor": "val_loss",
    # If set to `True`, will enforce that the value specified 'monitor'
    # is available when the scheduler is updated, thus stopping
    # training if not found. If set to `False`, it will only produce a warning
    "strict": True,
    # If using the `LearningRateMonitor` callback to monitor the
    # learning rate progress, this keyword can be used to specify
    # a custom logged name
    "name": None,
}
```

When there are schedulers in which the `.step()` method is conditioned on a value, such as the `torch.optim.lr_scheduler.ReduceLROnPlateau` scheduler, Lightning requires that the `lr_scheduler_config` contains the keyword `"monitor"` set to the metric name that the scheduler should be conditioned on.

Metrics can be made available to monitor by simply logging it using `self.log('metric_to_track', metric_val)` in your `LightningModule`.

Note: Some things to know:

- Lightning calls `.backward()` and `.step()` automatically in case of automatic optimization.
- If a learning rate scheduler is specified in `configure_optimizers()` with key `"interval"` (default "epoch") in the scheduler configuration, Lightning will call the scheduler's `.step()` method automatically in case of automatic optimization.
- If you use 16-bit precision (`precision=16`), Lightning will automatically handle the optimizer.
- If you use `torch.optim.LBFGS`, Lightning handles the closure function automatically for you.
- If you use multiple optimizers, you will have to switch to 'manual optimization' mode and step them yourself.
- If you need to control how often the optimizer steps, override the `optimizer_step()` hook.

---

class `dicee.models.base_model.`**`BaseKGE`**(*args: dict*)

Bases: *BaseKGELightning*

Base class for all neural network modules.

Your models should also subclass this class.

Modules can also contain other Modules, allowing to nest them in a tree structure. You can assign the submodules as regular attributes:

```
import torch.nn as nn
import torch.nn.functional as F

class Model(nn.Module):
    def __init__(self):
        super().__init__()
        self.conv1 = nn.Conv2d(1, 20, 5)
        self.conv2 = nn.Conv2d(20, 20, 5)

    def forward(self, x):
        x = F.relu(self.conv1(x))
        return F.relu(self.conv2(x))
```

Submodules assigned in this way will be registered, and will have their parameters converted too when you call `to()`, etc.

Note: As per the example above, an `__init__()` call to the parent class must be made before assignment on the child.

Variables

training (*bool*) – Boolean represents whether this module is in training or evaluation mode.

forward_byte_pair_encoded_k_vs_all(*x: torch.LongTensor*)

Parameters

x (*B x 2 x T*) –

forward_byte_pair_encoded_triple(*x: Tuple[torch.LongTensor, torch.LongTensor]*)

byte pair encoded neural link predictors

Parameters

------- –

init_params_with_sanity_checking()

forward(*x: torch.LongTensor | Tuple[torch.LongTensor, torch.LongTensor], y_idx: torch.LongTensor = None*)

Parameters

- **x** –
- **y_idx** –
- **ordered_bpe_entities** –

forward_triples(*x: torch.LongTensor*) → torch.Tensor

Parameters

x –

forward_k_vs_all(**args, **kwargs*)

forward_k_vs_sample(**args, **kwargs*)

get_triple_representation(*idx_hrt*)

get_head_relation_representation(*indexed_triple*)

get_sentence_representation(*x: torch.LongTensor*)

Parameters

- **(b** (*x shape*) –
- **3** –
- **t)** –

get_bpe_head_and_relation_representation(*x: torch.LongTensor*)
→ Tuple[torch.FloatTensor, torch.FloatTensor]

Parameters

x (*B x 2 x T*) –

get_embeddings() → Tuple[numpy.ndarray, numpy.ndarray]

class dicee.models.base_model.**IdentityClass**(*args=None*)

Bases: `torch.nn.Module`

Base class for all neural network modules.

Your models should also subclass this class.

Modules can also contain other Modules, allowing to nest them in a tree structure. You can assign the submodules as regular attributes:

```
import torch.nn as nn
import torch.nn.functional as F

class Model(nn.Module):
    def __init__(self):
        super().__init__()
        self.conv1 = nn.Conv2d(1, 20, 5)
        self.conv2 = nn.Conv2d(20, 20, 5)

    def forward(self, x):
        x = F.relu(self.conv1(x))
        return F.relu(self.conv2(x))
```

Submodules assigned in this way will be registered, and will have their parameters converted too when you call `to()`, etc.

Note: As per the example above, an `__init__()` call to the parent class must be made before assignment on the child.

Variables

training (*bool*) – Boolean represents whether this module is in training or evaluation mode.

static forward(*x*)

`dicee.models.clifford`

Module Contents

Classes

CMult	Cl_(0,0) => Real Numbers
Keci	Base class for all neural network modules.
KeciBase	Without learning dimension scaling
DeCaL	Base class for all neural network modules.

class `dicee.models.clifford.`**`CMult`**(*args*)

Bases: *dicee.models.base_model.BaseKGE*

Cl_(0,0) => Real Numbers

Cl_(0,1) =>

A multivector mathbf{a} = a_0 + a_1 e_1 A multivector mathbf{b} = b_0 + b_1 e_1

multiplication is isomorphic to the product of two complex numbers

mathbf{a} imes mathbf{b} = a_0 b_0 + a_0b_1 e1 + a_1 b_1 e_1 e_1

= (a_0 b_0 - a_1 b_1) + (a_0 b_1 + a_1 b_0) e_1

Cl_(2,0) =>

A multivector mathbf{a} = a_0 + a_1 e_1 + a_2 e_2 + a_{12} e_1 e_2 A multivector mathbf{b} = b_0 + b_1 e_1 + b_2 e_2 + b_{12} e_1 e_2

mathbf{a} imes mathbf{b} = a_0b_0 + a_0b_1 e_1 + a_0b_2e_2 + a_0 b_12 e_1 e_2

- a_1 b_0 e_1 + a_1b_1 e_1_e1 ..

Cl_(0,2) => Quaternions

`clifford_mul`(*x: torch.FloatTensor*, *y: torch.FloatTensor*, *p: int*, *q: int*) → tuple

Clifford multiplication Cl_{p,q} (mathbb{R})

ei ^2 = +1 for i =< i =< p ej ^2 = -1 for p < j =< p+q ei ej = -eje1 for i

eq j

x: torch.FloatTensor with (n,d) shape

y: torch.FloatTensor with (n,d) shape

p: a non-negative integer p>= 0 q: a non-negative integer q>= 0

`score`(*head_ent_emb*, *rel_ent_emb*, *tail_ent_emb*)

`forward_triples`(*x: torch.LongTensor*) → torch.FloatTensor

Compute batch triple scores

Parameter

x: torch.LongTensor with shape n by 3

rtype
torch.LongTensor with shape n

forward_k_vs_all(*x: torch.Tensor*) → torch.FloatTensor

Compute batch KvsAll triple scores

Parameter

x: torch.LongTensor with shape n by 3

rtype
torch.LongTensor with shape n

class dicee.models.clifford.**Keci**(*args*)

Bases: *dicee.models.base_model.BaseKGE*

Base class for all neural network modules.

Your models should also subclass this class.

Modules can also contain other Modules, allowing to nest them in a tree structure. You can assign the submodules as regular attributes:

```
import torch.nn as nn
import torch.nn.functional as F

class Model(nn.Module):
    def __init__(self):
        super().__init__()
        self.conv1 = nn.Conv2d(1, 20, 5)
        self.conv2 = nn.Conv2d(20, 20, 5)

    def forward(self, x):
        x = F.relu(self.conv1(x))
        return F.relu(self.conv2(x))
```

Submodules assigned in this way will be registered, and will have their parameters converted too when you call `to()`, etc.

Note: As per the example above, an `__init__()` call to the parent class must be made before assignment on the child.

Variables
training (*bool*) – Boolean represents whether this module is in training or evaluation mode.

compute_sigma_pp(*hp*, *rp*)

Compute sigma_{pp} = sum_{i=1}^{p-1} sum_{k=i+1}^p (h_i r_k - h_k r_i) e_i e_k

sigma_{pp} captures the interactions between along p bases For instance, let p e_1, e_2, e_3, we compute interactions between e_1 e_2, e_1 e_3 , and e_2 e_3 This can be implemented with a nested two for loops

results = [] for i in range(p - 1):

for k in range(i + 1, p):
results.append(hp[:, :, i] * rp[:, :, k] - hp[:, :, k] * rp[:, :, i])

sigma_pp = torch.stack(results, dim=2) assert sigma_pp.shape == (b, r, int((p * (p - 1)) / 2))

Yet, this computation would be quite inefficient. Instead, we compute interactions along all p, e.g., e1e1, e1e2, e1e3,

e2e1, e2e2, e2e3, e3e1, e3e2, e3e3

Then select the triangular matrix without diagonals: e1e2, e1e3, e2e3.

compute_sigma_qq(*hq*, *rq*)

Compute sigma_{qq} = sum_{j=1}^{p+q-1} sum_{k=j+1}^{p+q} (h_j r_k - h_k r_j) e_j e_k sigma_{q} captures the interactions between along q bases For instance, let q e_1, e_2, e_3, we compute interactions between e_1 e_2, e_1 e_3 , and e_2 e_3 This can be implemented with a nested two for loops

results = [] for j in range(q - 1):

for k in range(j + 1, q):
results.append(hq[:, :, j] * rq[:, :, k] - hq[:, :, k] * rq[:, :, j])

sigma_qq = torch.stack(results, dim=2) assert sigma_qq.shape == (b, r, int((q * (q - 1)) / 2))

Yet, this computation would be quite inefficient. Instead, we compute interactions along all p, e.g., e1e1, e1e2, e1e3,

e2e1, e2e2, e2e3, e3e1, e3e2, e3e3

Then select the triangular matrix without diagonals: e1e2, e1e3, e2e3.

compute_sigma_pq(*, *hp*, *hq*, *rp*, *rq*)

sum_{i=1}^{p} sum_{j=p+1}^{p+q} (h_i r_j - h_j r_i) e_i e_j

results = [] sigma_pq = torch.zeros(b, r, p, q) for i in range(p):

for j in range(q):
sigma_pq[:, :, i, j] = hp[:, :, i] * rq[:, :, j] - hq[:, :, j] * rp[:, :, i]

print(sigma_pq.shape)

apply_coefficients(*h0*, *hp*, *hq*, *r0*, *rp*, *rq*)

Multiplying a base vector with its scalar coefficient

clifford_multiplication(*h0*, *hp*, *hq*, *r0*, *rp*, *rq*)

Compute our CL multiplication

h = h_0 + sum_{i=1}^p h_i e_i + sum_{j=p+1}^{p+q} h_j e_j r = r_0 + sum_{i=1}^p r_i e_i + sum_{j=p+1}^{p+q} r_j e_j

ei ^2 = +1 for i =< i =< p ej ^2 = -1 for p < j =< p+q ei ej = -eje1 for i

eq j

h r = sigma_0 + sigma_p + sigma_q + sigma_{pp} + sigma_{q}+ sigma_{pq} where

(1) sigma_0 = h_0 r_0 + sum_{i=1}^p (h_0 r_i) e_i - sum_{j=p+1}^{p+q} (h_j r_j) e_j

(2) sigma_p = sum_{i=1}^p (h_0 r_i + h_i r_0) e_i

(3) sigma_q = sum_{j=p+1}^{p+q} (h_0 r_j + h_j r_0) e_j

(4) sigma_{pp} = sum_{i=1}^{p-1} sum_{k=i+1}^p (h_i r_k - h_k r_i) e_i e_k

(5) sigma_{qq} = sum_{j=1}^{p+q-1} sum_{k=j+1}^{p+q} (h_j r_k - h_k r_j) e_j e_k

(6) sigma_{pq} = sum_{i=1}^{p} sum_{j=p+1}^{p+q} (h_i r_j - h_j r_i) e_i e_j

construct_cl_multivector (*x: torch.FloatTensor*, *r: int*, *p: int*, *q: int*) → tuple[torch.FloatTensor, torch.FloatTensor, torch.FloatTensor]

Construct a batch of multivectors Cl_{p,q}(mathbb{R}^d)

Parameter

x: torch.FloatTensor with (n,d) shape

returns

- **a0** (*torch.FloatTensor with (n,r) shape*)
- **ap** (*torch.FloatTensor with (n,r,p) shape*)
- **aq** (*torch.FloatTensor with (n,r,q) shape*)

forward_k_vs_with_explicit (*x: torch.Tensor*)

k_vs_all_score (*bpe_head_ent_emb*, *bpe_rel_ent_emb*, *E*)

forward_k_vs_all (*x: torch.Tensor*) → torch.FloatTensor

Kvsall training

(1) Retrieve real-valued embedding vectors for heads and relations mathbb{R}^d .

(2) Construct head entity and relation embeddings according to Cl_{p,q}(mathbb{R}^d) .

(3) Perform Cl multiplication

(4) Inner product of (3) and all entity embeddings

forward_k_vs_with_explicit and this funcitons are identical Parameter ——— x: torch.LongTensor with (n,2) shape :rtype: torch.FloatTensor with (n, |E|) shape

forward_k_vs_sample (*x: torch.LongTensor*, *target_entity_idx: torch.LongTensor*) → torch.FloatTensor

Kvsall training

(1) Retrieve real-valued embedding vectors for heads and relations mathbb{R}^d .

(2) Construct head entity and relation embeddings according to Cl_{p,q}(mathbb{R}^d) .

(3) Perform Cl multiplication

(4) Inner product of (3) and all entity embeddings

Parameter

x: torch.LongTensor with (n,2) shape

rtype

torch.FloatTensor with (n, |E|) shape

score (*h*, *r*, *t*)

forward_triples (*x: torch.Tensor*) → torch.FloatTensor

Parameter

x: torch.LongTensor with (n,3) shape

rtype
torch.FloatTensor with (n) shape

class dicee.models.clifford.**KeciBase**(*args*)

Bases: *Keci*

Without learning dimension scaling

class dicee.models.clifford.**DeCaL**(*args*)

Bases: *dicee.models.base_model.BaseKGE*

Base class for all neural network modules.

Your models should also subclass this class.

Modules can also contain other Modules, allowing to nest them in a tree structure. You can assign the submodules as regular attributes:

```
import torch.nn as nn
import torch.nn.functional as F

class Model(nn.Module):
    def __init__(self):
        super().__init__()
        self.conv1 = nn.Conv2d(1, 20, 5)
        self.conv2 = nn.Conv2d(20, 20, 5)

    def forward(self, x):
        x = F.relu(self.conv1(x))
        return F.relu(self.conv2(x))
```

Submodules assigned in this way will be registered, and will have their parameters converted too when you call `to()`, etc.

Note: As per the example above, an `__init__()` call to the parent class must be made before assignment on the child.

Variables
training (*bool*) – Boolean represents whether this module is in training or evaluation mode.

forward_triples(*x: torch.Tensor*) → torch.FloatTensor

Parameter

x: torch.LongTensor with (n,3) shape

rtype
torch.FloatTensor with (n) shape

cl_pqr (*a*)

Input: tensor(batch_size, emb_dim) —-> output: tensor with 1+p+q+r components with size (batch_size, emb_dim/(1+p+q+r)) each.

1) takes a tensor of size (batch_size, emb_dim), split it into 1 + p + q +r components, hence 1+p+q+r must be a divisor of the emb_dim. 2) Return a list of the 1+p+q+r components vectors, each are tensors of size (batch_size, emb_dim/(1+p+q+r))

compute_sigmas_single (*list_h_emb*, *list_r_emb*, *list_t_emb*)

here we compute all the sums with no others vectors interaction taken with the scalar product with t, that is, 1) s0 = h_0r_0t_0 2) s1 = sum_{i=1}^{p}h_ir_it_0 3) s2 = sum_{j=p+1}^{p+q}h_jr_jt_0 4) s3 = sum_{i=1}^{q}(h_0r_it_i + h_ir_0t_i) 5) s4 = sum_{i=p+1}^{p+q}(h_0r_it_i + h_ir_0t_i) 5) s5 = sum_{i=p+q+1}^{p+q+r}(h_0r_it_i + h_ir_0t_i)

and return:

*) sigma_0t = sigma_0 cdot t_0 = s0 + s1 -s2 *) s3, s4 and s5

compute_sigmas_multivect (*list_h_emb*, *list_r_emb*)

Here we compute and return all the sums with vectors interaction for the same and different bases.

For same bases vectors interaction we have

1) sigma_pp = sum_{i=1}^{p-1}sum_{i'=i+1}^{p}(h_ir_{i'}-h_{i'}r_i) (models the interactions between e_i and e_i' for 1 <= i, i' <= p)
2) sigma_qq = sum_{j=p+1}^{p+q-1}sum_{j'=j+1}^{p+q}(h_jr_{j'}-h_{j'} (models the interactions between e_j and e_j' for p+1 <= j, j' <= p+q)
3) sigma_rr = sum_{k=p+q+1}^{p+q+r-1}sum_{k'=k+1}^{p}(h_kr_{k'}-h_{k'}r_k) (models the interactions between e_k and e_k' for p+q+1 <= k, k' <= p+q+r)

For different base vector interactions, we have

4) sigma_pq = sum_{i=1}^{p}sum_{j=p+1}^{p+q}(h_ir_j - h_jr_i) (interactionsn between e_i and e_j for 1<=i <=p and p+1<= j <= p+q)
5) sigma_pr = sum_{i=1}^{p}sum_{k=p+q+1}^{p+q+r}(h_ir_k - h_kr_i) (interactionsn between e_i and e_k for 1<=i <=p and p+q+1<= k <= p+q+r)
6) sigma_qr = sum_{j=p+1}^{p+q}sum_{j=p+q+1}^{p+q+r}(h_jr_k - h_kr_j) (interactionsn between e_j and e_k for p+1 <= j <=p+q and p+q+1<= j <= p+q+r)

forward_k_vs_all (*x: torch.Tensor*) → torch.FloatTensor

Kvsall training

(1) Retrieve real-valued embedding vectors for heads and relations mathbb{R}^d .
(2) Construct head entity and relation embeddings according to Cl_{p,q}(mathbb{R}^d) .
(3) Perform Cl multiplication
(4) Inner product of (3) and all entity embeddings

forward_k_vs_with_explicit and this funcitons are identical Parameter ——— x: torch.LongTensor with (n,2) shape :rtype: torch.FloatTensor with (n, |E|) shape

apply_coefficients(*h0*, *hp*, *hq*, *hk*, *r0*, *rp*, *rq*, *rk*)

Multiplying a base vector with its scalar coefficient

construct_cl_multivector(*x: torch.FloatTensor*, *re: int*, *p: int*, *q: int*, *r: int*) → tuple[torch.FloatTensor, torch.FloatTensor, torch.FloatTensor]

Construct a batch of multivectors Cl_{p,q,r}(mathbb{R}^d)

Parameter

x: torch.FloatTensor with (n,d) shape

returns

- **a0** (*torch.FloatTensor*)
- **ap** (*torch.FloatTensor*)
- **aq** (*torch.FloatTensor*)
- **ar** (*torch.FloatTensor*)

compute_sigma_pp(*hp*, *rp*)

sigma_{p,p}^* = sum_{i=1}^{p-1}sum_{i'=i+1}^{p}(x_iy_{i'}-x_{i'}y_i)

sigma_{pp} captures the interactions between along p bases For instance, let p e_1, e_2, e_3, we compute interactions between e_1 e_2, e_1 e_3 , and e_2 e_3 This can be implemented with a nested two for loops

results = [] for i in range(p - 1):

for k in range(i + 1, p):
results.append(hp[:, :, i] * rp[:, :, k] - hp[:, :, k] * rp[:, :, i])

sigma_pp = torch.stack(results, dim=2) assert sigma_pp.shape == (b, r, int((p * (p - 1)) / 2))

Yet, this computation would be quite inefficient. Instead, we compute interactions along all p, e.g., e1e1, e1e2, e1e3,

e2e1, e2e2, e2e3, e3e1, e3e2, e3e3

Then select the triangular matrix without diagonals: e1e2, e1e3, e2e3.

compute_sigma_qq(*hq*, *rq*)

Compute sigma_{q,q}^* = sum_{j=p+1}^{p+q-1}sum_{j'=j+1}^{p+q}(x_jy_{j'}-x_{j'}y_j) Eq. 16 sigma_{q} captures the interactions between along q bases For instance, let q e_1, e_2, e_3, we compute interactions between e_1 e_2, e_1 e_3 , and e_2 e_3 This can be implemented with a nested two for loops

results = [] for j in range(q - 1):

for k in range(j + 1, q):
results.append(hq[:, :, j] * rq[:, :, k] - hq[:, :, k] * rq[:, :, j])

sigma_qq = torch.stack(results, dim=2) assert sigma_qq.shape == (b, r, int((q * (q - 1)) / 2))

Yet, this computation would be quite inefficient. Instead, we compute interactions along all p, e.g., e1e1, e1e2, e1e3,

e2e1, e2e2, e2e3, e3e1, e3e2, e3e3

Then select the triangular matrix without diagonals: e1e2, e1e3, e2e3.

compute_sigma_rr(*hk*, *rk*)

sigma_{r,r}^* = sum_{k=p+q+1}^{p+q+r-1}sum_{k'=k+1}^{p}(x_ky_{k'}-x_{k'}y_k)

compute_sigma_pq(*, *hp*, *hq*, *rp*, *rq*)

sum_{i=1}^{p} sum_{j=p+1}^{p+q} (h_i r_j - h_j r_i) e_i e_j

results = [] sigma_pq = torch.zeros(b, r, p, q) for i in range(p):

for j in range(q):
sigma_pq[:, :, i, j] = hp[:, :, i] * rq[:, :, j] - hq[:, :, j] * rp[:, :, i]

print(sigma_pq.shape)

compute_sigma_pr(*, *hp*, *hk*, *rp*, *rk*)

sum_{i=1}^{p} sum_{j=p+1}^{p+q} (h_i r_j - h_j r_i) e_i e_j

results = [] sigma_pq = torch.zeros(b, r, p, q) for i in range(p):

for j in range(q):
sigma_pq[:, :, i, j] = hp[:, :, i] * rq[:, :, j] - hq[:, :, j] * rp[:, :, i]

print(sigma_pq.shape)

compute_sigma_qr(*, *hq*, *hk*, *rq*, *rk*)

sum_{i=1}^{p} sum_{j=p+1}^{p+q} (h_i r_j - h_j r_i) e_i e_j

results = [] sigma_pq = torch.zeros(b, r, p, q) for i in range(p):

for j in range(q):
sigma_pq[:, :, i, j] = hp[:, :, i] * rq[:, :, j] - hq[:, :, j] * rp[:, :, i]

print(sigma_pq.shape)

dicee.models.complex

Module Contents

Classes

ConEx	Convolutional ComplEx Knowledge Graph Embeddings
AConEx	Additive Convolutional ComplEx Knowledge Graph Embeddings
ComplEx	Base class for all neural network modules.

class dicee.models.complex.**ConEx**(*args*)

Bases: *dicee.models.base_model.BaseKGE*

Convolutional ComplEx Knowledge Graph Embeddings

residual_convolution(*C_1: Tuple[torch.Tensor, torch.Tensor]*, *C_2: Tuple[torch.Tensor, torch.Tensor]*) → torch.FloatTensor

Compute residual score of two complex-valued embeddings. :param C_1: a tuple of two pytorch tensors that corresponds complex-valued embeddings :param C_2: a tuple of two pytorch tensors that corresponds complex-valued embeddings :return:

forward_k_vs_all(*x: torch.Tensor*) → torch.FloatTensor

forward_triples(*x: torch.Tensor*) → torch.FloatTensor

Parameters
x –

forward_k_vs_sample(*x: torch.Tensor*, *target_entity_idx: torch.Tensor*)

class dicee.models.complex.**AConEx**(*args*)
Bases: *dicee.models.base_model.BaseKGE*

Additive Convolutional ComplEx Knowledge Graph Embeddings

residual_convolution(*C_1: Tuple[torch.Tensor, torch.Tensor]*, *C_2: Tuple[torch.Tensor, torch.Tensor]*) → torch.FloatTensor

Compute residual score of two complex-valued embeddings. :param C_1: a tuple of two pytorch tensors that corresponds complex-valued embeddings :param C_2: a tuple of two pytorch tensors that corresponds complex-valued embeddings :return:

forward_k_vs_all(*x: torch.Tensor*) → torch.FloatTensor

forward_triples(*x: torch.Tensor*) → torch.FloatTensor

Parameters
x –

forward_k_vs_sample(*x: torch.Tensor*, *target_entity_idx: torch.Tensor*)

class dicee.models.complex.**ComplEx**(*args*)
Bases: *dicee.models.base_model.BaseKGE*

Base class for all neural network modules.

Your models should also subclass this class.

Modules can also contain other Modules, allowing to nest them in a tree structure. You can assign the submodules as regular attributes:

```
import torch.nn as nn
import torch.nn.functional as F

class Model(nn.Module):
    def __init__(self):
        super().__init__()
        self.conv1 = nn.Conv2d(1, 20, 5)
        self.conv2 = nn.Conv2d(20, 20, 5)

    def forward(self, x):
        x = F.relu(self.conv1(x))
        return F.relu(self.conv2(x))
```

Submodules assigned in this way will be registered, and will have their parameters converted too when you call `to()`, etc.

Note: As per the example above, an `__init__()` call to the parent class must be made before assignment on the child.

Variables
training (*bool*) – Boolean represents whether this module is in training or evaluation mode.

static score(*head_ent_emb: torch.FloatTensor*, *rel_ent_emb: torch.FloatTensor*, *tail_ent_emb: torch.FloatTensor*)

static k_vs_all_score(*emb_h: torch.FloatTensor*, *emb_r: torch.FloatTensor*, *emb_E: torch.FloatTensor*)

Parameters

- **emb_h** –
- **emb_r** –
- **emb_E** –

forward_k_vs_all(*x: torch.LongTensor*) → torch.FloatTensor

dicee.models.function_space

Module Contents

Classes

FMult	Learning Knowledge Neural Graphs
GFMult	Learning Knowledge Neural Graphs
FMult2	Learning Knowledge Neural Graphs
LFMult1	Embedding with trigonometric functions. We represent all entities and relations in the complex number space as:
LFMult	Embedding with polynomial functions. We represent all entities and relations in the polynomial space as:

class dicee.models.function_space.**FMult**(*args*)

Bases: *dicee.models.base_model.BaseKGE*

Learning Knowledge Neural Graphs

compute_func(*weights: torch.FloatTensor*, *x*) → torch.FloatTensor

chain_func(*weights*, *x: torch.FloatTensor*)

forward_triples(*idx_triple: torch.Tensor*) → torch.Tensor

Parameters

x –

class dicee.models.function_space.**GFMult**(*args*)

Bases: *dicee.models.base_model.BaseKGE*

Learning Knowledge Neural Graphs

compute_func(*weights: torch.FloatTensor*, *x*) → torch.FloatTensor

chain_func(*weights*, *x: torch.FloatTensor*)

forward_triples(*idx_triple: torch.Tensor*) → torch.Tensor

Parameters

x –

class dicee.models.function_space.**FMult2**(*args*)

Bases: *dicee.models.base_model.BaseKGE*

Learning Knowledge Neural Graphs

build_func(*Vec*)

build_chain_funcs(*list_Vec*)

compute_func(*W*, *b*, *x*) → torch.FloatTensor

function(*list_W*, *list_b*)

trapezoid(*list_W*, *list_b*)

forward_triples(*idx_triple: torch.Tensor*) → torch.Tensor

Parameters

x –

class dicee.models.function_space.**LFMult1**(*args*)

Bases: *dicee.models.base_model.BaseKGE*

Embedding with trigonometric functions. We represent all entities and relations in the complex number space as: f(x) = sum_{k=0}^{k=d-1}wk e^{kix}. and use the three differents scoring function as in the paper to evaluate the score

forward_triples(*idx_triple*)

Parameters

x –

tri_score(*h*, *r*, *t*)

vtp_score(*h*, *r*, *t*)

class dicee.models.function_space.**LFMult**(*args*)

Bases: *dicee.models.base_model.BaseKGE*

Embedding with polynomial functions. We represent all entities and relations in the polynomial space as: f(x) = sum_{i=0}^{d-1} a_k x^{i%d} and use the three differents scoring function as in the paper to evaluate the score. We also consider combining with Neural Networks.

forward_triples(*idx_triple*)

Parameters

x –

construct_multi_coeff(*x*)

poly_NN(*x*, *coefh*, *coefr*, *coeft*)

Constructing a 2 layers NN to represent the embeddings. h = sigma(wh^T x + bh), r = sigma(wr^T x + br), t = sigma(wt^T x + bt)

linear(*x*, *w*, *b*)

scalar_batch_NN(*a*, *b*, *c*)

element wise multiplication between a,b and c: Inputs : a, b, c ====> torch.tensor of size batch_size x m x d Output : a tensor of size batch_size x d

tri_score (*coeff_h*, *coeff_r*, *coeff_t*)

this part implement the trilinear scoring techniques:

score(h,r,t) = int_{0}{1} h(x)r(x)t(x) dx = sum_{i,j,k = 0}^{d-1} dfrac{a_i*b_j*c_k}{1+(i+j+k)%d}

1. generate the range for i,j and k from [0 d-1]

2. perform dfrac{a_i*b_j*c_k}{1+(i+j+k)%d} in parallel for every batch

3. take the sum over each batch

vtp_score (*h*, *r*, *t*)

this part implement the vector triple product scoring techniques:

score(h,r,t) = int_{0}{1} h(x)r(x)t(x) dx = sum_{i,j,k = 0}^{d-1} dfrac{a_i*c_j*b_k - b_i*c_j*a_k}{(1+(i+j)%d)(1+k)}

1. generate the range for i,j and k from [0 d-1]
2. Compute the first and second terms of the sum
3. Multiply with then denominator and take the sum
4. take the sum over each batch

comp_func (*h*, *r*, *t*)

this part implement the function composition scoring techniques: i.e. score = <hor, t>

polynomial (*coeff*, *x*, *degree*)

This function takes a matrix tensor of coefficients (coeff), a tensor vector of points x and range of integer [0,1,…d] and return a vector tensor (coeff[0][0] + coeff[0][1]x +…+ coeff[0][d]x^d,

coeff[1][0] + coeff[1][1]x +…+ coeff[1][d]x^d)

pop (*coeff*, *x*, *degree*)

This function allow us to evaluate the composition of two polynomes without for loops :) it takes a matrix tensor of coefficients (coeff), a matrix tensor of points x and range of integer [0,1,…d]

and return a tensor (coeff[0][0] + coeff[0][1]x +…+ coeff[0][d]x^d,

coeff[1][0] + coeff[1][1]x +…+ coeff[1][d]x^d)

dicee.models.octonion

Module Contents

Classes

OMult	Base class for all neural network modules.
ConvO	Base class for all neural network modules.
AConvO	Additive Convolutional Octonion Knowledge Graph Embeddings

Functions

octonion_mul(*, O_1, O_2)	
octonion_mul_norm(*, O_1, O_2)	

dicee.models.octonion.**octonion_mul**(*, *O_1*, *O_2*)

dicee.models.octonion.**octonion_mul_norm**(*, *O_1*, *O_2*)

class dicee.models.octonion.**OMult**(*args*)

Bases: *dicee.models.base_model.BaseKGE*

Base class for all neural network modules.

Your models should also subclass this class.

Modules can also contain other Modules, allowing to nest them in a tree structure. You can assign the submodules as regular attributes:

```
import torch.nn as nn
import torch.nn.functional as F

class Model(nn.Module):
    def __init__(self):
        super().__init__()
        self.conv1 = nn.Conv2d(1, 20, 5)
        self.conv2 = nn.Conv2d(20, 20, 5)

    def forward(self, x):
        x = F.relu(self.conv1(x))
        return F.relu(self.conv2(x))
```

Submodules assigned in this way will be registered, and will have their parameters converted too when you call `to()`, etc.

Note: As per the example above, an `__init__()` call to the parent class must be made before assignment on the child.

Variables

training (*bool*) – Boolean represents whether this module is in training or evaluation mode.

static octonion_normalizer(*emb_rel_e0*, *emb_rel_e1*, *emb_rel_e2*, *emb_rel_e3*, *emb_rel_e4*, *emb_rel_e5*, *emb_rel_e6*, *emb_rel_e7*)

score(*head_ent_emb: torch.FloatTensor*, *rel_ent_emb: torch.FloatTensor*, *tail_ent_emb: torch.FloatTensor*)

k_vs_all_score(*bpe_head_ent_emb*, *bpe_rel_ent_emb*, *E*)

forward_k_vs_all(*x*)

Completed. Given a head entity and a relation (h,r), we compute scores for all possible triples,i.e., [score(h,r,x)|x in Entities] => [0.0,0.1,…,0.8], shape=> (1, **|Entities|**) Given a batch of head entities and relations => shape (size of batch,| Entities|)

class dicee.models.octonion.**ConvO**(*args: dict*)

Bases: *dicee.models.base_model.BaseKGE*

Base class for all neural network modules.

Your models should also subclass this class.

Modules can also contain other Modules, allowing to nest them in a tree structure. You can assign the submodules as regular attributes:

```
import torch.nn as nn
import torch.nn.functional as F

class Model(nn.Module):
    def __init__(self):
        super().__init__()
        self.conv1 = nn.Conv2d(1, 20, 5)
        self.conv2 = nn.Conv2d(20, 20, 5)

    def forward(self, x):
        x = F.relu(self.conv1(x))
        return F.relu(self.conv2(x))
```

Submodules assigned in this way will be registered, and will have their parameters converted too when you call `to()`, etc.

Note: As per the example above, an `__init__()` call to the parent class must be made before assignment on the child.

Variables

training (*bool*) – Boolean represents whether this module is in training or evaluation mode.

static octonion_normalizer(*emb_rel_e0, emb_rel_e1, emb_rel_e2, emb_rel_e3, emb_rel_e4, emb_rel_e5, emb_rel_e6, emb_rel_e7*)

residual_convolution(*O_1, O_2*)

forward_triples(*x: torch.Tensor*) → torch.Tensor

Parameters

x –

forward_k_vs_all(*x: torch.Tensor*)

Given a head entity and a relation (h,r), we compute scores for all entities. [score(h,r,x)|x in Entities] => [0.0,0.1,…,0.8], shape=> (1, |Entities|) Given a batch of head entities and relations => shape (size of batch,| Entities|)

class dicee.models.octonion.**AConvO**(*args: dict*)

Bases: *dicee.models.base_model.BaseKGE*

Additive Convolutional Octonion Knowledge Graph Embeddings

static octonion_normalizer(*emb_rel_e0, emb_rel_e1, emb_rel_e2, emb_rel_e3, emb_rel_e4, emb_rel_e5, emb_rel_e6, emb_rel_e7*)

residual_convolution(*O_1, O_2*)

forward_triples (*x: torch.Tensor*) → torch.Tensor

Parameters

x –

forward_k_vs_all (*x: torch.Tensor*)

Given a head entity and a relation (h,r), we compute scores for all entities. [score(h,r,x)|x in Entities] => [0.0,0.1,…,0.8], shape=> (1, **|Entities|**) Given a batch of head entities and relations => shape (size of batch,| Entities|)

dicee.models.pykeen_models

Module Contents

Classes

PykeenKGE	A class for using knowledge graph embedding models implemented in Pykeen

class dicee.models.pykeen_models.**PykeenKGE** (*args: dict*)

Bases: *dicee.models.base_model.BaseKGE*

A class for using knowledge graph embedding models implemented in Pykeen

Notes: Pykeen_DistMult: C Pykeen_ComplEx: Pykeen_QuatE: Pykeen_MuRE: Pykeen_CP: Pykeen_HolE: Pykeen_HolE:

forward_k_vs_all (*x: torch.LongTensor*)

=> Explicit version by this we can apply bn and dropout

(1) Retrieve embeddings of heads and relations + apply Dropout & Normalization if given. h, r = self.get_head_relation_representation(x) # (2) Reshape (1). if self.last_dim > 0:

h = h.reshape(len(x), self.embedding_dim, self.last_dim) r = r.reshape(len(x), self.embedding_dim, self.last_dim)

(3) Reshape all entities. if self.last_dim > 0:

t = self.entity_embeddings.weight.reshape(self.num_entities, self.embedding_dim, self.last_dim)

else:

t = self.entity_embeddings.weight

(4) Call the score_t from interactions to generate triple scores. return self.interaction.score_t(h=h, r=r, all_entities=t, slice_size=1)

forward_triples (*x: torch.LongTensor*) → torch.FloatTensor

=> Explicit version by this we can apply bn and dropout

(1) Retrieve embeddings of heads, relations and tails and apply Dropout & Normalization if given. h, r, t = self.get_triple_representation(x) # (2) Reshape (1). if self.last_dim > 0:

h = h.reshape(len(x), self.embedding_dim, self.last_dim) r = r.reshape(len(x), self.embedding_dim, self.last_dim) t = t.reshape(len(x), self.embedding_dim, self.last_dim)

(3) Compute the triple score return self.interaction.score(h=h, r=r, t=t, slice_size=None, slice_dim=0)

abstract forward_k_vs_sample (*x: torch.LongTensor*, *target_entity_idx*)

dicee.models.quaternion

Module Contents

Classes

QMult	Base class for all neural network modules.
ConvQ	Convolutional Quaternion Knowledge Graph Embeddings
AConvQ	Additive Convolutional Quaternion Knowledge Graph Embeddings

Functions

quaternion_mul_with_unit_norm(*, Q_1, Q_2)	

dicee.models.quaternion.**quaternion_mul_with_unit_norm**(*, *Q_1*, *Q_2*)

class dicee.models.quaternion.**QMult**(*args*)

Bases: *dicee.models.base_model.BaseKGE*

Base class for all neural network modules.

Your models should also subclass this class.

Modules can also contain other Modules, allowing to nest them in a tree structure. You can assign the submodules as regular attributes:

```
import torch.nn as nn
import torch.nn.functional as F

class Model(nn.Module):
    def __init__(self):
        super().__init__()
        self.conv1 = nn.Conv2d(1, 20, 5)
        self.conv2 = nn.Conv2d(20, 20, 5)

    def forward(self, x):
        x = F.relu(self.conv1(x))
        return F.relu(self.conv2(x))
```

Submodules assigned in this way will be registered, and will have their parameters converted too when you call `to()`, etc.

Note: As per the example above, an `__init__()` call to the parent class must be made before assignment on the child.

Variables

training (*bool*) – Boolean represents whether this module is in training or evaluation mode.

quaternion_multiplication_followed_by_inner_product (*h*, *r*, *t*)

Parameters

- **h** – shape: (**batch_dims*, dim) The head representations.
- **r** – shape: (**batch_dims*, dim) The head representations.
- **t** – shape: (**batch_dims*, dim) The tail representations.

Returns

Triple scores.

static **quaternion_normalizer** (*x: torch.FloatTensor*) → torch.FloatTensor

Normalize the length of relation vectors, if the forward constraint has not been applied yet.

Absolute value of a quaternion

$$|a + bi + cj + dk| = \sqrt{a^2 + b^2 + c^2 + d^2}$$

L2 norm of quaternion vector:

$$\|x\|^2 = \sum_{i=1}^{d} |x_i|^2 = \sum_{i=1}^{d} (x_i.re^2 + x_i.im_1^2 + x_i.im_2^2 + x_i.im_3^2)$$

Parameters

x – The vector.

Returns

The normalized vector.

score (*head_ent_emb: torch.FloatTensor*, *rel_ent_emb: torch.FloatTensor*, *tail_ent_emb: torch.FloatTensor*)

k_vs_all_score (*bpe_head_ent_emb*, *bpe_rel_ent_emb*, *E*)

Parameters

- **bpe_head_ent_emb** –
- **bpe_rel_ent_emb** –
- **E** –

forward_k_vs_all (*x*)

Parameters

x –

forward_k_vs_sample (*x*, *target_entity_idx*)

Completed. Given a head entity and a relation (h,r), we compute scores for all possible triples,i.e., [score(h,r,x)|x in Entities] => [0.0,0.1,…,0.8], shape=> (1, **|Entities|**) Given a batch of head entities and relations => shape (size of batch,| Entities|)

class dicee.models.quaternion.**ConvQ** (*args*)

Bases: *dicee.models.base_model.BaseKGE*

Convolutional Quaternion Knowledge Graph Embeddings

residual_convolution(*Q_1*, *Q_2*)

forward_triples(*indexed_triple: torch.Tensor*) → torch.Tensor

Parameters

x –

forward_k_vs_all(*x: torch.Tensor*)

Given a head entity and a relation (h,r), we compute scores for all entities. [score(h,r,x)|x in Entities] => [0.0,0.1,…,0.8], shape=> (1, **|Entities|**) Given a batch of head entities and relations => shape (size of batch,| Entities|)

class dicee.models.quaternion.**AConvQ**(*args*)

Bases: *dicee.models.base_model.BaseKGE*

Additive Convolutional Quaternion Knowledge Graph Embeddings

residual_convolution(*Q_1*, *Q_2*)

forward_triples(*indexed_triple: torch.Tensor*) → torch.Tensor

Parameters

x –

forward_k_vs_all(*x: torch.Tensor*)

Given a head entity and a relation (h,r), we compute scores for all entities. [score(h,r,x)|x in Entities] => [0.0,0.1,…,0.8], shape=> (1, **|Entities|**) Given a batch of head entities and relations => shape (size of batch,| Entities|)

dicee.models.real

Module Contents

Classes

DistMult	Embedding Entities and Relations for Learning and Inference in Knowledge Bases
TransE	Translating Embeddings for Modeling
Shallom	A shallow neural model for relation prediction (https://arxiv.org/abs/2101.09090)
Pyke	A Physical Embedding Model for Knowledge Graphs

class dicee.models.real.**DistMult**(*args*)

Bases: *dicee.models.base_model.BaseKGE*

Embedding Entities and Relations for Learning and Inference in Knowledge Bases https://arxiv.org/abs/1412.6575

k_vs_all_score(*emb_h: torch.FloatTensor*, *emb_r: torch.FloatTensor*, *emb_E: torch.FloatTensor*)

Parameters

- **emb_h** –
- **emb_r** –

- **emb_E** –

forward_k_vs_all(*x: torch.LongTensor*)

forward_k_vs_sample(*x: torch.LongTensor*, *target_entity_idx: torch.LongTensor*)

score(*h*, *r*, *t*)

class dicee.models.real.**TransE**(*args*)

Bases: *dicee.models.base_model.BaseKGE*

Translating Embeddings for Modeling Multi-relational Data https://proceedings.neurips.cc/paper/2013/file/1cecc7a77928ca8133fa24680a88d2f9-Paper.pdf

score(*head_ent_emb*, *rel_ent_emb*, *tail_ent_emb*)

forward_k_vs_all(*x: torch.Tensor*) → torch.FloatTensor

class dicee.models.real.**Shallom**(*args*)

Bases: *dicee.models.base_model.BaseKGE*

A shallow neural model for relation prediction (https://arxiv.org/abs/2101.09090)

get_embeddings() → Tuple[numpy.ndarray, None]

forward_k_vs_all(*x*) → torch.FloatTensor

forward_triples(*x*) → torch.FloatTensor

Parameters
x –

Returns

class dicee.models.real.**Pyke**(*args*)

Bases: *dicee.models.base_model.BaseKGE*

A Physical Embedding Model for Knowledge Graphs

forward_triples(*x: torch.LongTensor*)

Parameters
x –

dicee.models.static_funcs

Module Contents

Functions

quaternion_mul(→ torch.Tensor, ...)	Tuple[torch.Tensor,	Perform quaternion multiplication

dicee.models.static_funcs.**quaternion_mul**(*, *Q_1*, *Q_2*) → Tuple[torch.Tensor, torch.Tensor, torch.Tensor, torch.Tensor]

Perform quaternion multiplication :param Q_1: :param Q_2: :return:

`dicee.models.transformers`

Module Contents

Classes

BytE	Base class for all neural network modules.
LayerNorm	LayerNorm but with an optional bias. PyTorch doesn't support simply bias=False
CausalSelfAttention	Base class for all neural network modules.
MLP	Base class for all neural network modules.
Block	Base class for all neural network modules.
GPTConfig	
GPT	Base class for all neural network modules.

class dicee.models.transformers.**BytE**(**args*, ***kwargs*)

Bases: *dicee.models.base_model.BaseKGE*

Base class for all neural network modules.

Your models should also subclass this class.

Modules can also contain other Modules, allowing to nest them in a tree structure. You can assign the submodules as regular attributes:

```
import torch.nn as nn
import torch.nn.functional as F

class Model(nn.Module):
    def __init__(self):
        super().__init__()
        self.conv1 = nn.Conv2d(1, 20, 5)
        self.conv2 = nn.Conv2d(20, 20, 5)

    def forward(self, x):
        x = F.relu(self.conv1(x))
        return F.relu(self.conv2(x))
```

Submodules assigned in this way will be registered, and will have their parameters converted too when you call `to()`, etc.

Note: As per the example above, an `__init__()` call to the parent class must be made before assignment on the child.

Variables

training (*bool*) – Boolean represents whether this module is in training or evaluation mode.

loss_function(*yhat_batch*, *y_batch*)

Parameters

- **yhat_batch** –

- **y_batch** –

forward (*x: torch.LongTensor*)

Parameters
x (*B by T tensor*) –

generate (*idx*, *max_new_tokens*, *temperature=1.0*, *top_k=None*)

Take a conditioning sequence of indices idx (LongTensor of shape (b,t)) and complete the sequence max_new_tokens times, feeding the predictions back into the model each time. Most likely you'll want to make sure to be in model.eval() mode of operation for this.

training_step (*batch*, *batch_idx=None*)

Here you compute and return the training loss and some additional metrics for e.g. the progress bar or logger.

Parameters

- **batch** – The output of your data iterable, normally a `DataLoader`.
- **batch_idx** – The index of this batch.
- **dataloader_idx** – The index of the dataloader that produced this batch. (only if multiple dataloaders used)

Returns

- `Tensor` - The loss tensor
- `dict` - A dictionary which can include any keys, but must include the key `'loss'` in the case of automatic optimization.
- `None` - In automatic optimization, this will skip to the next batch (but is not supported for multi-GPU, TPU, or DeepSpeed). For manual optimization, this has no special meaning, as returning the loss is not required.

In this step you'd normally do the forward pass and calculate the loss for a batch. You can also do fancier things like multiple forward passes or something model specific.

Example:

```
def training_step(self, batch, batch_idx):
    x, y, z = batch
    out = self.encoder(x)
    loss = self.loss(out, x)
    return loss
```

To use multiple optimizers, you can switch to 'manual optimization' and control their stepping:

```
def __init__(self):
    super().__init__()
    self.automatic_optimization = False


# Multiple optimizers (e.g.: GANs)
def training_step(self, batch, batch_idx):
    opt1, opt2 = self.optimizers()

    # do training_step with encoder
    ...
    opt1.step()
    # do training_step with decoder
```

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```
    ...
    opt2.step()
```

Note: When `accumulate_grad_batches` > 1, the loss returned here will be automatically normalized by `accumulate_grad_batches` internally.

class `dicee.models.transformers.`**LayerNorm**(*ndim*, *bias*)

Bases: `torch.nn.Module`

LayerNorm but with an optional bias. PyTorch doesn't support simply bias=False

forward(*input*)

class `dicee.models.transformers.`**CausalSelfAttention**(*config*)

Bases: `torch.nn.Module`

Base class for all neural network modules.

Your models should also subclass this class.

Modules can also contain other Modules, allowing to nest them in a tree structure. You can assign the submodules as regular attributes:

```
import torch.nn as nn
import torch.nn.functional as F

class Model(nn.Module):
    def __init__(self):
        super().__init__()
        self.conv1 = nn.Conv2d(1, 20, 5)
        self.conv2 = nn.Conv2d(20, 20, 5)

    def forward(self, x):
        x = F.relu(self.conv1(x))
        return F.relu(self.conv2(x))
```

Submodules assigned in this way will be registered, and will have their parameters converted too when you call `to()`, etc.

Note: As per the example above, an `__init__()` call to the parent class must be made before assignment on the child.

Variables

training (*bool*) – Boolean represents whether this module is in training or evaluation mode.

forward(*x*)

class `dicee.models.transformers.`**MLP**(*config*)

Bases: `torch.nn.Module`

Base class for all neural network modules.

Your models should also subclass this class.

Modules can also contain other Modules, allowing to nest them in a tree structure. You can assign the submodules as regular attributes:

```
import torch.nn as nn
import torch.nn.functional as F

class Model(nn.Module):
    def __init__(self):
        super().__init__()
        self.conv1 = nn.Conv2d(1, 20, 5)
        self.conv2 = nn.Conv2d(20, 20, 5)

    def forward(self, x):
        x = F.relu(self.conv1(x))
        return F.relu(self.conv2(x))
```

Submodules assigned in this way will be registered, and will have their parameters converted too when you call `to()`, etc.

Note: As per the example above, an `__init__()` call to the parent class must be made before assignment on the child.

Variables

training (*bool*) – Boolean represents whether this module is in training or evaluation mode.

forward(*x*)

class dicee.models.transformers.**Block**(*config*)

Bases: `torch.nn.Module`

Base class for all neural network modules.

Your models should also subclass this class.

Modules can also contain other Modules, allowing to nest them in a tree structure. You can assign the submodules as regular attributes:

```
import torch.nn as nn
import torch.nn.functional as F

class Model(nn.Module):
    def __init__(self):
        super().__init__()
        self.conv1 = nn.Conv2d(1, 20, 5)
        self.conv2 = nn.Conv2d(20, 20, 5)

    def forward(self, x):
        x = F.relu(self.conv1(x))
        return F.relu(self.conv2(x))
```

Submodules assigned in this way will be registered, and will have their parameters converted too when you call `to()`, etc.

Note: As per the example above, an `__init__()` call to the parent class must be made before assignment on the child.

Variables

training (*bool*) – Boolean represents whether this module is in training or evaluation mode.

forward(*x*)

class dicee.models.transformers.**GPTConfig**

block_size: int = 1024

vocab_size: int = 50304

n_layer: int = 12

n_head: int = 12

n_embd: int = 768

dropout: float = 0.0

bias: bool = False

class dicee.models.transformers.**GPT**(*config*)

Bases: torch.nn.Module

Base class for all neural network modules.

Your models should also subclass this class.

Modules can also contain other Modules, allowing to nest them in a tree structure. You can assign the submodules as regular attributes:

```
import torch.nn as nn
import torch.nn.functional as F

class Model(nn.Module):
    def __init__(self):
        super().__init__()
        self.conv1 = nn.Conv2d(1, 20, 5)
        self.conv2 = nn.Conv2d(20, 20, 5)

    def forward(self, x):
        x = F.relu(self.conv1(x))
        return F.relu(self.conv2(x))
```

Submodules assigned in this way will be registered, and will have their parameters converted too when you call to(), etc.

Note: As per the example above, an __init__() call to the parent class must be made before assignment on the child.

Variables

training (*bool*) – Boolean represents whether this module is in training or evaluation mode.

get_num_params(*non_embedding=True*)

Return the number of parameters in the model. For non-embedding count (default), the position embeddings get subtracted. The token embeddings would too, except due to the parameter sharing these params are actually used as weights in the final layer, so we include them.

forward(*idx*, *targets=None*)

crop_block_size(*block_size*)

classmethod from_pretrained(*model_type*, *override_args=None*)

configure_optimizers(*weight_decay*, *learning_rate*, *betas*, *device_type*)

estimate_mfu(*fwdbwd_per_iter*, *dt*)

estimate model flops utilization (MFU) in units of A100 bfloat16 peak FLOPS

Package Contents

Classes

BaseKGELightning	Base class for all neural network modules.
BaseKGE	Base class for all neural network modules.
IdentityClass	Base class for all neural network modules.
BaseKGE	Base class for all neural network modules.
DistMult	Embedding Entities and Relations for Learning and Inference in Knowledge Bases
TransE	Translating Embeddings for Modeling
Shallom	A shallow neural model for relation prediction (https://arxiv.org/abs/2101.09090)
Pyke	A Physical Embedding Model for Knowledge Graphs
BaseKGE	Base class for all neural network modules.
ConEx	Convolutional ComplEx Knowledge Graph Embeddings
AConEx	Additive Convolutional ComplEx Knowledge Graph Embeddings
ComplEx	Base class for all neural network modules.
BaseKGE	Base class for all neural network modules.
IdentityClass	Base class for all neural network modules.
QMult	Base class for all neural network modules.
ConvQ	Convolutional Quaternion Knowledge Graph Embeddings
AConvQ	Additive Convolutional Quaternion Knowledge Graph Embeddings
BaseKGE	Base class for all neural network modules.
IdentityClass	Base class for all neural network modules.
OMult	Base class for all neural network modules.
ConvO	Base class for all neural network modules.
AConvO	Additive Convolutional Octonion Knowledge Graph Embeddings
Keci	Base class for all neural network modules.
KeciBase	Without learning dimension scaling
CMult	Cl_(0,0) => Real Numbers
DeCaL	Base class for all neural network modules.
BaseKGE	Base class for all neural network modules.
PykeenKGE	A class for using knowledge graph embedding models implemented in Pykeen
BaseKGE	Base class for all neural network modules.

continues on next page

Table 1 – continued from previous page

FMult	Learning Knowledge Neural Graphs
GFMult	Learning Knowledge Neural Graphs
FMult2	Learning Knowledge Neural Graphs
LFMult1	Embedding with trigonometric functions. We represent all entities and relations in the complex number space as:
LFMult	Embedding with polynomial functions. We represent all entities and relations in the polynomial space as:

Functions

quaternion_mul(→ Tuple[torch.Tensor, torch.Tensor, ...)	Perform quaternion multiplication
quaternion_mul_with_unit_norm(*, Q_1, Q_2)	
octonion_mul(*, O_1, O_2)	
octonion_mul_norm(*, O_1, O_2)	

class dicee.models.**BaseKGELightning**(**args*, ***kwargs*)

Bases: `lightning.LightningModule`

Base class for all neural network modules.

Your models should also subclass this class.

Modules can also contain other Modules, allowing to nest them in a tree structure. You can assign the submodules as regular attributes:

```
import torch.nn as nn
import torch.nn.functional as F

class Model(nn.Module):
    def __init__(self):
        super().__init__()
        self.conv1 = nn.Conv2d(1, 20, 5)
        self.conv2 = nn.Conv2d(20, 20, 5)

    def forward(self, x):
        x = F.relu(self.conv1(x))
        return F.relu(self.conv2(x))
```

Submodules assigned in this way will be registered, and will have their parameters converted too when you call `to()`, etc.

Note: As per the example above, an `__init__()` call to the parent class must be made before assignment on the child.

Variables

training (*bool*) – Boolean represents whether this module is in training or evaluation mode.

mem_of_model() → Dict

Size of model in MB and number of params

training_step(*batch*, *batch_idx=None*)

Here you compute and return the training loss and some additional metrics for e.g. the progress bar or logger.

Parameters

- **batch** – The output of your data iterable, normally a `DataLoader`.
- **batch_idx** – The index of this batch.
- **dataloader_idx** – The index of the dataloader that produced this batch. (only if multiple dataloaders used)

Returns

- `Tensor` - The loss tensor
- `dict` - A dictionary which can include any keys, but must include the key `'loss'` in the case of automatic optimization.
- `None` - In automatic optimization, this will skip to the next batch (but is not supported for multi-GPU, TPU, or DeepSpeed). For manual optimization, this has no special meaning, as returning the loss is not required.

In this step you'd normally do the forward pass and calculate the loss for a batch. You can also do fancier things like multiple forward passes or something model specific.

Example:

```
def training_step(self, batch, batch_idx):
    x, y, z = batch
    out = self.encoder(x)
    loss = self.loss(out, x)
    return loss
```

To use multiple optimizers, you can switch to 'manual optimization' and control their stepping:

```
def __init__(self):
    super().__init__()
    self.automatic_optimization = False


# Multiple optimizers (e.g.: GANs)
def training_step(self, batch, batch_idx):
    opt1, opt2 = self.optimizers()

    # do training_step with encoder
    ...
    opt1.step()
    # do training_step with decoder
    ...
    opt2.step()
```

Note: When `accumulate_grad_batches` > 1, the loss returned here will be automatically normalized by `accumulate_grad_batches` internally.

loss_function(*yhat_batch: torch.FloatTensor*, *y_batch: torch.FloatTensor*)

Parameters

- **yhat_batch** –
- **y_batch** –

on_train_epoch_end(**args*, ***kwargs*)

Called in the training loop at the very end of the epoch.

To access all batch outputs at the end of the epoch, you can cache step outputs as an attribute of the `LightningModule` and access them in this hook:

```
class MyLightningModule(L.LightningModule):
    def __init__(self):
        super().__init__()
        self.training_step_outputs = []

    def training_step(self):
        loss = ...
        self.training_step_outputs.append(loss)
        return loss

    def on_train_epoch_end(self):
        # do something with all training_step outputs, for example:
        epoch_mean = torch.stack(self.training_step_outputs).mean()
        self.log("training_epoch_mean", epoch_mean)
        # free up the memory
        self.training_step_outputs.clear()
```

test_epoch_end(*outputs: List[Any]*)

test_dataloader() → None

An iterable or collection of iterables specifying test samples.

For more information about multiple dataloaders, see this section.

For data processing use the following pattern:

- download in `prepare_data()`
- process and split in `setup()`

However, the above are only necessary for distributed processing.

Warning: do not assign state in prepare_data

- `test()`
- `prepare_data()`
- `setup()`

Note: Lightning tries to add the correct sampler for distributed and arbitrary hardware. There is no need to set it yourself.

Note: If you don't need a test dataset and a `test_step()`, you don't need to implement this method.

`val_dataloader``()` → None

An iterable or collection of iterables specifying validation samples.

For more information about multiple dataloaders, see this section.

The dataloader you return will not be reloaded unless you set **:paramref:`~lightning.pytorch.trainer.trainer.Trainer.reload_dataloaders_every_n_epochs`** to a positive integer.

It's recommended that all data downloads and preparation happen in `prepare_data()`.

- `fit()`
- `validate()`
- `prepare_data()`
- `setup()`

Note: Lightning tries to add the correct sampler for distributed and arbitrary hardware There is no need to set it yourself.

Note: If you don't need a validation dataset and a `validation_step()`, you don't need to implement this method.

`predict_dataloader``()` → None

An iterable or collection of iterables specifying prediction samples.

For more information about multiple dataloaders, see this section.

It's recommended that all data downloads and preparation happen in `prepare_data()`.

- `predict()`
- `prepare_data()`
- `setup()`

Note: Lightning tries to add the correct sampler for distributed and arbitrary hardware There is no need to set it yourself.

Returns

A `torch.utils.data.DataLoader` or a sequence of them specifying prediction samples.

`train_dataloader``()` → None

An iterable or collection of iterables specifying training samples.

For more information about multiple dataloaders, see this section.

The dataloader you return will not be reloaded unless you set **:paramref:`~lightning.pytorch.trainer.trainer.Trainer.reload_dataloaders_every_n_epochs`** to a positive integer.

For data processing use the following pattern:

- download in `prepare_data()`
- process and split in `setup()`

However, the above are only necessary for distributed processing.

> **Warning:** do not assign state in prepare_data

- `fit()`
- `prepare_data()`
- `setup()`

Note: Lightning tries to add the correct sampler for distributed and arbitrary hardware. There is no need to set it yourself.

`configure_optimizers`(*parameters=None*)

Choose what optimizers and learning-rate schedulers to use in your optimization. Normally you'd need one. But in the case of GANs or similar you might have multiple. Optimization with multiple optimizers only works in the manual optimization mode.

Returns

Any of these 6 options.

- **Single optimizer**.
- **List or Tuple** of optimizers.
- **Two lists** - The first list has multiple optimizers, and the second has multiple LR schedulers (or multiple `lr_scheduler_config`).
- **Dictionary**, with an `"optimizer"` key, and (optionally) a `"lr_scheduler"` key whose value is a single LR scheduler or `lr_scheduler_config`.
- **None** - Fit will run without any optimizer.

The `lr_scheduler_config` is a dictionary which contains the scheduler and its associated configuration. The default configuration is shown below.

```
lr_scheduler_config = {
    # REQUIRED: The scheduler instance
    "scheduler": lr_scheduler,
    # The unit of the scheduler's step size, could also be 'step'.
    # 'epoch' updates the scheduler on epoch end whereas 'step'
    # updates it after a optimizer update.
    "interval": "epoch",
    # How many epochs/steps should pass between calls to
    # `scheduler.step()`. 1 corresponds to updating the learning
    # rate after every epoch/step.
    "frequency": 1,
    # Metric to to monitor for schedulers like `ReduceLROnPlateau`
    "monitor": "val_loss",
    # If set to `True`, will enforce that the value specified 'monitor'
    # is available when the scheduler is updated, thus stopping
```

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```
    # training if not found. If set to `False`, it will only produce a warning
    "strict": True,
    # If using the `LearningRateMonitor` callback to monitor the
    # learning rate progress, this keyword can be used to specify
    # a custom logged name
    "name": None,
}
```

When there are schedulers in which the `.step()` method is conditioned on a value, such as the `torch.optim.lr_scheduler.ReduceLROnPlateau` scheduler, Lightning requires that the `lr_scheduler_config` contains the keyword `"monitor"` set to the metric name that the scheduler should be conditioned on.

Metrics can be made available to monitor by simply logging it using `self.log('metric_to_track', metric_val)` in your `LightningModule`.

Note: Some things to know:

- Lightning calls `.backward()` and `.step()` automatically in case of automatic optimization.
- If a learning rate scheduler is specified in `configure_optimizers()` with key `"interval"` (default "epoch") in the scheduler configuration, Lightning will call the scheduler's `.step()` method automatically in case of automatic optimization.
- If you use 16-bit precision (`precision=16`), Lightning will automatically handle the optimizer.
- If you use `torch.optim.LBFGS`, Lightning handles the closure function automatically for you.
- If you use multiple optimizers, you will have to switch to 'manual optimization' mode and step them yourself.
- If you need to control how often the optimizer steps, override the `optimizer_step()` hook.

---

class dicee.models.**BaseKGE**(*args: dict*)

Bases: *BaseKGELightning*

Base class for all neural network modules.

Your models should also subclass this class.

Modules can also contain other Modules, allowing to nest them in a tree structure. You can assign the submodules as regular attributes:

```
import torch.nn as nn
import torch.nn.functional as F

class Model(nn.Module):
    def __init__(self):
        super().__init__()
        self.conv1 = nn.Conv2d(1, 20, 5)
        self.conv2 = nn.Conv2d(20, 20, 5)

    def forward(self, x):
        x = F.relu(self.conv1(x))
        return F.relu(self.conv2(x))
```

Submodules assigned in this way will be registered, and will have their parameters converted too when you call `to()`, etc.

Note: As per the example above, an `__init__()` call to the parent class must be made before assignment on the child.

Variables

training (*bool*) – Boolean represents whether this module is in training or evaluation mode.

forward_byte_pair_encoded_k_vs_all (*x: torch.LongTensor*)

Parameters

x (*B x 2 x T*) –

forward_byte_pair_encoded_triple (*x: Tuple[torch.LongTensor, torch.LongTensor]*)

byte pair encoded neural link predictors

Parameters

------- –

init_params_with_sanity_checking ()

forward (*x: torch.LongTensor | Tuple[torch.LongTensor, torch.LongTensor], y_idx: torch.LongTensor = None*)

Parameters

- **x** –
- **y_idx** –
- **ordered_bpe_entities** –

forward_triples (*x: torch.LongTensor*) → torch.Tensor

Parameters

x –

forward_k_vs_all (**args, **kwargs*)

forward_k_vs_sample (**args, **kwargs*)

get_triple_representation (*idx_hrt*)

get_head_relation_representation (*indexed_triple*)

get_sentence_representation (*x: torch.LongTensor*)

Parameters

- **(b** (*x shape*) –
- **3** –
- **t)** –

get_bpe_head_and_relation_representation (*x: torch.LongTensor*) → Tuple[torch.FloatTensor, torch.FloatTensor]

Parameters

x (*B x 2 x T*) –

get_embeddings () → Tuple[numpy.ndarray, numpy.ndarray]

class dicee.models.**IdentityClass**(*args=None*)

Bases: `torch.nn.Module`

Base class for all neural network modules.

Your models should also subclass this class.

Modules can also contain other Modules, allowing to nest them in a tree structure. You can assign the submodules as regular attributes:

```
import torch.nn as nn
import torch.nn.functional as F

class Model(nn.Module):
    def __init__(self):
        super().__init__()
        self.conv1 = nn.Conv2d(1, 20, 5)
        self.conv2 = nn.Conv2d(20, 20, 5)

    def forward(self, x):
        x = F.relu(self.conv1(x))
        return F.relu(self.conv2(x))
```

Submodules assigned in this way will be registered, and will have their parameters converted too when you call `to()`, etc.

Note: As per the example above, an `__init__()` call to the parent class must be made before assignment on the child.

Variables

training (*bool*) – Boolean represents whether this module is in training or evaluation mode.

static forward(*x*)

class dicee.models.**BaseKGE**(*args: dict*)

Bases: *BaseKGELightning*

Base class for all neural network modules.

Your models should also subclass this class.

Modules can also contain other Modules, allowing to nest them in a tree structure. You can assign the submodules as regular attributes:

```
import torch.nn as nn
import torch.nn.functional as F

class Model(nn.Module):
    def __init__(self):
        super().__init__()
        self.conv1 = nn.Conv2d(1, 20, 5)
        self.conv2 = nn.Conv2d(20, 20, 5)

    def forward(self, x):
        x = F.relu(self.conv1(x))
        return F.relu(self.conv2(x))
```

Submodules assigned in this way will be registered, and will have their parameters converted too when you call `to()`, etc.

Note: As per the example above, an `__init__()` call to the parent class must be made before assignment on the child.

Variables

training (*bool*) – Boolean represents whether this module is in training or evaluation mode.

forward_byte_pair_encoded_k_vs_all(*x: torch.LongTensor*)

Parameters

x (*B x 2 x T*) –

forward_byte_pair_encoded_triple(*x: Tuple[torch.LongTensor, torch.LongTensor]*)

byte pair encoded neural link predictors

Parameters

------- –

init_params_with_sanity_checking()

forward(*x: torch.LongTensor | Tuple[torch.LongTensor, torch.LongTensor], y_idx: torch.LongTensor = None*)

Parameters

- **x** –
- **y_idx** –
- **ordered_bpe_entities** –

forward_triples(*x: torch.LongTensor*) → torch.Tensor

Parameters

x –

forward_k_vs_all(**args, **kwargs*)

forward_k_vs_sample(**args, **kwargs*)

get_triple_representation(*idx_hrt*)

get_head_relation_representation(*indexed_triple*)

get_sentence_representation(*x: torch.LongTensor*)

Parameters

- **(b** (*x shape*) –
- **3** –
- **t)** –

get_bpe_head_and_relation_representation(*x: torch.LongTensor*) → Tuple[torch.FloatTensor, torch.FloatTensor]

Parameters

x (*B x 2 x T*) –

get_embeddings() → Tuple[numpy.ndarray, numpy.ndarray]

class dicee.models.**DistMult**(*args*)

Bases: *dicee.models.base_model.BaseKGE*

Embedding Entities and Relations for Learning and Inference in Knowledge Bases https://arxiv.org/abs/1412.6575

k_vs_all_score(*emb_h: torch.FloatTensor*, *emb_r: torch.FloatTensor*, *emb_E: torch.FloatTensor*)

Parameters

- **emb_h** –
- **emb_r** –
- **emb_E** –

forward_k_vs_all(*x: torch.LongTensor*)

forward_k_vs_sample(*x: torch.LongTensor*, *target_entity_idx: torch.LongTensor*)

score(*h*, *r*, *t*)

class dicee.models.**TransE**(*args*)

Bases: *dicee.models.base_model.BaseKGE*

Translating Embeddings for Modeling Multi-relational Data https://proceedings.neurips.cc/paper/2013/file/1cecc7a77928ca8133fa24680a88d2f9-Paper.pdf

score(*head_ent_emb*, *rel_ent_emb*, *tail_ent_emb*)

forward_k_vs_all(*x: torch.Tensor*) → torch.FloatTensor

class dicee.models.**Shallom**(*args*)

Bases: *dicee.models.base_model.BaseKGE*

A shallow neural model for relation prediction (https://arxiv.org/abs/2101.09090)

get_embeddings() → Tuple[numpy.ndarray, None]

forward_k_vs_all(*x*) → torch.FloatTensor

forward_triples(*x*) → torch.FloatTensor

Parameters

x –

Returns

class dicee.models.**Pyke**(*args*)

Bases: *dicee.models.base_model.BaseKGE*

A Physical Embedding Model for Knowledge Graphs

forward_triples(*x: torch.LongTensor*)

Parameters

x –

class dicee.models.**BaseKGE**(*args: dict*)

Bases: *BaseKGELightning*

Base class for all neural network modules.

Your models should also subclass this class.

Modules can also contain other Modules, allowing to nest them in a tree structure. You can assign the submodules as regular attributes:

```
import torch.nn as nn
import torch.nn.functional as F

class Model(nn.Module):
    def __init__(self):
        super().__init__()
        self.conv1 = nn.Conv2d(1, 20, 5)
        self.conv2 = nn.Conv2d(20, 20, 5)

    def forward(self, x):
        x = F.relu(self.conv1(x))
        return F.relu(self.conv2(x))
```

Submodules assigned in this way will be registered, and will have their parameters converted too when you call `to()`, etc.

Note: As per the example above, an `__init__()` call to the parent class must be made before assignment on the child.

Variables

training (*bool*) – Boolean represents whether this module is in training or evaluation mode.

forward_byte_pair_encoded_k_vs_all(*x: torch.LongTensor*)

Parameters

x (*B x 2 x T*) –

forward_byte_pair_encoded_triple(*x: Tuple[torch.LongTensor, torch.LongTensor]*)

byte pair encoded neural link predictors

Parameters

------- –

init_params_with_sanity_checking()

forward(*x: torch.LongTensor | Tuple[torch.LongTensor, torch.LongTensor], y_idx: torch.LongTensor = None*)

Parameters

- **x** –
- **y_idx** –
- **ordered_bpe_entities** –

forward_triples (*x: torch.LongTensor*) → torch.Tensor

Parameters

x –

forward_k_vs_all (**args*, ***kwargs*)

forward_k_vs_sample (**args*, ***kwargs*)

get_triple_representation (*idx_hrt*)

get_head_relation_representation (*indexed_triple*)

get_sentence_representation (*x: torch.LongTensor*)

Parameters

- **(b** (*x shape*) –
- **3** –
- **t)** –

get_bpe_head_and_relation_representation (*x: torch.LongTensor*) → Tuple[torch.FloatTensor, torch.FloatTensor]

Parameters

x (*B x 2 x T*) –

get_embeddings () → Tuple[numpy.ndarray, numpy.ndarray]

class dicee.models.**ConEx** (*args*)

Bases: *dicee.models.base_model.BaseKGE*

Convolutional ComplEx Knowledge Graph Embeddings

residual_convolution (*C_1: Tuple[torch.Tensor, torch.Tensor]*, *C_2: Tuple[torch.Tensor, torch.Tensor]*) → torch.FloatTensor

Compute residual score of two complex-valued embeddings. :param C_1: a tuple of two pytorch tensors that corresponds complex-valued embeddings :param C_2: a tuple of two pytorch tensors that corresponds complex-valued embeddings :return:

forward_k_vs_all (*x: torch.Tensor*) → torch.FloatTensor

forward_triples (*x: torch.Tensor*) → torch.FloatTensor

Parameters

x –

forward_k_vs_sample (*x: torch.Tensor*, *target_entity_idx: torch.Tensor*)

class dicee.models.**AConEx** (*args*)

Bases: *dicee.models.base_model.BaseKGE*

Additive Convolutional ComplEx Knowledge Graph Embeddings

residual_convolution (*C_1: Tuple[torch.Tensor, torch.Tensor]*, *C_2: Tuple[torch.Tensor, torch.Tensor]*) → torch.FloatTensor

Compute residual score of two complex-valued embeddings. :param C_1: a tuple of two pytorch tensors that corresponds complex-valued embeddings :param C_2: a tuple of two pytorch tensors that corresponds complex-valued embeddings :return:

forward_k_vs_all(*x: torch.Tensor*) → torch.FloatTensor

forward_triples(*x: torch.Tensor*) → torch.FloatTensor

Parameters
x –

forward_k_vs_sample(*x: torch.Tensor*, *target_entity_idx: torch.Tensor*)

class dicee.models.**ComplEx**(*args*)

Bases: *dicee.models.base_model.BaseKGE*

Base class for all neural network modules.

Your models should also subclass this class.

Modules can also contain other Modules, allowing to nest them in a tree structure. You can assign the submodules as regular attributes:

```
import torch.nn as nn
import torch.nn.functional as F

class Model(nn.Module):
    def __init__(self):
        super().__init__()
        self.conv1 = nn.Conv2d(1, 20, 5)
        self.conv2 = nn.Conv2d(20, 20, 5)

    def forward(self, x):
        x = F.relu(self.conv1(x))
        return F.relu(self.conv2(x))
```

Submodules assigned in this way will be registered, and will have their parameters converted too when you call `to()`, etc.

Note: As per the example above, an `__init__()` call to the parent class must be made before assignment on the child.

Variables
training (*bool*) – Boolean represents whether this module is in training or evaluation mode.

static score(*head_ent_emb: torch.FloatTensor*, *rel_ent_emb: torch.FloatTensor*, *tail_ent_emb: torch.FloatTensor*)

static k_vs_all_score(*emb_h: torch.FloatTensor*, *emb_r: torch.FloatTensor*, *emb_E: torch.FloatTensor*)

Parameters

- **emb_h** –
- **emb_r** –
- **emb_E** –

forward_k_vs_all(*x: torch.LongTensor*) → torch.FloatTensor dicee.models.**quaternion_mul**(*, *Q_1*, *Q_2*) → Tuple[torch.Tensor, torch.Tensor, torch.Tensor, torch.Tensor]

Perform quaternion multiplication :param Q_1: :param Q_2: :return:

class dicee.models.**BaseKGE**(*args: dict*)

Bases: *BaseKGELightning*

Base class for all neural network modules.

Your models should also subclass this class.

Modules can also contain other Modules, allowing to nest them in a tree structure. You can assign the submodules as regular attributes:

```
import torch.nn as nn
import torch.nn.functional as F

class Model(nn.Module):
    def __init__(self):
        super().__init__()
        self.conv1 = nn.Conv2d(1, 20, 5)
        self.conv2 = nn.Conv2d(20, 20, 5)

    def forward(self, x):
        x = F.relu(self.conv1(x))
        return F.relu(self.conv2(x))
```

Submodules assigned in this way will be registered, and will have their parameters converted too when you call to(), etc.

Note: As per the example above, an __init__() call to the parent class must be made before assignment on the child.

Variables

training (*bool*) – Boolean represents whether this module is in training or evaluation mode.

forward_byte_pair_encoded_k_vs_all(*x: torch.LongTensor*)

Parameters

x (*B x 2 x T*) –

forward_byte_pair_encoded_triple(*x: Tuple[torch.LongTensor, torch.LongTensor]*)

byte pair encoded neural link predictors

Parameters

------- –

init_params_with_sanity_checking()

forward(*x: torch.LongTensor | Tuple[torch.LongTensor, torch.LongTensor]*, *y_idx: torch.LongTensor = None*)

Parameters

- **x** –
- **y_idx** –
- **ordered_bpe_entities** –

forward_triples (*x: torch.LongTensor*) → torch.Tensor

Parameters
x –

forward_k_vs_all (**args, **kwargs*)

forward_k_vs_sample (**args, **kwargs*)

get_triple_representation (*idx_hrt*)

get_head_relation_representation (*indexed_triple*)

get_sentence_representation (*x: torch.LongTensor*)

Parameters

- **(b** (*x shape*) –
- **3** –
- **t)** –

get_bpe_head_and_relation_representation (*x: torch.LongTensor*)
→ Tuple[torch.FloatTensor, torch.FloatTensor]

Parameters
x (*B x 2 x T*) –

get_embeddings () → Tuple[numpy.ndarray, numpy.ndarray]

class dicee.models.**IdentityClass** (*args=None*)

Bases: `torch.nn.Module`

Base class for all neural network modules.

Your models should also subclass this class.

Modules can also contain other Modules, allowing to nest them in a tree structure. You can assign the submodules as regular attributes:

```
import torch.nn as nn
import torch.nn.functional as F

class Model(nn.Module):
    def __init__(self):
        super().__init__()
        self.conv1 = nn.Conv2d(1, 20, 5)
        self.conv2 = nn.Conv2d(20, 20, 5)

    def forward(self, x):
        x = F.relu(self.conv1(x))
        return F.relu(self.conv2(x))
```

Submodules assigned in this way will be registered, and will have their parameters converted too when you call `to()`, etc.

Note: As per the example above, an `__init__()` call to the parent class must be made before assignment on the child.

Variables

training (*bool*) – Boolean represents whether this module is in training or evaluation mode.

static forward (*x*)

dicee.models.**quaternion_mul_with_unit_norm** (*, *Q_1*, *Q_2*)

class dicee.models.**QMult** (*args*)

Bases: *dicee.models.base_model.BaseKGE*

Base class for all neural network modules.

Your models should also subclass this class.

Modules can also contain other Modules, allowing to nest them in a tree structure. You can assign the submodules as regular attributes:

```
import torch.nn as nn
import torch.nn.functional as F

class Model(nn.Module):
    def __init__(self):
        super().__init__()
        self.conv1 = nn.Conv2d(1, 20, 5)
        self.conv2 = nn.Conv2d(20, 20, 5)

    def forward(self, x):
        x = F.relu(self.conv1(x))
        return F.relu(self.conv2(x))
```

Submodules assigned in this way will be registered, and will have their parameters converted too when you call `to()`, etc.

Note: As per the example above, an `__init__()` call to the parent class must be made before assignment on the child.

Variables

training (*bool*) – Boolean represents whether this module is in training or evaluation mode.

quaternion_multiplication_followed_by_inner_product (*h*, *r*, *t*)

Parameters

- **h** – shape: (**batch_dims*, dim) The head representations.
- **r** – shape: (**batch_dims*, dim) The head representations.
- **t** – shape: (**batch_dims*, dim) The tail representations.

Returns

Triple scores.

static quaternion_normalizer (*x: torch.FloatTensor*) → torch.FloatTensor

Normalize the length of relation vectors, if the forward constraint has not been applied yet.

Absolute value of a quaternion

$$|a + bi + cj + dk| = \sqrt{a^2 + b^2 + c^2 + d^2}$$

L2 norm of quaternion vector:

$$\|x\|^2 = \sum_{i=1}^{d} |x_i|^2 = \sum_{i=1}^{d} (x_i.re^2 + x_i.im_1^2 + x_i.im_2^2 + x_i.im_3^2)$$

Parameters
x – The vector.

Returns
The normalized vector.

score (*head_ent_emb: torch.FloatTensor*, *rel_ent_emb: torch.FloatTensor*, *tail_ent_emb: torch.FloatTensor*)

k_vs_all_score (*bpe_head_ent_emb*, *bpe_rel_ent_emb*, *E*)

Parameters

- **bpe_head_ent_emb** –
- **bpe_rel_ent_emb** –
- **E** –

forward_k_vs_all (*x*)

Parameters
x –

forward_k_vs_sample (*x*, *target_entity_idx*)

Completed. Given a head entity and a relation (h,r), we compute scores for all possible triples,i.e., [score(h,r,x)|x in Entities] => [0.0,0.1,…,0.8], shape=> (1, **|Entities|**) Given a batch of head entities and relations => shape (size of batch,| Entities|)

class dicee.models.**ConvQ** (*args*)

Bases: *dicee.models.base_model.BaseKGE*

Convolutional Quaternion Knowledge Graph Embeddings

residual_convolution (*Q_1*, *Q_2*)

forward_triples (*indexed_triple: torch.Tensor*) → torch.Tensor

Parameters
x –

forward_k_vs_all (*x: torch.Tensor*)

Given a head entity and a relation (h,r), we compute scores for all entities. [score(h,r,x)|x in Entities] => [0.0,0.1,…,0.8], shape=> (1, **|Entities|**) Given a batch of head entities and relations => shape (size of batch,| Entities|)

class dicee.models.**AConvQ** (*args*)

Bases: *dicee.models.base_model.BaseKGE*

Additive Convolutional Quaternion Knowledge Graph Embeddings

residual_convolution (*Q_1*, *Q_2*)

forward_triples (*indexed_triple: torch.Tensor*) → torch.Tensor

Parameters
x –

forward_k_vs_all (*x: torch.Tensor*)

Given a head entity and a relation (h,r), we compute scores for all entities. [score(h,r,x)|x in Entities] => [0.0,0.1,…,0.8], shape=> (1, **|Entities|**) Given a batch of head entities and relations => shape (size of batch,| Entities|)

class dicee.models.**BaseKGE** (*args: dict*)

Bases: *BaseKGELightning*

Base class for all neural network modules.

Your models should also subclass this class.

Modules can also contain other Modules, allowing to nest them in a tree structure. You can assign the submodules as regular attributes:

```
import torch.nn as nn
import torch.nn.functional as F

class Model(nn.Module):
    def __init__(self):
        super().__init__()
        self.conv1 = nn.Conv2d(1, 20, 5)
        self.conv2 = nn.Conv2d(20, 20, 5)

    def forward(self, x):
        x = F.relu(self.conv1(x))
        return F.relu(self.conv2(x))
```

Submodules assigned in this way will be registered, and will have their parameters converted too when you call `to()`, etc.

Note: As per the example above, an `__init__()` call to the parent class must be made before assignment on the child.

Variables

training (*bool*) – Boolean represents whether this module is in training or evaluation mode.

forward_byte_pair_encoded_k_vs_all (*x: torch.LongTensor*)

Parameters

x (*B x 2 x T*) –

forward_byte_pair_encoded_triple (*x: Tuple[torch.LongTensor, torch.LongTensor]*)

byte pair encoded neural link predictors

Parameters

------- –

init_params_with_sanity_checking ()

forward (*x: torch.LongTensor | Tuple[torch.LongTensor, torch.LongTensor], y_idx: torch.LongTensor = None*)

Parameters

- **x** –
- **y_idx** –

- **ordered_bpe_entities** –

forward_triples (*x: torch.LongTensor*) → torch.Tensor

Parameters
x –

forward_k_vs_all (**args, **kwargs*)

forward_k_vs_sample (**args, **kwargs*)

get_triple_representation (*idx_hrt*)

get_head_relation_representation (*indexed_triple*)

get_sentence_representation (*x: torch.LongTensor*)

Parameters

- **(b** (*x shape*) –
- **3** –
- **t)** –

get_bpe_head_and_relation_representation (*x: torch.LongTensor*)
→ Tuple[torch.FloatTensor, torch.FloatTensor]

Parameters
x (*B x 2 x T*) –

get_embeddings () → Tuple[numpy.ndarray, numpy.ndarray]

class dicee.models.**IdentityClass** (*args=None*)

Bases: torch.nn.Module

Base class for all neural network modules.

Your models should also subclass this class.

Modules can also contain other Modules, allowing to nest them in a tree structure. You can assign the submodules as regular attributes:

```
import torch.nn as nn
import torch.nn.functional as F

class Model(nn.Module):
    def __init__(self):
        super().__init__()
        self.conv1 = nn.Conv2d(1, 20, 5)
        self.conv2 = nn.Conv2d(20, 20, 5)

    def forward(self, x):
        x = F.relu(self.conv1(x))
        return F.relu(self.conv2(x))
```

Submodules assigned in this way will be registered, and will have their parameters converted too when you call to(), etc.

Note: As per the example above, an __init__() call to the parent class must be made before assignment on the child.

Variables

training (*bool*) – Boolean represents whether this module is in training or evaluation mode.

static forward (*x*)

dicee.models.**octonion_mul** (**, O_1, O_2*)

dicee.models.**octonion_mul_norm** (**, O_1, O_2*)

class dicee.models.**OMult** (*args*)

Bases: *dicee.models.base_model.BaseKGE*

Base class for all neural network modules.

Your models should also subclass this class.

Modules can also contain other Modules, allowing to nest them in a tree structure. You can assign the submodules as regular attributes:

```
import torch.nn as nn
import torch.nn.functional as F

class Model(nn.Module):
    def __init__(self):
        super().__init__()
        self.conv1 = nn.Conv2d(1, 20, 5)
        self.conv2 = nn.Conv2d(20, 20, 5)

    def forward(self, x):
        x = F.relu(self.conv1(x))
        return F.relu(self.conv2(x))
```

Submodules assigned in this way will be registered, and will have their parameters converted too when you call `to()`, etc.

Note: As per the example above, an `__init__()` call to the parent class must be made before assignment on the child.

Variables

training (*bool*) – Boolean represents whether this module is in training or evaluation mode.

static octonion_normalizer (*emb_rel_e0, emb_rel_e1, emb_rel_e2, emb_rel_e3, emb_rel_e4, emb_rel_e5, emb_rel_e6, emb_rel_e7*)

score (*head_ent_emb: torch.FloatTensor, rel_ent_emb: torch.FloatTensor, tail_ent_emb: torch.FloatTensor*)

k_vs_all_score (*bpe_head_ent_emb, bpe_rel_ent_emb, E*)

forward_k_vs_all (*x*)

Completed. Given a head entity and a relation (h,r), we compute scores for all possible triples,i.e., [score(h,r,x)|x in Entities] => [0.0,0.1,…,0.8], shape=> (1, **|Entities|**) Given a batch of head entities and relations => shape (size of batch,| Entities|)

class dicee.models.**ConvO**(*args: dict*)

Bases: *dicee.models.base_model.BaseKGE*

Base class for all neural network modules.

Your models should also subclass this class.

Modules can also contain other Modules, allowing to nest them in a tree structure. You can assign the submodules as regular attributes:

```
import torch.nn as nn
import torch.nn.functional as F

class Model(nn.Module):
    def __init__(self):
        super().__init__()
        self.conv1 = nn.Conv2d(1, 20, 5)
        self.conv2 = nn.Conv2d(20, 20, 5)

    def forward(self, x):
        x = F.relu(self.conv1(x))
        return F.relu(self.conv2(x))
```

Submodules assigned in this way will be registered, and will have their parameters converted too when you call `to()`, etc.

Note: As per the example above, an `__init__()` call to the parent class must be made before assignment on the child.

Variables

training (*bool*) – Boolean represents whether this module is in training or evaluation mode.

static octonion_normalizer(*emb_rel_e0*, *emb_rel_e1*, *emb_rel_e2*, *emb_rel_e3*, *emb_rel_e4*, *emb_rel_e5*, *emb_rel_e6*, *emb_rel_e7*)

residual_convolution(*O_1*, *O_2*)

forward_triples(*x: torch.Tensor*) → torch.Tensor

Parameters

x –

forward_k_vs_all(*x: torch.Tensor*)

Given a head entity and a relation (h,r), we compute scores for all entities. [score(h,r,x)|x in Entities] => [0.0,0.1,…,0.8], shape=> (1, **|Entities|**) Given a batch of head entities and relations => shape (size of batch,| Entities|)

class dicee.models.**AConvO**(*args: dict*)

Bases: *dicee.models.base_model.BaseKGE*

Additive Convolutional Octonion Knowledge Graph Embeddings

static octonion_normalizer(*emb_rel_e0*, *emb_rel_e1*, *emb_rel_e2*, *emb_rel_e3*, *emb_rel_e4*, *emb_rel_e5*, *emb_rel_e6*, *emb_rel_e7*)

residual_convolution(*O_1*, *O_2*)

forward_triples (*x: torch.Tensor*) → torch.Tensor

Parameters
x –

forward_k_vs_all (*x: torch.Tensor*)

Given a head entity and a relation (h,r), we compute scores for all entities. [score(h,r,x)|x in Entities] => [0.0,0.1,…,0.8], shape=> (1, **|Entities|**) Given a batch of head entities and relations => shape (size of batch,| Entities|)

class dicee.models.**Keci** (*args*)

Bases: `dicee.models.base_model.BaseKGE`

Base class for all neural network modules.

Your models should also subclass this class.

Modules can also contain other Modules, allowing to nest them in a tree structure. You can assign the submodules as regular attributes:

```
import torch.nn as nn
import torch.nn.functional as F

class Model(nn.Module):
    def __init__(self):
        super().__init__()
        self.conv1 = nn.Conv2d(1, 20, 5)
        self.conv2 = nn.Conv2d(20, 20, 5)

    def forward(self, x):
        x = F.relu(self.conv1(x))
        return F.relu(self.conv2(x))
```

Submodules assigned in this way will be registered, and will have their parameters converted too when you call `to()`, etc.

Note: As per the example above, an `__init__()` call to the parent class must be made before assignment on the child.

Variables
training (*bool*) – Boolean represents whether this module is in training or evaluation mode.

compute_sigma_pp (*hp, rp*)

Compute sigma_{pp} = sum_{i=1}^{p-1} sum_{k=i+1}^p (h_i r_k - h_k r_i) e_i e_k

sigma_{pp} captures the interactions between along p bases For instance, let p e_1, e_2, e_3, we compute interactions between e_1 e_2, e_1 e_3 , and e_2 e_3 This can be implemented with a nested two for loops

results = [] for i in range(p - 1):

for k in range(i + 1, p):
results.append(hp[:, :, i] * rp[:, :, k] - hp[:, :, k] * rp[:, :, i])

sigma_pp = torch.stack(results, dim=2) assert sigma_pp.shape == (b, r, int((p * (p - 1)) / 2))

Yet, this computation would be quite inefficient. Instead, we compute interactions along all p, e.g., e1e1, e1e2, e1e3,

e2e1, e2e2, e2e3, e3e1, e3e2, e3e3

Then select the triangular matrix without diagonals: e1e2, e1e3, e2e3.

compute_sigma_qq (*hq*, *rq*)

Compute sigma_{qq} = sum_{j=1}^{p+q-1} sum_{k=j+1}^{p+q} (h_j r_k - h_k r_j) e_j e_k sigma_{q} captures the interactions between along q bases For instance, let q e_1, e_2, e_3, we compute interactions between e_1 e_2, e_1 e_3 , and e_2 e_3 This can be implemented with a nested two for loops

results = [] for j in range(q - 1):

for k in range(j + 1, q):
results.append(hq[:, :, j] * rq[:, :, k] - hq[:, :, k] * rq[:, :, j])

sigma_qq = torch.stack(results, dim=2) assert sigma_qq.shape == (b, r, int((q * (q - 1)) / 2))

Yet, this computation would be quite inefficient. Instead, we compute interactions along all p, e.g., e1e1, e1e2, e1e3,

e2e1, e2e2, e2e3, e3e1, e3e2, e3e3

Then select the triangular matrix without diagonals: e1e2, e1e3, e2e3.

compute_sigma_pq (*, *hp*, *hq*, *rp*, *rq*)

sum_{i=1}^{p} sum_{j=p+1}^{p+q} (h_i r_j - h_j r_i) e_i e_j

results = [] sigma_pq = torch.zeros(b, r, p, q) for i in range(p):

for j in range(q):
sigma_pq[:, :, i, j] = hp[:, :, i] * rq[:, :, j] - hq[:, :, j] * rp[:, :, i]

print(sigma_pq.shape)

apply_coefficients (*h0*, *hp*, *hq*, *r0*, *rp*, *rq*)

Multiplying a base vector with its scalar coefficient

clifford_multiplication (*h0*, *hp*, *hq*, *r0*, *rp*, *rq*)

Compute our CL multiplication

h = h_0 + sum_{i=1}^p h_i e_i + sum_{j=p+1}^{p+q} h_j e_j r = r_0 + sum_{i=1}^p r_i e_i + sum_{j=p+1}^{p+q} r_j e_j

ei ^2 = +1 for i =< i =< p ej ^2 = -1 for p < j =< p+q ei ej = -eje1 for i

eq j

h r = sigma_0 + sigma_p + sigma_q + sigma_{pp} + sigma_{q}+ sigma_{pq} where

(1) sigma_0 = h_0 r_0 + sum_{i=1}^p (h_0 r_i) e_i - sum_{j=p+1}^{p+q} (h_j r_j) e_j

(2) sigma_p = sum_{i=1}^p (h_0 r_i + h_i r_0) e_i

(3) sigma_q = sum_{j=p+1}^{p+q} (h_0 r_j + h_j r_0) e_j

(4) sigma_{pp} = sum_{i=1}^{p-1} sum_{k=i+1}^p (h_i r_k - h_k r_i) e_i e_k

(5) sigma_{qq} = sum_{j=1}^{p+q-1} sum_{k=j+1}^{p+q} (h_j r_k - h_k r_j) e_j e_k

(6) sigma_{pq} = sum_{i=1}^{p} sum_{j=p+1}^{p+q} (h_i r_j - h_j r_i) e_i e_j

construct_cl_multivector (*x: torch.FloatTensor*, *r: int*, *p: int*, *q: int*)
→ tuple[torch.FloatTensor, torch.FloatTensor, torch.FloatTensor]

Construct a batch of multivectors Cl_{p,q}(mathbb{R}^d)

Parameter

x: torch.FloatTensor with (n,d) shape

returns

- **a0** (*torch.FloatTensor with (n,r) shape*)
- **ap** (*torch.FloatTensor with (n,r,p) shape*)
- **aq** (*torch.FloatTensor with (n,r,q) shape*)

forward_k_vs_with_explicit (*x: torch.Tensor*)

k_vs_all_score (*bpe_head_ent_emb, bpe_rel_ent_emb, E*)

forward_k_vs_all (*x: torch.Tensor*) → torch.FloatTensor

Kvsall training

(1) Retrieve real-valued embedding vectors for heads and relations mathbb{R}^d .

(2) Construct head entity and relation embeddings according to Cl_{p,q}(mathbb{R}^d) .

(3) Perform Cl multiplication

(4) Inner product of (3) and all entity embeddings

forward_k_vs_with_explicit and this funcitons are identical Parameter ——— x: torch.LongTensor with (n,2) shape :rtype: torch.FloatTensor with (n, **|E|**) shape

forward_k_vs_sample (*x: torch.LongTensor, target_entity_idx: torch.LongTensor*) → torch.FloatTensor

Kvsall training

(1) Retrieve real-valued embedding vectors for heads and relations mathbb{R}^d .

(2) Construct head entity and relation embeddings according to Cl_{p,q}(mathbb{R}^d) .

(3) Perform Cl multiplication

(4) Inner product of (3) and all entity embeddings

Parameter

x: torch.LongTensor with (n,2) shape

rtype

torch.FloatTensor with (n, **|E|**) shape

score (*h, r, t*)

forward_triples (*x: torch.Tensor*) → torch.FloatTensor

Parameter

x: torch.LongTensor with (n,3) shape

rtype
torch.FloatTensor with (n) shape

class dicee.models.**KeciBase**(*args*)

Bases: *Keci*

Without learning dimension scaling

class dicee.models.**CMult**(*args*)

Bases: *dicee.models.base_model.BaseKGE*

Cl_(0,0) => Real Numbers

Cl_(0,1) =>
A multivector mathbf{a} = a_0 + a_1 e_1 A multivector mathbf{b} = b_0 + b_1 e_1

multiplication is isomorphic to the product of two complex numbers

mathbf{a} imes mathbf{b} = a_0 b_0 + a_0b_1 e1 + a_1 b_1 e_1 e_1
= (a_0 b_0 - a_1 b_1) + (a_0 b_1 + a_1 b_0) e_1

Cl_(2,0) =>
A multivector mathbf{a} = a_0 + a_1 e_1 + a_2 e_2 + a_{12} e_1 e_2 A multivector mathbf{b} = b_0 + b_1 e_1 + b_2 e_2 + b_{12} e_1 e_2

mathbf{a} imes mathbf{b} = a_0b_0 + a_0b_1 e_1 + a_0b_2e_2 + a_0 b_12 e_1 e_2

- a_1 b_0 e_1 + a_1b_1 e_1_e1 ..

Cl_(0,2) => Quaternions

clifford_mul(*x: torch.FloatTensor*, *y: torch.FloatTensor*, *p: int*, *q: int*) → tuple

Clifford multiplication Cl_{p,q} (mathbb{R})

ei ^2 = +1 for i =< i =< p ej ^2 = -1 for p < j =< p+q ei ej = -eje1 for i

eq j

x: torch.FloatTensor with (n,d) shape

y: torch.FloatTensor with (n,d) shape

p: a non-negative integer p>= 0 q: a non-negative integer q>= 0

score(*head_ent_emb*, *rel_ent_emb*, *tail_ent_emb*)

forward_triples(*x: torch.LongTensor*) → torch.FloatTensor
Compute batch triple scores

Parameter

x: torch.LongTensor with shape n by 3

rtype
torch.LongTensor with shape n

forward_k_vs_all(*x: torch.Tensor*) → torch.FloatTensor

Compute batch KvsAll triple scores

Parameter

x: torch.LongTensor with shape n by 3

rtype
torch.LongTensor with shape n

class dicee.models.**DeCaL**(*args*)

Bases: *dicee.models.base_model.BaseKGE*

Base class for all neural network modules.

Your models should also subclass this class.

Modules can also contain other Modules, allowing to nest them in a tree structure. You can assign the submodules as regular attributes:

```
import torch.nn as nn
import torch.nn.functional as F

class Model(nn.Module):
    def __init__(self):
        super().__init__()
        self.conv1 = nn.Conv2d(1, 20, 5)
        self.conv2 = nn.Conv2d(20, 20, 5)

    def forward(self, x):
        x = F.relu(self.conv1(x))
        return F.relu(self.conv2(x))
```

Submodules assigned in this way will be registered, and will have their parameters converted too when you call `to()`, etc.

Note: As per the example above, an `__init__()` call to the parent class must be made before assignment on the child.

Variables
training (*bool*) – Boolean represents whether this module is in training or evaluation mode.

forward_triples(*x: torch.Tensor*) → torch.FloatTensor

Parameter

x: torch.LongTensor with (n,3) shape

rtype
torch.FloatTensor with (n) shape

cl_pqr (*a*)

Input: tensor(batch_size, emb_dim) —-> output: tensor with 1+p+q+r components with size (batch_size, emb_dim/(1+p+q+r)) each.

1) takes a tensor of size (batch_size, emb_dim), split it into 1 + p + q +r components, hence 1+p+q+r must be a divisor of the emb_dim. 2) Return a list of the 1+p+q+r components vectors, each are tensors of size (batch_size, emb_dim/(1+p+q+r))

compute_sigmas_single (*list_h_emb, list_r_emb, list_t_emb*)

here we compute all the sums with no others vectors interaction taken with the scalar product with t, that is, 1) s0 = h_0r_0t_0 2) s1 = sum_{i=1}^{p}h_ir_it_0 3) s2 = sum_{j=p+1}^{p+q}h_jr_jt_0 4) s3 = sum_{i=1}^{q}(h_0r_it_i + h_ir_0t_i) 5) s4 = sum_{i=p+1}^{p+q}(h_0r_it_i + h_ir_0t_i) 5) s5 = sum_{i=p+q+1}^{p+q+r}(h_0r_it_i + h_ir_0t_i)

and return:

*) sigma_0t = sigma_0 cdot t_0 = s0 + s1 -s2 *) s3, s4 and s5

compute_sigmas_multivect (*list_h_emb, list_r_emb*)

Here we compute and return all the sums with vectors interaction for the same and different bases.

For same bases vectors interaction we have

1) sigma_pp = sum_{i=1}^{p-1}sum_{i'=i+1}^{p}(h_ir_{i'}-h_{i'}r_i) (models the interactions between e_i and e_i' for 1 <= i, i' <= p)
2) sigma_qq = sum_{j=p+1}^{p+q-1}sum_{j'=j+1}^{p+q}(h_jr_{j'}-h_{j'} (models the interactions between e_j and e_j' for p+1 <= j, j' <= p+q)
3) sigma_rr = sum_{k=p+q+1}^{p+q+r-1}sum_{k'=k+1}^{p}(h_kr_{k'}-h_{k'}r_k) (models the interactions between e_k and e_k' for p+q+1 <= k, k' <= p+q+r)

For different base vector interactions, we have

4) sigma_pq = sum_{i=1}^{p}sum_{j=p+1}^{p+q}(h_ir_j - h_jr_i) (interactionsn between e_i and e_j for 1<=i <=p and p+1<= j <= p+q)
5) sigma_pr = sum_{i=1}^{p}sum_{k=p+q+1}^{p+q+r}(h_ir_k - h_kr_i) (interactionsn between e_i and e_k for 1<=i <=p and p+q+1<= k <= p+q+r)
6) sigma_qr = sum_{j=p+1}^{p+q}sum_{j=p+q+1}^{p+q+r}(h_jr_k - h_kr_j) (interactionsn between e_j and e_k for p+1 <= j <=p+q and p+q+1<= j <= p+q+r)

forward_k_vs_all (*x: torch.Tensor*) → torch.FloatTensor

Kvsall training

(1) Retrieve real-valued embedding vectors for heads and relations mathbb{R}^d .
(2) Construct head entity and relation embeddings according to Cl_{p,q}(mathbb{R}^d) .
(3) Perform Cl multiplication
(4) Inner product of (3) and all entity embeddings

forward_k_vs_with_explicit and this funcitons are identical Parameter ——— x: torch.LongTensor with (n,2) shape :rtype: torch.FloatTensor with (n, **|E|**) shape

apply_coefficients (*h0*, *hp*, *hq*, *hk*, *r0*, *rp*, *rq*, *rk*)

Multiplying a base vector with its scalar coefficient

construct_cl_multivector (*x: torch.FloatTensor*, *re: int*, *p: int*, *q: int*, *r: int*) → tuple[torch.FloatTensor, torch.FloatTensor, torch.FloatTensor]

Construct a batch of multivectors Cl_{p,q,r}(mathbb{R}^d)

Parameter

x: torch.FloatTensor with (n,d) shape

returns

- **a0** (*torch.FloatTensor*)
- **ap** (*torch.FloatTensor*)
- **aq** (*torch.FloatTensor*)
- **ar** (*torch.FloatTensor*)

compute_sigma_pp (*hp*, *rp*)

sigma_{p,p}^* = sum_{i=1}^{p-1}sum_{i'=i+1}^{p}(x_iy_{i'}-x_{i'}y_i)

sigma_{pp} captures the interactions between along p bases For instance, let p e_1, e_2, e_3, we compute interactions between e_1 e_2, e_1 e_3 , and e_2 e_3 This can be implemented with a nested two for loops

results = [] for i in range(p - 1):

for k in range(i + 1, p):
results.append(hp[:, :, i] * rp[:, :, k] - hp[:, :, k] * rp[:, :, i])

sigma_pp = torch.stack(results, dim=2) assert sigma_pp.shape == (b, r, int((p * (p - 1)) / 2))

Yet, this computation would be quite inefficient. Instead, we compute interactions along all p, e.g., e1e1, e1e2, e1e3,

e2e1, e2e2, e2e3, e3e1, e3e2, e3e3

Then select the triangular matrix without diagonals: e1e2, e1e3, e2e3.

compute_sigma_qq (*hq*, *rq*)

Compute sigma_{q,q}^* = sum_{j=p+1}^{p+q-1}sum_{j'=j+1}^{p+q}(x_jy_{j'}-x_{j'}y_j) Eq. 16 sigma_{q} captures the interactions between along q bases For instance, let q e_1, e_2, e_3, we compute interactions between e_1 e_2, e_1 e_3 , and e_2 e_3 This can be implemented with a nested two for loops

results = [] for j in range(q - 1):

for k in range(j + 1, q):
results.append(hq[:, :, j] * rq[:, :, k] - hq[:, :, k] * rq[:, :, j])

sigma_qq = torch.stack(results, dim=2) assert sigma_qq.shape == (b, r, int((q * (q - 1)) / 2))

Yet, this computation would be quite inefficient. Instead, we compute interactions along all p, e.g., e1e1, e1e2, e1e3,

e2e1, e2e2, e2e3, e3e1, e3e2, e3e3

Then select the triangular matrix without diagonals: e1e2, e1e3, e2e3.

compute_sigma_rr (*hk*, *rk*)

sigma_{r,r}^* = sum_{k=p+q+1}^{p+q+r-1}sum_{k'=k+1}^{p}(x_ky_{k'}-x_{k'}y_k)

compute_sigma_pq(*, *hp*, *hq*, *rp*, *rq*)

sum_{i=1}^{p} sum_{j=p+1}^{p+q} (h_i r_j - h_j r_i) e_i e_j

results = [] sigma_pq = torch.zeros(b, r, p, q) for i in range(p):

for j in range(q):
sigma_pq[:, :, i, j] = hp[:, :, i] * rq[:, :, j] - hq[:, :, j] * rp[:, :, i]

print(sigma_pq.shape)

compute_sigma_pr(*, *hp*, *hk*, *rp*, *rk*)

sum_{i=1}^{p} sum_{j=p+1}^{p+q} (h_i r_j - h_j r_i) e_i e_j

results = [] sigma_pq = torch.zeros(b, r, p, q) for i in range(p):

for j in range(q):
sigma_pq[:, :, i, j] = hp[:, :, i] * rq[:, :, j] - hq[:, :, j] * rp[:, :, i]

print(sigma_pq.shape)

compute_sigma_qr(*, *hq*, *hk*, *rq*, *rk*)

sum_{i=1}^{p} sum_{j=p+1}^{p+q} (h_i r_j - h_j r_i) e_i e_j

results = [] sigma_pq = torch.zeros(b, r, p, q) for i in range(p):

for j in range(q):
sigma_pq[:, :, i, j] = hp[:, :, i] * rq[:, :, j] - hq[:, :, j] * rp[:, :, i]

print(sigma_pq.shape)

class dicee.models.**BaseKGE**(*args: dict*)

Bases: *BaseKGELightning*

Base class for all neural network modules.

Your models should also subclass this class.

Modules can also contain other Modules, allowing to nest them in a tree structure. You can assign the submodules as regular attributes:

```
import torch.nn as nn
import torch.nn.functional as F

class Model(nn.Module):
    def __init__(self):
        super().__init__()
        self.conv1 = nn.Conv2d(1, 20, 5)
        self.conv2 = nn.Conv2d(20, 20, 5)

    def forward(self, x):
        x = F.relu(self.conv1(x))
        return F.relu(self.conv2(x))
```

Submodules assigned in this way will be registered, and will have their parameters converted too when you call `to()`, etc.

Note: As per the example above, an `__init__()` call to the parent class must be made before assignment on the child.

Variables

training (*bool*) – Boolean represents whether this module is in training or evaluation mode.

forward_byte_pair_encoded_k_vs_all (*x: torch.LongTensor*)

Parameters

x (*B x 2 x T*) –

forward_byte_pair_encoded_triple (*x: Tuple[torch.LongTensor, torch.LongTensor]*)

byte pair encoded neural link predictors

Parameters

------- –

init_params_with_sanity_checking ()

forward (*x: torch.LongTensor | Tuple[torch.LongTensor, torch.LongTensor], y_idx: torch.LongTensor = None*)

Parameters

- **x** –
- **y_idx** –
- **ordered_bpe_entities** –

forward_triples (*x: torch.LongTensor*) → torch.Tensor

Parameters

x –

forward_k_vs_all (**args, **kwargs*)

forward_k_vs_sample (**args, **kwargs*)

get_triple_representation (*idx_hrt*)

get_head_relation_representation (*indexed_triple*)

get_sentence_representation (*x: torch.LongTensor*)

Parameters

- **(b** (*x shape*) –
- **3** –
- **t)** –

get_bpe_head_and_relation_representation (*x: torch.LongTensor*) → Tuple[torch.FloatTensor, torch.FloatTensor]

Parameters

x (*B x 2 x T*) –

get_embeddings () → Tuple[numpy.ndarray, numpy.ndarray]

class dicee.models.**PykeenKGE** (*args: dict*)

Bases: *dicee.models.base_model.BaseKGE*

A class for using knowledge graph embedding models implemented in Pykeen

Notes: Pykeen_DistMult: C Pykeen_ComplEx: Pykeen_QuatE: Pykeen_MuRE: Pykeen_CP: Pykeen_HolE: Pykeen_HolE:

forward_k_vs_all (*x: torch.LongTensor*)

=> Explicit version by this we can apply bn and dropout

(1) Retrieve embeddings of heads and relations + apply Dropout & Normalization if given. h, r = self.get_head_relation_representation(x) # (2) Reshape (1). if self.last_dim > 0:

h = h.reshape(len(x), self.embedding_dim, self.last_dim) r = r.reshape(len(x), self.embedding_dim, self.last_dim)

(3) Reshape all entities. if self.last_dim > 0:

t = self.entity_embeddings.weight.reshape(self.num_entities, self.embedding_dim, self.last_dim)

else:

t = self.entity_embeddings.weight

(4) Call the score_t from interactions to generate triple scores. return self.interaction.score_t(h=h, r=r, all_entities=t, slice_size=1)

forward_triples (*x: torch.LongTensor*) → torch.FloatTensor

=> Explicit version by this we can apply bn and dropout

(1) Retrieve embeddings of heads, relations and tails and apply Dropout & Normalization if given. h, r, t = self.get_triple_representation(x) # (2) Reshape (1). if self.last_dim > 0:

h = h.reshape(len(x), self.embedding_dim, self.last_dim) r = r.reshape(len(x), self.embedding_dim, self.last_dim) t = t.reshape(len(x), self.embedding_dim, self.last_dim)

(3) Compute the triple score return self.interaction.score(h=h, r=r, t=t, slice_size=None, slice_dim=0)

abstract forward_k_vs_sample (*x: torch.LongTensor, target_entity_idx*)

class dicee.models.**BaseKGE** (*args: dict*)

Bases: *BaseKGELightning*

Base class for all neural network modules.

Your models should also subclass this class.

Modules can also contain other Modules, allowing to nest them in a tree structure. You can assign the submodules as regular attributes:

```
import torch.nn as nn
import torch.nn.functional as F

class Model(nn.Module):
    def __init__(self):
        super().__init__()
        self.conv1 = nn.Conv2d(1, 20, 5)
        self.conv2 = nn.Conv2d(20, 20, 5)

    def forward(self, x):
        x = F.relu(self.conv1(x))
        return F.relu(self.conv2(x))
```

Submodules assigned in this way will be registered, and will have their parameters converted too when you call `to()`, etc.

Note: As per the example above, an `__init__()` call to the parent class must be made before assignment on the child.

Variables
: **training** (*bool*) – Boolean represents whether this module is in training or evaluation mode.

forward_byte_pair_encoded_k_vs_all (*x: torch.LongTensor*)

Parameters
: **x** (*B x 2 x T*) –

forward_byte_pair_encoded_triple (*x: Tuple[torch.LongTensor, torch.LongTensor]*)

byte pair encoded neural link predictors

Parameters
: **-------** –

init_params_with_sanity_checking ()

forward (*x: torch.LongTensor | Tuple[torch.LongTensor, torch.LongTensor], y_idx: torch.LongTensor = None*)

Parameters

- **x** –
- **y_idx** –
- **ordered_bpe_entities** –

forward_triples (*x: torch.LongTensor*) → torch.Tensor

Parameters
: **x** –

forward_k_vs_all (**args, **kwargs*)

forward_k_vs_sample (**args, **kwargs*)

get_triple_representation (*idx_hrt*)

get_head_relation_representation (*indexed_triple*)

get_sentence_representation (*x: torch.LongTensor*)

Parameters

- **(b** (*x shape*) –
- **3** –
- **t)** –

get_bpe_head_and_relation_representation (*x: torch.LongTensor*) → Tuple[torch.FloatTensor, torch.FloatTensor]

Parameters
: **x** (*B x 2 x T*) –

get_embeddings () → Tuple[numpy.ndarray, numpy.ndarray]

class dicee.models.**FMult**(*args*)

Bases: *dicee.models.base_model.BaseKGE*

Learning Knowledge Neural Graphs

compute_func(*weights: torch.FloatTensor*, *x*) → torch.FloatTensor

chain_func(*weights*, *x: torch.FloatTensor*)

forward_triples(*idx_triple: torch.Tensor*) → torch.Tensor

Parameters
x –

class dicee.models.**GFMult**(*args*)

Bases: *dicee.models.base_model.BaseKGE*

Learning Knowledge Neural Graphs

compute_func(*weights: torch.FloatTensor*, *x*) → torch.FloatTensor

chain_func(*weights*, *x: torch.FloatTensor*)

forward_triples(*idx_triple: torch.Tensor*) → torch.Tensor

Parameters
x –

class dicee.models.**FMult2**(*args*)

Bases: *dicee.models.base_model.BaseKGE*

Learning Knowledge Neural Graphs

build_func(*Vec*)

build_chain_funcs(*list_Vec*)

compute_func(*W*, *b*, *x*) → torch.FloatTensor

function(*list_W*, *list_b*)

trapezoid(*list_W*, *list_b*)

forward_triples(*idx_triple: torch.Tensor*) → torch.Tensor

Parameters
x –

class dicee.models.**LFMult1**(*args*)

Bases: *dicee.models.base_model.BaseKGE*

Embedding with trigonometric functions. We represent all entities and relations in the complex number space as: f(x) = sum_{k=0}^{k=d-1}wk e^{kix}. and use the three differents scoring function as in the paper to evaluate the score

forward_triples(*idx_triple*)

Parameters
x –

tri_score(*h*, *r*, *t*)

vtp_score (*h*, *r*, *t*)

class dicee.models.**LFMult** (*args*)

Bases: *dicee.models.base_model.BaseKGE*

Embedding with polynomial functions. We represent all entities and relations in the polynomial space as: f(x) = sum_{i=0}^{d-1} a_k x^{i%d} and use the three differents scoring function as in the paper to evaluate the score. We also consider combining with Neural Networks.

forward_triples (*idx_triple*)

Parameters
x –

construct_multi_coeff (*x*)

poly_NN (*x*, *coefh*, *coefr*, *coeft*)

Constructing a 2 layers NN to represent the embeddings. h = sigma(wh^T x + bh), r = sigma(wr^T x + br), t = sigma(wt^T x + bt)

linear (*x*, *w*, *b*)

scalar_batch_NN (*a*, *b*, *c*)

element wise multiplication between a,b and c: Inputs : a, b, c ====> torch.tensor of size batch_size x m x d Output : a tensor of size batch_size x d

tri_score (*coeff_h*, *coeff_r*, *coeff_t*)

this part implement the trilinear scoring techniques:

score(h,r,t) = int_{0}{1} h(x)r(x)t(x) dx = sum_{i,j,k = 0}^{d-1} dfrac{a_i*b_j*c_k}{1+(i+j+k)%d}

1. generate the range for i,j and k from [0 d-1]
2. perform dfrac{a_i*b_j*c_k}{1+(i+j+k)%d} in parallel for every batch
3. take the sum over each batch

vtp_score (*h*, *r*, *t*)

this part implement the vector triple product scoring techniques:

score(h,r,t) = int_{0}{1} h(x)r(x)t(x) dx = sum_{i,j,k = 0}^{d-1} dfrac{a_i*c_j*b_k - b_i*c_j*a_k}{(1+(i+j)%d)(1+k)}

1. generate the range for i,j and k from [0 d-1]
2. Compute the first and second terms of the sum
3. Multiply with then denominator and take the sum
4. take the sum over each batch

comp_func (*h*, *r*, *t*)

this part implement the function composition scoring techniques: i.e. score = <hor, t>

polynomial (*coeff*, *x*, *degree*)

This function takes a matrix tensor of coefficients (coeff), a tensor vector of points x and range of integer [0,1,…d] and return a vector tensor (coeff[0][0] + coeff[0][1]x +…+ coeff[0][d]x^d,

coeff[1][0] + coeff[1][1]x +…+ coeff[1][d]x^d)

pop(*coeff*, *x*, *degree*)

This function allow us to evaluate the composition of two polynomes without for loops :) it takes a matrix tensor of coefficients (coeff), a matrix tensor of points x and range of integer [0,1,…d]

and return a tensor (coeff[0][0] + coeff[0][1]x +…+ coeff[0][d]x^d,

coeff[1][0] + coeff[1][1]x +…+ coeff[1][d]x^d)

dicee.read_preprocess_save_load_kg

Submodules

dicee.read_preprocess_save_load_kg.preprocess

Module Contents

Classes

PreprocessKG	Preprocess the data in memory

class dicee.read_preprocess_save_load_kg.preprocess.**PreprocessKG**(*kg*)

Preprocess the data in memory

start() → None

Preprocess train, valid and test datasets stored in knowledge graph instance

Parameter

rtype

None

preprocess_with_byte_pair_encoding()

preprocess_with_byte_pair_encoding_with_padding() → None

preprocess_with_pandas() → None

Preprocess train, valid and test datasets stored in knowledge graph instance with pandas

(1) Add reciprioal or noisy triples

(2) Construct vocabulary

(3) Index datasets

Parameter

rtype
None

preprocess_with_polars() → None

sequential_vocabulary_construction() → None

(1) Read input data into memory

(2) Remove triples with a condition

(3) **Serialize vocabularies in a pandas dataframe where**
=> the index is integer and => a single column is string (e.g. URI)

remove_triples_from_train_with_condition()

dicee.read_preprocess_save_load_kg.read_from_disk

Module Contents

Classes

ReadFromDisk	Read the data from disk into memory

class dicee.read_preprocess_save_load_kg.read_from_disk.**ReadFromDisk**(*kg*)

Read the data from disk into memory

start() → None

Read a knowledge graph from disk into memory

Data will be available at the train_set, test_set, valid_set attributes.

Parameter

None

rtype
None

add_noisy_triples_into_training()

dicee.read_preprocess_save_load_kg.save_load_disk

Module Contents

Classes

LoadSaveToDisk

class dicee.read_preprocess_save_load_kg.save_load_disk.**LoadSaveToDisk**(*kg*)

save()

load()

dicee.read_preprocess_save_load_kg.util

Module Contents

Functions

apply_reciprical_or_noise(add_reciprical, eval_model)	(1) Add reciprocal triples (2) Add noisy triples
timeit(func)	
read_with_polars(→ polars.DataFrame)	Load and Preprocess via Polars
read_with_pandas(data_path[, read_only_few, ...])	
read_from_disk(data_path[, read_only_few, ...])	
read_from_triple_store([endpoint])	Read triples from triple store into pandas dataframe
get_er_vocab(data[, file_path])	
get_re_vocab(data[, file_path])	
get_ee_vocab(data[, file_path])	
create_constraints(triples[, file_path])	(1) Extract domains and ranges of relations
load_with_pandas(→ None)	Deserialize data
save_numpy_ndarray(*, data, file_path)	
load_numpy_ndarray(*, file_path)	
save_pickle(*, data[, file_path])	
load_pickle(*[, file_path])	
create_recipriocal_triples(x)	Add inverse triples into dask dataframe
index_triples_with_pandas(→ pandas.core.frame.DataFrame)	**param train_set** pandas dataframe
dataset_sanity_checking(→ None)	**param train_set**

`dicee.read_preprocess_save_load_kg.util.`**`apply_reciprical_or_noise`**`(`*add_reciprical: bool*, *eval_model: str*, *df: object = None*, *info: str = None*`)`

(1) Add reciprocal triples (2) Add noisy triples

`dicee.read_preprocess_save_load_kg.util.`**`timeit`**`(`*func*`)`

`dicee.read_preprocess_save_load_kg.util.`**`read_with_polars`**`(`*data_path*, *read_only_few: int = None*, *sample_triples_ratio: float = None*`)` → polars.DataFrame

Load and Preprocess via Polars

`dicee.read_preprocess_save_load_kg.util.`**`read_with_pandas`**`(`*data_path*, *read_only_few: int = None*, *sample_triples_ratio: float = None*`)` `dicee.read_preprocess_save_load_kg.util.`**`read_from_disk`**`(`*data_path: str*, *read_only_few: int = None*, *sample_triples_ratio: float = None*, *backend=None*`)`

`dicee.read_preprocess_save_load_kg.util.`**`read_from_triple_store`**`(`*endpoint: str = None*`)`

Read triples from triple store into pandas dataframe

`dicee.read_preprocess_save_load_kg.util.`**`get_er_vocab`**`(`*data*, *file_path: str = None*`)`

`dicee.read_preprocess_save_load_kg.util.`**`get_re_vocab`**`(`*data*, *file_path: str = None*`)`

`dicee.read_preprocess_save_load_kg.util.`**`get_ee_vocab`**`(`*data*, *file_path: str = None*`)`

`dicee.read_preprocess_save_load_kg.util.`**`create_constraints`**`(`*triples*, *file_path: str = None*`)`

(1) Extract domains and ranges of relations

(2) Store a mapping from relations to entities that are outside of the domain and range. Crete constrainted entities based on the range of relations :param triples: :return: Tuple[dict, dict]

`dicee.read_preprocess_save_load_kg.util.`**`load_with_pandas`**`(`*self*`)` → None

Deserialize data

`dicee.read_preprocess_save_load_kg.util.`**`save_numpy_ndarray`**`(`*, *data: numpy.ndarray*, *file_path: str*`)`

`dicee.read_preprocess_save_load_kg.util.`**`load_numpy_ndarray`**`(`*, *file_path: str*`)`

`dicee.read_preprocess_save_load_kg.util.`**`save_pickle`**`(`*, *data: object*, *file_path=str*`)`

`dicee.read_preprocess_save_load_kg.util.`**`load_pickle`**`(`*, *file_path=str*`)`

`dicee.read_preprocess_save_load_kg.util.`**`create_recipriocal_triples`**`(`*x*`)`

Add inverse triples into dask dataframe :param x: :return:

`dicee.read_preprocess_save_load_kg.util.`**`index_triples_with_pandas`**`(`*train_set*, *entity_to_idx: dict*, *relation_to_idx: dict*`)` → pandas.core.frame.DataFrame

Parameters

- **`train_set`** – pandas dataframe
- **`entity_to_idx`** – a mapping from str to integer index
- **`relation_to_idx`** – a mapping from str to integer index
- **`num_core`** – number of cores to be used

Returns

indexed triples, i.e., pandas dataframe

`dicee.read_preprocess_save_load_kg.util.`**`dataset_sanity_checking`**`(`*train_set: numpy.ndarray*, *num_entities: int*, *num_relations: int*`)` → None

Parameters

- **`train_set`** –
- **`num_entities`** –
- **`num_relations`** –

Returns

Package Contents

Classes

PreprocessKG	Preprocess the data in memory
LoadSaveToDisk	
ReadFromDisk	Read the data from disk into memory

class dicee.read_preprocess_save_load_kg.**PreprocessKG**(*kg*)

Preprocess the data in memory

start() → None

Preprocess train, valid and test datasets stored in knowledge graph instance

Parameter

rtype
None

preprocess_with_byte_pair_encoding()

preprocess_with_byte_pair_encoding_with_padding() → None

preprocess_with_pandas() → None

Preprocess train, valid and test datasets stored in knowledge graph instance with pandas

(1) Add recipriocal or noisy triples

(2) Construct vocabulary

(3) Index datasets

Parameter

rtype
None

preprocess_with_polars() → None

sequential_vocabulary_construction() → None

(1) Read input data into memory

(2) Remove triples with a condition

(3) **Serialize vocabularies in a pandas dataframe where**
=> the index is integer and => a single column is string (e.g. URI)

remove_triples_from_train_with_condition()

class dicee.read_preprocess_save_load_kg.**LoadSaveToDisk**(*kg*)

save()

load()

class dicee.read_preprocess_save_load_kg.**ReadFromDisk**(*kg*)

Read the data from disk into memory

start() → None

Read a knowledge graph from disk into memory

Data will be available at the train_set, test_set, valid_set attributes.

Parameter

None

rtype
None

add_noisy_triples_into_training()

dicee.scripts

Submodules

dicee.scripts.index

Module Contents

Functions

get_default_arguments()	
main()	

dicee.scripts.index.**get_default_arguments**()

dicee.scripts.index.**main**()

dicee.scripts.run

Module Contents

Functions

get_default_arguments([description])	Extends pytorch_lightning Trainer's arguments with ours
main()	

dicee.scripts.run.**get_default_arguments**(*description=None*)

Extends pytorch_lightning Trainer's arguments with ours

dicee.scripts.run.**main**()

dicee.scripts.serve

Module Contents

Classes

NeuralSearcher	

Functions

get_default_arguments()	
root()	
search_embeddings(q)	
retrieve_embeddings(q)	
main()	

Attributes

app	
neural_searcher	

dicee.scripts.serve.**app**

dicee.scripts.serve.**neural_searcher**

dicee.scripts.serve.**get_default_arguments**()

async dicee.scripts.serve.**root**()

async dicee.scripts.serve.**search_embeddings**(*q: str*)

async dicee.scripts.serve.**retrieve_embeddings**(*q: str*)

class dicee.scripts.serve.**NeuralSearcher**(*args*)

get(*entity: str*)

search(*entity: str*)

dicee.scripts.serve.**main**()

dicee.trainer

Submodules

dicee.trainer.dice_trainer

Module Contents

Classes

DICE_Trainer	DICE_Trainer implement

Functions

initialize_trainer(args, callbacks)	
get_callbacks(args)	

dicee.trainer.dice_trainer.**initialize_trainer**(*args*, *callbacks*)

dicee.trainer.dice_trainer.**get_callbacks**(*args*)

class dicee.trainer.dice_trainer.**DICE_Trainer**(*args*, *is_continual_training*, *storage_path*, *evaluator=None*)

DICE_Trainer implement

1- Pytorch Lightning trainer (https://pytorch-lightning.readthedocs.io/en/stable/common/trainer.html) 2- Multi-GPU Trainer(https://pytorch.org/docs/stable/generated/torch.nn.parallel.DistributedDataParallel.html) 3- CPU Trainer

args

is_continual_training:bool

storage_path:str

evaluator:

report:dict

continual_start()

(1) Initialize training.

(2) Load model

(3) Load trainer (3) Fit model

Parameter

returns

- *model*
- **form_of_labelling** (*str*)

initialize_trainer(*callbacks: List*) → lightning.Trainer

Initialize Trainer from input arguments

initialize_or_load_model()

initialize_dataloader(*dataset: torch.utils.data.Dataset*) → torch.utils.data.DataLoader

initialize_dataset(*dataset: dicee.knowledge_graph.KG*, *form_of_labelling*) → torch.utils.data.Dataset

start(*knowledge_graph: dicee.knowledge_graph.KG*) → Tuple[*dicee.models.base_model.BaseKGE*, str]

Train selected model via the selected training strategy

k_fold_cross_validation(*dataset*) → Tuple[*dicee.models.base_model.BaseKGE*, str]

Perform K-fold Cross-Validation

1. Obtain K train and test splits.
2. **For each split,**
   2.1 initialize trainer and model 2.2. Train model with configuration provided in args. 2.3. Compute the mean reciprocal rank (MRR) score of the model on the test respective split.
3. Report the mean and average MRR .

Parameters

- **self** –
- **dataset** –

Returns

model

dicee.trainer.torch_trainer

Module Contents

Classes

TorchTrainer	TorchTrainer for using single GPU or multi CPUs on a single node

class dicee.trainer.torch_trainer.**TorchTrainer**(*args*, *callbacks*)

Bases: *dicee.abstracts.AbstractTrainer*

TorchTrainer for using single GPU or multi CPUs on a single node

Arguments

callbacks: list of Abstract callback instances

fit(**args*, *train_dataloaders*, ***kwargs*) → None

Training starts

Arguments

kwargs:Tuple
empty dictionary

Return type
batch loss (float)

forward_backward_update(*x_batch: torch.Tensor*, *y_batch: torch.Tensor*) → torch.Tensor

Compute forward, loss, backward, and parameter update

Arguments

Return type
batch loss (float)

extract_input_outputs_set_device(*batch: list*) → Tuple

Construct inputs and outputs from a batch of inputs with outputs From a batch of inputs and put

Arguments

Return type
(tuple) mini-batch on select device

dicee.trainer.torch_trainer_ddp

Module Contents

Classes

TorchDDPTrainer	A Trainer based on torch.nn.parallel.DistributedDataParallel
NodeTrainer	
DDPTrainer	

Functions

`print_peak_memory`(prefix, device)	

`dicee.trainer.torch_trainer_ddp.`**`print_peak_memory`**(*prefix*, *device*)

class `dicee.trainer.torch_trainer_ddp.`**`TorchDDPTrainer`**(*args*, *callbacks*)

Bases: `dicee.abstracts.AbstractTrainer`

A Trainer based on torch.nn.parallel.DistributedDataParallel

Arguments

entity_idxs
mapping.

relation_idxs
mapping.

form
?

store
?

label_smoothing_rate
Using hard targets (0,1) drives weights to infinity. An outlier produces enormous gradients.

Return type
torch.utils.data.Dataset

`fit`(**args*, ***kwargs*)

Train model

class `dicee.trainer.torch_trainer_ddp.`**`NodeTrainer`**(*trainer*, *model: torch.nn.Module*, *train_dataset_loader: torch.utils.data.DataLoader*, *optimizer: torch.optim.Optimizer*, *callbacks*, *num_epochs: int*)

`extract_input_outputs`(*z: list*)

`train`()

Training loop for DDP

class `dicee.trainer.torch_trainer_ddp.`**`DDPTrainer`**(*model: torch.nn.Module*, *train_dataset_loader: torch.utils.data.DataLoader*, *optimizer: torch.optim.Optimizer*, *gpu_id: int*, *callbacks*, *num_epochs*)

`extract_input_outputs`(*z: list*)

`train`()

Package Contents

Classes

DICE_Trainer	DICE_Trainer implement

class dicee.trainer.**DICE_Trainer**(*args*, *is_continual_training*, *storage_path*, *evaluator=None*)

DICE_Trainer implement

1- Pytorch Lightning trainer (https://pytorch-lightning.readthedocs.io/en/stable/common/trainer.html) 2- Multi-GPU Trainer(https://pytorch.org/docs/stable/generated/torch.nn.parallel.DistributedDataParallel.html) 3- CPU Trainer

args

is_continual_training:bool

storage_path:str

evaluator:

report:dict

continual_start()

(1) Initialize training.

(2) Load model

(3) Load trainer (3) Fit model

Parameter

returns

- *model*
- **form_of_labelling** (*str*)

initialize_trainer(*callbacks: List*) → lightning.Trainer

Initialize Trainer from input arguments

initialize_or_load_model()

initialize_dataloader(*dataset: torch.utils.data.Dataset*) → torch.utils.data.DataLoader

initialize_dataset(*dataset: dicee.knowledge_graph.KG*, *form_of_labelling*) → torch.utils.data.Dataset

start(*knowledge_graph: dicee.knowledge_graph.KG*) → Tuple[*dicee.models.base_model.BaseKGE*, str]

Train selected model via the selected training strategy

k_fold_cross_validation(*dataset*) → Tuple[*dicee.models.base_model.BaseKGE*, str]

Perform K-fold Cross-Validation

1. Obtain K train and test splits.

2. **For each split,**
   2.1 initialize trainer and model 2.2. Train model with configuration provided in args. 2.3. Compute the mean reciprocal rank (MRR) score of the model on the test respective split.
3. Report the mean and average MRR .

Parameters

- **self** –
- **dataset** –

Returns
model

13.2 Submodules

dicee.abstracts

Module Contents

Classes

AbstractTrainer	Abstract class for Trainer class for knowledge graph embedding models
BaseInteractiveKGE	Abstract/base class for using knowledge graph embedding models interactively.
AbstractCallback	Abstract class for Callback class for knowledge graph embedding models
AbstractPPECallback	Abstract class for Callback class for knowledge graph embedding models

class dicee.abstracts.**AbstractTrainer**(*args*, *callbacks*)

Abstract class for Trainer class for knowledge graph embedding models

Parameter

args
[str] ?

callbacks: list
?

on_fit_start(**args*, ***kwargs*)

A function to call callbacks before the training starts.

Parameter

args

kwargs

rtype
None

on_fit_end(**args*, ***kwargs*)
A function to call callbacks at the ned of the training.

Parameter

args

kwargs

rtype
None

on_train_epoch_end(**args*, ***kwargs*)
A function to call callbacks at the end of an epoch.

Parameter

args

kwargs

rtype
None

on_train_batch_end(**args*, ***kwargs*)
A function to call callbacks at the end of each mini-batch during training.

Parameter

args

kwargs

rtype
None

static save_checkpoint(*full_path: str*, *model*) → None
A static function to save a model into disk

Parameter

full_path : str

model:

rtype
None

class dicee.abstracts.**BaseInteractiveKGE**(*path: str = None*, *url: str = None*, *construct_ensemble: bool = False*, *model_name: str = None*, *apply_semantic_constraint: bool = False*)

Abstract/base class for using knowledge graph embedding models interactively.

Parameter

path_of_pretrained_model_dir
[str] ?

construct_ensemble: boolean
?

model_name: str apply_semantic_constraint : boolean

property name

get_eval_report() → dict

get_bpe_token_representation(*str_entity_or_relation: List[str] | str*) → List[List[int]] | List[int]

Parameters
str_entity_or_relation(*corresponds to a str or a list of strings to be tokenized via BPE and shaped.*) –

Return type
A list integer(s) or a list of lists containing integer(s)

get_padded_bpe_triple_representation(*triples: List[List[str]]*) → Tuple[List, List, List]

Parameters
triples –

get_domain_of_relation(*rel: str*) → List[str]

get_range_of_relation(*rel: str*) → List[str]

set_model_train_mode() → None

Setting the model into training mode

Parameter

set_model_eval_mode() → None

Setting the model into eval mode

Parameter

sample_entity(*n: int*) → List[str]

sample_relation(*n: int*) → List[str]

is_seen(*entity: str = None*, *relation: str = None*) → bool

save() → None

get_entity_index(*x: str*)

get_relation_index(*x: str*)

index_triple(*head_entity: List[str]*, *relation: List[str]*, *tail_entity: List[str]*) → Tuple[torch.LongTensor, torch.LongTensor, torch.LongTensor]

Index Triple

Parameter

head_entity: List[str]

String representation of selected entities.

relation: List[str]

String representation of selected relations.

tail_entity: List[str]

String representation of selected entities.

Returns: Tuple

pytorch tensor of triple score

add_new_entity_embeddings(*entity_name: str = None*, *embeddings: torch.FloatTensor = None*)

get_entity_embeddings(*items: List[str]*)

Return embedding of an entity given its string representation

Parameter

items:
entities

get_relation_embeddings(*items: List[str]*)

Return embedding of a relation given its string representation

Parameter

items:
relations

construct_input_and_output(*head_entity: List[str]*, *relation: List[str]*, *tail_entity: List[str]*, *labels*)

Construct a data point :param head_entity: :param relation: :param tail_entity: :param labels: :return:

parameters()

class dicee.abstracts.**AbstractCallback**

Bases: `abc.ABC`, `lightning.pytorch.callbacks.Callback`

Abstract class for Callback class for knowledge graph embedding models

Parameter

on_init_start(**args*, ***kwargs*)

Parameter

trainer:

model:

rtype
None

on_init_end(**args*, ***kwargs*)

Call at the beginning of the training.

Parameter

trainer:

model:

rtype
None

on_fit_start(*trainer*, *model*)

Call at the beginning of the training.

Parameter

trainer:

model:

rtype
None

on_train_epoch_end(*trainer*, *model*)
Call at the end of each epoch during training.

Parameter

trainer:

model:

rtype
None

on_train_batch_end(**args*, ***kwargs*)
Call at the end of each mini-batch during the training.

Parameter

trainer:

model:

rtype
None

on_fit_end(**args*, ***kwargs*)
Call at the end of the training.

Parameter

trainer:

model:

rtype
None

class dicee.abstracts.**AbstractPPECallback**(*num_epochs*, *path*, *epoch_to_start*, *last_percent_to_consider*)
Bases: *AbstractCallback*

Abstract class for Callback class for knowledge graph embedding models

Parameter

on_fit_start (*trainer*, *model*)

Call at the beginning of the training.

Parameter

trainer:

model:

rtype
None

on_fit_end (*trainer*, *model*)

Call at the end of the training.

Parameter

trainer:

model:

rtype
None

store_ensemble (*param_ensemble*) → None

dicee.analyse_experiments

This script should be moved to dicee/scripts

Module Contents

Classes

Experiment

Functions

get_default_arguments()
analyse(args)

dicee.analyse_experiments.**get_default_arguments**()

class dicee.analyse_experiments.**Experiment**

save_experiment(*x*)

to_df()

dicee.analyse_experiments.**analyse**(*args*)

dicee.callbacks

Module Contents

Classes

AccumulateEpochLossCallback	Abstract class for Callback class for knowledge graph embedding models
PrintCallback	Abstract class for Callback class for knowledge graph embedding models
KGESaveCallback	Abstract class for Callback class for knowledge graph embedding models
PseudoLabellingCallback	Abstract class for Callback class for knowledge graph embedding models
ASWA	Adaptive stochastic weight averaging
Eval	Abstract class for Callback class for knowledge graph embedding models
KronE	Abstract class for Callback class for knowledge graph embedding models
Perturb	A callback for a three-Level Perturbation

Functions

estimate_q(eps)	estimate rate of convergence q from sequence esp
compute_convergence(seq, i)	

class dicee.callbacks.**AccumulateEpochLossCallback**(*path: str*)

Bases: *dicee.abstracts.AbstractCallback*

Abstract class for Callback class for knowledge graph embedding models

Parameter

on_fit_end(*trainer*, *model*) → None

Store epoch loss

Parameter

trainer:

model:

rtype
None

class dicee.callbacks.**PrintCallback**

Bases: *dicee.abstracts.AbstractCallback*

Abstract class for Callback class for knowledge graph embedding models

Parameter

on_fit_start(*trainer*, *pl_module*)

Call at the beginning of the training.

Parameter

trainer:

model:

rtype
None

on_fit_end(*trainer*, *pl_module*)

Call at the end of the training.

Parameter

trainer:

model:

rtype
None

on_train_batch_end(**args*, ***kwargs*)

Call at the end of each mini-batch during the training.

Parameter

trainer:

model:

rtype
None

on_train_epoch_end(**args*, ***kwargs*)
Call at the end of each epoch during training.

Parameter

trainer:

model:

rtype
None

class dicee.callbacks.**KGESaveCallback**(*every_x_epoch: int*, *max_epochs: int*, *path: str*)
Bases: *dicee.abstracts.AbstractCallback*

Abstract class for Callback class for knowledge graph embedding models

Parameter

on_train_batch_end(**args*, ***kwargs*)
Call at the end of each mini-batch during the training.

Parameter

trainer:

model:

rtype
None

on_fit_start(*trainer*, *pl_module*)
Call at the beginning of the training.

Parameter

trainer:

model:

rtype
None

on_train_epoch_end(**args*, ***kwargs*)
Call at the end of each epoch during training.

Parameter

trainer:

model:

rtype
None

on_fit_end(**args*, ***kwargs*)
Call at the end of the training.

Parameter

trainer:

model:

rtype
None

on_epoch_end(*model*, *trainer*, ***kwargs*)

class dicee.callbacks.**PseudoLabellingCallback**(*data_module*, *kg*, *batch_size*)
Bases: *dicee.abstracts.AbstractCallback*

Abstract class for Callback class for knowledge graph embedding models

Parameter

create_random_data()

on_epoch_end(*trainer*, *model*)

dicee.callbacks.**estimate_q**(*eps*)
estimate rate of convergence q from sequence esp

dicee.callbacks.**compute_convergence**(*seq*, *i*)

class dicee.callbacks.**ASWA**(*num_epochs*, *path*)
Bases: *dicee.abstracts.AbstractCallback*

Adaptive stochastic weight averaging ASWE keeps track of the validation performance and update s the ensemble model accordingly.

on_fit_end(*trainer*, *model*)
Call at the end of the training.

Parameter

trainer:

model:

rtype
None

static compute_mrr (*trainer*, *model*) → float

get_aswa_state_dict (*model*)

decide (*running_model_state_dict*, *ensemble_state_dict*, *val_running_model*, *mrr_updated_ensemble_model*)

Perform Hard Update, software or rejection

Parameters

- **running_model_state_dict** –
- **ensemble_state_dict** –
- **val_running_model** –
- **mrr_updated_ensemble_model** –

on_train_epoch_end (*trainer*, *model*)

Call at the end of each epoch during training.

Parameter

trainer:

model:

rtype
None

class dicee.callbacks.**Eval** (*path*, *epoch_ratio: int = None*)

Bases: *dicee.abstracts.AbstractCallback*

Abstract class for Callback class for knowledge graph embedding models

Parameter

on_fit_start (*trainer*, *model*)

Call at the beginning of the training.

Parameter

trainer:

model:

rtype
None

on_fit_end(*trainer*, *model*)

Call at the end of the training.

Parameter

trainer:

model:

rtype
None

on_train_epoch_end(*trainer*, *model*)

Call at the end of each epoch during training.

Parameter

trainer:

model:

rtype
None

on_train_batch_end(**args*, ***kwargs*)

Call at the end of each mini-batch during the training.

Parameter

trainer:

model:

rtype
None

class dicee.callbacks.**KronE**

Bases: *dicee.abstracts.AbstractCallback*

Abstract class for Callback class for knowledge graph embedding models

Parameter

static batch_kronecker_product(*a*, *b*)

Kronecker product of matrices a and b with leading batch dimensions. Batch dimensions are broadcast. The number of them mush :type a: torch.Tensor :type b: torch.Tensor :rtype: torch.Tensor

get_kronecker_triple_representation(*indexed_triple: torch.LongTensor*)

Get kronecker embeddings

on_fit_start(*trainer*, *model*)

Call at the beginning of the the training.

Parameter

trainer:

model:

rtype
None

class dicee.callbacks.**Perturb**(*level: str = 'input'*, *ratio: float = 0.0*, *method: str = None*, *scaler: float = None*, *frequency=None*)

Bases: `dicee.abstracts.AbstractCallback`

A callback for a three-Level Perturbation

Input Perturbation: During training an input x is perturbed by randomly replacing its element. In the context of knowledge graph embedding models, x can denote a triple, a tuple of an entity and a relation, or a tuple of two entities. A perturbation means that a component of x is randomly replaced by an entity or a relation.

Parameter Perturbation:

Output Perturbation:

on_train_batch_start(*trainer*, *model*, *batch*, *batch_idx*)

Called when the train batch begins.

dicee.config

Module Contents

Classes

`Namespace`	Simple object for storing attributes.

class dicee.config.**Namespace**(***kwargs*)

Bases: `argparse.Namespace`

Simple object for storing attributes.

Implements equality by attribute names and values, and provides a simple string representation.

dataset_dir: str
The path of a folder containing train.txt, and/or valid.txt and/or test.txt

save_embeddings_as_csv: bool = False
Embeddings of entities and relations are stored into CSV files to facilitate easy usage.

storage_path: str = 'Experiments'
A directory named with time of execution under –storage_path that contains related data about embeddings.

path_to_store_single_run: str
A single directory created that contains related data about embeddings.

path_single_kg
Path of a file corresponding to the input knowledge graph

sparql_endpoint
An endpoint of a triple store.

model: str = 'Keci'
KGE model

optim: str = 'Adam'
Optimizer

embedding_dim: int = 64
Size of continuous vector representation of an entity/relation

num_epochs: int = 150
Number of pass over the training data

batch_size: int = 1024
Mini-batch size if it is None, an automatic batch finder technique applied

lr: float = 0.1
Learning rate

add_noise_rate: float
The ratio of added random triples into training dataset

gpus
Number GPUs to be used during training

callbacks
10}}

Type
Callbacks, e.g., {"PPE"

Type
{ "last_percent_to_consider"

backend: str = 'pandas'
Backend to read, process, and index input knowledge graph. pandas, polars and rdflib available

trainer: str = 'torchCPUTrainer'
Trainer for knowledge graph embedding model

scoring_technique: str = 'KvsAll'
Scoring technique for knowledge graph embedding models

neg_ratio: int = 0
Negative ratio for a true triple in NegSample training_technique

weight_decay: float = 0.0
Weight decay for all trainable params

normalization: str = 'None'
LayerNorm, BatchNorm1d, or None

init_param: str
xavier_normal or None

gradient_accumulation_steps: int = 0
Not tested e

num_folds_for_cv: int = 0
Number of folds for CV

eval_model: str = 'train_val_test'
["None", "train", "train_val", "train_val_test", "test"]

Type
Evaluate trained model choices

save_model_at_every_epoch: int
Not tested

num_core: int = 0
Number of CPUs to be used in the mini-batch loading process

random_seed: int = 0
Random Seed

sample_triples_ratio: float
Read some triples that are uniformly at random sampled. Ratio being between 0 and 1

read_only_few: int
Read only first few triples

pykeen_model_kwargs
Additional keyword arguments for pykeen models

kernel_size: int = 3
Size of a square kernel in a convolution operation

num_of_output_channels: int = 32
Number of slices in the generated feature map by convolution.

p: int = 0
P parameter of Clifford Embeddings

q: int = 1
Q parameter of Clifford Embeddings

input_dropout_rate: float = 0.0
Dropout rate on embeddings of input triples

hidden_dropout_rate: float = 0.0
Dropout rate on hidden representations of input triples

feature_map_dropout_rate: float = 0.0

Dropout rate on a feature map generated by a convolution operation

byte_pair_encoding: bool = False

Byte pair encoding

Type

WIP

adaptive_swa: bool = False

Adaptive stochastic weight averaging

swa: bool = False

Stochastic weight averaging

block_size: int

block size of LLM

__iter__()

dicee.dataset_classes

Module Contents

Classes

BPE_NegativeSamplingDataset	An abstract class representing a `Dataset`.
MultiLabelDataset	An abstract class representing a `Dataset`.
MultiClassClassificationDataset	Dataset for the 1vsALL training strategy
OnevsAllDataset	Dataset for the 1vsALL training strategy
KvsAll	Creates a dataset for KvsAll training by inheriting from torch.utils.data.Dataset.
AllvsAll	Creates a dataset for AllvsAll training by inheriting from torch.utils.data.Dataset.
KvsSampleDataset	KvsSample a Dataset:
NegSampleDataset	An abstract class representing a `Dataset`.
TriplePredictionDataset	Triple Dataset
CVDataModule	Create a Dataset for cross validation

Functions

reload_dataset(path, form_of_labelling, ...)	Reload the files from disk to construct the Pytorch dataset
construct_dataset(→ torch.utils.data.Dataset)	

dicee.dataset_classes.**reload_dataset**(*path: str*, *form_of_labelling*, *scoring_technique*, *neg_ratio*, *label_smoothing_rate*)

Reload the files from disk to construct the Pytorch dataset dicee.dataset_classes.**construct_dataset**(*, *train_set: numpy.ndarray | list*, *valid_set=None*, *test_set=None*, *ordered_bpe_entities=None*, *train_target_indices=None*, *target_dim: int = None*, *entity_to_idx: dict*, *relation_to_idx: dict*, *form_of_labelling: str*, *scoring_technique: str*, *neg_ratio: int*, *label_smoothing_rate: float*, *byte_pair_encoding=None*, *block_size: int = None*) → torch.utils.data.Dataset

class dicee.dataset_classes.**BPE_NegativeSamplingDataset**(*train_set: torch.LongTensor*, *ordered_shaped_bpe_entities: torch.LongTensor*, *neg_ratio: int*)

Bases: `torch.utils.data.Dataset`

An abstract class representing a `Dataset`.

All datasets that represent a map from keys to data samples should subclass it. All subclasses should overwrite `__getitem__()`, supporting fetching a data sample for a given key. Subclasses could also optionally overwrite `__len__()`, which is expected to return the size of the dataset by many `Sampler` implementations and the default options of `DataLoader`. Subclasses could also optionally implement `__getitems__()`, for speedup batched samples loading. This method accepts list of indices of samples of batch and returns list of samples.

Note: `DataLoader` by default constructs an index sampler that yields integral indices. To make it work with a map-style dataset with non-integral indices/keys, a custom sampler must be provided.

__len__()

__getitem__(*idx*)

collate_fn(*batch_shaped_bpe_triples: List[Tuple[torch.Tensor, torch.Tensor]]*)

class dicee.dataset_classes.**MultiLabelDataset**(*train_set: torch.LongTensor*, *train_indices_target: torch.LongTensor*, *target_dim: int*, *torch_ordered_shaped_bpe_entities: torch.LongTensor*)

Bases: `torch.utils.data.Dataset`

An abstract class representing a `Dataset`.

All datasets that represent a map from keys to data samples should subclass it. All subclasses should overwrite `__getitem__()`, supporting fetching a data sample for a given key. Subclasses could also optionally overwrite `__len__()`, which is expected to return the size of the dataset by many `Sampler` implementations and the default options of `DataLoader`. Subclasses could also optionally implement `__getitems__()`, for speedup batched samples loading. This method accepts list of indices of samples of batch and returns list of samples.

Note: `DataLoader` by default constructs an index sampler that yields integral indices. To make it work with a map-style dataset with non-integral indices/keys, a custom sampler must be provided.

__len__()

__getitem__(*idx*)

class dicee.dataset_classes.**MultiClassClassificationDataset**(*subword_units: numpy.ndarray*, *block_size: int = 8*)

Bases: `torch.utils.data.Dataset`

Dataset for the 1vsALL training strategy

Parameters

- **train_set_idx** – Indexed triples for the training.

- **entity_idxs** – mapping.
- **relation_idxs** – mapping.
- **form** – ?
- **num_workers** – int for https://pytorch.org/docs/stable/data.html#torch.utils.data.DataLoader

Return type
torch.utils.data.Dataset

__len__()

__getitem__(*idx*)

class dicee.dataset_classes.**OnevsAllDataset**(*train_set_idx: numpy.ndarray*, *entity_idxs*)

Bases: `torch.utils.data.Dataset`

Dataset for the 1vsALL training strategy

Parameters

- **train_set_idx** – Indexed triples for the training.
- **entity_idxs** – mapping.
- **relation_idxs** – mapping.
- **form** – ?
- **num_workers** – int for https://pytorch.org/docs/stable/data.html#torch.utils.data.DataLoader

Return type
torch.utils.data.Dataset

__len__()

__getitem__(*idx*)

class dicee.dataset_classes.**KvsAll**(*train_set_idx: numpy.ndarray*, *entity_idxs*, *relation_idxs*, *form*, *store=None*, *label_smoothing_rate: float = 0.0*)

Bases: `torch.utils.data.Dataset`

Creates a dataset for KvsAll training by inheriting from torch.utils.data.Dataset.
Let D denote a dataset for KvsAll training and be defined as D:= {(x,y)_i}_i ^N, where x: (h,r) is an unique tuple of an entity h in E and a relation r in R that has been seed in the input graph. y: denotes a multi-label vector in [0,1]^{|E|} is a binary label.

orall y_i =1 s.t. (h r E_i) in KG

Note: TODO

---

train_set_idx
[numpy.ndarray] n by 3 array representing n triples

entity_idxs
[dictonary] string representation of an entity to its integer id

relation_idxs
[dictonary] string representation of a relation to its integer id

self : torch.utils.data.Dataset

```
>>> a = KvsAll()
>>> a
? array([0, 1, 2, 3, 4, 5, 6, 7, 8, 9])
```

__len__()

__getitem__(*idx*)

class dicee.dataset_classes.**AllvsAll**(*train_set_idx: numpy.ndarray*, *entity_idxs*, *relation_idxs*, *label_smoothing_rate=0.0*)

Bases: torch.utils.data.Dataset

Creates a dataset for AllvsAll training by inheriting from torch.utils.data.Dataset.

Let D denote a dataset for AllvsAll training and be defined as D:= {(x,y)_i}_i ^N, where x: (h,r) is a possible unique tuple of an entity h in E and a relation r in R. Hence N = |E| x |R| y: denotes a multi-label vector in [0,1]^{|E|} is a binary label.

orall y_i =1 s.t. (h r E_i) in KG

Note:

AllvsAll extends KvsAll via none existing (h,r). Hence, it adds data points that are labelled without 1s,

only with 0s.

---

train_set_idx

[numpy.ndarray] n by 3 array representing n triples

entity_idxs

[dictonary] string representation of an entity to its integer id

relation_idxs

[dictonary] string representation of a relation to its integer id

self : torch.utils.data.Dataset

```
>>> a = AllvsAll()
>>> a
? array([0, 1, 2, 3, 4, 5, 6, 7, 8, 9])
```

__len__()

__getitem__(*idx*)

class dicee.dataset_classes.**KvsSampleDataset**(*train_set: numpy.ndarray*, *num_entities*, *num_relations*, *neg_sample_ratio: int = None*, *label_smoothing_rate: float = 0.0*)

Bases: torch.utils.data.Dataset

KvsSample a Dataset:

D:= {(x,y)_i}_i ^N, where

. x:(h,r) is a unique h in E and a relation r in R and . y in [0,1]^{|E|} is a binary label.

orall y_i =1 s.t. (h r E_i) in KG

At each mini-batch construction, we subsample(y), hence n

|new_y| << |E| new_y contains all 1's if sum(y)< neg_sample ratio new_y contains

train_set_idx
Indexed triples for the training.

entity_idxs
mapping.

relation_idxs
mapping.

form
?

store
?

label_smoothing_rate
?

torch.utils.data.Dataset

`__len__`()

`__getitem__`(*idx*)

class dicee.dataset_classes.**NegSampleDataset**(*train_set: numpy.ndarray*, *num_entities: int*, *num_relations: int*, *neg_sample_ratio: int = 1*)

Bases: `torch.utils.data.Dataset`

An abstract class representing a `Dataset`.

All datasets that represent a map from keys to data samples should subclass it. All subclasses should overwrite `__getitem__()`, supporting fetching a data sample for a given key. Subclasses could also optionally overwrite `__len__()`, which is expected to return the size of the dataset by many `Sampler` implementations and the default options of `DataLoader`. Subclasses could also optionally implement `__getitems__()`, for speedup batched samples loading. This method accepts list of indices of samples of batch and returns list of samples.

Note: `DataLoader` by default constructs an index sampler that yields integral indices. To make it work with a map-style dataset with non-integral indices/keys, a custom sampler must be provided.

`__len__`()

`__getitem__`(*idx*)

class dicee.dataset_classes.**TriplePredictionDataset**(*train_set: numpy.ndarray*, *num_entities: int*, *num_relations: int*, *neg_sample_ratio: int = 1*, *label_smoothing_rate: float = 0.0*)

Bases: `torch.utils.data.Dataset`

Triple Dataset

D:= {(x)_i}_i ^N, where
. x:(h,r, t) in KG is a unique h in E and a relation r in R and . collact_fn => Generates negative triples

collect_fn:

orall (h,r,t) in G obtain, create negative triples{(h,r,x),(,r,t),(h,m,t)} y:labels are represented in torch.float16

train_set_idx
Indexed triples for the training.

entity_idxs
mapping.

relation_idxs
mapping.

form
?

store
?

label_smoothing_rate

collate_fn: batch:List[torch.IntTensor] Returns ——- torch.utils.data.Dataset

`__len__``()`

`__getitem__``(`*idx*`)`

`collate_fn``(`*batch: List[torch.Tensor]*`)`

`class` `dicee.dataset_classes.`**`CVDataModule`**`(`*train_set_idx: numpy.ndarray*, *num_entities*, *num_relations*, *neg_sample_ratio*, *batch_size*, *num_workers*`)`

Bases: `pytorch_lightning.LightningDataModule`

Create a Dataset for cross validation

Parameters

- **`train_set_idx`** – Indexed triples for the training.
- **`num_entities`** – entity to index mapping.
- **`num_relations`** – relation to index mapping.
- **`batch_size`** – int
- **`form`** – ?
- **`num_workers`** – int for https://pytorch.org/docs/stable/data.html#torch.utils.data.DataLoader

Return type

?

`train_dataloader``()` → torch.utils.data.DataLoader

An iterable or collection of iterables specifying training samples.

For more information about multiple dataloaders, see this section.

The dataloader you return will not be reloaded unless you set **:paramref:`~pytorch_lightning.trainer.trainer.Trainer.reload_dataloaders_every_n_epochs`** to a positive integer.

For data processing use the following pattern:

- download in *`prepare_data()`*

- process and split in *setup()*

However, the above are only necessary for distributed processing.

Warning: do not assign state in prepare_data

- `fit()`
- *prepare_data()*
- *setup()*

Note: Lightning tries to add the correct sampler for distributed and arbitrary hardware. There is no need to set it yourself.

---

setup(**args*, ***kwargs*)

Called at the beginning of fit (train + validate), validate, test, or predict. This is a good hook when you need to build models dynamically or adjust something about them. This hook is called on every process when using DDP.

Parameters

stage – either `'fit'`, `'validate'`, `'test'`, or `'predict'`

Example:

```
class LitModel(...):
    def __init__(self):
        self.l1 = None

    def prepare_data(self):
        download_data()
        tokenize()

        # don't do this
        self.something = else

    def setup(self, stage):
        data = load_data(...)
        self.l1 = nn.Linear(28, data.num_classes)
```

transfer_batch_to_device(**args*, ***kwargs*)

Override this hook if your `DataLoader` returns tensors wrapped in a custom data structure.

The data types listed below (and any arbitrary nesting of them) are supported out of the box:

- `torch.Tensor` or anything that implements *.to(…)*
- `list`
- `dict`
- `tuple`

For anything else, you need to define how the data is moved to the target device (CPU, GPU, TPU, …).

Note: This hook should only transfer the data and not modify it, nor should it move the data to any other device than the one passed in as argument (unless you know what you are doing). To check the current state of execution of this hook you can use `self.trainer.training/testing/validating/predicting` so that you can add different logic as per your requirement.

Parameters

- **batch** – A batch of data that needs to be transferred to a new device.
- **device** – The target device as defined in PyTorch.
- **dataloader_idx** – The index of the dataloader to which the batch belongs.

Returns
A reference to the data on the new device.

Example:

```
def transfer_batch_to_device(self, batch, device, dataloader_idx):
    if isinstance(batch, CustomBatch):
        # move all tensors in your custom data structure to the device
        batch.samples = batch.samples.to(device)
        batch.targets = batch.targets.to(device)
    elif dataloader_idx == 0:
        # skip device transfer for the first dataloader or anything you wish
        pass
    else:
        batch = super().transfer_batch_to_device(batch, device, dataloader_
↪idx)
    return batch
```

Raises
MisconfigurationException – If using IPUs, `Trainer(accelerator='ipu')`.

See also:

- `move_data_to_device()`
- `apply_to_collection()`

prepare_data(**args*, ***kwargs*)

Use this to download and prepare data. Downloading and saving data with multiple processes (distributed settings) will result in corrupted data. Lightning ensures this method is called only within a single process, so you can safely add your downloading logic within.

> **Warning:** DO NOT set state to the model (use `setup` instead) since this is NOT called on every device

Example:

```
def prepare_data(self):
    # good
    download_data()
    tokenize()
    etc()

    # bad
```

(continues on next page)

(continued from previous page)

```
    self.split = data_split
    self.some_state = some_other_state()
```

In a distributed environment, `prepare_data` can be called in two ways (using prepare_data_per_node)

1. Once per node. This is the default and is only called on LOCAL_RANK=0.
2. Once in total. Only called on GLOBAL_RANK=0.

Example:

```
# DEFAULT
# called once per node on LOCAL_RANK=0 of that node
class LitDataModule(LightningDataModule):
    def __init__(self):
        super().__init__()
        self.prepare_data_per_node = True


# call on GLOBAL_RANK=0 (great for shared file systems)
class LitDataModule(LightningDataModule):
    def __init__(self):
        super().__init__()
        self.prepare_data_per_node = False
```

This is called before requesting the dataloaders:

```
model.prepare_data()
initialize_distributed()
model.setup(stage)
model.train_dataloader()
model.val_dataloader()
model.test_dataloader()
model.predict_dataloader()
```

`dicee.eval_static_funcs`

Module Contents

Functions

evaluate_link_prediction_performance(→ Dict)	**param model**
evaluate_link_prediction_performance_w	
evaluate_link_prediction_performance_w	
evaluate_link_prediction_performance_w ...)	**param model**
evaluate_lp_bpe_k_vs_all(model, triples[, er_vocab, ...])	

dicee.eval_static_funcs.**evaluate_link_prediction_performance**(*model: dicee.knowledge_graph_embeddings.KGE*, *triples*, *er_vocab: Dict[Tuple, List]*, *re_vocab: Dict[Tuple, List]*) → Dict

Parameters

- **model** –
- **triples** –
- **er_vocab** –
- **re_vocab** –

dicee.eval_static_funcs.**evaluate_link_prediction_performance_with_reciprocals**(*model: dicee.knowledge_graph_embeddings.KGE*, *triples*, *er_vocab: Dict[Tuple, List]*)

dicee.eval_static_funcs.**evaluate_link_prediction_performance_with_bpe_reciprocals**(*model: dicee.knowledge_graph_embeddings.KGE*, *within_entities: List[str]*, *triples: List[List[str]]*, *er_vocab: Dict[Tuple, List]*)

dicee.eval_static_funcs.**evaluate_link_prediction_performance_with_bpe**(*model: dicee.knowledge_graph_embeddings.KGE*, *within_entities: List[str]*, *triples: List[Tuple[str]]*, *er_vocab: Dict[Tuple, List]*, *re_vocab: Dict[Tuple, List]*)

Parameters

- **model** –
- **triples** –
- **within_entities** –
- **er_vocab** –
- **re_vocab** –

dicee.eval_static_funcs.**evaluate_lp_bpe_k_vs_all**(*model*, *triples: List[List[str]]*, *er_vocab=None*, *batch_size=None*, *func_triple_to_bpe_representation: Callable = None*, *str_to_bpe_entity_to_idx=None*)

dicee.evaluator

Module Contents

Classes

Evaluator	Evaluator class to evaluate KGE models in various downstream tasks

class dicee.evaluator.**Evaluator**(*args*, *is_continual_training=None*)

Evaluator class to evaluate KGE models in various downstream tasks

Arguments

vocab_preparation (*dataset*) → None

A function to wait future objects for the attributes of executor

Return type
None

eval (*dataset: dicee.knowledge_graph.KG*, *trained_model*, *form_of_labelling*, *during_training=False*) → None

eval_rank_of_head_and_tail_entity (***, *train_set*, *valid_set=None*, *test_set=None*, *trained_model*)

eval_rank_of_head_and_tail_byte_pair_encoded_entity (***, *train_set=None*, *valid_set=None*, *test_set=None*, *ordered_bpe_entities*, *trained_model*)

eval_with_byte (***, *raw_train_set*, *raw_valid_set=None*, *raw_test_set=None*, *trained_model*, *form_of_labelling*) → None

Evaluate model after reciprocal triples are added

eval_with_bpe_vs_all (***, *raw_train_set*, *raw_valid_set=None*, *raw_test_set=None*, *trained_model*, *form_of_labelling*) → None

Evaluate model after reciprocal triples are added

eval_with_vs_all (***, *train_set*, *valid_set=None*, *test_set=None*, *trained_model*, *form_of_labelling*) → None

Evaluate model after reciprocal triples are added

evaluate_lp_k_vs_all (*model*, *triple_idx*, *info=None*, *form_of_labelling=None*)

Filtered link prediction evaluation. :param model: :param triple_idx: test triples :param info: :param form_of_labelling: :return:

evaluate_lp_with_byte (*model*, *triples: List[List[str]]*, *info=None*)

evaluate_lp_bpe_k_vs_all (*model*, *triples: List[List[str]]*, *info=None*, *form_of_labelling=None*)

Parameters

- **model** –
- **triples** (*List of lists*) –
- **info** –
- **form_of_labelling** –

evaluate_lp (*model*, *triple_idx*, *info: str*)

dummy_eval (*trained_model*, *form_of_labelling: str*)

eval_with_data (*dataset*, *trained_model*, *triple_idx: numpy.ndarray*, *form_of_labelling: str*)

dicee.executer

Module Contents

Classes

`Execute`	A class for Training, Retraining and Evaluation a model.
`ContinuousExecute`	A subclass of Execute Class for retraining

class dicee.executer.**Execute**(*args*, *continuous_training=False*)

A class for Training, Retraining and Evaluation a model.

(1) Loading & Preprocessing & Serializing input data.

(2) Training & Validation & Testing

(3) Storing all necessary info

read_or_load_kg()

read_preprocess_index_serialize_data() → None

Read & Preprocess & Index & Serialize Input Data

(1) Read or load the data from disk into memory.

(2) Store the statistics of the data.

Parameter

rtype
None

load_indexed_data() → None

Load the indexed data from disk into memory

Parameter

rtype
None

save_trained_model() → None

Save a knowledge graph embedding model

(1) Send model to eval mode and cpu.

(2) Store the memory footprint of the model.

(3) Save the model into disk.

(4) Update the stats of KG again ?

Parameter

rtype
None

`end(form_of_labelling: str)` → dict

End training

(1) Store trained model.

(2) Report runtimes.

(3) Eval model if required.

Parameter

rtype
A dict containing information about the training and/or evaluation

`write_report()` → None

Report training related information in a report.json file

`start()` → dict

Start training

(1) Loading the Data # (2) Create an evaluator object. # (3) Create a trainer object. # (4) Start the training

Parameter

rtype
A dict containing information about the training and/or evaluation

class `dicee.executer.ContinuousExecute(args)`

Bases: `Execute`

A subclass of Execute Class for retraining

(1) Loading & Preprocessing & Serializing input data.

(2) Training & Validation & Testing

(3) Storing all necessary info

`continual_start()` → dict

Start Continual Training

(1) Initialize training.

(2) Start continual training.

(3) Save trained model.

Parameter

rtype
A dict containing information about the training and/or evaluation

dicee.knowledge_graph

Module Contents

Classes

KG	Knowledge Graph

class dicee.knowledge_graph.**KG**(*dataset_dir: str = None*, *byte_pair_encoding: bool = False*, *padding: bool = False*, *add_noise_rate: float = None*, *sparql_endpoint: str = None*, *path_single_kg: str = None*, *path_for_deserialization: str = None*, *add_reciprical: bool = None*, *eval_model: str = None*, *read_only_few: int = None*, *sample_triples_ratio: float = None*, *path_for_serialization: str = None*, *entity_to_idx=None*, *relation_to_idx=None*, *backend=None*, *training_technique: str = None*)

Knowledge Graph

property entities_str: List

property relations_str: List

func_triple_to_bpe_representation(*triple: List[str]*)

dicee.knowledge_graph_embeddings

Module Contents

Classes

KGE	Knowledge Graph Embedding Class for interactive usage of pre-trained models

class dicee.knowledge_graph_embeddings.**KGE**(*path=None*, *url=None*, *construct_ensemble=False*, *model_name=None*, *apply_semantic_constraint=False*)

Bases: *dicee.abstracts.BaseInteractiveKGE*

Knowledge Graph Embedding Class for interactive usage of pre-trained models

get_transductive_entity_embeddings(*indices: torch.LongTensor | List[str]*, *as_pytorch=False*, *as_numpy=False*, *as_list=True*) → torch.FloatTensor | numpy.ndarray | List[float]

create_vector_database(*collection_name: str*, *distance: str*, *location: str = 'localhost'*, *port: int = 6333*)

generate (*h=''*, *r=''*)

__str__ ()

Return str(self).

eval_lp_performance (*dataset=List[Tuple[str, str, str]]*, *filtered=True*)

predict_missing_head_entity (*relation: List[str] | str*, *tail_entity: List[str] | str*, *within=None*) → Tuple

Given a relation and a tail entity, return top k ranked head entity.

argmax_{e in E } f(e,r,t), where r in R, t in E.

Parameter

relation: Union[List[str], str]

String representation of selected relations.

tail_entity: Union[List[str], str]

String representation of selected entities.

k: int

Highest ranked k entities.

Returns: Tuple

Highest K scores and entities

predict_missing_relations (*head_entity: List[str] | str*, *tail_entity: List[str] | str*, *within=None*) → Tuple

Given a head entity and a tail entity, return top k ranked relations.

argmax_{r in R } f(h,r,t), where h, t in E.

Parameter

head_entity: List[str]

String representation of selected entities.

tail_entity: List[str]

String representation of selected entities.

k: int

Highest ranked k entities.

Returns: Tuple

Highest K scores and entities

predict_missing_tail_entity(*head_entity: List[str] | str*, *relation: List[str] | str*, *within: List[str] = None*) → torch.FloatTensor

Given a head entity and a relation, return top k ranked entities

argmax_{e in E } f(h,r,e), where h in E and r in R.

Parameter

head_entity: List[str]

String representation of selected entities.

tail_entity: List[str]

String representation of selected entities.

Returns: Tuple

scores

predict(***, *h: List[str] | str = None*, *r: List[str] | str = None*, *t: List[str] | str = None*, *within=None*, *logits=True*) → torch.FloatTensor

Parameters

- **logits** –
- **h** –
- **r** –
- **t** –
- **within** –

predict_topk(***, *h: List[str] = None*, *r: List[str] = None*, *t: List[str] = None*, *topk: int = 10*, *within: List[str] = None*)

Predict missing item in a given triple.

Parameter

head_entity: List[str]

String representation of selected entities.

relation: List[str]

String representation of selected relations.

tail_entity: List[str]

String representation of selected entities.

k: int

Highest ranked k item.

Returns: Tuple

Highest K scores and items

triple_score (*h: List[str] | str = None*, *r: List[str] | str = None*, *t: List[str] | str = None*, *logits=False*) → torch.FloatTensor

Predict triple score

Parameter

head_entity: List[str]

String representation of selected entities.

relation: List[str]

String representation of selected relations.

tail_entity: List[str]

String representation of selected entities.

logits: bool

If logits is True, unnormalized score returned

Returns: Tuple

pytorch tensor of triple score

t_norm (*tens_1: torch.Tensor*, *tens_2: torch.Tensor*, *tnorm: str = 'min'*) → torch.Tensor

tensor_t_norm (*subquery_scores: torch.FloatTensor*, *tnorm: str = 'min'*) → torch.FloatTensor

Compute T-norm over [0,1] ^{n imes d} where n denotes the number of hops and d denotes number of entities

t_conorm (*tens_1: torch.Tensor*, *tens_2: torch.Tensor*, *tconorm: str = 'min'*) → torch.Tensor

negnorm (*tens_1: torch.Tensor*, *lambda_: float*, *neg_norm: str = 'standard'*) → torch.Tensor

return_multi_hop_query_results (*aggregated_query_for_all_entities*, *k: int*, *only_scores*)

single_hop_query_answering (*query: tuple*, *only_scores: bool = True*, *k: int = None*)

answer_multi_hop_query (*query_type: str = None*, *query: Tuple[str | Tuple[str, str], Ellipsis] = None*, *queries: List[Tuple[str | Tuple[str, str], Ellipsis]] = None*, *tnorm: str = 'prod'*, *neg_norm: str = 'standard'*, *lambda_: float = 0.0*, *k: int = 10*, *only_scores=False*) → List[Tuple[str, torch.Tensor]]

@TODO: Refactoring is needed # @TODO: Score computation for each query type should be done in a static function

Find an answer set for EPFO queries including negation and disjunction

Parameter

query_type: str The type of the query, e.g., "2p".

query: Union[str, Tuple[str, Tuple[str, str]]] The query itself, either a string or a nested tuple.

queries: List of Tuple[Union[str, Tuple[str, str]], …]

tnorm: str The t-norm operator.

neg_norm: str The negation norm.

lambda_: float lambda parameter for sugeno and yager negation norms

k: int The top-k substitutions for intermediate variables.

returns

- *List[Tuple[str, torch.Tensor]]*
- *Entities and corresponding scores sorted in the descening order of scores*

find_missing_triples (*confidence: float*, *entities: List[str] = None*, *relations: List[str] = None*, *topk: int = 10*, *at_most: int = sys.maxsize*) → Set

Find missing triples

Iterative over a set of entities E and a set of relation R :

orall e in E and orall r in R f(e,r,x)

Return (e,r,x)

otin G and f(e,r,x) > confidence

confidence: float

A threshold for an output of a sigmoid function given a triple.

topk: int

Highest ranked k item to select triples with f(e,r,x) > confidence .

at_most: int

Stop after finding at_most missing triples

{(e,r,x) | f(e,r,x) > confidence land (e,r,x)

otin G

deploy (*share: bool = False*, *top_k: int = 10*)

train_triples (*h: List[str]*, *r: List[str]*, *t: List[str]*, *labels: List[float]*, *iteration=2*, *optimizer=None*)

train_k_vs_all (*h*, *r*, *iteration=1*, *lr=0.001*)

Train k vs all :param head_entity: :param relation: :param iteration: :param lr: :return:

train (*kg*, *lr=0.1*, *epoch=10*, *batch_size=32*, *neg_sample_ratio=10*, *num_workers=1*) → None

Retrained a pretrain model on an input KG via negative sampling.

`dicee.query_generator`

Module Contents

Classes

QueryGenerator

class dicee.query_generator.**QueryGenerator**(*train_path*, *val_path: str*, *test_path: str*, *ent2id: Dict = None*, *rel2id: Dict = None*, *seed: int = 1*, *gen_valid: bool = False*, *gen_test: bool = True*)

list2tuple(*list_data*)

tuple2list(*x: List | Tuple*) → List | Tuple

Convert a nested tuple to a nested list.

set_global_seed(*seed: int*)

Set seed

construct_graph(*paths: List[str]*) → Tuple[Dict, Dict]

Construct graph from triples Returns dicts with incoming and outgoing edges

fill_query(*query_structure: List[str | List]*, *ent_in: Dict*, *ent_out: Dict*, *answer: int*) → bool

Private method for fill_query logic.

achieve_answer(*query: List[str | List]*, *ent_in: Dict*, *ent_out: Dict*) → set

Private method for achieve_answer logic. @TODO: Document the code

write_links(*ent_out*, *small_ent_out*)

ground_queries(*query_structure: List[str | List]*, *ent_in: Dict*, *ent_out: Dict*, *small_ent_in: Dict*, *small_ent_out: Dict*, *gen_num: int*, *query_name: str*)

Generating queries and achieving answers

unmap(*query_type*, *queries*, *tp_answers*, *fp_answers*, *fn_answers*)

unmap_query(*query_structure*, *query*, *id2ent*, *id2rel*)

generate_queries(*query_struct: List*, *gen_num: int*, *query_type: str*)

Passing incoming and outgoing edges to ground queries depending on mode [train valid or text] and getting queries and answers in return @ TODO: create a class for each single query struct

save_queries(*query_type: str*, *gen_num: int*, *save_path: str*)

abstract load_queries(*path*)

get_queries(*query_type: str*, *gen_num: int*)

static save_queries_and_answers(*path: str*, *data: List[Tuple[str, Tuple[collections.defaultdict]]]*) → None

Save Queries into Disk

static load_queries_and_answers(*path: str*) → List[Tuple[str, Tuple[collections.defaultdict]]]

Load Queries from Disk to Memory

dicee.sanity_checkers

Module Contents

Functions

is_sparql_endpoint_alive([sparql_endpoint])	
validate_knowledge_graph(args)	Validating the source of knowledge graph
sanity_checking_with_arguments(args)	

dicee.sanity_checkers.**is_sparql_endpoint_alive**(*sparql_endpoint: str = None*)

dicee.sanity_checkers.**validate_knowledge_graph**(*args*)

Validating the source of knowledge graph

dicee.sanity_checkers.**sanity_checking_with_arguments**(*args*)

dicee.static_funcs

Module Contents

Functions

create_recipriocal_triples(x)	Add inverse triples into dask dataframe
get_er_vocab(data[, file_path])	
get_re_vocab(data[, file_path])	
get_ee_vocab(data[, file_path])	
timeit(func)	
save_pickle(*[, data, file_path])	
load_pickle([file_path])	
select_model(args[, is_continual_training, storage_path])	
load_model(→ Tuple[object, Tuple[dict, dict]])	Load weights and initialize pytorch module from namespace arguments
load_model_ensemble(...)	Construct Ensemble Of weights and initialize pytorch module from namespace arguments
save_numpy_ndarray(*, data, file_path)	
numpy_data_type_changer(→ numpy.ndarray)	Detect most efficient data type for a given triples
save_checkpoint_model(→ None)	Store Pytorch model into disk

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Table 2 – continued from previous page

`store`(→ None)	Store trained_model model and save embeddings into csv file.
`add_noisy_triples`(→ pandas.DataFrame)	Add randomly constructed triples
`read_or_load_kg`(args, cls)	
`intialize_model`(→ Tuple[object, str])	
`load_json`(→ dict)	
`save_embeddings`(→ None)	Save it as CSV if memory allows.
`random_prediction`(pre_trained_kge)	
`deploy_triple_prediction`(pre_trained_kge, str_subject, ...)	
`deploy_tail_entity_prediction`(pre_trained_] ...)	
`deploy_head_entity_prediction`(pre_trained_] ...)	
`deploy_relation_prediction`(pre_trained_kge, ...)	
`vocab_to_parquet`(vocab_to_idx, name, ...)	
`create_experiment_folder`([folder_name])	
`continual_training_setup_executor`(→ None)	storage_path:str A path leading to a parent directory, where a subdirectory containing KGE related data
`exponential_function`(→ torch.FloatTensor)	
`load_numpy`(→ numpy.ndarray)	
`evaluate`(entity_to_idx, scores, easy_answers, hard_answers)	# @TODO: CD: Renamed this function
`download_file`(url[, destination_folder])	
`download_files_from_url`(base_url[, destination_folder])	
`download_pretrained_model`(→ str)	

`dicee.static_funcs.`**`create_recipriocal_triples`**(*x*)

Add inverse triples into dask dataframe :param x: :return:

`dicee.static_funcs.`**`get_er_vocab`**(*data, file_path: str = None*)

`dicee.static_funcs.`**`get_re_vocab`**(*data, file_path: str = None*)

`dicee.static_funcs.`**`get_ee_vocab`**(*data, file_path: str = None*)

`dicee.static_funcs.`**`timeit`**(*func*)

`dicee.static_funcs.`**`save_pickle`**(**, data: object = None, file_path=str*)

`dicee.static_funcs.`**`load_pickle`**(*file_path=str*) dicee.static_funcs.**select_model**(*args: dict*, *is_continual_training: bool = None*, *storage_path: str = None*)

dicee.static_funcs.**load_model**(*path_of_experiment_folder: str*, *model_name='model.pt'*, *verbose=0*) → Tuple[object, Tuple[dict, dict]]

Load weights and initialize pytorch module from namespace arguments

dicee.static_funcs.**load_model_ensemble**(*path_of_experiment_folder: str*) → Tuple[*dicee.models.base_model.BaseKGE*, Tuple[pandas.DataFrame, pandas.DataFrame]]

Construct Ensemble Of weights and initialize pytorch module from namespace arguments

(1) Detect models under given path

(2) Accumulate parameters of detected models

(3) Normalize parameters

(4) Insert (3) into model.

dicee.static_funcs.**save_numpy_ndarray**(*, *data: numpy.ndarray*, *file_path: str*)

dicee.static_funcs.**numpy_data_type_changer**(*train_set: numpy.ndarray*, *num: int*) → numpy.ndarray

Detect most efficient data type for a given triples :param train_set: :param num: :return:

dicee.static_funcs.**save_checkpoint_model**(*model*, *path: str*) → None

Store Pytorch model into disk

dicee.static_funcs.**store**(*trainer*, *trained_model*, *model_name: str = 'model'*, *full_storage_path: str = None*, *save_embeddings_as_csv=False*) → None

Store trained_model model and save embeddings into csv file. :param trainer: an instance of trainer class :param full_storage_path: path to save parameters. :param model_name: string representation of the name of the model. :param trained_model: an instance of BaseKGE see core.models.base_model . :param save_embeddings_as_csv: for easy access of embeddings. :return:

dicee.static_funcs.**add_noisy_triples**(*train_set: pandas.DataFrame*, *add_noise_rate: float*) → pandas.DataFrame

Add randomly constructed triples :param train_set: :param add_noise_rate: :return:

dicee.static_funcs.**read_or_load_kg**(*args*, *cls*)

dicee.static_funcs.**intialize_model**(*args: dict*, *verbose=0*) → Tuple[object, str]

dicee.static_funcs.**load_json**(*p: str*) → dict

dicee.static_funcs.**save_embeddings**(*embeddings: numpy.ndarray*, *indexes*, *path: str*) → None

Save it as CSV if memory allows. :param embeddings: :param indexes: :param path: :return:

dicee.static_funcs.**random_prediction**(*pre_trained_kge*)

dicee.static_funcs.**deploy_triple_prediction**(*pre_trained_kge*, *str_subject*, *str_predicate*, *str_object*)

dicee.static_funcs.**deploy_tail_entity_prediction**(*pre_trained_kge*, *str_subject*, *str_predicate*, *top_k*)

dicee.static_funcs.**deploy_head_entity_prediction**(*pre_trained_kge*, *str_object*, *str_predicate*, *top_k*) dicee.static_funcs.**deploy_relation_prediction**(*pre_trained_kge*, *str_subject*, *str_object*, *top_k*)

dicee.static_funcs.**vocab_to_parquet**(*vocab_to_idx*, *name*, *path_for_serialization*, *print_into*)

dicee.static_funcs.**create_experiment_folder**(*folder_name='Experiments'*)

dicee.static_funcs.**continual_training_setup_executor**(*executor*) → None

storage_path:str A path leading to a parent directory, where a subdirectory containing KGE related data

full_storage_path:str A path leading to a subdirectory containing KGE related data

dicee.static_funcs.**exponential_function**(*x: numpy.ndarray*, *lam: float*, *ascending_order=True*) → torch.FloatTensor

dicee.static_funcs.**load_numpy**(*path*) → numpy.ndarray

dicee.static_funcs.**evaluate**(*entity_to_idx*, *scores*, *easy_answers*, *hard_answers*)

@TODO: CD: Renamed this function Evaluate multi hop query answering on different query types

dicee.static_funcs.**download_file**(*url*, *destination_folder='.'*)

dicee.static_funcs.**download_files_from_url**(*base_url*, *destination_folder='.'*)

dicee.static_funcs.**download_pretrained_model**(*url: str*) → str

dicee.static_funcs_training

Module Contents

Functions

evaluate_lp(model, triple_idx, num_entities, er_vocab, ...)	Evaluate model in a standard link prediction task
evaluate_bpe_lp(model, triple_idx, ...[, info])	
efficient_zero_grad(model)	

dicee.static_funcs_training.**evaluate_lp**(*model*, *triple_idx*, *num_entities*, *er_vocab: Dict[Tuple, List]*, *re_vocab: Dict[Tuple, List]*, *info='Eval Starts'*)

Evaluate model in a standard link prediction task

for each triple the rank is computed by taking the mean of the filtered missing head entity rank and the filtered missing tail entity rank :param model: :param triple_idx: :param info: :return:

dicee.static_funcs_training.**evaluate_bpe_lp**(*model*, *triple_idx: List[Tuple]*, *all_bpe_shaped_entities*, *er_vocab: Dict[Tuple, List]*, *re_vocab: Dict[Tuple, List]*, *info='Eval Starts'*)

dicee.static_funcs_training.**efficient_zero_grad**(*model*)

dicee.static_preprocess_funcs

Module Contents

Functions

timeit(func)	
preprocesses_input_args(args)	Sanity Checking in input arguments
create_constraints(→ Tuple[dict, dict, dict, dict])	(1) Extract domains and ranges of relations
get_er_vocab(data)	
get_re_vocab(data)	
get_ee_vocab(data)	
mapping_from_first_two_cols_to_third(tra	

Attributes

enable_log

dicee.static_preprocess_funcs.**enable_log = False**

dicee.static_preprocess_funcs.**timeit**(*func*)

dicee.static_preprocess_funcs.**preprocesses_input_args**(*args*)

Sanity Checking in input arguments

dicee.static_preprocess_funcs.**create_constraints**(*triples: numpy.ndarray*)
→ Tuple[dict, dict, dict, dict]

(1) Extract domains and ranges of relations

(2) Store a mapping from relations to entities that are outside of the domain and range. Create constraints entities based on the range of relations :param triples: :return:

dicee.static_preprocess_funcs.**get_er_vocab**(*data*)

dicee.static_preprocess_funcs.**get_re_vocab**(*data*)

dicee.static_preprocess_funcs.**get_ee_vocab**(*data*)

dicee.static_preprocess_funcs.**mapping_from_first_two_cols_to_third**(
train_set_idx)

13.3 Package Contents

Classes

CMult	Cl_(0,0) => Real Numbers
Pyke	A Physical Embedding Model for Knowledge Graphs
DistMult	Embedding Entities and Relations for Learning and Inference in Knowledge Bases
KeciBase	Without learning dimension scaling
Keci	Base class for all neural network modules.
TransE	Translating Embeddings for Modeling
DeCaL	Base class for all neural network modules.
ComplEx	Base class for all neural network modules.
AConEx	Additive Convolutional ComplEx Knowledge Graph Embeddings
AConvO	Additive Convolutional Octonion Knowledge Graph Embeddings
AConvQ	Additive Convolutional Quaternion Knowledge Graph Embeddings
ConvQ	Convolutional Quaternion Knowledge Graph Embeddings
ConvO	Base class for all neural network modules.
ConEx	Convolutional ComplEx Knowledge Graph Embeddings
QMult	Base class for all neural network modules.
OMult	Base class for all neural network modules.
Shallom	A shallow neural model for relation prediction (https://arxiv.org/abs/2101.09090)
LFMult	Embedding with polynomial functions. We represent all entities and relations in the polynomial space as:
PykeenKGE	A class for using knowledge graph embedding models implemented in Pykeen
BytE	Base class for all neural network modules.
BaseKGE	Base class for all neural network modules.
DICE_Trainer	DICE_Trainer implement
KGE	Knowledge Graph Embedding Class for interactive usage of pre-trained models
Execute	A class for Training, Retraining and Evaluation a model.
BPE_NegativeSamplingDataset	An abstract class representing a `Dataset`.
MultiLabelDataset	An abstract class representing a `Dataset`.
MultiClassClassificationDataset	Dataset for the 1vsALL training strategy
OnevsAllDataset	Dataset for the 1vsALL training strategy
KvsAll	Creates a dataset for KvsAll training by inheriting from torch.utils.data.Dataset.
AllvsAll	Creates a dataset for AllvsAll training by inheriting from torch.utils.data.Dataset.
KvsSampleDataset	KvsSample a Dataset:
NegSampleDataset	An abstract class representing a `Dataset`.
TriplePredictionDataset	Triple Dataset
CVDataModule	Create a Dataset for cross validation
QueryGenerator	

Functions

create_reciprioical_triples(x)	Add inverse triples into dask dataframe
get_er_vocab(data[, file_path])	
get_re_vocab(data[, file_path])	
get_ee_vocab(data[, file_path])	
timeit(func)	
save_pickle(*[, data, file_path])	
load_pickle([file_path])	
select_model(args[, is_continual_training, storage_path])	
load_model(→ Tuple[object, Tuple[dict, dict]])	Load weights and initialize pytorch module from namespace arguments
load_model_ensemble(...)	Construct Ensemble Of weights and initialize pytorch module from namespace arguments
save_numpy_ndarray(*, data, file_path)	
numpy_data_type_changer(→ numpy.ndarray)	Detect most efficient data type for a given triples
save_checkpoint_model(→ None)	Store Pytorch model into disk
store(→ None)	Store trained_model model and save embeddings into csv file.
add_noisy_triples(→ pandas.DataFrame)	Add randomly constructed triples
read_or_load_kg(args, cls)	
intialize_model(→ Tuple[object, str])	
load_json(→ dict)	
save_embeddings(→ None)	Save it as CSV if memory allows.
random_prediction(pre_trained_kge)	
deploy_triple_prediction(pre_trained_kge, str_subject, ...)	
deploy_tail_entity_prediction(pre_trained_] ...)	
deploy_head_entity_prediction(pre_trained_] ...)	
deploy_relation_prediction(pre_trained_kge, ...)	
vocab_to_parquet(vocab_to_idx, name, ...)	
create_experiment_folder([folder_name])	

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Table 4 – continued from previous page

continual_training_setup_executor(→ None)	storage_path:str A path leading to a parent directory, where a subdirectory containing KGE related data
exponential_function(→ torch.FloatTensor)	
load_numpy(→ numpy.ndarray)	
evaluate(entity_to_idx, scores, easy_answers, hard_answers)	# @TODO: CD: Renamed this function
download_file(url[, destination_folder])	
download_files_from_url(base_url[, destination_folder])	
download_pretrained_model(→ str)	
mapping_from_first_two_cols_to_third(tra	
timeit(func)	
load_pickle([file_path])	
reload_dataset(path, form_of_labelling, ...)	Reload the files from disk to construct the Pytorch dataset
construct_dataset(→ torch.utils.data.Dataset)	

Attributes

`__version__`

class dicee.**CMult**(*args*)

Bases: `dicee.models.base_model.BaseKGE`

Cl_(0,0) => Real Numbers

Cl_(0,1) =>

A multivector mathbf{a} = a_0 + a_1 e_1 A multivector mathbf{b} = b_0 + b_1 e_1

multiplication is isomorphic to the product of two complex numbers

mathbf{a} imes mathbf{b} = a_0 b_0 + a_0b_1 e1 + a_1 b_1 e_1 e_1

= (a_0 b_0 - a_1 b_1) + (a_0 b_1 + a_1 b_0) e_1

Cl_(2,0) =>

A multivector mathbf{a} = a_0 + a_1 e_1 + a_2 e_2 + a_{12} e_1 e_2 A multivector mathbf{b} = b_0 + b_1 e_1 + b_2 e_2 + b_{12} e_1 e_2

mathbf{a} imes mathbf{b} = a_0b_0 + a_0b_1 e_1 + a_0b_2e_2 + a_0 b_12 e_1 e_2

- a_1 b_0 e_1 + a_1b_1 e_1_e1 ..

Cl_(0,2) => Quaternions

clifford_mul(*x: torch.FloatTensor*, *y: torch.FloatTensor*, *p: int*, *q: int*) → tuple

Clifford multiplication Cl_{p,q} (mathbb{R})

ei ^2 = +1 for i =< i =< p ej ^2 = -1 for p < j =< p+q ei ej = -eje1 for i

eq j

x: torch.FloatTensor with (n,d) shape

y: torch.FloatTensor with (n,d) shape

p: a non-negative integer p>= 0 q: a non-negative integer q>= 0

score (*head_ent_emb*, *rel_ent_emb*, *tail_ent_emb*)

forward_triples (*x: torch.LongTensor*) → torch.FloatTensor

Compute batch triple scores

Parameter

x: torch.LongTensor with shape n by 3

rtype
torch.LongTensor with shape n

forward_k_vs_all (*x: torch.Tensor*) → torch.FloatTensor

Compute batch KvsAll triple scores

Parameter

x: torch.LongTensor with shape n by 3

rtype
torch.LongTensor with shape n

class dicee.**Pyke** (*args*)

Bases: *dicee.models.base_model.BaseKGE*

A Physical Embedding Model for Knowledge Graphs

forward_triples (*x: torch.LongTensor*)

Parameters
x –

class dicee.**DistMult** (*args*)

Bases: *dicee.models.base_model.BaseKGE*

Embedding Entities and Relations for Learning and Inference in Knowledge Bases https://arxiv.org/abs/1412.6575

k_vs_all_score (*emb_h: torch.FloatTensor*, *emb_r: torch.FloatTensor*, *emb_E: torch.FloatTensor*)

Parameters

- **emb_h** –
- **emb_r** –
- **emb_E** –

forward_k_vs_all (*x: torch.LongTensor*)

forward_k_vs_sample (*x: torch.LongTensor*, *target_entity_idx: torch.LongTensor*)

score (*h*, *r*, *t*)

class dicee.**KeciBase** (*args*)

Bases: *Keci*

Without learning dimension scaling

class dicee.**Keci** (*args*)

Bases: *dicee.models.base_model.BaseKGE*

Base class for all neural network modules.

Your models should also subclass this class.

Modules can also contain other Modules, allowing to nest them in a tree structure. You can assign the submodules as regular attributes:

```
import torch.nn as nn
import torch.nn.functional as F

class Model(nn.Module):
    def __init__(self):
        super().__init__()
        self.conv1 = nn.Conv2d(1, 20, 5)
        self.conv2 = nn.Conv2d(20, 20, 5)

    def forward(self, x):
        x = F.relu(self.conv1(x))
        return F.relu(self.conv2(x))
```

Submodules assigned in this way will be registered, and will have their parameters converted too when you call `to()`, etc.

Note: As per the example above, an `__init__()` call to the parent class must be made before assignment on the child.

Variables

training (*bool*) – Boolean represents whether this module is in training or evaluation mode.

compute_sigma_pp (*hp*, *rp*)

Compute sigma_{pp} = sum_{i=1}^{p-1} sum_{k=i+1}^p (h_i r_k - h_k r_i) e_i e_k

sigma_{pp} captures the interactions between along p bases For instance, let p e_1, e_2, e_3, we compute interactions between e_1 e_2, e_1 e_3 , and e_2 e_3 This can be implemented with a nested two for loops

results = [] for i in range(p - 1):

for k in range(i + 1, p):
results.append(hp[:, :, i] * rp[:, :, k] - hp[:, :, k] * rp[:, :, i])

sigma_pp = torch.stack(results, dim=2) assert sigma_pp.shape == (b, r, int((p * (p - 1)) / 2))

Yet, this computation would be quite inefficient. Instead, we compute interactions along all p, e.g., e1e1, e1e2, e1e3, e2e1, e2e2, e2e3, e3e1, e3e2, e3e3

Then select the triangular matrix without diagonals: e1e2, e1e3, e2e3.

compute_sigma_qq (*hq*, *rq*)

Compute sigma_{qq} = sum_{j=1}^{p+q-1} sum_{k=j+1}^{p+q} (h_j r_k - h_k r_j) e_j e_k sigma_{q} captures the interactions between along q bases For instance, let q e_1, e_2, e_3, we compute interactions between e_1 e_2, e_1 e_3 , and e_2 e_3 This can be implemented with a nested two for loops

results = [] for j in range(q - 1):

for k in range(j + 1, q):
results.append(hq[:, :, j] * rq[:, :, k] - hq[:, :, k] * rq[:, :, j])

sigma_qq = torch.stack(results, dim=2) assert sigma_qq.shape == (b, r, int((q * (q - 1)) / 2))

Yet, this computation would be quite inefficient. Instead, we compute interactions along all p, e.g., e1e1, e1e2, e1e3,

e2e1, e2e2, e2e3, e3e1, e3e2, e3e3

Then select the triangular matrix without diagonals: e1e2, e1e3, e2e3.

compute_sigma_pq (*, *hp*, *hq*, *rp*, *rq*)

sum_{i=1}^{p} sum_{j=p+1}^{p+q} (h_i r_j - h_j r_i) e_i e_j

results = [] sigma_pq = torch.zeros(b, r, p, q) for i in range(p):

for j in range(q):
sigma_pq[:, :, i, j] = hp[:, :, i] * rq[:, :, j] - hq[:, :, j] * rp[:, :, i]

print(sigma_pq.shape)

apply_coefficients (*h0*, *hp*, *hq*, *r0*, *rp*, *rq*)

Multiplying a base vector with its scalar coefficient

clifford_multiplication (*h0*, *hp*, *hq*, *r0*, *rp*, *rq*)

Compute our CL multiplication

h = h_0 + sum_{i=1}^p h_i e_i + sum_{j=p+1}^{p+q} h_j e_j r = r_0 + sum_{i=1}^p r_i e_i + sum_{j=p+1}^{p+q} r_j e_j

ei ^2 = +1 for i =< i =< p ej ^2 = -1 for p < j =< p+q ei ej = -eje1 for i

eq j

h r = sigma_0 + sigma_p + sigma_q + sigma_{pp} + sigma_{q}+ sigma_{pq} where

(1) sigma_0 = h_0 r_0 + sum_{i=1}^p (h_0 r_i) e_i - sum_{j=p+1}^{p+q} (h_j r_j) e_j

(2) sigma_p = sum_{i=1}^p (h_0 r_i + h_i r_0) e_i

(3) sigma_q = sum_{j=p+1}^{p+q} (h_0 r_j + h_j r_0) e_j

(4) sigma_{pp} = sum_{i=1}^{p-1} sum_{k=i+1}^p (h_i r_k - h_k r_i) e_i e_k

(5) sigma_{qq} = sum_{j=1}^{p+q-1} sum_{k=j+1}^{p+q} (h_j r_k - h_k r_j) e_j e_k

(6) sigma_{pq} = sum_{i=1}^{p} sum_{j=p+1}^{p+q} (h_i r_j - h_j r_i) e_i e_j

construct_cl_multivector (*x: torch.FloatTensor*, *r: int*, *p: int*, *q: int*)
→ tuple[torch.FloatTensor, torch.FloatTensor, torch.FloatTensor]

Construct a batch of multivectors Cl_{p,q}(mathbb{R}^d)

Parameter

x: torch.FloatTensor with (n,d) shape

returns

- **a0** (*torch.FloatTensor with (n,r) shape*)
- **ap** (*torch.FloatTensor with (n,r,p) shape*)
- **aq** (*torch.FloatTensor with (n,r,q) shape*)

forward_k_vs_with_explicit (*x: torch.Tensor*)

k_vs_all_score (*bpe_head_ent_emb, bpe_rel_ent_emb, E*)

forward_k_vs_all (*x: torch.Tensor*) → torch.FloatTensor

Kvsall training

(1) Retrieve real-valued embedding vectors for heads and relations mathbb{R}^d .

(2) Construct head entity and relation embeddings according to Cl_{p,q}(mathbb{R}^d) .

(3) Perform Cl multiplication

(4) Inner product of (3) and all entity embeddings

forward_k_vs_with_explicit and this funcitons are identical Parameter ——— x: torch.LongTensor with (n,2) shape :rtype: torch.FloatTensor with (n, **|E|**) shape

forward_k_vs_sample (*x: torch.LongTensor, target_entity_idx: torch.LongTensor*) → torch.FloatTensor

Kvsall training

(1) Retrieve real-valued embedding vectors for heads and relations mathbb{R}^d .

(2) Construct head entity and relation embeddings according to Cl_{p,q}(mathbb{R}^d) .

(3) Perform Cl multiplication

(4) Inner product of (3) and all entity embeddings

Parameter

x: torch.LongTensor with (n,2) shape

rtype

torch.FloatTensor with (n, **|E|**) shape

score (*h, r, t*)

forward_triples (*x: torch.Tensor*) → torch.FloatTensor

Parameter

x: torch.LongTensor with (n,3) shape

rtype
torch.FloatTensor with (n) shape

class dicee.**TransE**(*args*)

Bases: *dicee.models.base_model.BaseKGE*

Translating Embeddings for Modeling Multi-relational Data https://proceedings.neurips.cc/paper/2013/file/1cecc7a77928ca8133fa24680a88d2f9-Paper.pdf

score(*head_ent_emb*, *rel_ent_emb*, *tail_ent_emb*)

forward_k_vs_all(*x: torch.Tensor*) → torch.FloatTensor

class dicee.**DeCaL**(*args*)

Bases: *dicee.models.base_model.BaseKGE*

Base class for all neural network modules.

Your models should also subclass this class.

Modules can also contain other Modules, allowing to nest them in a tree structure. You can assign the submodules as regular attributes:

```
import torch.nn as nn
import torch.nn.functional as F

class Model(nn.Module):
    def __init__(self):
        super().__init__()
        self.conv1 = nn.Conv2d(1, 20, 5)
        self.conv2 = nn.Conv2d(20, 20, 5)

    def forward(self, x):
        x = F.relu(self.conv1(x))
        return F.relu(self.conv2(x))
```

Submodules assigned in this way will be registered, and will have their parameters converted too when you call `to()`, etc.

Note: As per the example above, an `__init__()` call to the parent class must be made before assignment on the child.

Variables
training (*bool*) – Boolean represents whether this module is in training or evaluation mode.

forward_triples(*x: torch.Tensor*) → torch.FloatTensor

Parameter

x: torch.LongTensor with (n,3) shape

rtype
torch.FloatTensor with (n) shape

cl_pqr (*a*)

Input: tensor(batch_size, emb_dim) —-> output: tensor with 1+p+q+r components with size (batch_size, emb_dim/(1+p+q+r)) each.

1) takes a tensor of size (batch_size, emb_dim), split it into 1 + p + q +r components, hence 1+p+q+r must be a divisor of the emb_dim. 2) Return a list of the 1+p+q+r components vectors, each are tensors of size (batch_size, emb_dim/(1+p+q+r))

compute_sigmas_single (*list_h_emb*, *list_r_emb*, *list_t_emb*)

here we compute all the sums with no others vectors interaction taken with the scalar product with t, that is, 1) s0 = h_0r_0t_0 2) s1 = sum_{i=1}^{p}h_ir_it_0 3) s2 = sum_{j=p+1}^{p+q}h_jr_jt_0 4) s3 = sum_{i=1}^{q}(h_0r_it_i + h_ir_0t_i) 5) s4 = sum_{i=p+1}^{p+q}(h_0r_it_i + h_ir_0t_i) 5) s5 = sum_{i=p+q+1}^{p+q+r}(h_0r_it_i + h_ir_0t_i)

and return:

*) sigma_0t = sigma_0 cdot t_0 = s0 + s1 -s2 *) s3, s4 and s5

compute_sigmas_multivect (*list_h_emb*, *list_r_emb*)

Here we compute and return all the sums with vectors interaction for the same and different bases.

For same bases vectors interaction we have

1) sigma_pp = sum_{i=1}^{p-1}sum_{i'=i+1}^{p}(h_ir_{i'}-h_{i'}r_i) (models the interactions between e_i and e_i' for 1 <= i, i' <= p)
2) sigma_qq = sum_{j=p+1}^{p+q-1}sum_{j'=j+1}^{p+q}(h_jr_{j'}-h_{j'} (models the interactions between e_j and e_j' for p+1 <= j, j' <= p+q)
3) sigma_rr = sum_{k=p+q+1}^{p+q+r-1}sum_{k'=k+1}^{p}(h_kr_{k'}-h_{k'}r_k) (models the interactions between e_k and e_k' for p+q+1 <= k, k' <= p+q+r)

For different base vector interactions, we have

4) sigma_pq = sum_{i=1}^{p}sum_{j=p+1}^{p+q}(h_ir_j - h_jr_i) (interactionsn between e_i and e_j for 1<=i <=p and p+1<= j <= p+q)
5) sigma_pr = sum_{i=1}^{p}sum_{k=p+q+1}^{p+q+r}(h_ir_k - h_kr_i) (interactionsn between e_i and e_k for 1<=i <=p and p+q+1<= k <= p+q+r)
6) sigma_qr = sum_{j=p+1}^{p+q}sum_{j=p+q+1}^{p+q+r}(h_jr_k - h_kr_j) (interactionsn between e_j and e_k for p+1 <= j <=p+q and p+q+1<= j <= p+q+r)

forward_k_vs_all (*x: torch.Tensor*) → torch.FloatTensor

Kvsall training

(1) Retrieve real-valued embedding vectors for heads and relations mathbb{R}^d .
(2) Construct head entity and relation embeddings according to Cl_{p,q}(mathbb{R}^d) .
(3) Perform Cl multiplication
(4) Inner product of (3) and all entity embeddings

forward_k_vs_with_explicit and this funcitons are identical Parameter ——— x: torch.LongTensor with (n,2) shape :rtype: torch.FloatTensor with (n, **|E|**) shape

apply_coefficients (*h0*, *hp*, *hq*, *hk*, *r0*, *rp*, *rq*, *rk*)

Multiplying a base vector with its scalar coefficient

construct_cl_multivector (*x: torch.FloatTensor*, *re: int*, *p: int*, *q: int*, *r: int*) → tuple[torch.FloatTensor, torch.FloatTensor, torch.FloatTensor]

Construct a batch of multivectors Cl_{p,q,r}(mathbb{R}^d)

Parameter

x: torch.FloatTensor with (n,d) shape

returns

- **a0** (*torch.FloatTensor*)
- **ap** (*torch.FloatTensor*)
- **aq** (*torch.FloatTensor*)
- **ar** (*torch.FloatTensor*)

compute_sigma_pp (*hp*, *rp*)

sigma_{p,p}^* = sum_{i=1}^{p-1}sum_{i'=i+1}^{p}(x_iy_{i'}-x_{i'}y_i)

sigma_{pp} captures the interactions between along p bases For instance, let p e_1, e_2, e_3, we compute interactions between e_1 e_2, e_1 e_3 , and e_2 e_3 This can be implemented with a nested two for loops

results = [] for i in range(p - 1):

for k in range(i + 1, p):
results.append(hp[:, :, i] * rp[:, :, k] - hp[:, :, k] * rp[:, :, i])

sigma_pp = torch.stack(results, dim=2) assert sigma_pp.shape == (b, r, int((p * (p - 1)) / 2))

Yet, this computation would be quite inefficient. Instead, we compute interactions along all p, e.g., e1e1, e1e2, e1e3,

e2e1, e2e2, e2e3, e3e1, e3e2, e3e3

Then select the triangular matrix without diagonals: e1e2, e1e3, e2e3.

compute_sigma_qq (*hq*, *rq*)

Compute sigma_{q,q}^* = sum_{j=p+1}^{p+q-1}sum_{j'=j+1}^{p+q}(x_jy_{j'}-x_{j'}y_j) Eq. 16 sigma_{q} captures the interactions between along q bases For instance, let q e_1, e_2, e_3, we compute interactions between e_1 e_2, e_1 e_3 , and e_2 e_3 This can be implemented with a nested two for loops

results = [] for j in range(q - 1):

for k in range(j + 1, q):
results.append(hq[:, :, j] * rq[:, :, k] - hq[:, :, k] * rq[:, :, j])

sigma_qq = torch.stack(results, dim=2) assert sigma_qq.shape == (b, r, int((q * (q - 1)) / 2))

Yet, this computation would be quite inefficient. Instead, we compute interactions along all p, e.g., e1e1, e1e2, e1e3,

e2e1, e2e2, e2e3, e3e1, e3e2, e3e3

Then select the triangular matrix without diagonals: e1e2, e1e3, e2e3.

compute_sigma_rr (*hk*, *rk*)

sigma_{r,r}^* = sum_{k=p+q+1}^{p+q+r-1}sum_{k'=k+1}^{p}(x_ky_{k'}-x_{k'}y_k)

compute_sigma_pq (*, *hp*, *hq*, *rp*, *rq*)

sum_{i=1}^{p} sum_{j=p+1}^{p+q} (h_i r_j - h_j r_i) e_i e_j

results = [] sigma_pq = torch.zeros(b, r, p, q) for i in range(p):

for j in range(q):
sigma_pq[:, :, i, j] = hp[:, :, i] * rq[:, :, j] - hq[:, :, j] * rp[:, :, i]

print(sigma_pq.shape)

compute_sigma_pr (*, *hp*, *hk*, *rp*, *rk*)

sum_{i=1}^{p} sum_{j=p+1}^{p+q} (h_i r_j - h_j r_i) e_i e_j

results = [] sigma_pq = torch.zeros(b, r, p, q) for i in range(p):

for j in range(q):
sigma_pq[:, :, i, j] = hp[:, :, i] * rq[:, :, j] - hq[:, :, j] * rp[:, :, i]

print(sigma_pq.shape)

compute_sigma_qr (*, *hq*, *hk*, *rq*, *rk*)

sum_{i=1}^{p} sum_{j=p+1}^{p+q} (h_i r_j - h_j r_i) e_i e_j

results = [] sigma_pq = torch.zeros(b, r, p, q) for i in range(p):

for j in range(q):
sigma_pq[:, :, i, j] = hp[:, :, i] * rq[:, :, j] - hq[:, :, j] * rp[:, :, i]

print(sigma_pq.shape)

class dicee.**ComplEx** (*args*)

Bases: *dicee.models.base_model.BaseKGE*

Base class for all neural network modules.

Your models should also subclass this class.

Modules can also contain other Modules, allowing to nest them in a tree structure. You can assign the submodules as regular attributes:

```
import torch.nn as nn
import torch.nn.functional as F

class Model(nn.Module):
    def __init__(self):
        super().__init__()
        self.conv1 = nn.Conv2d(1, 20, 5)
        self.conv2 = nn.Conv2d(20, 20, 5)

    def forward(self, x):
        x = F.relu(self.conv1(x))
        return F.relu(self.conv2(x))
```

Submodules assigned in this way will be registered, and will have their parameters converted too when you call `to()`, etc.

Note: As per the example above, an `__init__()` call to the parent class must be made before assignment on the child.

Variables

training (*bool*) – Boolean represents whether this module is in training or evaluation mode.

static score (*head_ent_emb: torch.FloatTensor*, *rel_ent_emb: torch.FloatTensor*, *tail_ent_emb: torch.FloatTensor*)

static k_vs_all_score (*emb_h: torch.FloatTensor*, *emb_r: torch.FloatTensor*, *emb_E: torch.FloatTensor*)

Parameters

- **emb_h** –
- **emb_r** –
- **emb_E** –

forward_k_vs_all (*x: torch.LongTensor*) → torch.FloatTensor

class dicee.**AConEx** (*args*)

Bases: *dicee.models.base_model.BaseKGE*

Additive Convolutional ComplEx Knowledge Graph Embeddings

residual_convolution (*C_1: Tuple[torch.Tensor, torch.Tensor]*, *C_2: Tuple[torch.Tensor, torch.Tensor]*) → torch.FloatTensor

Compute residual score of two complex-valued embeddings. :param C_1: a tuple of two pytorch tensors that corresponds complex-valued embeddings :param C_2: a tuple of two pytorch tensors that corresponds complex-valued embeddings :return:

forward_k_vs_all (*x: torch.Tensor*) → torch.FloatTensor

forward_triples (*x: torch.Tensor*) → torch.FloatTensor

Parameters

x –

forward_k_vs_sample (*x: torch.Tensor*, *target_entity_idx: torch.Tensor*)

class dicee.**AConvO** (*args: dict*)

Bases: *dicee.models.base_model.BaseKGE*

Additive Convolutional Octonion Knowledge Graph Embeddings

static octonion_normalizer (*emb_rel_e0*, *emb_rel_e1*, *emb_rel_e2*, *emb_rel_e3*, *emb_rel_e4*, *emb_rel_e5*, *emb_rel_e6*, *emb_rel_e7*)

residual_convolution (*O_1*, *O_2*)

forward_triples (*x: torch.Tensor*) → torch.Tensor

Parameters

x –

forward_k_vs_all (*x: torch.Tensor*)

Given a head entity and a relation (h,r), we compute scores for all entities. [score(h,r,x)|x in Entities] => [0.0,0.1,…,0.8], shape=> (1, **|Entities|**) Given a batch of head entities and relations => shape (size of batch,| Entities|)

class dicee.**AConvQ**(*args*)

Bases: *dicee.models.base_model.BaseKGE*

Additive Convolutional Quaternion Knowledge Graph Embeddings

residual_convolution(*Q_1*, *Q_2*)

forward_triples(*indexed_triple: torch.Tensor*) → torch.Tensor

Parameters

x –

forward_k_vs_all(*x: torch.Tensor*)

Given a head entity and a relation (h,r), we compute scores for all entities. [score(h,r,x)|x in Entities] => [0.0,0.1,…,0.8], shape=> (1, **|Entities|**) Given a batch of head entities and relations => shape (size of batch,| Entities|)

class dicee.**ConvQ**(*args*)

Bases: *dicee.models.base_model.BaseKGE*

Convolutional Quaternion Knowledge Graph Embeddings

residual_convolution(*Q_1*, *Q_2*)

forward_triples(*indexed_triple: torch.Tensor*) → torch.Tensor

Parameters

x –

forward_k_vs_all(*x: torch.Tensor*)

Given a head entity and a relation (h,r), we compute scores for all entities. [score(h,r,x)|x in Entities] => [0.0,0.1,…,0.8], shape=> (1, **|Entities|**) Given a batch of head entities and relations => shape (size of batch,| Entities|)

class dicee.**ConvO**(*args: dict*)

Bases: *dicee.models.base_model.BaseKGE*

Base class for all neural network modules.

Your models should also subclass this class.

Modules can also contain other Modules, allowing to nest them in a tree structure. You can assign the submodules as regular attributes:

```
import torch.nn as nn
import torch.nn.functional as F

class Model(nn.Module):
    def __init__(self):
        super().__init__()
        self.conv1 = nn.Conv2d(1, 20, 5)
        self.conv2 = nn.Conv2d(20, 20, 5)

    def forward(self, x):
        x = F.relu(self.conv1(x))
        return F.relu(self.conv2(x))
```

Submodules assigned in this way will be registered, and will have their parameters converted too when you call `to()`, etc.

Note: As per the example above, an `__init__()` call to the parent class must be made before assignment on the child.

Variables
training (*bool*) – Boolean represents whether this module is in training or evaluation mode.

static octonion_normalizer(*emb_rel_e0*, *emb_rel_e1*, *emb_rel_e2*, *emb_rel_e3*, *emb_rel_e4*, *emb_rel_e5*, *emb_rel_e6*, *emb_rel_e7*)

residual_convolution(*O_1*, *O_2*)

forward_triples(*x: torch.Tensor*) → torch.Tensor

Parameters
x –

forward_k_vs_all(*x: torch.Tensor*)

Given a head entity and a relation (h,r), we compute scores for all entities. [score(h,r,x)|x in Entities] => [0.0,0.1,…,0.8], shape=> (1, **|Entities|**) Given a batch of head entities and relations => shape (size of batch,| Entities|)

class dicee.**ConEx**(*args*)

Bases: *dicee.models.base_model.BaseKGE*

Convolutional ComplEx Knowledge Graph Embeddings

residual_convolution(*C_1: Tuple[torch.Tensor, torch.Tensor]*, *C_2: Tuple[torch.Tensor, torch.Tensor]*) → torch.FloatTensor

Compute residual score of two complex-valued embeddings. :param C_1: a tuple of two pytorch tensors that corresponds complex-valued embeddings :param C_2: a tuple of two pytorch tensors that corresponds complex-valued embeddings :return:

forward_k_vs_all(*x: torch.Tensor*) → torch.FloatTensor

forward_triples(*x: torch.Tensor*) → torch.FloatTensor

Parameters
x –

forward_k_vs_sample(*x: torch.Tensor*, *target_entity_idx: torch.Tensor*)

class dicee.**QMult**(*args*)

Bases: *dicee.models.base_model.BaseKGE*

Base class for all neural network modules.

Your models should also subclass this class.

Modules can also contain other Modules, allowing to nest them in a tree structure. You can assign the submodules as regular attributes:

```
import torch.nn as nn
import torch.nn.functional as F

class Model(nn.Module):
    def __init__(self):
        super().__init__()
```

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```
        self.conv1 = nn.Conv2d(1, 20, 5)
        self.conv2 = nn.Conv2d(20, 20, 5)

    def forward(self, x):
        x = F.relu(self.conv1(x))
        return F.relu(self.conv2(x))
```

Submodules assigned in this way will be registered, and will have their parameters converted too when you call `to()`, etc.

Note: As per the example above, an `__init__()` call to the parent class must be made before assignment on the child.

Variables

training (*bool*) – Boolean represents whether this module is in training or evaluation mode.

quaternion_multiplication_followed_by_inner_product (*h*, *r*, *t*)

Parameters

- **h** – shape: (**batch_dims*, dim) The head representations.
- **r** – shape: (**batch_dims*, dim) The head representations.
- **t** – shape: (**batch_dims*, dim) The tail representations.

Returns

Triple scores.

static quaternion_normalizer (*x: torch.FloatTensor*) → torch.FloatTensor

Normalize the length of relation vectors, if the forward constraint has not been applied yet.

Absolute value of a quaternion

$$|a + bi + cj + dk| = \sqrt{a^2 + b^2 + c^2 + d^2}$$

L2 norm of quaternion vector:

$$\|x\|^2 = \sum_{i=1}^{d} |x_i|^2 = \sum_{i=1}^{d} (x_i.re^2 + x_i.im_1^2 + x_i.im_2^2 + x_i.im_3^2)$$

Parameters

x – The vector.

Returns

The normalized vector.

score (*head_ent_emb: torch.FloatTensor*, *rel_ent_emb: torch.FloatTensor*, *tail_ent_emb: torch.FloatTensor*)

k_vs_all_score (*bpe_head_ent_emb*, *bpe_rel_ent_emb*, *E*)

Parameters

- **bpe_head_ent_emb** –
- **bpe_rel_ent_emb** –
- **E** –

forward_k_vs_all(*x*)

Parameters

x –

forward_k_vs_sample(*x*, *target_entity_idx*)

Completed. Given a head entity and a relation (h,r), we compute scores for all possible triples,i.e., [score(h,r,x)|x in Entities] => [0.0,0.1,…,0.8], shape=> (1, **|Entities|**) Given a batch of head entities and relations => shape (size of batch,| Entities|)

class dicee.**OMult**(*args*)

Bases: *dicee.models.base_model.BaseKGE*

Base class for all neural network modules.

Your models should also subclass this class.

Modules can also contain other Modules, allowing to nest them in a tree structure. You can assign the submodules as regular attributes:

```
import torch.nn as nn
import torch.nn.functional as F

class Model(nn.Module):
    def __init__(self):
        super().__init__()
        self.conv1 = nn.Conv2d(1, 20, 5)
        self.conv2 = nn.Conv2d(20, 20, 5)

    def forward(self, x):
        x = F.relu(self.conv1(x))
        return F.relu(self.conv2(x))
```

Submodules assigned in this way will be registered, and will have their parameters converted too when you call `to()`, etc.

Note: As per the example above, an `__init__()` call to the parent class must be made before assignment on the child.

Variables

training (*bool*) – Boolean represents whether this module is in training or evaluation mode.

static octonion_normalizer(*emb_rel_e0*, *emb_rel_e1*, *emb_rel_e2*, *emb_rel_e3*, *emb_rel_e4*, *emb_rel_e5*, *emb_rel_e6*, *emb_rel_e7*)

score(*head_ent_emb: torch.FloatTensor*, *rel_ent_emb: torch.FloatTensor*, *tail_ent_emb: torch.FloatTensor*)

k_vs_all_score(*bpe_head_ent_emb*, *bpe_rel_ent_emb*, *E*)

forward_k_vs_all(*x*)

Completed. Given a head entity and a relation (h,r), we compute scores for all possible triples,i.e., [score(h,r,x)|x in Entities] => [0.0,0.1,…,0.8], shape=> (1, **|Entities|**) Given a batch of head entities and relations => shape (size of batch,| Entities|)

class dicee.**Shallom**(*args*)

Bases: *dicee.models.base_model.BaseKGE*

A shallow neural model for relation prediction (https://arxiv.org/abs/2101.09090)

get_embeddings() → Tuple[numpy.ndarray, None]

forward_k_vs_all(*x*) → torch.FloatTensor

forward_triples(*x*) → torch.FloatTensor

Parameters

x –

Returns

class dicee.**LFMult**(*args*)

Bases: *dicee.models.base_model.BaseKGE*

Embedding with polynomial functions. We represent all entities and relations in the polynomial space as: f(x) = sum_{i=0}^{d-1} a_k x^{i%d} and use the three differents scoring function as in the paper to evaluate the score. We also consider combining with Neural Networks.

forward_triples(*idx_triple*)

Parameters

x –

construct_multi_coeff(*x*)

poly_NN(*x, coefh, coefr, coeft*)

Constructing a 2 layers NN to represent the embeddings. h = sigma(wh^T x + bh), r = sigma(wr^T x + br), t = sigma(wt^T x + bt)

linear(*x, w, b*)

scalar_batch_NN(*a, b, c*)

element wise multiplication between a,b and c: Inputs : a, b, c ====> torch.tensor of size batch_size x m x d Output : a tensor of size batch_size x d

tri_score(*coeff_h, coeff_r, coeff_t*)

this part implement the trilinear scoring techniques:

score(h,r,t) = int_{0}{1} h(x)r(x)t(x) dx = sum_{i,j,k = 0}^{d-1} dfrac{a_i*b_j*c_k}{1+(i+j+k)%d}

1. generate the range for i,j and k from [0 d-1]

2. perform dfrac{a_i*b_j*c_k}{1+(i+j+k)%d} in parallel for every batch

3. take the sum over each batch

vtp_score(*h, r, t*)

this part implement the vector triple product scoring techniques:

score(h,r,t) = int_{0}{1} h(x)r(x)t(x) dx = sum_{i,j,k = 0}^{d-1} dfrac{a_i*c_j*b_k - b_i*c_j*a_k}{(1+(i+j)%d)(1+k)}

1. generate the range for i,j and k from [0 d-1]

2. Compute the first and second terms of the sum

3. Multiply with then denominator and take the sum

4. take the sum over each batch

comp_func (*h*, *r*, *t*)

this part implement the function composition scoring techniques: i.e. score = <hor, t>

polynomial (*coeff*, *x*, *degree*)

This function takes a matrix tensor of coefficients (coeff), a tensor vector of points x and range of integer [0,1,…d] and return a vector tensor (coeff[0][0] + coeff[0][1]x +…+ coeff[0][d]x^d,

coeff[1][0] + coeff[1][1]x +…+ coeff[1][d]x^d)

pop (*coeff*, *x*, *degree*)

This function allow us to evaluate the composition of two polynomes without for loops :) it takes a matrix tensor of coefficients (coeff), a matrix tensor of points x and range of integer [0,1,…d]

and return a tensor (coeff[0][0] + coeff[0][1]x +…+ coeff[0][d]x^d,

coeff[1][0] + coeff[1][1]x +…+ coeff[1][d]x^d)

class dicee.**PykeenKGE** (*args: dict*)

Bases: `dicee.models.base_model.BaseKGE`

A class for using knowledge graph embedding models implemented in Pykeen

Notes: Pykeen_DistMult: C Pykeen_ComplEx: Pykeen_QuatE: Pykeen_MuRE: Pykeen_CP: Pykeen_HolE: Pykeen_HolE:

forward_k_vs_all (*x: torch.LongTensor*)

=> Explicit version by this we can apply bn and dropout

(1) Retrieve embeddings of heads and relations + apply Dropout & Normalization if given. h, r = self.get_head_relation_representation(x) # (2) Reshape (1). if self.last_dim > 0:

h = h.reshape(len(x), self.embedding_dim, self.last_dim) r = r.reshape(len(x), self.embedding_dim, self.last_dim)

(3) Reshape all entities. if self.last_dim > 0:

t = self.entity_embeddings.weight.reshape(self.num_entities, self.embedding_dim, self.last_dim)

else:

t = self.entity_embeddings.weight

(4) Call the score_t from interactions to generate triple scores. return self.interaction.score_t(h=h, r=r, all_entities=t, slice_size=1)

forward_triples (*x: torch.LongTensor*) → torch.FloatTensor

=> Explicit version by this we can apply bn and dropout

(1) Retrieve embeddings of heads, relations and tails and apply Dropout & Normalization if given. h, r, t = self.get_triple_representation(x) # (2) Reshape (1). if self.last_dim > 0:

h = h.reshape(len(x), self.embedding_dim, self.last_dim) r = r.reshape(len(x), self.embedding_dim, self.last_dim) t = t.reshape(len(x), self.embedding_dim, self.last_dim)

(3) Compute the triple score return self.interaction.score(h=h, r=r, t=t, slice_size=None, slice_dim=0)

abstract forward_k_vs_sample (*x: torch.LongTensor*, *target_entity_idx*)

class dicee.**BytE** (**args*, ***kwargs*)

Bases: `dicee.models.base_model.BaseKGE`

Base class for all neural network modules.

Your models should also subclass this class.

Modules can also contain other Modules, allowing to nest them in a tree structure. You can assign the submodules as regular attributes:

```
import torch.nn as nn
import torch.nn.functional as F

class Model(nn.Module):
    def __init__(self):
        super().__init__()
        self.conv1 = nn.Conv2d(1, 20, 5)
        self.conv2 = nn.Conv2d(20, 20, 5)

    def forward(self, x):
        x = F.relu(self.conv1(x))
        return F.relu(self.conv2(x))
```

Submodules assigned in this way will be registered, and will have their parameters converted too when you call `to()`, etc.

Note: As per the example above, an `__init__()` call to the parent class must be made before assignment on the child.

Variables

training (*bool*) – Boolean represents whether this module is in training or evaluation mode.

loss_function (*yhat_batch*, *y_batch*)

Parameters

- **yhat_batch** –
- **y_batch** –

forward (*x: torch.LongTensor*)

Parameters

x (*B by T tensor*) –

generate (*idx*, *max_new_tokens*, *temperature=1.0*, *top_k=None*)

Take a conditioning sequence of indices idx (LongTensor of shape (b,t)) and complete the sequence max_new_tokens times, feeding the predictions back into the model each time. Most likely you'll want to make sure to be in model.eval() mode of operation for this.

training_step (*batch*, *batch_idx=None*)

Here you compute and return the training loss and some additional metrics for e.g. the progress bar or logger.

Parameters

- **batch** – The output of your data iterable, normally a `DataLoader`.
- **batch_idx** – The index of this batch.
- **dataloader_idx** – The index of the dataloader that produced this batch. (only if multiple dataloaders used)

Returns

- `Tensor` - The loss tensor

- dict - A dictionary which can include any keys, but must include the key 'loss' in the case of automatic optimization.
- None - In automatic optimization, this will skip to the next batch (but is not supported for multi-GPU, TPU, or DeepSpeed). For manual optimization, this has no special meaning, as returning the loss is not required.

In this step you'd normally do the forward pass and calculate the loss for a batch. You can also do fancier things like multiple forward passes or something model specific.

Example:

```
def training_step(self, batch, batch_idx):
    x, y, z = batch
    out = self.encoder(x)
    loss = self.loss(out, x)
    return loss
```

To use multiple optimizers, you can switch to 'manual optimization' and control their stepping:

```
def __init__(self):
    super().__init__()
    self.automatic_optimization = False


# Multiple optimizers (e.g.: GANs)
def training_step(self, batch, batch_idx):
    opt1, opt2 = self.optimizers()

    # do training_step with encoder
    ...
    opt1.step()
    # do training_step with decoder
    ...
    opt2.step()
```

Note: When accumulate_grad_batches > 1, the loss returned here will be automatically normalized by accumulate_grad_batches internally.

class dicee.**BaseKGE**(*args: dict*)

Bases: BaseKGELightning

Base class for all neural network modules.

Your models should also subclass this class.

Modules can also contain other Modules, allowing to nest them in a tree structure. You can assign the submodules as regular attributes:

```
import torch.nn as nn
import torch.nn.functional as F

class Model(nn.Module):
    def __init__(self):
        super().__init__()
        self.conv1 = nn.Conv2d(1, 20, 5)
        self.conv2 = nn.Conv2d(20, 20, 5)
```

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```
    def forward(self, x):
        x = F.relu(self.conv1(x))
        return F.relu(self.conv2(x))
```

Submodules assigned in this way will be registered, and will have their parameters converted too when you call `to()`, etc.

Note: As per the example above, an `__init__()` call to the parent class must be made before assignment on the child.

Variables

training (*bool*) – Boolean represents whether this module is in training or evaluation mode.

forward_byte_pair_encoded_k_vs_all (*x: torch.LongTensor*)

Parameters

x (*B x 2 x T*) –

forward_byte_pair_encoded_triple (*x: Tuple[torch.LongTensor, torch.LongTensor]*)

byte pair encoded neural link predictors

Parameters

-------- –

init_params_with_sanity_checking ()

forward (*x: torch.LongTensor | Tuple[torch.LongTensor, torch.LongTensor], y_idx: torch.LongTensor = None*)

Parameters

- **x** –
- **y_idx** –
- **ordered_bpe_entities** –

forward_triples (*x: torch.LongTensor*) → torch.Tensor

Parameters

x –

forward_k_vs_all (**args, **kwargs*)

forward_k_vs_sample (**args, **kwargs*)

get_triple_representation (*idx_hrt*)

get_head_relation_representation (*indexed_triple*)

get_sentence_representation (*x: torch.LongTensor*)

Parameters

- **(b** (*x shape*) –
- **3** –

- **t)** –

get_bpe_head_and_relation_representation(*x: torch.LongTensor*)
→ Tuple[torch.FloatTensor, torch.FloatTensor]

Parameters
x (`B x 2 x T`) –

get_embeddings() → Tuple[numpy.ndarray, numpy.ndarray]

dicee.**create_recipriocal_triples**(*x*)

Add inverse triples into dask dataframe :param x: :return:

dicee.**get_er_vocab**(*data*, *file_path: str = None*)

dicee.**get_re_vocab**(*data*, *file_path: str = None*)

dicee.**get_ee_vocab**(*data*, *file_path: str = None*)

dicee.**timeit**(*func*)

dicee.**save_pickle**(*, *data: object = None*, *file_path=str*)

dicee.**load_pickle**(*file_path=str*)

dicee.**select_model**(*args: dict*, *is_continual_training: bool = None*, *storage_path: str = None*)

dicee.**load_model**(*path_of_experiment_folder: str*, *model_name='model.pt'*, *verbose=0*)
→ Tuple[object, Tuple[dict, dict]]

Load weights and initialize pytorch module from namespace arguments

dicee.**load_model_ensemble**(*path_of_experiment_folder: str*)
→ Tuple[*dicee.models.base_model.BaseKGE*, Tuple[pandas.DataFrame, pandas.DataFrame]]

Construct Ensemble Of weights and initialize pytorch module from namespace arguments

(1) Detect models under given path

(2) Accumulate parameters of detected models

(3) Normalize parameters

(4) Insert (3) into model.

dicee.**save_numpy_ndarray**(*, *data: numpy.ndarray*, *file_path: str*)

dicee.**numpy_data_type_changer**(*train_set: numpy.ndarray*, *num: int*) → numpy.ndarray

Detect most efficient data type for a given triples :param train_set: :param num: :return:

dicee.**save_checkpoint_model**(*model*, *path: str*) → None

Store Pytorch model into disk

dicee.**store**(*trainer*, *trained_model*, *model_name: str = 'model'*, *full_storage_path: str = None*, *save_embeddings_as_csv=False*) → None

Store trained_model model and save embeddings into csv file. :param trainer: an instance of trainer class :param full_storage_path: path to save parameters. :param model_name: string representation of the name of the model. :param trained_model: an instance of BaseKGE see core.models.base_model . :param save_embeddings_as_csv: for easy access of embeddings. :return:

dicee.**add_noisy_triples**(*train_set: pandas.DataFrame*, *add_noise_rate: float*) → pandas.DataFrame

Add randomly constructed triples :param train_set: :param add_noise_rate: :return:

dicee.**read_or_load_kg**(*args*, *cls*)

dicee.**intialize_model**(*args: dict*, *verbose=0*) → Tuple[object, str]

dicee.**load_json**(*p: str*) → dict

dicee.**save_embeddings**(*embeddings: numpy.ndarray*, *indexes*, *path: str*) → None

Save it as CSV if memory allows. :param embeddings: :param indexes: :param path: :return:

dicee.**random_prediction**(*pre_trained_kge*)

dicee.**deploy_triple_prediction**(*pre_trained_kge*, *str_subject*, *str_predicate*, *str_object*)

dicee.**deploy_tail_entity_prediction**(*pre_trained_kge*, *str_subject*, *str_predicate*, *top_k*)

dicee.**deploy_head_entity_prediction**(*pre_trained_kge*, *str_object*, *str_predicate*, *top_k*)

dicee.**deploy_relation_prediction**(*pre_trained_kge*, *str_subject*, *str_object*, *top_k*)

dicee.**vocab_to_parquet**(*vocab_to_idx*, *name*, *path_for_serialization*, *print_into*)

dicee.**create_experiment_folder**(*folder_name='Experiments'*)

dicee.**continual_training_setup_executor**(*executor*) → None

storage_path:str A path leading to a parent directory, where a subdirectory containing KGE related data

full_storage_path:str A path leading to a subdirectory containing KGE related data

dicee.**exponential_function**(*x: numpy.ndarray*, *lam: float*, *ascending_order=True*)
→ torch.FloatTensor

dicee.**load_numpy**(*path*) → numpy.ndarray

dicee.**evaluate**(*entity_to_idx*, *scores*, *easy_answers*, *hard_answers*)

@TODO: CD: Renamed this function Evaluate multi hop query answering on different query types

dicee.**download_file**(*url*, *destination_folder='.'*)

dicee.**download_files_from_url**(*base_url*, *destination_folder='.'*)

dicee.**download_pretrained_model**(*url: str*) → str

class dicee.**DICE_Trainer**(*args*, *is_continual_training*, *storage_path*, *evaluator=None*)

DICE_Trainer implement

1- Pytorch Lightning trainer (https://pytorch-lightning.readthedocs.io/en/stable/common/trainer.html) 2- Multi-GPU Trainer(https://pytorch.org/docs/stable/generated/torch.nn.parallel.DistributedDataParallel.html) 3- CPU Trainer

args

is_continual_training:bool

storage_path:str

evaluator:

report:dict

continual_start()

(1) Initialize training.

(2) Load model

(3) Load trainer (3) Fit model

Parameter

returns

- *model*
- **form_of_labelling** (*str*)

initialize_trainer(*callbacks: List*) → lightning.Trainer

Initialize Trainer from input arguments

initialize_or_load_model()

initialize_dataloader(*dataset: torch.utils.data.Dataset*) → torch.utils.data.DataLoader

initialize_dataset(*dataset: dicee.knowledge_graph.KG*, *form_of_labelling*) → torch.utils.data.Dataset

start(*knowledge_graph: dicee.knowledge_graph.KG*) → Tuple[*dicee.models.base_model.BaseKGE*, str]

Train selected model via the selected training strategy

k_fold_cross_validation(*dataset*) → Tuple[*dicee.models.base_model.BaseKGE*, str]

Perform K-fold Cross-Validation

1. Obtain K train and test splits.
2. **For each split,**
   2.1 initialize trainer and model 2.2. Train model with configuration provided in args. 2.3. Compute the mean reciprocal rank (MRR) score of the model on the test respective split.
3. Report the mean and average MRR .

Parameters

- **self** –
- **dataset** –

Returns
model

class dicee.**KGE**(*path=None*, *url=None*, *construct_ensemble=False*, *model_name=None*, *apply_semantic_constraint=False*)

Bases: *dicee.abstracts.BaseInteractiveKGE*

Knowledge Graph Embedding Class for interactive usage of pre-trained models

get_transductive_entity_embeddings(*indices: torch.LongTensor | List[str]*, *as_pytorch=False*, *as_numpy=False*, *as_list=True*) → torch.FloatTensor | numpy.ndarray | List[float]

create_vector_database(*collection_name: str*, *distance: str*, *location: str = 'localhost'*, *port: int = 6333*)

generate(*h=''*, *r=''*)

__str__()

Return str(self).

eval_lp_performance(*dataset=List[Tuple[str, str, str]]*, *filtered=True*)

predict_missing_head_entity(*relation: List[str] | str*, *tail_entity: List[str] | str*, *within=None*) → Tuple

Given a relation and a tail entity, return top k ranked head entity.

argmax_{e in E } f(e,r,t), where r in R, t in E.

Parameter

relation: Union[List[str], str]

String representation of selected relations.

tail_entity: Union[List[str], str]

String representation of selected entities.

k: int

Highest ranked k entities.

Returns: Tuple

Highest K scores and entities

predict_missing_relations(*head_entity: List[str] | str*, *tail_entity: List[str] | str*, *within=None*) → Tuple

Given a head entity and a tail entity, return top k ranked relations.

argmax_{r in R } f(h,r,t), where h, t in E.

Parameter

head_entity: List[str]

String representation of selected entities.

tail_entity: List[str]

String representation of selected entities.

k: int

Highest ranked k entities.

Returns: Tuple

Highest K scores and entities

predict_missing_tail_entity(*head_entity: List[str] | str*, *relation: List[str] | str*, *within: List[str] = None*) → torch.FloatTensor

Given a head entity and a relation, return top k ranked entities

argmax_{e in E } f(h,r,e), where h in E and r in R.

Parameter

head_entity: List[str]

String representation of selected entities.

tail_entity: List[str]

String representation of selected entities.

Returns: Tuple

scores

predict(*, *h: List[str] | str = None*, *r: List[str] | str = None*, *t: List[str] | str = None*, *within=None*, *logits=True*) → torch.FloatTensor

Parameters

- **logits** –
- **h** –
- **r** –
- **t** –
- **within** –

predict_topk(*, *h: List[str] = None*, *r: List[str] = None*, *t: List[str] = None*, *topk: int = 10*, *within: List[str] = None*)

Predict missing item in a given triple.

Parameter

head_entity: List[str]

String representation of selected entities.

relation: List[str]

String representation of selected relations.

tail_entity: List[str]

String representation of selected entities.

k: int

Highest ranked k item.

Returns: Tuple

Highest K scores and items

triple_score (*h: List[str] | str = None*, *r: List[str] | str = None*, *t: List[str] | str = None*, *logits=False*) → torch.FloatTensor

Predict triple score

Parameter

head_entity: List[str]

String representation of selected entities.

relation: List[str]

String representation of selected relations.

tail_entity: List[str]

String representation of selected entities.

logits: bool

If logits is True, unnormalized score returned

Returns: Tuple

pytorch tensor of triple score

t_norm (*tens_1: torch.Tensor*, *tens_2: torch.Tensor*, *tnorm: str = 'min'*) → torch.Tensor

tensor_t_norm (*subquery_scores: torch.FloatTensor*, *tnorm: str = 'min'*) → torch.FloatTensor

Compute T-norm over [0,1] ^{n imes d} where n denotes the number of hops and d denotes number of entities

t_conorm (*tens_1: torch.Tensor*, *tens_2: torch.Tensor*, *tconorm: str = 'min'*) → torch.Tensor

negnorm (*tens_1: torch.Tensor*, *lambda_: float*, *neg_norm: str = 'standard'*) → torch.Tensor

return_multi_hop_query_results (*aggregated_query_for_all_entities*, *k: int*, *only_scores*)

single_hop_query_answering (*query: tuple*, *only_scores: bool = True*, *k: int = None*)

answer_multi_hop_query (*query_type: str = None*, *query: Tuple[str | Tuple[str, str], Ellipsis] = None*, *queries: List[Tuple[str | Tuple[str, str], Ellipsis]] = None*, *tnorm: str = 'prod'*, *neg_norm: str = 'standard'*, *lambda_: float = 0.0*, *k: int = 10*, *only_scores=False*) → List[Tuple[str, torch.Tensor]]

@TODO: Refactoring is needed # @TODO: Score computation for each query type should be done in a static function

Find an answer set for EPFO queries including negation and disjunction

Parameter

query_type: str The type of the query, e.g., "2p".

query: Union[str, Tuple[str, Tuple[str, str]]] The query itself, either a string or a nested tuple.

queries: List of Tuple[Union[str, Tuple[str, str]], ...]

tnorm: str The t-norm operator.

neg_norm: str The negation norm.

lambda_: float lambda parameter for sugeno and yager negation norms

k: int The top-k substitutions for intermediate variables.

returns

- *List[Tuple[str, torch.Tensor]]*
- *Entities and corresponding scores sorted in the descening order of scores*

find_missing_triples (*confidence: float*, *entities: List[str] = None*, *relations: List[str] = None*, *topk: int = 10*, *at_most: int = sys.maxsize*) → Set

Find missing triples

Iterative over a set of entities E and a set of relation R :

orall e in E and orall r in R f(e,r,x)

Return (e,r,x)

otin G and f(e,r,x) > confidence

confidence: float

A threshold for an output of a sigmoid function given a triple.

topk: int

Highest ranked k item to select triples with f(e,r,x) > confidence .

at_most: int

Stop after finding at_most missing triples

{(e,r,x) | f(e,r,x) > confidence land (e,r,x)

otin G

deploy (*share: bool = False*, *top_k: int = 10*)

train_triples (*h: List[str]*, *r: List[str]*, *t: List[str]*, *labels: List[float]*, *iteration=2*, *optimizer=None*)

train_k_vs_all (*h*, *r*, *iteration=1*, *lr=0.001*)

Train k vs all :param head_entity: :param relation: :param iteration: :param lr: :return:

train (*kg*, *lr=0.1*, *epoch=10*, *batch_size=32*, *neg_sample_ratio=10*, *num_workers=1*) → None

Retrained a pretrain model on an input KG via negative sampling.

class dicee.**Execute** (*args*, *continuous_training=False*)

A class for Training, Retraining and Evaluation a model.

(1) Loading & Preprocessing & Serializing input data.

(2) Training & Validation & Testing

(3) Storing all necessary info

read_or_load_kg()

read_preprocess_index_serialize_data() → None

Read & Preprocess & Index & Serialize Input Data

(1) Read or load the data from disk into memory.

(2) Store the statistics of the data.

Parameter

rtype

None

load_indexed_data() → None

Load the indexed data from disk into memory

Parameter

rtype

None

save_trained_model() → None

Save a knowledge graph embedding model

(1) Send model to eval mode and cpu.

(2) Store the memory footprint of the model.

(3) Save the model into disk.

(4) Update the stats of KG again ?

Parameter

rtype

None

end(*form_of_labelling: str*) → dict

End training

(1) Store trained model.

(2) Report runtimes.

(3) Eval model if required.

Parameter

rtype
A dict containing information about the training and/or evaluation

write_report() → None

Report training related information in a report.json file

start() → dict

Start training

(1) Loading the Data # (2) Create an evaluator object. # (3) Create a trainer object. # (4) Start the training

Parameter

rtype
A dict containing information about the training and/or evaluation

`dicee.`**mapping_from_first_two_cols_to_third**(*train_set_idx*)

`dicee.`**timeit**(*func*)

`dicee.`**load_pickle**(*file_path=str*)

`dicee.`**reload_dataset**(*path: str*, *form_of_labelling*, *scoring_technique*, *neg_ratio*, *label_smoothing_rate*)

Reload the files from disk to construct the Pytorch dataset

`dicee.`**construct_dataset**(*, *train_set: numpy.ndarray | list*, *valid_set=None*, *test_set=None*, *ordered_bpe_entities=None*, *train_target_indices=None*, *target_dim: int = None*, *entity_to_idx: dict*, *relation_to_idx: dict*, *form_of_labelling: str*, *scoring_technique: str*, *neg_ratio: int*, *label_smoothing_rate: float*, *byte_pair_encoding=None*, *block_size: int = None*) → torch.utils.data.Dataset

class `dicee.`**BPE_NegativeSamplingDataset**(*train_set: torch.LongTensor*, *ordered_shaped_bpe_entities: torch.LongTensor*, *neg_ratio: int*)

Bases: `torch.utils.data.Dataset`

An abstract class representing a `Dataset`.

All datasets that represent a map from keys to data samples should subclass it. All subclasses should overwrite `__getitem__()`, supporting fetching a data sample for a given key. Subclasses could also optionally overwrite `__len__()`, which is expected to return the size of the dataset by many `Sampler` implementations and the default options of `DataLoader`. Subclasses could also optionally implement `__getitems__()`, for speedup batched samples loading. This method accepts list of indices of samples of batch and returns list of samples.

Note: `DataLoader` by default constructs an index sampler that yields integral indices. To make it work with a map-style dataset with non-integral indices/keys, a custom sampler must be provided.

__len__()

__getitem__(*idx*)

collate_fn(*batch_shaped_bpe_triples: List[Tuple[torch.Tensor, torch.Tensor]]*)

class dicee.**MultiLabelDataset**(*train_set: torch.LongTensor*, *train_indices_target: torch.LongTensor*, *target_dim: int*, *torch_ordered_shaped_bpe_entities: torch.LongTensor*)

Bases: `torch.utils.data.Dataset`

An abstract class representing a `Dataset`.

All datasets that represent a map from keys to data samples should subclass it. All subclasses should overwrite `__getitem__()`, supporting fetching a data sample for a given key. Subclasses could also optionally overwrite `__len__()`, which is expected to return the size of the dataset by many `Sampler` implementations and the default options of `DataLoader`. Subclasses could also optionally implement `__getitems__()`, for speedup batched samples loading. This method accepts list of indices of samples of batch and returns list of samples.

Note: `DataLoader` by default constructs an index sampler that yields integral indices. To make it work with a map-style dataset with non-integral indices/keys, a custom sampler must be provided.

__len__()

__getitem__(*idx*)

class dicee.**MultiClassClassificationDataset**(*subword_units: numpy.ndarray*, *block_size: int = 8*)

Bases: `torch.utils.data.Dataset`

Dataset for the 1vsALL training strategy

Parameters

- **train_set_idx** – Indexed triples for the training.
- **entity_idxs** – mapping.
- **relation_idxs** – mapping.
- **form** – ?
- **num_workers** – int for https://pytorch.org/docs/stable/data.html#torch.utils.data.DataLoader

Return type

torch.utils.data.Dataset

__len__()

__getitem__(*idx*)

class dicee.**OnevsAllDataset**(*train_set_idx: numpy.ndarray*, *entity_idxs*)

Bases: `torch.utils.data.Dataset`

Dataset for the 1vsALL training strategy

Parameters

- **train_set_idx** – Indexed triples for the training.
- **entity_idxs** – mapping.
- **relation_idxs** – mapping.
- **form** – ?
- **num_workers** – int for https://pytorch.org/docs/stable/data.html#torch.utils.data.DataLoader

Return type
torch.utils.data.Dataset

__len__()

__getitem__(*idx*)

class dicee.**KvsAll**(*train_set_idx: numpy.ndarray*, *entity_idxs*, *relation_idxs*, *form*, *store=None*, *label_smoothing_rate: float = 0.0*)

Bases: `torch.utils.data.Dataset`

Creates a dataset for KvsAll training by inheriting from torch.utils.data.Dataset.
Let D denote a dataset for KvsAll training and be defined as D:= {(x,y)_i}_i ^N, where x: (h,r) is an unique tuple of an entity h in E and a relation r in R that has been seed in the input graph. y: denotes a multi-label vector in [0,1]^{**|E|**} is a binary label.

orall y_i =1 s.t. (h r E_i) in KG

Note: TODO

---

train_set_idx
[numpy.ndarray] n by 3 array representing n triples

entity_idxs
[dictonary] string representation of an entity to its integer id

relation_idxs
[dictonary] string representation of a relation to its integer id

self : torch.utils.data.Dataset

```
>>> a = KvsAll()
>>> a
? array([0, 1, 2, 3, 4, 5, 6, 7, 8, 9])
```

__len__()

__getitem__(*idx*)

class dicee.**AllvsAll**(*train_set_idx: numpy.ndarray*, *entity_idxs*, *relation_idxs*, *label_smoothing_rate=0.0*)

Bases: `torch.utils.data.Dataset`

Creates a dataset for AllvsAll training by inheriting from torch.utils.data.Dataset.
Let D denote a dataset for AllvsAll training and be defined as D:= {(x,y)_i}_i ^N, where x: (h,r) is a possible unique tuple of an entity h in E and a relation r in R. Hence N = **|E|** x **|R|** y: denotes a multi-label vector in [0,1]^{**|E|**} is a binary label.

orall y_i =1 s.t. (h r E_i) in KG

Note:

AllvsAll extends KvsAll via none existing (h,r). Hence, it adds data points that are labelled without 1s,
only with 0s.

---

train_set_idx
[numpy.ndarray] n by 3 array representing n triples

entity_idxs
[dictonary] string representation of an entity to its integer id

relation_idxs
[dictonary] string representation of a relation to its integer id

self : torch.utils.data.Dataset

```
>>> a = AllvsAll()
>>> a
? array([0, 1, 2, 3, 4, 5, 6, 7, 8, 9])
```

__len__()

__getitem__(*idx*)

class dicee.**KvsSampleDataset**(*train_set: numpy.ndarray*, *num_entities*, *num_relations*, *neg_sample_ratio: int = None*, *label_smoothing_rate: float = 0.0*)

Bases: torch.utils.data.Dataset

KvsSample a Dataset:

D:= {(x,y)_i}_i ^N, where
. x:(h,r) is a unique h in E and a relation r in R and . y in [0,1]^{|E|} is a binary label.

orall y_i =1 s.t. (h r E_i) in KG

At each mini-batch construction, we subsample(y), hence n
|new_y| << |E| new_y contains all 1's if sum(y)< neg_sample ratio new_y contains

train_set_idx
Indexed triples for the training.

entity_idxs
mapping.

relation_idxs
mapping.

form
?

store
?

label_smoothing_rate
?

torch.utils.data.Dataset

__len__()

__getitem__(*idx*)

class dicee.**NegSampleDataset**(*train_set: numpy.ndarray*, *num_entities: int*, *num_relations: int*, *neg_sample_ratio: int = 1*)

Bases: `torch.utils.data.Dataset`

An abstract class representing a `Dataset`.

All datasets that represent a map from keys to data samples should subclass it. All subclasses should overwrite `__getitem__()`, supporting fetching a data sample for a given key. Subclasses could also optionally overwrite `__len__()`, which is expected to return the size of the dataset by many `Sampler` implementations and the default options of `DataLoader`. Subclasses could also optionally implement `__getitems__()`, for speedup batched samples loading. This method accepts list of indices of samples of batch and returns list of samples.

Note: `DataLoader` by default constructs an index sampler that yields integral indices. To make it work with a map-style dataset with non-integral indices/keys, a custom sampler must be provided.

__len__()

__getitem__(*idx*)

class dicee.**TriplePredictionDataset**(*train_set: numpy.ndarray*, *num_entities: int*, *num_relations: int*, *neg_sample_ratio: int = 1*, *label_smoothing_rate: float = 0.0*)

Bases: `torch.utils.data.Dataset`

Triple Dataset

D:= {(x)_i}_i ^N, where

. x:(h,r, t) in KG is a unique h in E and a relation r in R and . collact_fn => Generates negative triples

collect_fn:

orall (h,r,t) in G obtain, create negative triples{(h,r,x),(,r,t),(h,m,t)}

y:labels are represented in torch.float16

train_set_idx
Indexed triples for the training.

entity_idxs
mapping.

relation_idxs
mapping.

form
?

store
?

label_smoothing_rate

collate_fn: batch:List[torch.IntTensor] Returns ——- torch.utils.data.Dataset

__len__()

__getitem__(*idx*)

collate_fn(*batch: List[torch.Tensor]*)

class dicee.**CVDataModule**(*train_set_idx: numpy.ndarray*, *num_entities*, *num_relations*, *neg_sample_ratio*, *batch_size*, *num_workers*)

Bases: `pytorch_lightning.LightningDataModule`

Create a Dataset for cross validation

Parameters

- **train_set_idx** – Indexed triples for the training.
- **num_entities** – entity to index mapping.
- **num_relations** – relation to index mapping.
- **batch_size** – int
- **form** – ?
- **num_workers** – int for https://pytorch.org/docs/stable/data.html#torch.utils.data.DataLoader

Return type

?

train_dataloader() → torch.utils.data.DataLoader

An iterable or collection of iterables specifying training samples.

For more information about multiple dataloaders, see this section.

The dataloader you return will not be reloaded unless you set **:paramref:`~pytorch_lightning.trainer.trainer.Trainer.reload_dataloaders_every_n_epochs`** to a positive integer.

For data processing use the following pattern:

- download in *prepare_data()*
- process and split in *setup()*

However, the above are only necessary for distributed processing.

Warning: do not assign state in prepare_data

- `fit()`
- *prepare_data()*
- *setup()*

Note: Lightning tries to add the correct sampler for distributed and arbitrary hardware. There is no need to set it yourself.

setup(**args*, ***kwargs*)

Called at the beginning of fit (train + validate), validate, test, or predict. This is a good hook when you need to build models dynamically or adjust something about them. This hook is called on every process when using DDP.

Parameters

stage – either `'fit'`, `'validate'`, `'test'`, or `'predict'`

Example:

```
class LitModel(...):
    def __init__(self):
        self.l1 = None

    def prepare_data(self):
        download_data()
        tokenize()

        # don't do this
        self.something = else

    def setup(self, stage):
        data = load_data(...)
        self.l1 = nn.Linear(28, data.num_classes)
```

transfer_batch_to_device (**args*, ***kwargs*)

Override this hook if your `DataLoader` returns tensors wrapped in a custom data structure.

The data types listed below (and any arbitrary nesting of them) are supported out of the box:

- `torch.Tensor` or anything that implements *.to(…)*
- `list`
- `dict`
- `tuple`

For anything else, you need to define how the data is moved to the target device (CPU, GPU, TPU, …).

Note: This hook should only transfer the data and not modify it, nor should it move the data to any other device than the one passed in as argument (unless you know what you are doing). To check the current state of execution of this hook you can use `self.trainer.training/testing/validating/predicting` so that you can add different logic as per your requirement.

Parameters

- **batch** – A batch of data that needs to be transferred to a new device.
- **device** – The target device as defined in PyTorch.
- **dataloader_idx** – The index of the dataloader to which the batch belongs.

Returns

A reference to the data on the new device.

Example:

```
def transfer_batch_to_device(self, batch, device, dataloader_idx):
    if isinstance(batch, CustomBatch):
        # move all tensors in your custom data structure to the device
        batch.samples = batch.samples.to(device)
        batch.targets = batch.targets.to(device)
    elif dataloader_idx == 0:
        # skip device transfer for the first dataloader or anything you wish
        pass
    else:
```

(continues on next page)

```
        batch = super().transfer_batch_to_device(batch, device, dataloader_
↪idx)
    return batch
```

Raises

MisconfigurationException – If using IPUs, `Trainer(accelerator='ipu')`.

See also:

- `move_data_to_device()`
- `apply_to_collection()`

prepare_data(**args*, ***kwargs*)

Use this to download and prepare data. Downloading and saving data with multiple processes (distributed settings) will result in corrupted data. Lightning ensures this method is called only within a single process, so you can safely add your downloading logic within.

> **Warning:** DO NOT set state to the model (use `setup` instead) since this is NOT called on every device

Example:

```
def prepare_data(self):
    # good
    download_data()
    tokenize()
    etc()

    # bad
    self.split = data_split
    self.some_state = some_other_state()
```

In a distributed environment, `prepare_data` can be called in two ways (using prepare_data_per_node)

1. Once per node. This is the default and is only called on LOCAL_RANK=0.
2. Once in total. Only called on GLOBAL_RANK=0.

Example:

```
# DEFAULT
# called once per node on LOCAL_RANK=0 of that node
class LitDataModule(LightningDataModule):
    def __init__(self):
        super().__init__()
        self.prepare_data_per_node = True


# call on GLOBAL_RANK=0 (great for shared file systems)
class LitDataModule(LightningDataModule):
    def __init__(self):
        super().__init__()
        self.prepare_data_per_node = False
```

This is called before requesting the dataloaders:

```
model.prepare_data()
initialize_distributed()
model.setup(stage)
model.train_dataloader()
model.val_dataloader()
model.test_dataloader()
model.predict_dataloader()
```

class dicee.**QueryGenerator**(*train_path*, *val_path: str*, *test_path: str*, *ent2id: Dict = None*, *rel2id: Dict = None*, *seed: int = 1*, *gen_valid: bool = False*, *gen_test: bool = True*)

list2tuple(*list_data*)

tuple2list(*x: List | Tuple*) → List | Tuple

Convert a nested tuple to a nested list.

set_global_seed(*seed: int*)

Set seed

construct_graph(*paths: List[str]*) → Tuple[Dict, Dict]

Construct graph from triples Returns dicts with incoming and outgoing edges

fill_query(*query_structure: List[str | List]*, *ent_in: Dict*, *ent_out: Dict*, *answer: int*) → bool

Private method for fill_query logic.

achieve_answer(*query: List[str | List]*, *ent_in: Dict*, *ent_out: Dict*) → set

Private method for achieve_answer logic. @TODO: Document the code

write_links(*ent_out*, *small_ent_out*)

ground_queries(*query_structure: List[str | List]*, *ent_in: Dict*, *ent_out: Dict*, *small_ent_in: Dict*, *small_ent_out: Dict*, *gen_num: int*, *query_name: str*)

Generating queries and achieving answers

unmap(*query_type*, *queries*, *tp_answers*, *fp_answers*, *fn_answers*)

unmap_query(*query_structure*, *query*, *id2ent*, *id2rel*)

generate_queries(*query_struct: List*, *gen_num: int*, *query_type: str*)

Passing incoming and outgoing edges to ground queries depending on mode [train valid or text] and getting queries and answers in return @ TODO: create a class for each single query struct

save_queries(*query_type: str*, *gen_num: int*, *save_path: str*)

abstract load_queries(*path*)

get_queries(*query_type: str*, *gen_num: int*)

static save_queries_and_answers(*path: str*, *data: List[Tuple[str, Tuple[collections.defaultdict]]]*) → None

Save Queries into Disk

static load_queries_and_answers(*path: str*) → List[Tuple[str, Tuple[collections.defaultdict]]]

Load Queries from Disk to Memory

dicee.**__version__ = '0.1.4'**

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