# 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

**Publisher and maintainer:** Caglar Demir[2]

**Contact**: caglar.demir@upb.de

**License:** OSI Approved :: MIT License

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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
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
```

## 12 Coverage Report

The coverage report is generated using coverage.py[12]:

```
Name                                                    Stmts   Miss  Cover   Missing
-------------------------------------------------------------------------------------
dicee/__init__.py                                           7      0   100%
dicee/abstracts.py                                        201     82    59%   104-105,␣
```

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[11] https://files.dice-research.org/projects/DiceEmbeddings/
[12] https://coverage.readthedocs.io/en/7.6.0/

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```
↪123, 146-147, 152, 165, 197, 240-254, 257-260, 263-266, 301, 314-317, 320-324, 364-
↪375, 390-398, 413, 424-428, 555-575, 581-585, 589-591
dicee/callbacks.py                                    245    102    58%   50-55,␣
↪67-73, 76, 88-93, 98-103, 106-109, 116-133, 138-142, 146-147, 276-280, 286-287, 305-
↪311, 314, 319-320, 332-338, 344-353, 358-360, 405, 416-429, 433-468, 480-486
dicee/config.py                                        93      2    98%   141-142
dicee/dataset_classes.py                              299     74    75%   41, 54,␣
↪87, 93, 99-106, 109, 112, 115-139, 195-201, 204, 207-209, 314, 325-328, 344, 410-
↪411, 429, 528-536, 539, 543-557, 700-707, 710-714
dicee/eval_static_funcs.py                            227     95    58%   101, 106,
↪ 111, 258-353, 360-411
dicee/evaluator.py                                    262     51    81%   46, 51,␣
↪56, 84, 89-90, 93, 109, 126, 137, 141, 146, 177-188, 195-206, 314, 344-367, 455,␣
↪465, 482-487
dicee/executer.py                                     113      4    96%   116, 258-
↪259, 291
dicee/knowledge_graph.py                               65      3    95%   79, 110,␣
↪114
dicee/knowledge_graph_embeddings.py                   636    443    30%   27, 30-
↪31, 39-52, 57-90, 93-127, 131-139, 170-184, 215-228, 254-274, 324-327, 330-333, 346,
↪ 381-426, 484-486, 502-503, 509-517, 522-525, 528-533, 538, 547, 592-598, 630, 688-
↪1053, 1084-1145, 1149-1177, 1200, 1227-1265
dicee/models/__init__.py                               9      0   100%
dicee/models/base_model.py                            234     31    87%   54, 56,␣
↪82, 88-103, 157, 190, 230, 236, 245, 248, 252, 259, 263, 265, 280, 288-289, 296-297,
↪ 351, 354, 427, 439
dicee/models/clifford.py                              556    357    36%   31-42,␣
↪68-117, 122-133, 156-168, 190-220, 235, 237, 241, 248-249, 276-280, 303-311, 325-
↪327, 332-333, 364-384, 406, 413, 417-478, 495-499, 511, 514, 519, 524, 571-607, 625-
↪631, 644, 647, 652, 657, 686-692, 705, 708, 713, 718, 728-737, 753-754, 774-845,␣
↪856-859, 884-909, 933-966, 1002-1006, 1019, 1029, 1032, 1037, 1042, 1047, 1051,␣
↪1055, 1064-1065, 1095, 1102, 1107, 1135-1139, 1167-1176, 1186-1194, 1212-1214, 1232-
↪1234, 1250-1252
dicee/models/complex.py                               151     15    90%   86-109
dicee/models/dualE.py                                  59     10    83%   93-102,␣
↪142-156
dicee/models/function_space.py                        262    221    16%   10-24,␣
↪28-37, 40-49, 53-70, 77-86, 89-98, 101-110, 114-126, 134-156, 159-165, 168-185, 188-
↪194, 197-205, 208, 213-234, 243-246, 250-254, 258-267, 271-292, 301-307, 311-328,␣
↪332-335, 344-352, 355, 366-372, 392-406, 424-438, 443-453, 461-465, 474-478
dicee/models/octonion.py                              227     83    63%   21-44,␣
↪320-329, 334-345, 348-370, 374-416, 426-474
dicee/models/pykeen_models.py                          50      5    90%   60-63,␣
↪118
dicee/models/quaternion.py                            192     69    64%   7-21, 30-
↪55, 68-72, 107, 185, 328-342, 345-364, 368-389, 399-426
dicee/models/real.py                                   61     12    80%   36-39,␣
↪66-69, 87, 103-106
dicee/models/static_funcs.py                           10      0   100%
dicee/models/transformers.py                          236    189    20%   24-43,␣
↪46, 60-75, 84-102, 105-116, 123-125, 128, 134-151, 155-180, 186-190, 193-197, 203-
↪207, 210-212, 229-256, 265-268, 271-276, 279-304, 310-315, 319-372, 376-398, 404-414
```

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```
dicee/query_generator.py                                  374    346     7%   18-52,␣
↪56, 62-65, 69-70, 78-92, 100-147, 155-188, 192-206, 212-269, 274-303, 307-443, 453-
↪472, 480-501, 508-512, 517, 522-528
dicee/read_preprocess_save_load_kg/__init__.py              3      0   100%
dicee/read_preprocess_save_load_kg/preprocess.py          256     41    84%   34, 40,␣
↪78, 102-127, 133, 138-151, 184, 214, 388-389, 444
dicee/read_preprocess_save_load_kg/read_from_disk.py       36     11    69%   33, 38-
↪40, 47, 55, 58-72
dicee/read_preprocess_save_load_kg/save_load_disk.py       45     18    60%   39-60
dicee/read_preprocess_save_load_kg/util.py                219    126    42%   65-67,␣
↪72-73, 91-97, 100-102, 107-109, 121, 134, 140-143, 148-156, 161-167, 172-177, 182-
↪187, 199-220, 226-282, 286-290, 294-295, 299, 303-304, 334, 351, 356, 363-364
dicee/sanity_checkers.py                                   54     23    57%   8-12, 21-
↪31, 46, 51, 58, 64-79, 85, 89, 96
dicee/static_funcs.py                                     418    163    61%   40, 50,␣
↪56-61, 83, 105-106, 115, 138, 152, 157-159, 163-165, 167, 194-198, 246, 254, 263-
↪268, 290-304, 316-336, 340-357, 362, 386-387, 392-393, 410-411, 413-414, 416-417,␣
↪419-420, 428, 446-450, 467-470, 474-479, 483-487, 491-492, 498-500, 526-527, 539-
↪542, 547-550, 559-610, 615-627, 644-658, 661-669
dicee/static_funcs_training.py                            123     63    49%   118-215,␣
↪223-224
dicee/static_preprocess_funcs.py                          100     44    56%   17-25,␣
↪52, 56, 64, 67, 78, 91-115, 120-123, 128-131, 136-139
dicee/trainer/__init__.py                                   1      0   100%
dicee/trainer/dice_trainer.py                             126     13    90%   27-32,␣
↪91, 98, 103-108, 147
dicee/trainer/torch_trainer.py                             79      4    95%   31, 196,␣
↪207-208
dicee/trainer/torch_trainer_ddp.py                        152    128    16%   13-14,␣
↪43, 47-72, 83-112, 131-137, 140-149, 164-194, 204-217, 226-246, 251-260, 263-272,␣
↪275-299, 302-309
-------------------------------------------------------------------------------------
TOTAL                                                    6181   2828    54%
```

## 13 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
```

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```
@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},
  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,
```

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```
  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

# 14 dicee

## 14.1 Subpackages

### dicee.models

### Submodules

### dicee.models.base_model

### 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. |

### Module Contents

**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:

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

class Model(nn.Module):
    def __init__(self) -> None:
        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.

**training_step_outputs = []**

**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()
```

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```
    # 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) -> None:
        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.

**args**

**embedding_dim = None**

**num_entities = None**

**num_relations = None**

**num_tokens = None**

**learning_rate = None**

**apply_unit_norm = None**

**input_dropout_rate = None**

**hidden_dropout_rate = None**

**optimizer_name = None**

**feature_map_dropout_rate = None**

**kernel_size = None**

**num_of_output_channels = None**

**weight_decay = None**

**loss**

**selected_optimizer = None**

**normalizer_class = None**

**normalize_head_entity_embeddings**

**normalize_relation_embeddings**

**normalize_tail_entity_embeddings**

**hidden_normalizer**

**param_init**

**input_dp_ent_real**

**input_dp_rel_real**

**hidden_dropout**

**loss_history = []**

**byte_pair_encoding**

**max_length_subword_tokens**

**block_size**

**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) -> None:
        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.

**args**

**__call__**(*x*)

**static forward**(*x*)

## dicee.models.clifford

## Classes

| | |
|---|---|
| *Keci* | Base class for all neural network modules. |
| *KeciBase* | Without learning dimension scaling |
| *DeCaL* | Base class for all neural network modules. |

## Module Contents

**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) -> None:
        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.

**name = 'Keci'**

**p**

**q**

**r**

**requires_grad_for_interactions = True**

**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**(*hp*, *hq*, *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

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

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

### Parameter

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

**returns**

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

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

### Parameter

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

target_entity_idx: torch.LongTensor with (n, k ) shape k denotes the selected number of examples.

**rtype**
torch.FloatTensor with (n, k) 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

**name = 'KeciBase'**

**requires_grad_for_interactions = False**

**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) -> None:
        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.

**name = 'DeCaL'**

**entity_embeddings**

**relation_embeddings**

**p**

**q**

**r**

**re**

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

**Parameter**

x: torch.LongTensor with (n, ) shape

**rtype**

torch.FloatTensor with (n) shape

**cl_pqr**(*a: torch.tensor*) → torch.tensor

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,

$$s0 = h_0 r_0 t_0 s1 = \sum_{i=1}^{p} h_i r_i t_0 s2 = \sum_{j=p+1}^{p+q} h_j r_j t_0 s3 = \sum_{i=1}^{q} (h_0 r_i t_i + h_i r_0 t_i) s4 = \sum_{i=p+1}^{p+q} (h_0 r_i t_i + h_i r_0 t_i) s5 = \sum_{i=p+q+1}^{p+q+r} (h_0 r_i t$$

and return:

$$sigma_0 t = \sigma_0 \cdot t_0 = s0 + s1 - s2 s3, s4 and s5$$

**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

$$\sigma_p p = \sum_{i=1}^{p-1} \sum_{i'=i+1}^{p} (h_i r_{i'} - h_{i'} r_i)(models the interactions between e_i and e_i' for 1 <= i, i' <= p) \sigma_q q = \sum_{j=p+1}^{p+q-1} \sum_{j'=j+1}^{p+q} (h_j r_{j'}$$

For different base vector interactions, we have

$$\sigma_p q = \sum_{i=1}^{p} \sum_{j=p+1}^{p+q} (h_i r_j - h_j r_i)(interactions n between e_i and e_j for 1 <= i <= p and p+1 <= j <= p+q) \sigma_p r = \sum_{i=}^{}$$

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

Kvsall training

(1) Retrieve real-valued embedding vectors for heads and relations

(2) Construct head entity and relation embeddings according to Cl_{p,q, r}(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, ) 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*)

Compute .. math:

```
\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

$$\sigma_{q,q}^* = \sum_{j=p+1}^{p+q-1} \sum_{j'=j+1}^{p+q} (x_j y_{j'} - x_{j'} y_j) Eq.16$$

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*)

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

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

Compute

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

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*)

Compute

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

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

## Classes

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

## Module Contents

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

Bases: *dicee.models.base_model.BaseKGE*

Convolutional ComplEx Knowledge Graph Embeddings

**name = 'ConEx'**

**conv2d**

**fc_num_input**

**fc1**

**norm_fc1**

**bn_conv2d**

**feature_map_dropout**

**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

**name = 'AConEx'**

**conv2d**

**fc_num_input**

**fc1**

**norm_fc1**

**bn_conv2d**

**feature_map_dropout**

**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) -> None:
        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.

**name = 'ComplEx'**

**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

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

## dicee.models.dualE

## Classes

| | |
|---|---|
| *DualE* | Dual Quaternion Knowledge Graph Embeddings (https://ojs.aaai.org/index.php/AAAI/article/download/16850/16657) |

## Module Contents

**class** dicee.models.dualE.**DualE**(*args*)

Bases: *dicee.models.base_model.BaseKGE*

Dual Quaternion Knowledge Graph Embeddings (https://ojs.aaai.org/index.php/AAAI/article/download/16850/16657)

**name = 'DualE'**

**entity_embeddings**

**relation_embeddings**

**num_ent**

**kvsall_score**(*e_1_h*, *e_2_h*, *e_3_h*, *e_4_h*, *e_5_h*, *e_6_h*, *e_7_h*, *e_8_h*, *e_1_t*, *e_2_t*, *e_3_t*, *e_4_t*, *e_5_t*, *e_6_t*, *e_7_t*, *e_8_t*, *r_1*, *r_2*, *r_3*, *r_4*, *r_5*, *r_6*, *r_7*, *r_8*) → torch.tensor

KvsAll scoring function

### Input

x: torch.LongTensor with (n, ) shape

### Output

torch.FloatTensor with (n) shape

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

Negative Sampling forward pass:

### Input

x: torch.LongTensor with (n, ) shape

### Output

torch.FloatTensor with (n) shape

**forward_k_vs_all**(*x*)

KvsAll forward pass

### Input

x: torch.LongTensor with (n, ) shape

### Output

torch.FloatTensor with (n) shape

**T**(*x: torch.tensor*) → torch.tensor

Transpose function

Input: Tensor with shape (nxm) Output: Tensor with shape (mxn)

## dicee.models.function_space

### 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: |

### Module Contents

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

Bases: *dicee.models.base_model.BaseKGE*

Learning Knowledge Neural Graphs

**name = 'FMult'**

**entity_embeddings**

**relation_embeddings**

**k**

**num_sample = 50**

**gamma**

**roots**

**weights**

**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

**name = 'GFMult'**

**entity_embeddings**

**relation_embeddings**

**k**

**num_sample = 250**

**roots**

**weights**

**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

**name = 'FMult2'**

**n_layers = 3**

**tuned_embedding_dim = False**

**k**

**n = 50**

**score_func = 'compositional'**

**discrete_points**

**entity_embeddings**

**relation_embeddings**

**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

**name = 'LFMult1'**

**entity_embeddings**

**relation_embeddings**

**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.

**name = 'LFMult'**

**entity_embeddings**

**relation_embeddings**

**degree**

**m**

**x_values**

**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

### 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) |

### Module Contents

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) -> None:
        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.

**name** = 'OMult'

**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) -> None:
        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.

**name = 'ConvO'**

**conv2d**

**fc_num_input**

**fc1**

**bn_conv2d**

**norm_fc1**

**feature_map_dropout**

**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

**name = 'AConvO'**

**conv2d**

**fc_num_input**

**fc1**

**bn_conv2d**

**norm_fc1**

**feature_map_dropout**

**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

## Classes

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

## Module Contents

**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:

**model_kwargs**

**name**

**model**

**loss_history = []**

**args**

**entity_embeddings = None**

**relation_embeddings = None**

**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

## 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) |

## Module Contents

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) -> None:
        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.

**name = 'QMult'**

**explicit = True**

**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

**name = 'ConvQ'**

**entity_embeddings**

**relation_embeddings**

**conv2d**

**fc_num_input**

**fc1**

**bn_conv1**

**bn_conv2**

**feature_map_dropout**

**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

**name = 'AConvQ'**

**entity_embeddings**

**relation_embeddings**

**conv2d**

**fc_num_input**

**fc1**

**bn_conv1**

**bn_conv2**

**feature_map_dropout**

**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

## 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 |

### Module Contents

**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

**name = 'DistMult'**

**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

**name = 'TransE'**

**margin = 4**

**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)

**name = 'Shallom'**

**shallom_width**

**shallom**

**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

**name = 'Pyke'**

**dist_func**

**margin = 1.0**

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

**Parameters**

**x**

## dicee.models.static_funcs

## Functions

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

## Module Contents

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

Full definition of a GPT Language Model, all of it in this single file. References: 1) the official GPT-2 TensorFlow implementation released by OpenAI: https://github.com/openai/gpt-2/blob/master/src/model.py 2) huggingface/transformers PyTorch implementation: https://github.com/huggingface/transformers/blob/main/src/transformers/models/gpt2/modeling_gpt2.py

## 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. |

## Module Contents

**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) -> None:
        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.

**name = 'BytE'**

**config**

**temperature = 0.5**

**topk = 2**

**transformer**

**lm_head**

**weight**

**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

**weight**

**bias**

**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) -> None:
        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.

**c_attn**

**c_proj**

**attn_dropout**

**resid_dropout**

**n_head**

**n_embd**

**dropout**

**flash**

**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) -> None:
        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.

**c_fc**

**gelu**

**c_proj**

**dropout**

**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) -> None:
        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.

**ln_1**

**attn**

**ln_2**

**mlp**

**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) -> None:
        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.

**config**

**transformer**

**lm_head**

**weight**

**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

## 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 |
| *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. |
| *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: |

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Table 1 – continued from previous page

| | |
|---|---|
| *LFMult* | Embedding with polynomial functions. We represent all entities and relations in the polynomial space as: |
| *DualE* | Dual Quaternion Knowledge Graph Embeddings (https://ojs.aaai.org/index.php/AAAI/article/download/16850/16657) |

### 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) | |

### Package Contents

**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) -> None:
        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.

**training_step_outputs = []**

**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
    # 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) -> None:
        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.

**args**

**embedding_dim = None**

**num_entities = None**

**num_relations = None**

**num_tokens = None**

**learning_rate = None**

**apply_unit_norm = None**

**input_dropout_rate = None**

**hidden_dropout_rate = None**

**optimizer_name = None**

**feature_map_dropout_rate = None**

**kernel_size = None**

**num_of_output_channels = None**

**weight_decay = None**

**loss**

**selected_optimizer = None**

**normalizer_class = None**

**normalize_head_entity_embeddings**

**normalize_relation_embeddings**

**normalize_tail_entity_embeddings**

**hidden_normalizer**

**param_init**

**input_dp_ent_real**

**input_dp_rel_real**

**hidden_dropout**

**loss_history = []**

**byte_pair_encoding**

**max_length_subword_tokens**

**block_size**

**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) -> None:
        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.

**args**

**__call__**(*x*)

**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) -> None:
        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.

**args**

**embedding_dim = None**

**num_entities = None**

**num_relations = None**

**num_tokens = None**

**learning_rate = None**

**apply_unit_norm = None**

**input_dropout_rate = None**

**hidden_dropout_rate = None**

**optimizer_name = None**

**feature_map_dropout_rate = None**

**kernel_size = None**

**num_of_output_channels = None**

**weight_decay = None**

**loss**

**selected_optimizer = None**

**normalizer_class = None**

**normalize_head_entity_embeddings**

**normalize_relation_embeddings**

**normalize_tail_entity_embeddings**

**hidden_normalizer**

**param_init**

**input_dp_ent_real**

**input_dp_rel_real**

**hidden_dropout**

**loss_history = []**

**byte_pair_encoding**

**max_length_subword_tokens**

**block_size**

**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

**name = 'DistMult'**

**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

**name = 'TransE'**

**margin = 4**

**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)

**name = 'Shallom'**

**shallom_width**

**shallom**

**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

**name = 'Pyke'**

**dist_func**

**margin = 1.0**

**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) -> None:
        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.

**`args`**

**`embedding_dim = None`**

**`num_entities = None`**

**`num_relations = None`**

**`num_tokens = None`**

**`learning_rate = None`**

**`apply_unit_norm = None`**

**`input_dropout_rate = None`**

**`hidden_dropout_rate = None`**

**`optimizer_name = None`**

**`feature_map_dropout_rate = None`**

**`kernel_size = None`**

**`num_of_output_channels = None`**

**`weight_decay = None`**

**`loss`**

**selected_optimizer = None**

**normalizer_class = None**

**normalize_head_entity_embeddings**

**normalize_relation_embeddings**

**normalize_tail_entity_embeddings**

**hidden_normalizer**

**param_init**

**input_dp_ent_real**

**input_dp_rel_real**

**hidden_dropout**

**loss_history = []**

**byte_pair_encoding**

**max_length_subword_tokens**

**block_size**

**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

**name = 'ConEx'**

**conv2d**

**fc_num_input**

**fc1**

**norm_fc1**

**bn_conv2d**

**feature_map_dropout**

**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

**name = 'AConEx'**

**conv2d**

**fc_num_input**

**fc1**

**norm_fc1**

**bn_conv2d**

**feature_map_dropout**

**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) -> None:
        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.

**name = 'ComplEx'**

**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

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

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) -> None:
        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.

**args**

**embedding_dim = None**

**num_entities = None**

**num_relations = None**

**num_tokens = None**

**learning_rate = None**

**apply_unit_norm = None**

**input_dropout_rate = None**

**hidden_dropout_rate = None**

**optimizer_name = None**

**feature_map_dropout_rate = None**

**kernel_size = None**

**num_of_output_channels = None**

**weight_decay = None**

**loss**

**selected_optimizer = None**

**normalizer_class = None**

**normalize_head_entity_embeddings**

**normalize_relation_embeddings**

**normalize_tail_entity_embeddings**

**hidden_normalizer**

**param_init**

**input_dp_ent_real**

**input_dp_rel_real**

**hidden_dropout**

**loss_history = []**

**byte_pair_encoding**

**max_length_subword_tokens**

**block_size**

**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) -> None:
        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.

**args**

**__call__**(*x*)

**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) -> None:
        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.

**`name = 'QMult'`**

**`explicit = True`**

**`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

**name = 'ConvQ'**

**entity_embeddings**

**relation_embeddings**

**conv2d**

**fc_num_input**

**fc1**

**bn_conv1**

**bn_conv2**

**feature_map_dropout**

**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

**name = 'AConvQ'**

**entity_embeddings**

**relation_embeddings**

**conv2d**

**fc_num_input**

**fc1**

**bn_conv1**

**bn_conv2**

**feature_map_dropout**

**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) -> None:
        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.

**args**

**embedding_dim = None**

**num_entities = None**

**num_relations = None**

**num_tokens = None**

**learning_rate = None**

**apply_unit_norm = None**

**input_dropout_rate = None**

**hidden_dropout_rate = None**

**optimizer_name = None**

**feature_map_dropout_rate = None**

**kernel_size = None**

**num_of_output_channels = None**

**weight_decay = None**

**loss**

**selected_optimizer = None**

**normalizer_class = None**

**normalize_head_entity_embeddings**

**normalize_relation_embeddings**

**normalize_tail_entity_embeddings**

**hidden_normalizer**

**param_init**

**input_dp_ent_real**

**input_dp_rel_real**

**hidden_dropout**

**loss_history = []**

**byte_pair_encoding**

**max_length_subword_tokens**

**block_size**

**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) -> None:
        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.

**args**

**__call__**(*x*)

**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) -> None:
        super().__init__()
        self.conv1 = nn.Conv2d(1, 20, 5)
        self.conv2 = nn.Conv2d(20, 20, 5)

    def forward(self, x):
```

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```
        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.

**name = 'OMult'**

**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) -> None:
        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.

**name = 'ConvO'**

**conv2d**

**fc_num_input**

**fc1**

**bn_conv2d**

**norm_fc1**

**feature_map_dropout**

**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

**name = 'AConvO'**

**conv2d**

**fc_num_input**

**fc1**

**bn_conv2d**

**norm_fc1**

**feature_map_dropout**

**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) -> None:
        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.

**name = 'Keci'**

**p**

**q**

**r**

**requires_grad_for_interactions = True**

**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**(*hp*, *hq*, *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

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

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

### Parameter

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

**returns**

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

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

### Parameter

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

target_entity_idx: torch.LongTensor with (n, k ) shape k denotes the selected number of examples.

**rtype**
torch.FloatTensor with (n, k) 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

**name = 'KeciBase'**

**requires_grad_for_interactions = False**

**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) -> None:
        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.

**name = 'DeCaL'**

**entity_embeddings**

**relation_embeddings**

**p**

**q**

**r**

**re**

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

### Parameter

x: torch.LongTensor with (n, ) shape

**rtype**

torch.FloatTensor with (n) shape

**cl_pqr**(*a: torch.tensor*) → torch.tensor

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,

$$s0 = h_0 r_0 t_0 s1 = \sum_{i=1}^{p} h_i r_i t_0 s2 = \sum_{j=p+1}^{p+q} h_j r_j t_0 s3 = \sum_{i=1}^{q} (h_0 r_i t_i + h_i r_0 t_i) s4 = \sum_{i=p+1}^{p+q} (h_0 r_i t_i + h_i r_0 t_i) s5 = \sum_{i=p+q+1}^{p+q+r} (h_0 r_i t$$

and return:

$$sigma_0 t = \sigma_0 \cdot t_0 = s0 + s1 - s2 s3, s4 and s5$$

**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

$$\sigma_p p = \sum_{i=1}^{p-1} \sum_{i'=i+1}^{p} (h_i r_{i'} - h_{i'} r_i)(models the interactions between e_i and e'_i for 1 <= i, i' <= p) \sigma_q q = \sum_{j=p+1}^{p+q-1} \sum_{j'=j+1}^{p+q} (h_j r_{j'}$$

For different base vector interactions, we have

$$\sigma_p q = \sum_{i=1}^{p} \sum_{j=p+1}^{p+q} (h_i r_j - h_j r_i)(interactions nbetween e_i and e_j for 1 <= i <= p and p+1 <= j <= p+q) \sigma_p r = \sum_{i=}^{}$$

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

Kvsall training

(1) Retrieve real-valued embedding vectors for heads and relations

(2) Construct head entity and relation embeddings according to Cl_{p,q, r}(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, ) 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*)

Compute .. math:

```
\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

$$\sigma^*_{q,q} = \sum_{j=p+1}^{p+q-1} \sum_{j'=j+1}^{p+q} (x_j y_{j'} - x_{j'} y_j) Eq.16$$

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*)

$$\sigma^*_{r,r} = \sum_{k=p+q+1}^{p+q+r-1} \sum_{k'=k+1}^{p} (x_k y_{k'} - x_{k'} y_k)$$

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

Compute

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

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*)

Compute

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

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) -> None:
        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.

**args**

**embedding_dim = None**

**num_entities = None**

**num_relations = None**

**num_tokens = None**

**learning_rate = None**

**apply_unit_norm = None**

**input_dropout_rate = None**

**hidden_dropout_rate = None**

**optimizer_name = None**

**feature_map_dropout_rate = None**

**kernel_size = None**

**num_of_output_channels = None**

**weight_decay = None**

**loss**

**selected_optimizer = None**

**normalizer_class = None**

**normalize_head_entity_embeddings**

**normalize_relation_embeddings**

**normalize_tail_entity_embeddings**

**hidden_normalizer**

**param_init**

**input_dp_ent_real**

**input_dp_rel_real**

**hidden_dropout**

**loss_history = []**

**byte_pair_encoding**

**max_length_subword_tokens**

**block_size**

**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:

**model_kwargs**

**name**

**model**

**loss_history = []**

**args**

**entity_embeddings = None**

**relation_embeddings = None**

**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) -> None:
        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.

**args**

**embedding_dim = None**

**num_entities = None**

**num_relations = None**

**num_tokens = None**

**learning_rate = None**

**apply_unit_norm = None**

**input_dropout_rate = None**

**hidden_dropout_rate = None**

**optimizer_name = None**

**feature_map_dropout_rate = None**

**kernel_size = None**

**num_of_output_channels = None**

**weight_decay = None**

**loss**

**selected_optimizer = None**

**normalizer_class = None**

**normalize_head_entity_embeddings**

**normalize_relation_embeddings**

**normalize_tail_entity_embeddings**

**hidden_normalizer**

**param_init**

**input_dp_ent_real**

**input_dp_rel_real**

**hidden_dropout**

**loss_history = []**

**byte_pair_encoding**

**max_length_subword_tokens**

**block_size**

**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

**name = 'FMult'**

**entity_embeddings**

**relation_embeddings**

**k**

**num_sample = 50**

**gamma**

**roots**

**weights**

**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

**name = 'GFMult'**

**entity_embeddings**

**relation_embeddings**

**k**

**num_sample = 250**

**roots**

**weights**

**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

**name = 'FMult2'**

**n_layers = 3**

**tuned_embedding_dim = False**

**k**

**n = 50**

**score_func = 'compositional'**

**discrete_points**

**entity_embeddings**

**relation_embeddings**

**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

**name = 'LFMult1'**

**entity_embeddings**

**relation_embeddings**

**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.

**name = 'LFMult'**

**entity_embeddings**

**relation_embeddings**

**degree**

**m**

**x_values**

**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.models.**DualE**(*args*)

Bases: *dicee.models.base_model.BaseKGE*

Dual Quaternion Knowledge Graph Embeddings (https://ojs.aaai.org/index.php/AAAI/article/download/16850/16657)

**name = 'DualE'**

**entity_embeddings**

**relation_embeddings**

**num_ent**

**kvsall_score**(*e_1_h*, *e_2_h*, *e_3_h*, *e_4_h*, *e_5_h*, *e_6_h*, *e_7_h*, *e_8_h*, *e_1_t*, *e_2_t*, *e_3_t*, *e_4_t*, *e_5_t*, *e_6_t*, *e_7_t*, *e_8_t*, *r_1*, *r_2*, *r_3*, *r_4*, *r_5*, *r_6*, *r_7*, *r_8*) → torch.tensor

KvsAll scoring function

#### Input

x: torch.LongTensor with (n, ) shape

#### Output

torch.FloatTensor with (n) shape

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

Negative Sampling forward pass:

#### Input

x: torch.LongTensor with (n, ) shape

#### Output

torch.FloatTensor with (n) shape

**forward_k_vs_all**(*x*)

KvsAll forward pass

#### Input

x: torch.LongTensor with (n, ) shape

#### Output

torch.FloatTensor with (n) shape

**T**(*x: torch.tensor*) → torch.tensor

Transpose function

Input: Tensor with shape (nxm) Output: Tensor with shape (mxn)

## dicee.read_preprocess_save_load_kg

## Submodules

## dicee.read_preprocess_save_load_kg.preprocess

## Classes

| | |
|---|---|
| *PreprocessKG* | Preprocess the data in memory |

### Module Contents

**class** dicee.read_preprocess_save_load_kg.preprocess.**PreprocessKG**(*kg*)

Preprocess the data in memory

**kg**

**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)

## dicee.read_preprocess_save_load_kg.read_from_disk

### Classes

| | |
|---|---|
| *ReadFromDisk* | Read the data from disk into memory |

### Module Contents

**class** dicee.read_preprocess_save_load_kg.read_from_disk.**ReadFromDisk**(*kg*)

Read the data from disk into memory

**kg**

**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

## Classes

| |
|---|
| *LoadSaveToDisk* |

## Module Contents

**class** dicee.read_preprocess_save_load_kg.save_load_disk.**LoadSaveToDisk**(*kg*)

**kg**

**save**()

**load**()

## dicee.read_preprocess_save_load_kg.util

## Functions

| | |
|---|---|
| *polars_dataframe_indexer*(→ polars.DataFrame) | Replaces 'subject', 'relation', and 'object' columns in the input Polars DataFrame with their corresponding index values |
| *apply_reciprical_or_noise*(add_reciprical, eval_model) | |
| *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]) | |
| *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) | |
| *dataset_sanity_checking*(→ None) | |

## Module Contents

dicee.read_preprocess_save_load_kg.util.**polars_dataframe_indexer**(
*df_polars: polars.DataFrame*, *idx_entity: polars.DataFrame*, *idx_relation: polars.DataFrame*)
→ polars.DataFrame

Replaces ‘subject’, ‘relation’, and ‘object’ columns in the input Polars DataFrame with their corresponding index values from the entity and relation index DataFrames.

This function processes the DataFrame in three main steps: 1. Replace the ‘relation’ values with the corresponding index from *idx_relation*. 2. Replace the ‘subject’ values with the corresponding index from *idx_entity*. 3. Replace the ‘object’ values with the corresponding index from *idx_entity*.

### Parameters:

**df_polars**
[polars.DataFrame] The input Polars DataFrame containing columns: 'subject', 'relation', and 'object'.

**idx_entity**
[polars.DataFrame] A Polars DataFrame that contains the mapping between entity names and their corresponding indices. Must have columns: 'entity' and 'index'.

**idx_relation**
[polars.DataFrame] A Polars DataFrame that contains the mapping between relation names and their corresponding indices. Must have columns: 'relation' and 'index'.

### Returns:

**polars.DataFrame**
A DataFrame with the 'subject', 'relation', and 'object' columns replaced by their corresponding indices.

### Example Usage:

```
>>> df_polars = pl.DataFrame({
        "subject": ["Alice", "Bob", "Charlie"],
        "relation": ["knows", "works_with", "lives_in"],
        "object": ["Dave", "Eve", "Frank"]
    })
>>> idx_entity = pl.DataFrame({
        "entity": ["Alice", "Bob", "Charlie", "Dave", "Eve", "Frank"],
        "index": [0, 1, 2, 3, 4, 5]
    })
>>> idx_relation = pl.DataFrame({
        "relation": ["knows", "works_with", "lives_in"],
        "index": [0, 1, 2]
    })
>>> polars_dataframe_indexer(df_polars, idx_entity, idx_relation)
```

### Steps:

1. Join the input DataFrame *df_polars* on the 'relation' column with *idx_relation* to replace the relations with their indices.
2. Join on 'subject' to replace it with the corresponding entity index using a left join on *idx_entity*.
3. Join on 'object' to replace it with the corresponding entity index using a left join on *idx_entity*.
4. Select only the 'subject', 'relation', and 'object' columns to return the final result.

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**

## Classes

| | |
|---|---|
| *PreprocessKG* | Preprocess the data in memory |
| *LoadSaveToDisk* | |
| *ReadFromDisk* | Read the data from disk into memory |

## Package Contents

**class** dicee.read_preprocess_save_load_kg.**PreprocessKG**(*kg*)

Preprocess the data in memory

**kg**

**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)

**class** dicee.read_preprocess_save_load_kg.**LoadSaveToDisk**(*kg*)

**kg**

**save**()

**load**()

**class** dicee.read_preprocess_save_load_kg.**ReadFromDisk**(*kg*)

Read the data from disk into memory

**kg**

**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

## Functions

| | |
|---|---|
| *get_default_arguments*() | |
| *main*() | |

## Module Contents

dicee.scripts.index.**get_default_arguments**()

dicee.scripts.index.**main**()

## dicee.scripts.run

## Functions

| | |
|---|---|
| *get_default_arguments*([description]) | Extends pytorch_lightning Trainer's arguments with ours |
| *main*() | |

## Module Contents

dicee.scripts.run.**get_default_arguments**(*description=None*)

Extends pytorch_lightning Trainer's arguments with ours

dicee.scripts.run.**main**()

## dicee.scripts.serve

### Attributes

| |
|---|
| *app* |
| *neural_searcher* |

### Classes

| |
|---|
| *NeuralSearcher* |

### Functions

| |
|---|
| *get_default_arguments*() |
| *root*() |
| *search_embeddings*(q) |
| *retrieve_embeddings*(q) |
| *main*() |

### Module Contents

dicee.scripts.serve.**app**

dicee.scripts.serve.**neural_searcher = None**

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*)

**collection_name**

**model**

**qdrant_client**

**get**(*entity: str*)

**search**(*entity: str*)

dicee.scripts.serve.**main**()

## dicee.trainer

## Submodules

## dicee.trainer.dice_trainer

## Classes

| | |
|---|---|
| *DICE_Trainer* | DICE_Trainer implement |

## Functions

| | |
|---|---|
| *initialize_trainer*(args, callbacks) | |
| *get_callbacks*(args) | |

## Module Contents

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

**report**

**args**

**trainer = None**

**is_continual_training**

**storage_path**

**evaluator**

**form_of_labelling = None**

**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

## Classes

| | |
|---|---|
| *TorchTrainer* | TorchTrainer for using single GPU or multi CPUs on a single node |

### Module Contents

**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

**loss_function = None**

**optimizer = None**

**model = None**

**train_dataloaders = None**

**training_step = None**

**process**

**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

### Classes

| | |
|---|---|
| *TorchDDPTrainer* | A Trainer based on torch.nn.parallel.DistributedDataParallel |
| *NodeTrainer* | |

### Functions

| | |
|---|---|
| *make_iterable_verbose*(→ Iterable) | |

### Module Contents

dicee.trainer.torch_trainer_ddp.**make_iterable_verbose**(*iterable_object*, *verbose*, *desc='Default'*, *position=None*, *leave=True*) → Iterable

**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*, *callbacks*, *num_epochs: int*)

**trainer**

**local_rank**

**global_rank**

**optimizer**

**train_dataset_loader**

**loss_func**

**callbacks**

**model**

**num_epochs**

**loss_history = []**

**extract_input_outputs**(*z: list*)

**train**()

Training loop for DDP

## Classes

| | |
|---|---|
| *DICE_Trainer* | DICE_Trainer implement |

## Package Contents

**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

**report**

**args**

**trainer = None**

**is_continual_training**

**storage_path**

**evaluator**

**form_of_labelling = None**

**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

## 14.2 Submodules

### dicee.__main__

### dicee.abstracts

## 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 |

## Module Contents

**class** dicee.abstracts.**AbstractTrainer**(*args*, *callbacks*)

Abstract class for Trainer class for knowledge graph embedding models

### Parameter

**args**
[str] ?

**callbacks: list**
?

**attributes**

**callbacks**

**is_global_zero = True**

**strategy = None**

**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

**construct_ensemble**

**apply_semantic_constraint**

**configs**

**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**

**set_model_train_mode**() → None

Setting the model into training mode

### Parameter

**set_model_eval_mode**() → None

Setting the model into eval mode

### Parameter

**property name**

**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

**num_epochs**

**path**

**sample_counter = 0**

**epoch_count = 0**

**alphas = None**

**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

### Classes

| |
|---|
| *Experiment* |

### Functions

| |
|---|
| *get_default_arguments*() |
| *analyse*(args) |

### Module Contents

dicee.analyse_experiments.**get_default_arguments**()

**class** dicee.analyse_experiments.**Experiment**

**model_name = []**

**callbacks = []**

**embedding_dim = []**

**num_params = []**

**num_epochs = []**

**batch_size = []**

**lr = []**

**byte_pair_encoding = []**

**aswa = []**

**path_dataset_folder = []**

**full_storage_path = []**

**pq = []**

**train_mrr = []**

**train_h1 = []**

**train_h3 = []**

**train_h10 = []**

**val_mrr = []**

**val_h1 = []**

**val_h3 = []**

**val_h10 = []**

**test_mrr = []**

**test_h1 = []**

**test_h3 = []**

**test_h10 = []**

**runtime = []**

**normalization = []**

**scoring_technique = []**

**save_experiment**($x$)

**to_df**()

dicee.analyse_experiments.**analyse**(*args*)

## dicee.callbacks

### 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) | |

### Module Contents

**class** dicee.callbacks.**AccumulateEpochLossCallback**(*path: str*)

Bases: *dicee.abstracts.AbstractCallback*

Abstract class for Callback class for knowledge graph embedding models

#### Parameter

**path**

**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

**start_time**

**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

**every_x_epoch**

**max_epochs**

**epoch_counter = 0**

**path**

**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

**data_module**

**kg**

**num_of_epochs = 0**

**unlabelled_size**

**batch_size**

**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.

**path**

**num_epochs**

**initial_eval_setting = None**

**epoch_count = 0**

**alphas = []**

**val_aswa**

**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

**path**

**reports = []**

**epoch_ratio**

**epoch_counter = 0**

**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

**f = None**

**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 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:

**level**

**ratio**

**method**

**scaler**

**frequency**

**on_train_batch_start**(*trainer*, *model*, *batch*, *batch_idx*)

Called when the train batch begins.

## dicee.config

## Classes

| | |
|---|---|
| *Namespace* | Simple object for storing attributes. |

## Module Contents

**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 = None**

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 = None**

A single directory created that contains related data about embeddings.

**path_single_kg = None**

Path of a file corresponding to the input knowledge graph

**sparql_endpoint = None**

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 = None**

The ratio of added random triples into training dataset

**gpus = None**

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 = None**

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 = None**

Not tested

**label_smoothing_rate: float = 0.0**

**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 = None**

Read some triples that are uniformly at random sampled. Ratio being between 0 and 1

**read_only_few: int = None**

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 = None**

block size of LLM

**continual_learning = None**

Path of a pretrained model size of LLM

**__iter__**()

## dicee.dataset_classes

### 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. |
| *OnevsSample* | A custom PyTorch Dataset class for knowledge graph embeddings, which includes |
| *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) | |

### Module Contents

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.

**train_set**

**ordered_bpe_entities**

**num_bpe_entities**

**neg_ratio**

**num_datapoints**

**__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.

**train_set**

**train_indices_target**

**target_dim**

**num_datapoints**

**torch_ordered_shaped_bpe_entities**

**collate_fn = None**

**__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

**train_data**

**block_size**

**num_of_data_points**

**collate_fn = None**

**__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

**train_data**

**target_dim**

**collate_fn = None**

**__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])
```

**train_data = None**

**train_target = None**

**label_smoothing_rate**

**collate_fn = None**

**__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])
```

**train_data = None**

**train_target = None**

**label_smoothing_rate**

**collate_fn = None**

**target_dim**

**store**

**__len__**()

**__getitem__**(*idx*)

**class** dicee.dataset_classes.**OnevsSample**(*train_set: numpy.ndarray*, *num_entities*, *num_relations*, *neg_sample_ratio: int = None*, *label_smoothing_rate: float = 0.0*)

Bases: `torch.utils.data.Dataset`

A custom PyTorch Dataset class for knowledge graph embeddings, which includes both positive and negative sampling for a given dataset for multi-class classification problem..

**Parameters**

- **train_set** (*np.ndarray*) – A numpy array containing triples of knowledge graph data. Each triple consists of (head_entity, relation, tail_entity).
- **num_entities** (*int*) – The number of unique entities in the knowledge graph.
- **num_relations** (*int*) – The number of unique relations in the knowledge graph.
- **neg_sample_ratio** (*int, optional*) – The number of negative samples to be generated per positive sample. Must be a positive integer and less than num_entities.
- **label_smoothing_rate** (*float, optional*) – A label smoothing rate to apply to the positive and negative labels. Defaults to 0.0.

**train_data**

The input data converted into a PyTorch tensor.

**Type**
torch.Tensor

**num_entities**

Number of entities in the dataset.

**Type**
int

**num_relations**

Number of relations in the dataset.

**Type**
int

**neg_sample_ratio**

Ratio of negative samples to be drawn for each positive sample.

**Type**
int

**label_smoothing_rate**

The smoothing factor applied to the labels.

**Type**
torch.Tensor

**collate_fn**

A function that can be used to collate data samples into batches (set to None by default).

**Type**
function, optional

**train_data**

**num_entities**

**num_relations**

**neg_sample_ratio**

**label_smoothing_rate**

**collate_fn = None**

**__len__**()

Returns the number of samples in the dataset.

**__getitem__**(*idx*)

Retrieves a single data sample from the dataset at the given index.

**Parameters**

**idx** (*int*) – The index of the sample to retrieve.

**Returns**

**A tuple consisting of:**

- x (torch.Tensor): The head and relation part of the triple.
- y_idx (torch.Tensor): The concatenated indices of the true object (tail entity) and the indices of the negative samples.
- y_vec (torch.Tensor): A vector containing the labels for the positive and negative samples, with label smoothing applied.

**Return type**

tuple

**class** dicee.dataset_classes.**KvsSampleDataset**(*train_set_idx: numpy.ndarray*, *entity_idxs*, *relation_idxs*, *form*, *store=None*, *neg_ratio=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

**train_data = None**

**train_target = None**

**neg_ratio**

**num_entities**

**label_smoothing_rate**

**collate_fn = None**

**store**

**max_num_of_classes**

**__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.

**neg_sample_ratio**

**train_set**

**length**

**num_entities**

**num_relations**

**__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

**label_smoothing_rate**

**neg_sample_ratio**

**train_set**

**length**

**num_entities**

**num_relations**

**__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_set_idx**

**num_entities**

**num_relations**

**neg_sample_ratio**

**batch_size**

**num_workers**

**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)
```

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```
    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
```

**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
```

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```
# 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

### Functions

| | |
|---|---|
| *evaluate_link_prediction_performance*(→ Dict) | |
| *evaluate_link_prediction_performance_with_* | |
| *evaluate_link_prediction_performance_with_* | |
| *evaluate_link_prediction_performance_with_* ...) | |
| *evaluate_lp_bpe_k_vs_all*(model, triples[, er_vocab, ...]) | |

### Module Contents

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

## Classes

| | |
|---|---|
| *Evaluator* | Evaluator class to evaluate KGE models in various downstream tasks |

## Module Contents

**class** dicee.evaluator.**Evaluator**(*args*, *is_continual_training=None*)

Evaluator class to evaluate KGE models in various downstream tasks

Arguments

**re_vocab = None**

**er_vocab = None**

**ee_vocab = None**

**func_triple_to_bpe_representation = None**

**is_continual_training**

**num_entities = None**

**num_relations = None**

**args**

**report**

**during_training = False**

**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

## Classes

| | |
|---|---|
| *Execute* | A class for Training, Retraining and Evaluation a model. |
| *ContinuousExecute* | A subclass of Execute Class for retraining |

## Module Contents

**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

**args**

**is_continual_training**

**trainer = None**

**trained_model = None**

**knowledge_graph = None**

**report**

**evaluator = None**

**start_time = None**

**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

During the continual learning we can only modify * **num_epochs** * parameter. Trained model stored in the same folder as the seed model for the training. Trained model is noted with the current time.

**previous_args**

**args**

**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

### Classes

| | |
|---|---|
| *KG* | Knowledge Graph |

### Module Contents

**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_reciprocal: 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

**dataset_dir**

**byte_pair_encoding**

**ordered_shaped_bpe_tokens = None**

**sparql_endpoint**

**add_noise_rate**

**num_entities = None**

**num_relations = None**

**path_single_kg**

**path_for_deserialization**

**add_reciprocal**

**eval_model**

**read_only_few**

**sample_triples_ratio**

**path_for_serialization**

**entity_to_idx**

**relation_to_idx**

**backend**

**training_technique**

**idx_entity_to_bpe_shaped**

**enc**

**num_tokens**

**num_bpe_entities = None**

**padding**

**dummy_id**

**max_length_subword_tokens = None**

**train_set_target = None**

**target_dim = None**

**train_target_indices = None**

**ordered_bpe_entities = None**

**property entities_str: List**

**property relations_str: List**

**exists**(*h: str*, *r: str*, *t: str*)

**__iter__**()

**__len__**()

**func_triple_to_bpe_representation**(*triple: List[str]*)

## dicee.knowledge_graph_embeddings

## Classes

| | |
|---|---|
| *KGE* | Knowledge Graph Embedding Class for interactive usage of pre-trained models |

## Module Contents

**class** dicee.knowledge_graph_embeddings.**KGE**(*path=None*, *url=None*, *construct_ensemble=False*, *model_name=None*)

Bases: *dicee.abstracts.BaseInteractiveKGE*

Knowledge Graph Embedding Class for interactive usage of pre-trained models

**__str__**()

**to**(*device: str*) → None

**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=''*)

**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: str | List[str] = None*, *r: str | List[str] = None*, *t: str | List[str] = None*, *topk: int = 10*, *within: List[str] = None*)

Predict missing item in a given triple.

### Parameter

head_entity: Union[str, List[str]]

String representation of selected entities.

relation: Union[str, List[str]]

String representation of selected relations.

tail_entity: Union[str, 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

## Classes

| |
|---|
| *QueryGenerator* |

## Module Contents

**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*)

**train_path**

**val_path**

**test_path**

**gen_valid**

**gen_test**

**seed**

**max_ans_num = 1000000.0**

**mode**

**ent2id**

**rel2id: Dict**

**ent_in: Dict**

**ent_out: Dict**

**query_name_to_struct**

**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

## Functions

| | |
|---|---|
| *is_sparql_endpoint_alive*([sparql_endpoint]) | |
| *validate_knowledge_graph*(args) | Validating the source of knowledge graph |
| *sanity_checking_with_arguments*(args) | |

### Module Contents

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

### 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]) | |
| *load_term_mapping*([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, ...) | |

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Table 2 – continued from previous page

| | |
|---|---|
| *deploy_tail_entity_prediction*(pre_trained_kge, ...) | |
| *deploy_head_entity_prediction*(pre_trained_kge, ...) | |
| *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*(→ None) | |
| *download_pretrained_model*(→ str) | |

## Module Contents

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.**load_term_mapping**(*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: str*, *destination_folder='.'*) → None

**Parameters**

- **base_url** (e.g. "https://files.dice-research.org/projects/DiceEmbeddings/KINSHIP-Keci-dim128-epoch256-KvsAll")
- **destination_folder** (*e.g. "KINSHIP-Keci-dim128-epoch256-KvsAll"*)

dicee.static_funcs.**download_pretrained_model**(*url: str*) → str

## dicee.static_funcs_training

### 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) | |

### Module Contents

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

### Attributes

| |
|---|
| *enable_log* |

### Functions

| | |
|---|---|
| *timeit*(func) | |
| *preprocesses_input_args*(args) | Sanity Checking in input arguments |
| *create_constraints*(→ Tuple[dict, dict, dict, dict]) | |
| *get_er_vocab*(data) | |
| *get_re_vocab*(data) | |
| *get_ee_vocab*(data) | |
| *mapping_from_first_two_cols_to_third*(train_se | |

### Module Contents

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*)

## 14.3 Attributes

| | |
|---|---|
| *__version__* | |

## 14.4 Classes

| | |
|---|---|
| *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 |

continues on next page

Table 3 – continued from previous page

| | |
|---|---|
| *Keci* | Base class for all neural network modules. |
| *TransE* | Translating Embeddings for Modeling |
| *DeCaL* | Base class for all neural network modules. |
| *DualE* | Dual Quaternion Knowledge Graph Embeddings (https://ojs.aaai.org/index.php/AAAI/article/download/16850/16657) |
| *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. |
| *OnevsSample* | A custom PyTorch Dataset class for knowledge graph embeddings, which includes |
| *KvsSampleDataset* | KvsSample a Dataset: |
| *NegSampleDataset* | An abstract class representing a `Dataset`. |
| *TriplePredictionDataset* | Triple Dataset |
| *CVDataModule* | Create a Dataset for cross validation |
| *QueryGenerator* | |

## 14.5 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]) | |
| *load_term_mapping*([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_kge, ...) | |
| *deploy_head_entity_prediction*(pre_trained_kge, ...) | |
| *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*(→ None) | |
| *download_pretrained_model*(→ str) | |
| *mapping_from_first_two_cols_to_third*(train_se | |
| *timeit*(func) | |
| *load_term_mapping*([file_path]) | |
| *reload_dataset*(path, form_of_labelling, ...) | Reload the files from disk to construct the Pytorch dataset |
| *construct_dataset*(→ torch.utils.data.Dataset) | |

## 14.6 Package Contents

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

Bases: *dicee.models.base_model.BaseKGE*

A Physical Embedding Model for Knowledge Graphs

**name = 'Pyke'**

**dist_func**

**margin = 1.0**

**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

**name = 'DistMult'**

**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

**name = 'KeciBase'**

**requires_grad_for_interactions = False**

**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) -> None:
        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.

**name = 'Keci'**

**p**

**q**

**r**

**requires_grad_for_interactions = True**

**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**(*hp*, *hq*, *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

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

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

### Parameter

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

**returns**

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

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

### Parameter

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

target_entity_idx: torch.LongTensor with (n, k ) shape k denotes the selected number of examples.

**rtype**
torch.FloatTensor with (n, k) 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

**name = 'TransE'**

**margin = 4**

**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) -> None:
        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.

**name = 'DeCaL'**

**entity_embeddings**

**relation_embeddings**

**p**

**q**

**r**

**re**

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

### Parameter

x: torch.LongTensor with (n, ) shape

**rtype**

torch.FloatTensor with (n) shape

**cl_pqr**(*a: torch.tensor*) → torch.tensor

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,

$$s0 = h_0 r_0 t_0 s1 = \sum_{i=1}^{p} h_i r_i t_0 s2 = \sum_{j=p+1}^{p+q} h_j r_j t_0 s3 = \sum_{i=1}^{q} (h_0 r_i t_i + h_i r_0 t_i) s4 = \sum_{i=p+1}^{p+q} (h_0 r_i t_i + h_i r_0 t_i) s5 = \sum_{i=p+q+1}^{p+q+r} (h_0 r_i t$$

and return:

$$sigma_0 t = \sigma_0 \cdot t_0 = s0 + s1 - s2 s3, s4 and s5$$

**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

$$\sigma_p p = \sum_{i=1}^{p-1} \sum_{i'=i+1}^{p} (h_i r_{i'} - h_{i'} r_i) (models the interactions between e_i and e'_i for 1 <= i, i' <= p) \sigma_q q = \sum_{j=p+1}^{p+q-1} \sum_{j'=j+1}^{p+q} (h_j r_{j'}$$

For different base vector interactions, we have

$$\sigma_p q = \sum_{i=1}^{p} \sum_{j=p+1}^{p+q} (h_i r_j - h_j r_i)(interactionsnbetweene_i and e_j for 1 <= i <= p and p+1 <= j <= p+q) \sigma_p r = \sum_{i=}^{1}$$

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

Kvsall training

(1) Retrieve real-valued embedding vectors for heads and relations

(2) Construct head entity and relation embeddings according to Cl_{p,q, r}(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, ) 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*)

Compute .. math:

```
\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

$$\sigma^*_{q,q} = \sum_{j=p+1}^{p+q-1} \sum_{j'=j+1}^{p+q} (x_j y_{j'} - x_{j'} y_j) Eq.16$$

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*)

$$\sigma^*_{r,r} = \sum_{k=p+q+1}^{p+q+r-1} \sum_{k'=k+1}^{p} (x_k y_{k'} - x_{k'} y_k)$$

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

Compute

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

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*)

Compute

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

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.**DualE**(*args*)

Bases: *dicee.models.base_model.BaseKGE*

Dual Quaternion Knowledge Graph Embeddings (https://ojs.aaai.org/index.php/AAAI/article/download/16850/16657)

**name = 'DualE'**

**entity_embeddings**

**relation_embeddings**

**num_ent**

**kvsall_score**(*e_1_h*, *e_2_h*, *e_3_h*, *e_4_h*, *e_5_h*, *e_6_h*, *e_7_h*, *e_8_h*, *e_1_t*, *e_2_t*, *e_3_t*, *e_4_t*, *e_5_t*, *e_6_t*, *e_7_t*, *e_8_t*, *r_1*, *r_2*, *r_3*, *r_4*, *r_5*, *r_6*, *r_7*, *r_8*) → torch.tensor

KvsAll scoring function

### Input

x: torch.LongTensor with (n, ) shape

### Output

torch.FloatTensor with (n) shape

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

Negative Sampling forward pass:

### Input

x: torch.LongTensor with (n, ) shape

### Output

torch.FloatTensor with (n) shape

**forward_k_vs_all**(*x*)

KvsAll forward pass

### Input

x: torch.LongTensor with (n, ) shape

### Output

torch.FloatTensor with (n) shape

**T**(*x: torch.tensor*) → torch.tensor

Transpose function

Input: Tensor with shape (nxm) Output: Tensor with shape (mxn)

**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) -> None:
        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.

**name = 'ComplEx'**

**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

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

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

Bases: *dicee.models.base_model.BaseKGE*

Additive Convolutional ComplEx Knowledge Graph Embeddings

**name = 'AConEx'**

**conv2d**

**fc_num_input**

**fc1**

**norm_fc1**

**bn_conv2d**

**feature_map_dropout**

**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

**name = 'AConvO'**

**conv2d**

**fc_num_input**

**fc1**

**bn_conv2d**

**norm_fc1**

**feature_map_dropout**

**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

**name = 'AConvQ'**

**entity_embeddings**

**relation_embeddings**

**conv2d**

**fc_num_input**

**fc1**

**bn_conv1**

**bn_conv2**

**feature_map_dropout**

**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

**name = 'ConvQ'**

**entity_embeddings**

**relation_embeddings**

**conv2d**

**fc_num_input**

**fc1**

**bn_conv1**

**bn_conv2**

**feature_map_dropout**

**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) -> None:
        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.

**name = 'ConvO'**

**conv2d**

**fc_num_input**

**fc1**

**bn_conv2d**

**norm_fc1**

**feature_map_dropout**

**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

**name = 'ConEx'**

**conv2d**

**fc_num_input**

**fc1**

**norm_fc1**

**bn_conv2d**

**feature_map_dropout**

**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) -> None:
        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.

**name = 'QMult'**

**explicit = True**

**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) -> None:
        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.

**name = 'OMult'**

**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)

**name = 'Shallom'**

**shallom_width**

**shallom**

**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.

**name = 'LFMult'**

**entity_embeddings**

**relation_embeddings**

**degree**

**m**

**x_values**

**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:

**model_kwargs**

**name**

**model**

**loss_history = []**

**args**

**entity_embeddings = None**

**relation_embeddings = None**

**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) -> None:
        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.

**name = 'ByteE'**

**config**

**temperature = 0.5**

**topk = 2**

**transformer**

**lm_head**

**weight**

**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) -> None:
        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.

**args**

**embedding_dim = None**

**num_entities = None**

**num_relations = None**

**num_tokens = None**

**learning_rate = None**

**apply_unit_norm = None**

**input_dropout_rate = None**

**hidden_dropout_rate = None**

**optimizer_name = None**

**feature_map_dropout_rate = None**

**kernel_size = None**

**num_of_output_channels = None**

**weight_decay = None**

**loss**

**selected_optimizer = None**

**normalizer_class = None**

**normalize_head_entity_embeddings**

**normalize_relation_embeddings**

**normalize_tail_entity_embeddings**

**hidden_normalizer**

**param_init**

**input_dp_ent_real**

**input_dp_rel_real**

**hidden_dropout**

**loss_history = []**

**byte_pair_encoding**

**max_length_subword_tokens**

**block_size**

**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.**load_term_mapping**(*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: str*, *destination_folder='.'*) → None

**Parameters**

- **base_url** (e.g. "https://files.dice-research.org/projects/DiceEmbeddings/KINSHIP-Keci-dim128-epoch256-KvsAll")
- **destination_folder** (*e.g. "KINSHIP-Keci-dim128-epoch256-KvsAll"*)

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

**report**

**args**

**trainer = None**

**is_continual_training**

**storage_path**

**evaluator**

**form_of_labelling = None**

**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*)

Bases: *dicee.abstracts.BaseInteractiveKGE*

Knowledge Graph Embedding Class for interactive usage of pre-trained models

**__str__**()

**to**(*device: str*) → None

**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=''*)

**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: str | List[str] = None*, *r: str | List[str] = None*, *t: str | List[str] = None*, *topk: int = 10*, *within: List[str] = None*)

Predict missing item in a given triple.

### Parameter

head_entity: Union[str, List[str]]

String representation of selected entities.

relation: Union[str, List[str]]

String representation of selected relations.

tail_entity: Union[str, 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

**args**

**is_continual_training**

**trainer = None**

**trained_model = None**

**knowledge_graph = None**

**report**

**evaluator = None**

**start_time = None**

**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_term_mapping**(*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.

**train_set**

**ordered_bpe_entities**

**num_bpe_entities**

**neg_ratio**

**num_datapoints**

**__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.

**train_set**

**train_indices_target**

**target_dim**

**num_datapoints**

**torch_ordered_shaped_bpe_entities**

**collate_fn = None**

**__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

**train_data**

**block_size**

**num_of_data_points**

**collate_fn = None**

**__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

**train_data**

**target_dim**

**collate_fn = None**

**__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])
```

**train_data = None**

**train_target = None**

**label_smoothing_rate**

**collate_fn = None**

**__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])
```

**train_data = None**

**train_target = None**

**label_smoothing_rate**

**collate_fn = None**

**target_dim**

**store**

**__len__**()

**__getitem__**(*idx*)

**class** dicee.**OnevsSample**(*train_set: numpy.ndarray*, *num_entities*, *num_relations*, *neg_sample_ratio: int = None*, *label_smoothing_rate: float = 0.0*)

Bases: `torch.utils.data.Dataset`

A custom PyTorch Dataset class for knowledge graph embeddings, which includes both positive and negative sampling for a given dataset for multi-class classification problem..

**Parameters**

- **train_set** (*np.ndarray*) – A numpy array containing triples of knowledge graph data. Each triple consists of (head_entity, relation, tail_entity).
- **num_entities** (*int*) – The number of unique entities in the knowledge graph.
- **num_relations** (*int*) – The number of unique relations in the knowledge graph.
- **neg_sample_ratio** (*int, optional*) – The number of negative samples to be generated per positive sample. Must be a positive integer and less than num_entities.
- **label_smoothing_rate** (*float, optional*) – A label smoothing rate to apply to the positive and negative labels. Defaults to 0.0.

**train_data**

The input data converted into a PyTorch tensor.

**Type**
torch.Tensor

**num_entities**

Number of entities in the dataset.

**Type**
int

**num_relations**

Number of relations in the dataset.

**Type**
int

**neg_sample_ratio**

Ratio of negative samples to be drawn for each positive sample.

**Type**
int

**label_smoothing_rate**

The smoothing factor applied to the labels.

**Type**
torch.Tensor

**collate_fn**

A function that can be used to collate data samples into batches (set to None by default).

**Type**
function, optional

**train_data**

**num_entities**

**num_relations**

**neg_sample_ratio**

**label_smoothing_rate**

**collate_fn = None**

**__len__**()

Returns the number of samples in the dataset.

**__getitem__**(*idx*)

Retrieves a single data sample from the dataset at the given index.

**Parameters**
**idx** (*int*) – The index of the sample to retrieve.

**Returns**

**A tuple consisting of:**

- x (torch.Tensor): The head and relation part of the triple.

- y_idx (torch.Tensor): The concatenated indices of the true object (tail entity) and the indices of the negative samples.
- y_vec (torch.Tensor): A vector containing the labels for the positive and negative samples, with label smoothing applied.

**Return type**
tuple

**class** dicee.**KvsSampleDataset**(*train_set_idx: numpy.ndarray*, *entity_idxs*, *relation_idxs*, *form*, *store=None*, *neg_ratio=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

**train_data = None**

**train_target = None**

**neg_ratio**

**num_entities**

**label_smoothing_rate**

**collate_fn = None**

**store**

**max_num_of_classes**

**__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.

**neg_sample_ratio**

**train_set**

**length**

**num_entities**

**num_relations**

**__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

**label_smoothing_rate**

**neg_sample_ratio**

**train_set**

**length**

**num_entities**

**num_relations**

**__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_set_idx**

**num_entities**

**num_relations**

**neg_sample_ratio**

**batch_size**

**num_workers**

**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
```

**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*)

**train_path**

**val_path**

**test_path**

**gen_valid**

**gen_test**

**seed**

**max_ans_num = 1000000.0**

**mode**

**ent2id**

**rel2id: Dict**

**ent_in: Dict**

**ent_out: Dict**

**query_name_to_struct**

**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__ = '0.1.5'**

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