# **DICE Embeddings**

Release 0.1.3.2

## **Caglar Demir**

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DICE Embeddings<sup>1</sup>: 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<sup>2</sup>

Contact: caglar.demir@upb.de

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

Why Pandas<sup>6</sup> & 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<sup>7</sup> & 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<sup>8</sup> & PytorchLightning<sup>9</sup>. 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<sup>10</sup>? Deploy a pre-trained embedding model without writing a single line of code.

- <sup>1</sup> https://github.com/dice-group/dice-embeddings
- <sup>2</sup> https://github.com/Demirrr
- 3 https://pandas.pydata.org/
- 4 https://pytorch.org/
- <sup>5</sup> https://huggingface.co/
- 6 https://pandas.pydata.org/
- <sup>7</sup> 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["Trest"]["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
# {'H01': 0.9518788343558282, 'H03': 0.9988496932515337, 'H010': 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
# {'H01': 0.6951588502269289, 'H03': 0.9039334341906202, 'H010': 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
# {'H01': 0.9518788343558282, 'H03': 0.9988496932515337, 'H010': 1.0, 'MRR': 0.
\leftrightarrow 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

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 --
wmodel Keci --p 0 --q 1 --embedding_dim 32 --adaptive_swa
```

#### 6.2 Loading Embeddings into Qdrant Vector Database

#### 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://0.0.0.8000/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
```

```
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,
\hookrightarrow 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://
\rightarrowwww.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/<sup>11</sup>

### 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<sup>12</sup>:

Name	Stmts	Miss	Cover	Missing
dicee/initpy	7		100%	
dicee/abstracts.py	201	82		104–105, Litinues on next page)

<sup>11</sup> https://files.dice-research.org/projects/DiceEmbeddings/

<sup>12</sup> https://coverage.readthedocs.io/en/7.6.0/

```
→123, 146-147, 152, 165, 197, 240-254, 257-260, 263-266, 301, 314-317, 320-324, 364-
\Rightarrow375, 390-398, 413, 424-428, 555-575, 581-585, 589-591
dicee/callbacks.py
                                                           245
                                                                  102
\hookrightarrow67-73, 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
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dicee/dataset_classes.py
                                                           299
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→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
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→ 111, 258-353, 360-411
dicee/evaluator.py
                                                           262
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                                                                         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
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                                                           113
⇒259, 291
dicee/knowledge_graph.py
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⇔114
dicee/knowledge_graph_embeddings.py
                                                           636
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→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
                                                                        100%
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dicee/models/base_model.py
                                                                                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
                                                                  357
→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
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dicee/models/dualE.py
                                                            59
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→142-156
                                                           262
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dicee/models/function_space.py
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\Rightarrow28-37, 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
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                                                                         63%
dicee/models/octonion.py
                                                                                21-44,_
\Rightarrow320-329, 334-345, 348-370, 374-416, 426-474
dicee/models/pykeen_models.py
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dicee/models/quaternion.py
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                                                           192
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→55, 68-72, 107, 185, 328-342, 345-364, 368-389, 399-426
dicee/models/real.py
                                                            61
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\leftrightarrow 66-69, 87, 103-106
dicee/models/static_funcs.py
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dicee/models/transformers.py
                                                           236
                                                                  189
→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
```

```
dicee/query_generator.py
                                                              374
                                                                      346
                                                                               7%
                                                                                    18-52,_
\hookrightarrow56, 62-65, 69-70, 78-92, 100-147, 155-188, 192-206, 212-269, 274-303, 307-443, 453-
\hookrightarrow472, 480-501, 508-512, 517, 522-528
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dicee/read_preprocess_save_load_kg/__init__.py
dicee/read_preprocess_save_load_kg/preprocess.py
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\hookrightarrow78, 102-127, 133, 138-151, 184, 214, 388-389, 444
dicee/read_preprocess_save_load_kg/read_from_disk.py
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\hookrightarrow40, 47, 55, 58-72
dicee/read_preprocess_save_load_kg/save_load_disk.py
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dicee/read_preprocess_save_load_kg/util.py
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→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
                                                                       23
                                                                             57%
dicee/sanity_checkers.py
                                                               54
                                                                                    8-12, 21-
\rightarrow31, 46, 51, 58, 64-79, 85, 89, 96
dicee/static_funcs.py
                                                                      163
                                                                             61%
                                                                                    40, 50, ...
                                                              418
→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-
\hookrightarrow 542, 547-550, 559-610, 615-627, 644-658, 661-669
dicee/static_funcs_training.py
                                                              123
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⇔223-224
dicee/static_preprocess_funcs.py
                                                              100
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\hookrightarrow 52, 56, 64, 67, 78, 91-115, 120-123, 128-131, 136-139
dicee/trainer/__init__.py
                                                                        0
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                                                                1
dicee/trainer/dice_trainer.py
                                                              126
                                                                       13
                                                                             90%
                                                                                    27-32, _
\hookrightarrow 91, 98, 103-108, 147
dicee/trainer/torch_trainer.py
                                                               79
                                                                              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:)

```
@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,
                   {Convolutional Hypercomplex Embeddings for Link Prediction},
 title =
                 {Demir, Caglar and Moussallem, Diego and Heindorf, Stefan and Ngonga
 author =
→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 \text{ Nov}\},
 publisher =
                 {PMLR},
                 {https://proceedings.mlr.press/v157/demir21a/demir21a.pdf},
 pdf =
 url =
                 {https://proceedings.mlr.press/v157/demir21a.html},
# ConEx
@inproceedings{demir2021convolutional,
title={Convolutional Complex Knowledge Graph Embeddings},
author={Caglar Demir and Axel-Cyrille Ngonga Ngomo},
booktitle={Eighteenth Extended Semantic Web Conference - Research Track},
year={2021},
url={https://openreview.net/forum?id=6T45-4TFqaX}}
# Shallom
@inproceedings{demir2021shallow,
```

```
title={A shallow neural model for relation prediction},
author={Demir, Caglar and Moussallem, Diego and Ngomo, Axel-Cyrille Ngonga},
booktitle={2021 IEEE 15th International Conference on Semantic Computing (ICSC)},
pages={179--182},
year={2021},
organization={IEEE}
```

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

### 14 dicee

#### 14.1 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.

```
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) \rightarrow 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.
```

```
path_of_pretrained_model_dir
     [str]?
construct_ensemble: boolean
model_name: str apply_semantic_constraint : boolean
construct_ensemble
apply_semantic_constraint
configs
\texttt{get\_eval\_report}() \rightarrow dict
\texttt{get\_bpe\_token\_representation} (\textit{str\_entity\_or\_relation: List[str] | str}) \rightarrow \texttt{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)
\texttt{get\_padded\_bpe\_triple\_representation} (triples: List[List[str]]) \rightarrow Tuple[List, List, List]
          Parameters
               triples
\verb"set_model_train_mode"() \to None
      Setting the model into training mode
      Parameter
\mathtt{set}\_\mathtt{model}\_\mathtt{eval}\_\mathtt{mode}\,(\,) \, \to None
      Setting the model into eval mode
      Parameter
property name
sample\_entity(n:int) \rightarrow List[str]
{\tt sample\_relation}\,(\textit{n:int})\,\to List[\textit{str}]
is\_seen(entity: str = None, relation: str = None) \rightarrow bool
\mathbf{save}\,(\,)\,\to 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
```

```
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) \rightarrow 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
      \verb"on_fit_start" (\textit{trainer}, \textit{pl}\_\textit{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: \ \textit{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
```

on\_fit\_start (trainer, model)

Call at the beginning of the training.

```
trainer:
          model:
              rtype
                  None
     \verb|static compute_mrr|(trainer, model)| \rightarrow \verb|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
```

```
Parameter
           trainer:
           model:
               rtype
                   None
     on_fit_end(trainer, model)
           Call at the end of the training.
           Parameter
           trainer:
           model:
               rtype
                   None
     \verb"on_train_epoch_end" (\textit{trainer}, \textit{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
```

```
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:
               rtvpe
                   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"
             { "last_percent_to_consider"
backend: str = 'pandas'
     Backend to read, process, and index input knowledge graph. pandas, polars and rdflib available
separator: str = '\\s+'
     separator for extracting head, relation and tail from a triple
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
$construct\_dataset(\rightarrow torch.utils.data.Dataset)$	

#### **Module Contents**

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
```

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.



DataLoader by default constructs an index sampler that yields integral indices. To make it work with a mapstyle 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.

#### 1 Note

**Parameters** 

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)
{\tt class} \ {\tt dicee.dataset\_classes.} \\ {\tt 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 - ?
                                                 https://pytorch.org/docs/stable/data.html#torch.utils.data.
                • num_workers - int
                  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
```

- 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)
```

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



**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 AllysAll training and be defined as  $D := \{(x,y)_i\}_i ^n N$ , where x: (h,r) is a possible unique tuple of an entity h in E and a relation r in R. Hence  $N = |E| \times |R|$  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



#### 1 Note

AllvsAll extends KvsAll via none existing (h,r). Hence, it adds data points that are labelled

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()
```

```
train_data = None
train_target = None
label_smoothing_rate
collate_fn = None
target_dim
__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..

- 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
                    lnew_yl << |E| new_y contains all 1's if sum(y)< neg_sample ratio new_y contains</pre>
           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
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.

#### 1 Note

DataLoader by default constructs an index sampler that yields integral indices. To make it work with a mapstyle 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, \text{ 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: \verb"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 - ?
                                      int for https://pytorch.org/docs/stable/data.html#torch.utils.data.
                • num workers -
                  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 **:param-ref:~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.

# **A** Warning

do not assign state in prepare\_data

- fit()
- prepare\_data()
- setup()

# **1** 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
```

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```
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, ...).

# **1** 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_
```

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```
→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()
```

# 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]) <math>\rightarrow Dict
```

### **Parameters**

- model
- triples
- er\_vocab
- re\_vocab

### **Parameters**

- model
- triples

- within\_entities
- er\_vocab
- re\_vocab

### 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) \rightarrow 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)
     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)
```

```
\begin{tabular}{ll} \textbf{eval\_with\_byte} (*, raw\_train\_set, raw\_valid\_set=None, raw\_test\_set=None, trained\_model,\\ form\_of\_labelling) &\rightarrow None \end{tabular}
```

Evaluate model after reciprocal triples are added

 $\begin{tabular}{ll} \textbf{eval\_with\_bpe\_vs\_all} (*, raw\_train\_set, raw\_valid\_set=None, raw\_test\_set=None, trained\_model, \\ form\_of\_labelling) \rightarrow None \\ \end{tabular}$ 

Evaluate model after reciprocal triples are added

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)

 $\textbf{evaluate\_lp\_bpe\_k\_vs\_all} \ (model, \ triples: \ List[List[str]], \ info=None, \ form\_of\_labelling=None)$ 

### **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**

 $\verb"class" dicee.executer. \verb"Execute" (args, continuous\_training = False)$ 

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
setup_executor() \( \rightarrow \) None
dept_read_preprocess_index_serialize_data() \( \rightarrow \) None
    Read & Preprocess & Index & Serialize Input Data
```

Read & 1 reprocess & fildex & Serialize input Data

- (1) Read or load the data from disk into memory.
- (2) Store the statistics of the data.

### **Parameter**

rtype

None

```
save\_trained\_model() \rightarrow 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  $(form\_of\_labelling: str) \rightarrow dict$ 

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

 $\textbf{write\_report} \; () \; \rightarrow None$ 

Report training related information in a report.json file

 $\mathtt{start}() \rightarrow \mathrm{dict}$ 

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.

 $continual\_start() \rightarrow dict$ 

**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**

```
sparql_endpoint
path_single_kg
byte_pair_encoding
```

```
ordered_shaped_bpe_tokens = None
add_noise_rate
num_entities = None
num_relations = None
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
separator
description_of_input = None
\texttt{describe}\,()\,\to 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) \rightarrow None
      get_transductive_entity_embeddings (indices: torch.LongTensor | List[str], as_pytorch=False,
                   as\_numpy = False, as\_list = True) \rightarrow 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)
                    \rightarrow 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
```

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

```
{\tt predict\_missing\_tail\_entity}.\ \textit{List[str]} \ | \ \textit{str}, \ \textit{relation: List[str]} \ | \ \textit{str}, \\
```

*within:* List[str] = None  $\rightarrow$  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

 $predict(*, h: List[str] | str = None, r: List[str] | str = None, t: List[str] | str = None, within=None, logits=True) <math>\rightarrow$  torch.FloatTensor

### **Parameters**

- logits
- h
- r
- t
- within

```
predict_topk(*, h: str \mid List[str] = None, r: str \mid List[str] = None, t: str \mid 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)
               \rightarrow torch.FloatTensor
```

# Parameter

head\_entity: List[str]

Predict triple score

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

 $t_norm(tens\_1: torch.Tensor, tens\_2: torch.Tensor, tnorm: str = 'min') \rightarrow torch.Tensor$ 

 $tensor\_t\_norm$  ( $subquery\_scores$ : torch.FloatTensor, tnorm: str = 'min')  $\rightarrow$  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')  $\rightarrow$  torch.Tensor

 $negnorm(tens\_1: torch.Tensor, lambda\_: float, neg\_norm: str = 'standard') \rightarrow torch.Tensor$ 

```
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) \rightarrow 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) > \text{confidence}.
          at most: int
          Stop after finding at most missing triples
          \{(e,r,x) \mid f(e,r,x) > \text{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,  $batch\_size=32$ ,  $neg\_sample\_ratio=10$ ,  $num\_workers=1$ )  $\rightarrow$  None Retrained a pretrain model on an input KG via negative sampling.

### 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.

### 1 Note

As per the example above, an \_\_init\_\_() call to the parent class must be made before assignment on the child

### Variables

**training**  $(b \circ o 1)$  – Boolean represents whether this module is in training or evaluation mode.

```
\label{eq:training_step_outputs} \begin{tabular}{ll} training_step_outputs = [] \\ \\ mem_of_model() \rightarrow Dict \\ \end{tabular}
```

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()
```

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 Light-ningModule 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])

### $\texttt{test\_dataloader}\,()\,\to None$

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.

# Λ

# Warning

do not assign state in prepare\_data

• test()

- prepare\_data()
- setup()

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

# 1 Note

If you don't need a test dataset and a test\_step(), you don't need to implement this method.

# ${\tt val\_dataloader}\,()\,\to None$

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 **:param-ref:** "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()

### 1 Note

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

### 1 Note

If you don't need a validation dataset and a  $validation\_step()$ , you don't need to implement this method.

# $\texttt{predict\_dataloader}\,() \, \to None$

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()

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.

### $\texttt{train\_dataloader}\,()\,\to None$

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 **:param-ref: ~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.

# **A** Warning

do not assign state in prepare\_data

- fit()
- prepare\_data()
- setup()

### 1 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.

# 1 Note

Some things to know:

- Lightning calls .backward() and .step() automatically in case of automatic optimization.
- If a learning rate scheduler is specified in <code>configure\_optimizers()</code> with key "interval" (default "epoch") in the scheduler configuration, Lightning will call the scheduler's <code>.step()</code> 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.

# 1 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) \rightarrow 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)
     \texttt{get\_embeddings} \ () \ \rightarrow 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)

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.

As per the example above, an <u>\_\_init\_\_()</u> call to the parent class must be made before assignment on the child.

### Variables

**training**  $(b \circ \circ 1)$  – 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)

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.

As per the example above, an \_\_init\_\_() call to the parent class must be made before assignment on the child.

### **Variables**

**training**  $(b \circ o 1)$  – Boolean represents whether this module is in training or evaluation mode.

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.

```
\texttt{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.

```
\texttt{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):

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

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

eq j

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

$$(1) \ sigma\_0 = h\_0 \ r\_0 + sum\_\{i=1\}^p \ (h\_0 \ r\_i) \ e\_i - sum\_\{j=p+1\}^p \ (h\_j \ r\_j) \ e\_j$$

(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 
$$\{qq\} = sum \{j=1\}^{p+q-1} sum \{k=j+1\}^{p+q} (h jr k-h kr j) e je k$$

(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)

 $forward_k_vs_all(x: torch.Tensor) \rightarrow torch.FloatTensor$ 

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 functions 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) \rightarrow 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) \rightarrow torch.FloatTensor
           Parameter
           x: torch.LongTensor with (n,3) shape
                   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
```

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```
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.

# 1 Note

As per the example above, an <u>\_\_init\_\_()</u> 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)  $\rightarrow$  torch.tensor

Input: tensor(batch\_size, emb\_dim)  $\longrightarrow$  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_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_i + h_i r_0 t_i) s4 = \sum_{i=p+q+1}^{p+q+r} (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_i + h_i r_0 t_i) s4 = \sum_{i=p+q+1}^{p+q+r} (h_0 r_i t_i + h_i r_0 t_i) s4 = \sum_{i=p+q+1}^{p+q+r} (h_0 r_i t_i + h_i r_0 t_i) s4 = \sum_{i=p+q+1}^{p+q+r} (h_0 r_i t_i + h_i r_0 t_i) s4 = \sum_{i=p+q+1}^{p+q+r} (h_0 r_i t_i + h_i r_0 t_i) s4 = \sum_{i=p+q+1}^{p+q+r} (h_0 r_i t_i + h_i r_0 t_i) s4 = \sum_{i=p+q+1}^{p+q+r} (h_0 r_i t_i + h_i r_0 t_i) s4 = \sum_{i=p+q+1}^{p+q+r} (h_0 r_i t_i + h_i r_0 t_i) s4 = \sum_{i=p+q+1}^{p+q+r} (h_0 r_i t_i + h_i r_0 t_i) s4 = \sum_{i=p+q+1}^{p+q+r} (h_0 r_i t_i + h_i r_0 t_i) s4 = \sum_{i=p+q+1}^{p+q+r} (h_0 r_i t_i + h_i r_0 t_i) s4 = \sum_{i=p+q+1}^{p+q+r} (h_0 r_i t_i + h_i r_0 t_i) s4 = \sum_{i=p+q+1}^{p+q+r} (h_0 r_i t_i + h_i r_0 t_i) s4 = \sum_{i=p+q+1}^{p+q+r} (h_0 r_i t_i + h_i r_0 t_i) s4 = \sum_{i=p+q+1}^{p+q+r} (h_0 r_i t_i + h_i r_0 t_i) s4 = \sum_{i=p+q+1}^{p+q+r} (h_0 r_i t_i + h_i r_0 t_i) s4 = \sum_{i=p+q+1}^{p+q+r} (h_0 r_i t_i + h_i r_0 t_i) s4 = \sum_{i=p+q+1}^{p+q+r} (h_0 r_i t_i + h_i r_0 t_i) s4 = \sum_{i=p+q+r}^{p+q+r} (h_0 r_i t_i + h_i r_0 t_i) s4 = \sum_{i=p+q+r}^{p+q+r} (h_0 r_i t_i + h_i r_0 t_i) s4 = \sum_{i=p+q+r}^{p+q+r} (h_0 r_i t_i + h_i r_0 t_i) s4 = \sum_{i=p+q+r}^{p+q+r} (h_0 r_i t_i + h_i r_0 t_i) s4 = \sum_{i=p+q+r}^{p+q+r} (h_0 r_i t_i + h_i r_0 t_i) s4 = \sum_{i=p+q+r}^{p+q+r} (h_0 r_i t_i + h_i r_0 t_i) s4 = \sum_{i=p+q+r}^{p+q+r} (h_0 r_i t_i + h_i r_0 t_i) s4 = \sum_{i=p+q+r}^{p+q+r} (h_0 r_i t_i + h_i r_0 t_i) s4 = \sum_{i=p+q+r}^{p+q+r} (h_0 r_i t_i + h_i r_0 t_i) s4 = \sum_{i=p+q+r}^{p+q+r} (h_0 r_i t_i + h_i r_0 t_i) s4 = \sum_{i=p+q+r}^{p+q+r} (h_0 r_i t_i + h_i r_0 t_i) s4 = \sum_{i=p+q+r}^{p+q+r} (h_0 r_i t_i + h_i r_0 t_i) s4 = \sum_{i=p+q+r}^{p+q+r} (h_0 r_i t_i + h_i r_0 t_i) s4 = \sum_{i=p+q+r}^{p+q+r}$$

and return:

$$sigma_0t = \sigma_0 \cdot t_0 = s0 + s1 - s2s3, s4ands5$$

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

For different base vector interactions, we have

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

 $\textbf{forward\_k\_vs\_all} \ (\textit{x: torch.Tensor}) \ \rightarrow \text{torch.FloatTensor}$ 

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:

$$\label{eq:sigma_pp}^* = \sum_{i=1}^{p-1}\sum_{i'=i+1}^{p} (x_{i'}-x_{i'}y_{i})$$

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):

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

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

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[:, :, 
$$i$$
] \* rq[:, :,  $k$ ] - hq[:, :,  $k$ ] \* rq[:, :,  $i$ ])

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

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

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 Em-
	beddings
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]) \rightarrow 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) \rightarrow torch.FloatTensor
     forward\_triples(x: torch.Tensor) \rightarrow torch.FloatTensor
               Parameters
     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]) \rightarrow 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) \rightarrow torch.FloatTensor
     forward\_triples(x: torch.Tensor) \rightarrow torch.FloatTensor
               Parameters
     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.

# **1** 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.

- emb\_h
- emb\_r
- emb\_E

 $\textbf{forward\_k\_vs\_all} \ (\textit{x: torch.LongTensor}) \ \rightarrow \ torch.FloatTensor$ 

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
                     {\tt 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\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e_4\_t,e_4\_t,e_4\_t,e_4\_t,e_4\_t,e_4\_t,e_4\_t,e_4\_t,e_4\_t,e_4\_t,e_4\_t,e_4\_t,e_4\_t,e_4\_t,e_4\_t,e_4\_t,e_4\_t,e_4\_t,e_4\_t,e_4\_t,e_4\_t,e_4\_t,e_4\_t,e_4\_t,e_4\_t,e_4\_t,e_4\_t,e_4\_t,e_4\_t,e_4\_t,e_4\_t,e_4\_t,e_4\_t,e_4\_t,e_4\_t,e_4\_t,e_4\_t,e_4\_t,e_4\_t,e_4\_t,e_4\_t,e_4\_t,e_4\_t,e_4\_t,e_4\_t,e_4\_t,e_4\_t,e_4\_t,e_4\_t,e_4\_t,e_4\_t,e_4\_t,e_4\_t,e_4\_t,e_4\_t,e_4\_t,e_4\_t,e_4\_t,e_4\_t,e_4\_t,e_4\_t,e_4\_t,e_4\_t,e_4\_t,e_4\_t,e_4\_t,e_4\_t,e_4\_t,e_4\_t,e_4\_t,e_4\_t,e_4\_t,e_4\_t,e_4\_t,e_4\_t,e_4\_t,e_4\_t,e_4\_t,e_4\_t,e_4\_t,e_4\_t,e_4\_t,e_4\_t,e_4\_t,e_4\_
                                                                    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) \rightarrow \text{torch.tensor}
                                        KvsAll scoring function
                                        Input
                                        x: torch.LongTensor with (n, ) shape
                                         Output
                                         torch.FloatTensor with (n) shape
                     forward\_triples(idx\_triple: torch.tensor) \rightarrow 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) \rightarrow 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
      num_sample = 50
      gamma
      roots
      weights
      \verb|compute_func| (\textit{weights: torch.FloatTensor}, \textit{x}) \rightarrow \textit{torch.FloatTensor}
      chain_func(weights, x: torch.FloatTensor)
      \textbf{forward\_triples} \ (\textit{idx\_triple: torch.Tensor}) \ \rightarrow \textbf{torch.Tensor}) \ \rightarrow \textbf{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
      num_sample = 250
```

```
roots
     weights
     compute\_func(weights: torch.FloatTensor, x) \rightarrow torch.FloatTensor
     chain_func (weights, x: torch.FloatTensor)
     forward_triples (idx\_triple: torch.Tensor) \rightarrow torch.Tensor
               Parameters
class dicee.models.function_space.FMult2(args)
     Bases: dicee.models.base_model.BaseKGE
     Learning Knowledge Neural Graphs
     name = 'FMult2'
     n_{ayers} = 3
     n = 50
     score_func = 'compositional'
     discrete_points
     entity_embeddings
     relation_embeddings
     build_func(Vec)
     build_chain_funcs (list_Vec)
     compute\_func(W, b, x) \rightarrow torch.FloatTensor
     function (list\_W, list\_b)
     trapezoid(list_W, list_b)
     forward\_triples(idx\_triple: torch.Tensor) \rightarrow torch.Tensor
               Parameters
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=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)
     \mathtt{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
                   ×
     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 $[0][0] + \text{coeff}[0][1]x + ... + \text{coeff}[0][d]x^d$ ,

```
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.
AConv0	Additive Convolutional Octonion Knowledge Graph Embeddings

# **Functions**

```
 \begin{array}{l} \textit{octonion\_mul(*, O\_1, O\_2)} \\ \textit{octonion\_mul\_norm(*, O\_1, O\_2)} \end{array}
```

# **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.

# 1 Note

As per the example above, an \_\_init\_\_() call to the parent class must be made before assignment on the child.

#### Variables

**training**  $(b \circ o 1)$  – 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)
{\tt forward\_k\_vs\_all}\;(\mathcal{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.



conv2d

# 1 Note

As per the example above, an \_\_init\_\_() call to the parent class must be made before assignment on the child.

### Variables

**training**  $(b \circ o 1)$  – 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) \rightarrow 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'
```

```
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) \rightarrow 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
```

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,  $r = self.get_head_relation_representation(x) # (2) Reshape (1). if <math>self.last_dim > 0$ :
  - $h = h.reshape(len(x), self.embedding\_dim, self.last\_dim) r = r.reshape(len(x), self.embedding\_dim, self.last\_dim)$
- # (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) $\rightarrow$ 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.



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.

```
\label{eq:name} \begin{tabular}{ll} name = 'QMult' \\ \\ explicit = True \\ \\ quaternion_multiplication_followed_by_inner_product $(h,r,t)$ \\ \\ \end{tabular}
```

# **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.

 $\verb|static quaternion_normalizer| (x: torch.FloatTensor)| \rightarrow torch.FloatTensor|$ 

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:

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

```
Parameters
                   \mathbf{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
     {\tt forward\_k\_vs\_all}\;(\mathcal{X})
               Parameters
     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 \text{ 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) \rightarrow 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] =>
```

Entities<sub>()</sub>

[0.0,0.1,...,0.8], shape=> (1, |Entities|) Given a batch of head entities and relations => shape (size of batch,)

```
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
     \verb"residual_convolution" (Q\_1, Q\_2)
     forward\_triples (indexed_triple: torch.Tensor) \rightarrow torch.Tensor
               Parameters
     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,|
```

# dicee.models.real

Entities()

### **Classes**

DistMult	Embedding Entities and Relations for Learning and Infer-
	ence 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/
     1 cecc 7a 779 28 ca 8133 fa 2468 0a 88d 2f 9-Paper.pdf\\
     name = 'TransE'
     margin = 4
     score (head_ent_emb, rel_ent_emb, tail_ent_emb)
     \textbf{forward\_k\_vs\_all} \ (\textit{x: torch.Tensor}) \ \rightarrow \text{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
     \texttt{get\_embeddings}\,() \, \to Tuple[numpy.ndarray,\,None]
     forward_k_vs_all (x) \rightarrow \text{torch.FloatTensor}
     forward\_triples(x) \rightarrow torch.FloatTensor
               Parameters
               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( \rightarrow Tuple[torch.Tensor, torch.Tensor, Perform quaternion multiplication ...)
```

### **Module Contents**

```
\label{eq:dicee.models.static_funcs.quaternion_mul} (*, Q_1, Q_2) \\ \rightarrow 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) hugging-face/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.



### 1 Note

As per the example above, an \_\_init\_\_() call to the parent class must be made before assignment on the child.

#### Variables

name = 'BytE'

**training**  $(b \circ o 1)$  – Boolean represents whether this module is in training or evaluation mode.

```
config
temperature = 0.5
topk = 2
transformer
lm_head
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()
```

#### 1 Note

When accumulate\_grad\_batches > 1, the loss returned here will be automatically normalized by accumulate\_grad\_batches internally.

```
{\tt class} \ {\tt dicee.models.transformers.LayerNorm} \, (\textit{ndim}, \textit{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.

# 1 Note

As per the example above, an \_\_init\_\_() call to the parent class must be made before assignment on the child.

#### **Variables**

**training**  $(b \circ o 1)$  – 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.

# 1 Note

As per the example above, an \_\_init\_\_() call to the parent class must be made before assignment on the child.

#### **Variables**

**training**  $(b \circ o 1)$  – 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.

# 1 Note

As per the example above, an \_\_init\_\_() call to the parent class must be made before assignment on the child.

### Variables

**training**  $(b \circ \circ 1)$  – 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.

# 1 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

```
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.

### **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 Infer-
	ence in Knowledge Bases
TransE	Translating Embeddings for Modeling

Table 1 - continued from previous page

	Table 1 - Continued Iron previous page
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.
AConv0	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:
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**

```
\begin{array}{ll} \textit{quaternion\_mul}(\rightarrow \text{Tuple[torch.Tensor, torch.Tensor,} & \textit{Perform quaternion multiplication} \\ \textit{...}) \\ \textit{quaternion\_mul\_with\_unit\_norm}(*, Q\_1, Q\_2) \\ \textit{octonion\_mul}(*, O\_1, O\_2) \\ \textit{octonion\_mul\_norm}(*, O\_1, O\_2) \\ \end{array}
```

## **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.

# **1** Note

As per the example above, an \_\_init\_\_() call to the parent class must be made before assignment on the child.

#### Variables

**training**  $(b \circ o 1)$  – Boolean represents whether this module is in training or evaluation mode.

```
training_step_outputs = []
```

```
{\tt mem\_of\_model}\,()\,\to 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()
```

### 1 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 Light-ningModule 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])

#### $\texttt{test\_dataloader}() \rightarrow None$

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.

# **Marning**

do not assign state in prepare\_data

- test()
- prepare\_data()
- setup()

### **1** Note

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

### 1 Note

If you don't need a test dataset and a test\_step(), you don't need to implement this method.

### ${\tt val\_dataloader}\,()\,\to None$

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 :param-ref:`~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()

### **1** Note

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

# **1** Note

If you don't need a validation dataset and a  $validation\_step()$ , you don't need to implement this method.

### $predict\_dataloader() \rightarrow None$

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()

# **1** Note

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

### Returns

 $A \; {\tt torch.utils.data.DataLoader} \; or \; a \; sequence \; of \; them \; specifying \; prediction \; samples.$ 

### $train\_dataloader() \rightarrow None$

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 **:param-ref:** `**-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()



### 1 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.

### **1** Note

Some things to know:

- Lightning calls .backward() and .step() automatically in case of automatic optimization.
- If a learning rate scheduler is specified in <code>configure\_optimizers()</code> with key "interval" (default "epoch") in the scheduler configuration, Lightning will call the scheduler's <code>.step()</code> 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.

# **1** 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) \rightarrow torch.Tensor
        Parameters
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)
```

```
\begin{tabular}{ll} \tt get\_bpe\_head\_and\_relation\_representation~(x:torch.LongTensor)\\ &\rightarrow Tuple[torch.FloatTensor, torch.FloatTensor]\\ \hline & {\bf Parameters}\\ & {\bf x}~(B~x~2~x~T)\\ \hline & \tt get\_embeddings~() \rightarrow Tuple[numpy.ndarray, numpy.ndarray]\\ \hline \end{tabular}
```

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.

# **1** Note

As per the example above, an \_\_init\_\_() call to the parent class must be made before assignment on the child.

#### Variables

**training**  $(b \circ o 1)$  – 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.

# 1 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
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) \rightarrow torch.Tensor
        Parameters
forward_k_vs_all(*args, **kwargs)
forward_k_vs_sample(*args, **kwargs)
get_triple_representation(idx_hrt)
{\tt 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)
     \mathtt{get\_embeddings}() \rightarrow \mathsf{Tuple}[\mathsf{numpy}.\mathsf{ndarray}, \mathsf{numpy}.\mathsf{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) \rightarrow 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
     get_embeddings() → Tuple[numpy.ndarray, None]
     forward_k_vs_all (x) \rightarrow \text{torch.FloatTensor}
     forward_triples (x) \rightarrow \text{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
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.

# 1 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) \rightarrow torch.Tensor
              Parameters
     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
```

```
fc1
     norm_fc1
     bn_conv2d
     feature_map_dropout
     residual_convolution(C_1: Tuple[torch.Tensor, torch.Tensor],
                  C_2: Tuple[torch.Tensor, torch.Tensor]) \rightarrow 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) \rightarrow torch.FloatTensor
     forward\_triples(x: torch.Tensor) \rightarrow torch.FloatTensor
               Parameters
     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]) \rightarrow 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) \rightarrow torch.FloatTensor
     forward_triples (x: torch.Tensor) \rightarrow torch.FloatTensor
               Parameters
     forward_k_vs_sample (x: torch.Tensor, target_entity_idx: torch.Tensor)
```

fc\_num\_input

```
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.

# 1 Note

As per the example above, an \_\_init\_\_() call to the parent class must be made before assignment on the child.

#### Variables

**training**  $(b \circ \circ 1)$  – Boolean represents whether this module is in training or evaluation mode.

### **Parameters**

- emb\_h
- emb\_r
- emb E

 $\textbf{forward\_k\_vs\_all} \ (\textit{x: torch.LongTensor}) \ \rightarrow \ torch.FloatTensor$ 

forward\_k\_vs\_sample (x: torch.LongTensor, target\_entity\_idx: torch.LongTensor)

```
dicee.models.quaternion_mul(*,Q_1,Q_2)
```

 $\rightarrow Tuple[torch.Tensor, torch.Tensor, torch.Tensor, torch.Tensor]$ 

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.

# 1 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) \rightarrow 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)
     \mathtt{get\_embeddings}() \rightarrow 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.

# 1 Note

As per the example above, an \_\_init\_\_() call to the parent class must be made before assignment on the child.

### **Variables**

**training**  $(b \circ o 1)$  – 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.

# 1 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.

 $static quaternion\_normalizer(x: torch.FloatTensor) \rightarrow torch.FloatTensor$ 

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:

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

### **Parameters**

 $\mathbf{x}$  – The vector.

### Returns

The normalized vector.

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
     {\tt residual\_convolution}\,(Q\_1,\,Q\_2)
     forward\_triples (indexed\_triple: torch.Tensor) \rightarrow torch.Tensor
               Parameters
     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
     {\tt residual\_convolution}\,(Q\_I,\,Q\_2)
     forward\_triples (indexed\_triple: torch.Tensor) \rightarrow torch.Tensor
               Parameters
     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.

# 1 Note

As per the example above, an <u>\_\_init\_\_\_()</u> 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) \rightarrow 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)
     \mathtt{get\_embeddings}() \rightarrow 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.

# 1 Note

As per the example above, an \_\_init\_\_() call to the parent class must be made before assignment on the child.

### **Variables**

**training**  $(b \circ o 1)$  – 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):
        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.

# 1 Note

As per the example above, an \_\_init\_\_() call to the parent class must be made before assignment on the child.

### Variables

**training**  $(b \circ o 1)$  – Boolean represents whether this module is in training or evaluation mode.

name = 'OMult'

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.

# **1** 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) \rightarrow torch.Tensor
               Parameters
     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 l)
class dicee.models.AConvO(args: dict)
     Bases: dicee.models.base_model.BaseKGE
     Additive Convolutional Octonion Knowledge Graph Embeddings
     name = 'AConvO'
     conv2d
     fc_num_input
     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) \rightarrow torch.Tensor
               Parameters
     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.
```

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

Your models should also subclass this class.

```
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.

# 1 Note

As per the example above, an \_\_init\_\_() call to the parent class must be made before assignment on the child.

### Variables

**training**  $(b \circ o 1)$  – 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_q = 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 i 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 h_j e_j r = r_0 + sum_{i=1}^p r_i e_i + sum_{j=p+1}^n h_j e_j r = r_0 + sum_{i=1}^n h_j e_j r = r_0 + sum_{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 ir j-h jr i) e ie 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) \rightarrow 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) \rightarrow 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.
                    torch.FloatTensor with (n, k) shape
      score (h, r, t)
      forward\_triples(x: torch.Tensor) \rightarrow 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.

# **1** Note

As per the example above, an \_\_init\_\_() call to the parent class must be made before assignment on the child.

### Variables

**training**  $(b \circ o 1)$  – 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) \rightarrow torch.FloatTensor
```

### **Parameter**

x: torch.LongTensor with (n, ) shape

### rtype

torch.FloatTensor with (n) shape

 $cl\_pqr(a: torch.tensor) \rightarrow torch.tensor$ 

Input: tensor(batch\_size, emb\_dim)  $\longrightarrow$  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_i + h_i r_0 t_i) s4 = \sum_{i=p+1}^{p+q+r} (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_i + h_i r_0 t_i) s4 = \sum_{i=p+q+1}^{p+q+r} (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_i + h_i r_0 t_i) s4 = \sum_{i=p+q+1}^{p+q+r} (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_i + h_i r_0 t_i) s4 = \sum_{i=p+q+1}^{p+q+r} (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_i + h_i r_0 t_i) s5 = \sum_{i=p+q+1}^{p+q+r} (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_i + h_i r_0 t_i) s5 = \sum_{i=p+q+1}^{p+q+r} (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_i + h_i r_0 t_i) s5 = \sum_{i=p+q+1}^{p+q+r} (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_i + h_i r_0 t_i) s5 = \sum_{i=p+q+1}^{p+q+r} (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_i + h_i r_0 t_i) s5 = \sum_{i=p+q+1}^{p+q+r} (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_i + h_i r_0 t_i) s5 = \sum_{i=p+q+1}^{p+q+r} (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_i + h_i r_0 t_i) s5 = \sum_{i=p+q+1}^{p+q+r} (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_i + h_i r_0 t_i) s5 = \sum_{i=p+q+r}^{p+q+r} (h_0 r_i t_i + h_i r_0 t_i) s5 = \sum_{i=p+q+r}^{p+q+r} (h_0 r_i t_i + h_i r_0 t_i) s5 = \sum_{i=p+q+r}^{p+q+r} (h_0 r_i t_i + h_i r_0 t_i) s5 = \sum_{i=p+q+r}^{p+q+r} (h_0 r_i t_i + h_i r_0 t_i) s5 = \sum_{i=p+q+r}^{p+q+r} (h_0 r_i t_i + h_i r_0 t_i) s5 = \sum_{i=p+q+r}^{p+q+r} (h_0 r_i t_i + h_i r_0 t_i) s5 = \sum_{i=p+q+r}^{p+q+r} (h_0 r_i t_i + h_i r_0 t_i) s5 = \sum_{i=p+q+r}^{p+q+r} (h_0 r_i t_i + h_i r_0 t_i) s5 = \sum_{i=p+q+r}^{p+q+r} (h_0 r_i t_i + h_i r_0 t_i) s5 = \sum_{i=p+q+r}^{p+q+r} (h_0 r_i t_i + h_i r_0 t_i) s5 = \sum_{i=p+q+r}^{p+q+r} (h_0 r_i t_i + h_i r_0 t_i) s5 = \sum_{i=p+q+r}^{p+q+r} (h_0 r_i t_i + h_i r_0 t_i) s5 = \sum_{i=p+q+r}^{p+q+$$

and return:

$$sigma_0t = \sigma_0 \cdot t_0 = s0 + s1 - s2s3, s4ands5$$

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

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

For different base vector interactions, we have

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

 $forward_k_vs_all(x: torch.Tensor) \rightarrow torch.FloatTensor$ 

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:

```
\label{eq:sigma_p} $$ \sum_{p,p}^* = \sum_{i=1}^{p-1}\sum_{i'=i+1}^{p} (x_iy_{i'}-x_{i'}y_i) $$
```

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,

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):

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

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

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.



# 1 Note

As per the example above, an \_\_init\_\_() call to the parent class must be made before assignment on the

### **Variables**

**training**  $(b \circ \circ 1)$  – 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) \rightarrow torch.Tensor
        Parameters
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: Py-
            keen_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.embeddin
                                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) \rightarrow 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 <math>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.

# 1 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
\textbf{forward\_triples}~(\textit{x:torch.LongTensor})~\rightarrow torch.Tensor
        Parameters
forward_k_vs_all(*args, **kwargs)
forward_k_vs_sample(*args, **kwargs)
{\tt get\_triple\_representation}\,(idx\_hrt)
```

```
get_head_relation_representation(indexed_triple)
     get_sentence_representation(x: torch.LongTensor)
              Parameters
                  • (b (x shape)
                  • 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
     num_sample = 50
     gamma
     roots
     weights
     \verb|compute_func| (\textit{weights: torch.FloatTensor}, \textit{x}) \rightarrow \textit{torch.FloatTensor}
     chain_func (weights, x: torch.FloatTensor)
     forward\_triples (idx\_triple: torch.Tensor) \rightarrow torch.Tensor
              Parameters
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) \rightarrow torch.FloatTensor
     chain_func (weights, x: torch.FloatTensor)
     forward_triples (idx\_triple: torch.Tensor) \rightarrow torch.Tensor
               Parameters
class dicee.models.FMult2(args)
     Bases: dicee.models.base_model.BaseKGE
     Learning Knowledge Neural Graphs
     name = 'FMult2'
     n layers = 3
     n = 50
     score_func = 'compositional'
     discrete_points
     entity_embeddings
     relation_embeddings
     build_func(Vec)
     build_chain_funcs (list_Vec)
     compute\_func(W, b, x) \rightarrow torch.FloatTensor
     function(list_W, list_b)
     trapezoid(list_W, list_b)
     forward\_triples(idx\_triple: torch.Tensor) \rightarrow torch.Tensor
               Parameters
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=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)
     \mathtt{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
```

```
\mathtt{vtp\_score}(h, r, t)
```

this part implement the vector triple product scoring techniques:

```
score(h,r,t) = int_{0}{1} \quad h(x)r(x)t(x) \quad dx = sum_{i,j,k} = 0^{d-1} \quad 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*) 
$$\rightarrow$$
 torch.tensor

KvsAll scoring function

# Input

x: torch.LongTensor with (n, ) shape

# Output

torch.FloatTensor with (n) shape

 $forward\_triples(idx\_triple: torch.tensor) \rightarrow torch.tensor$ 

Negative Sampling forward pass:

# Input

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

# **Output**

torch.FloatTensor with (n) shape

```
{\tt forward\_k\_vs\_all}\;(\mathcal{X})
```

KvsAll forward pass

# Input

x: torch.LongTensor with (n, ) shape

# **Output**

torch.FloatTensor with (n) shape

**T** (x: torch.tensor)  $\rightarrow$  torch.tensor

Transpose function

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

# dicee.query\_generator

# **Classes**

QueryGenerator

# **Module Contents**

rel2id: Dict

```
ent_in: Dict
      ent_out: Dict
      query_name_to_struct
      list2tuple (list_data)
      tuple2list(x: List | Tuple) \rightarrow List | Tuple
           Convert a nested tuple to a nested list.
      set_global_seed (seed: int)
           Set seed
      construct\_graph(paths: List[str]) \rightarrow 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) \rightarrow 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]]])
                    \rightarrow None
           Save Queries into Disk
      static load\_queries\_and\_answers (path: str) \rightarrow List[Tuple[str, Tuple[collections.defaultdict]]]
           Load Queries from Disk to Memory
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
     \mathtt{start}() \to \mathrm{None}
           Preprocess train, valid and test datasets stored in knowledge graph instance
           Parameter
               rtype
                   None
     preprocess_with_byte_pair_encoding()
     {\tt preprocess\_with\_byte\_pair\_encoding\_with\_padding}\,()\,\to None
     {\tt preprocess\_with\_pandas}\,()\,\to 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
     {\tt preprocess\_with\_polars}\,()\,\to None
     \verb"sequential_vocabulary_construction"\ () \ \to 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
```

ReadFromDisk

**Classes** 

Read the data from disk into memory

# **Module Contents**

```
{\tt class} \  \, {\tt dice.read\_preprocess\_save\_load\_kg.read\_from\_disk.ReadFromDisk} \, (kg) \\  \  \, {\tt Read} \  \, {\tt the} \  \, {\tt data} \  \, {\tt from} \  \, {\tt disk} \  \, {\tt into} \  \, {\tt memory} \\  \  \, {\tt 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
```

LoadSaveToDisk

**Classes** 

# **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
<pre>pandas_dataframe_indexer(→ pandas.DataFrame)</pre>	Replaces 'subject', 'relation', and 'object' columns in the input Pandas DataFrame with their corresponding index values
<pre>apply_reciprical_or_noise(add_reciprical, eval_model)</pre>	
timeit(func)	
$read\_with\_polars(\rightarrow polars.DataFrame)$	Load and Preprocess via Polars
read_with_pandas(data_path[, read_only_few,])	
read_from_disk(→ Tuple[polars.DataFrame, pan-das.DataFrame])	
read_from_triple_store([endpoint])	Read triples from triple store into pandas dataframe
get_er_vocab(data[, file_path])	parameter and parameter
<pre>get_re_vocab(data[, file_path])</pre>	
<pre>get_ee_vocab(data[, file_path])</pre>	
<pre>create_constraints(triples[, file_path])</pre>	
$load\_with\_pandas(\rightarrow None)$	Deserialize data
<pre>save_numpy_ndarray(*, data, file_path)</pre>	
load_numpy_ndarray(*, file_path)	
<pre>save_pickle(*, data[, file_path])</pre>	
<pre>load_pickle(*[, file_path])</pre>	
<pre>create_recipriocal_triples(X)</pre>	Add inverse triples into dask 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) <math>\rightarrow 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.pandas_dataframe_indexer( df_pandas: pandas.DataFrame, idx_entity: pandas.DataFrame, idx_relation: pandas.DataFrame) <math>\rightarrow pandas.DataFrame
```

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

### **Parameters:**

# df\_pandas

[pd.DataFrame] The input Pandas DataFrame containing columns: 'subject', 'relation', and 'object'.

# idx\_entity

[pd.DataFrame] A Pandas DataFrame that contains the mapping between entity names and their corresponding indices. Must have columns: 'entity' and 'index'.

### idx relation

[pd.DataFrame] A Pandas DataFrame that contains the mapping between relation names and their corresponding indices. Must have columns: 'relation' and 'index'.

### **Returns:**

# pd.DataFrame

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

```
dicee.read_preprocess_save_load_kg.util.apply_reciprical_or_noise (add_reciprical: bool, eval_model: str, df: object = None, info: str = None)
```

read\_only\_few: int = None, sample\_triples\_ratio: float = None, separator: 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,
```

 $\rightarrow$  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, separator: str = 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: str = None, separator: str = None) → Tuple[polars.DataFrame, pandas.DataFrame]
```

```
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_kq.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) \rightarrow None
```

Deserialize data

### **Classes**

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

# **Package Contents**

(2) Construct vocabulary

(3) Index datasets

```
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
```

# **Parameter**

```
rtvpe
                   None
     {\tt preprocess\_with\_polars}\, () \, \to None
     \verb|sequential_vocabulary_construction|()| \to 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
     \mathtt{start}() \rightarrow \mathrm{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.sanity checkers

### **Functions**

### **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.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.serve

### **Attributes**

```
app
neural_searcher
```

### **Classes**

*NeuralSearcher* 

### **Functions**

```
get_default_arguments()

root()

search_embeddings(q)

retrieve_embeddings(q)

main()
```

# **Module Contents**

# dicee.static\_funcs

### **Functions**

create\_recipriocal\_triples(x)

Add inverse triples into dask dataframe

Table 2 - continued from previous page

```
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])
                         is_continual_training,
select_model(args[,
                                                 stor-
age path])
load_model(→ Tuple[object, Tuple[dict, dict]])
                                                        Load weights and initialize pytorch module from names-
                                                        pace arguments
                                                        Construct Ensemble Of weights and initialize pytorch
load_model_ensemble(...)
                                                        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(\rightarrow None)
                                                        Store Pytorch model into disk
store(\rightarrow None)
                                                        Store trained_model model and save embeddings into csv
add\_noisy\_triples(\rightarrow pandas.DataFrame)
                                                        Add randomly constructed triples
read_or_load_kg(args, cls)
intialize\_model(\rightarrow Tuple[object, str])
load_json(\rightarrow dict)
                                                        Save it as CSV if memory allows.
save\_embeddings(\rightarrow None)
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])
continual\_training\_setup\_executor(\rightarrow None)
exponential_function(\rightarrow torch.FloatTensor)
```

```
load_numpy(\rightarrow numpy.ndarray)
                                                          # @TODO: CD: Renamed this function
evaluate(entity to idx,
                              scores,
                                          easy answers,
hard answers)
download_file(url[, destination_folder])
download\_files\_from\_url(\rightarrow None)
download\_pretrained\_model(\rightarrow 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)
             \rightarrow 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) \rightarrow 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) \rightarrow 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)
             \rightarrow 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) \rightarrow Tuple[object, str]
dicee.static_funcs.load_json(p: str) \rightarrow dict
dicee.static_funcs.save embeddings (embeddings: numpy.ndarray, indexes, path: str) \rightarrow 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,
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) \rightarrow None
dicee.static_funcs.exponential_function(x: numpy.ndarray, lam: float, ascending_order=True)
             \rightarrow torch.FloatTensor
dicee.static_funcs.load_numpy(path) \rightarrow 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='.') \rightarrow 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(\mathit{url}: \mathit{str}) \to str
```

# dicee.static funcs training

#### **Functions**

### **Module Contents**

```
dicee.static_funcs_training.make_iterable_verbose (iterable_object, verbose, desc='Default', position=None, leave=True) → Iterable

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\_preprocess\_funcs

### **Attributes**

enable\_log

### **Functions**

```
timeit(func)
preprocesses\_input\_args(args)
create\_constraints(\rightarrow Tuple[dict, dict, dict])
get\_er\_vocab(data)
get\_re\_vocab(data)
get\_ee\_vocab(data)
mapping\_from\_first\_two\_cols\_to\_third(train\_se)
Sanity Checking in input arguments
get\_er\_vocab(data)
```

### **Module Contents**

- (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)
```

#### dicee.trainer

### **Submodules**

dicee.trainer.dice\_trainer

# **Classes**

EnsembleKGE	
DICE_Trainer	DICE_Trainer implement

### **Functions**

```
load_term_mapping([file_path])
initialize_trainer(...)
get_callbacks(args)
```

### **Module Contents**

```
class dicee.trainer.dice_trainer.EnsembleKGE(model)
     models = []
     optimizers = []
     __iter__()
     __len__()
     __call__(*args, **kwargs)
     __getattr__(name)
     __str__()
dicee.trainer.dice_trainer.load_term_mapping(file_path=str)
dicee.trainer.dice_trainer.initialize_trainer(args, callbacks)
            → dicee.trainer.torch_trainer.TorchTrainer | dicee.trainer.model_parallelism.MP | dicee.trainer.torch_trainer_ddp.TorchDDF
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 (knowledge_graph)
              (1) Initialize training.
              (2) Load model
              (3) Load trainer (3) Fit model
              Parameter
                         returns

    model

                                    • form_of_labelling (str)
initialize_trainer(callbacks: List)
                                   \rightarrow lightning.Trainer | dicee.trainer.model_parallelism.MP | dicee.trainer.torch_trainer.TorchTrainer | dicee.trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_tra
              Initialize Trainer from input arguments
initialize_or_load_model()
init_dataloader (dataset: torch.utils.data.Dataset) → torch.utils.data.DataLoader
init_dataset() → torch.utils.data.Dataset
start (knowledge_graph: dicee.knowledge_graph.KG | numpy.memmap)
                                   → Tuple[dicee.models.base_model.BaseKGE, str]
              Start the training
              (1) Initialize Trainer
              (2) Initialize or load a pretrained KGE model
              in DDP setup, we need to load the memory map of already read/index KG.
k\_fold\_cross\_validation(dataset) \rightarrow 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.model\_parallelism

### **Classes**

MP	Abstract class for Trainer class for knowledge graph em-
	bedding models

# **Module Contents**

```
class dicee.trainer.model_parallelism.MP (args, callbacks)
Bases: dicee.abstracts.AbstractTrainer
```

Abstract class for Trainer class for knowledge graph embedding models

### **Parameter**

```
args
    [str] ?

callbacks: list
    ?

get_ensemble()

fit(*args, **kwargs)
    Train model

extract_input_outputs(z: list)
```

# dicee.trainer.torch\_trainer

### **Classes**

xMP	Abstract class for Trainer class for knowledge graph embedding models
TorchTrainer	TorchTrainer for using single GPU or multi CPUs on a single node

# **Module Contents**

```
class dicee.trainer.torch_trainer.xMP (args, callbacks)
    Bases: dicee.abstracts.AbstractTrainer
```

Abstract class for Trainer class for knowledge graph embedding models

### **Parameter**

```
args
[str] ?
callbacks: list
```

```
loss_function = None
     optimizer = None
     model = None
     train_dataloaders = None
     training_step = None
     available_gpus
     process
     fit (*args, train\_dataloaders, **kwargs) \rightarrow None
               Training starts
               Arguments
           kwargs:Tuple
               empty dictionary
               Return type
                   batch loss (float)
     forward_backward_update (x\_batch: torch. Tensor, y\_batch: torch. Tensor) \rightarrow torch. Tensor
               Compute forward, loss, backward, and parameter update
               Arguments
               Return type
                   batch loss (float)
     \verb|extract_input_outputs_set_device| (\textit{batch: list}) \rightarrow 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
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

 $fit (*args, train\_dataloaders, **kwargs) \rightarrow None$ 

Training starts

Arguments

# kwargs:Tuple

empty dictionary

# Return type

batch loss (float)

 $forward\_backward\_update(x\_batch: torch.Tensor, y\_batch: torch.Tensor) \rightarrow torch.Tensor$ 

Compute forward, loss, backward, and parameter update

Arguments

### **Return type**

batch loss (float)

 $\verb|extract_input_outputs_set_device| (\textit{batch: list}) \rightarrow Tuple$ 

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**

 $make\_iterable\_verbose( \rightarrow Iterable)$ 

# **Module Contents**

dicee.trainer.torch\_trainer\_ddp.make\_iterable\_verbose (iterable\_object, verbose,  $desc='Default', position=None, leave=True) \rightarrow Iterable$ 

```
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 = []
     ctx
     scaler
     extract_input_outputs (z: list)
     train()
          Training loop for DDP
```

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 (knowledge_graph)
           (1) Initialize training.
           (2) Load model
           (3) Load trainer (3) Fit model
           Parameter
               returns

    model

                   • form_of_labelling (str)
```

initialize\_trainer(callbacks: List)

 $\rightarrow$  lightning.Trainer | dicee.trainer.model\_parallelism.MP | dicee.trainer.torch\_trainer.TorchTrainer | dicee.trainer.torch\_tra Initialize Trainer from input arguments

```
initialize_or_load_model()
```

 $init\_dataloader$  (dataset: torch.utils.data.Dataset)  $\rightarrow$  torch.utils.data.DataLoader

 $init\_dataset() \rightarrow torch.utils.data.Dataset$ 

 $\begin{tabular}{ll} \textbf{start} & (knowledge\_graph: dicee.knowledge\_graph.KG \mid numpy.memmap) \\ & \rightarrow \textbf{Tuple}[dicee.models.base\_model.BaseKGE, str] \\ \end{tabular}$ 

Start the training

- (1) Initialize Trainer
- (2) Initialize or load a pretrained KGE model

in DDP setup, we need to load the memory map of already read/index KG.

 $k\_fold\_cross\_validation(dataset) \rightarrow Tuple[dicee.models.base\_model.BaseKGE, str]$ 

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 Attributes

\_\_version\_\_

# 14.3 Classes

Pyke	A Physical Embedding Model for Knowledge Graphs
DistMult	Embedding Entities and Relations for Learning and Infer-
	ence in Knowledge Bases
KeciBase	Without learning dimension scaling
Keci	Base class for all neural network modules.
TransE	Translating Embeddings for Modeling
DeCaL	Base class for all neural network modules.
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 Em-
	beddings
AConv0	Additive Convolutional Octonion Knowledge Graph Em-
	beddings

Table 3 - continued from previous page

AConvQ	Additive Convolutional Quaternion Knowledge Graph Embeddings
ConvQ	Convolutional Quaternion Knowledge Graph Embeddings
Conv0	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	

# 14.4 Functions

create_recipriocal_triples(x)	Add inverse triples into dask dataframe
<pre>get_er_vocab(data[, file_path])</pre>	
<pre>get_re_vocab(data[, file_path])</pre>	
<pre>get_ee_vocab(data[, file_path])</pre>	
timeit(func)	
<pre>save_pickle(*[, data, file_path])</pre>	

Table 4 - continued from previous page

```
load_pickle([file_path])
load_term_mapping([file_path])
                         is_continual_training,
select_model(args[,
                                                 stor-
age_path])
load_model(→ Tuple[object, Tuple[dict, dict]])
                                                        Load weights and initialize pytorch module from names-
                                                        pace arguments
                                                        Construct Ensemble Of weights and initialize pytorch
load_model_ensemble(...)
                                                        module from namespace arguments
save_numpy_ndarray(*, data, file_path)
                                                        Detect most efficient data type for a given triples
numpy_data_type_changer(→ numpy.ndarray)
                                                        Store Pytorch model into disk
save\_checkpoint\_model(\rightarrow None)
store(\rightarrow None)
                                                        Store trained_model model and save embeddings into csv
add\_noisy\_triples(\rightarrow pandas.DataFrame)
                                                        Add randomly constructed triples
read_or_load_kg(args, cls)
intialize\_model(\rightarrow Tuple[object, str])
load_json(\rightarrow dict)
save\_embeddings(\rightarrow 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])
continual\_training\_setup\_executor(\rightarrow None)
exponential\_function( \rightarrow torch.FloatTensor)
load_numpy(→ numpy.ndarray)
                                                        # @TODO: CD: Renamed this function
evaluate(entity_to_idx,
                             scores,
                                        easy_answers,
hard_answers)
download_file(url[, destination_folder])
download\_files\_from\_url(\rightarrow None)
download\_pretrained\_model(\rightarrow str)
```

Table 4 - continued from previous page

```
{\it mapping\_from\_first\_two\_cols\_to\_third} (train\_se
timeit(func)
load_term_mapping([file_path])
                                                         Reload the files from disk to construct the Pytorch dataset
reload_dataset(path, form_of_labelling, ...)
construct_dataset(→ torch.utils.data.Dataset)
```

# 14.5 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
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.

# 1 Note

As per the example above, an \_\_init\_\_() call to the parent class must be made before assignment on the child.

#### Variables

**training**  $(b \circ o 1)$  – 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} = saptures 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] * 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_q = 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 ir j-h jr i) e ie 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 h_j e_j r = r_0 + sum_{i=1}^p r_i e_i + sum_{j=p+1}^p h_j e_j r = r_0 + sum_{i=1}^p r_i e_i + sum_{j=p+1}^p h_j e_j r = r_0 + sum_{i=1}^p h_j e_j r = r_0 + sum_{i=1}^p h_j e_i + sum_{i=1}^p h_j e_j r = r_0 + sum_{i=1}^p h_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

 $h r = sigma_0 + sigma_p + sigma_q + sigma_{pp} + sigma_{q} + sig$ 

- (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)

 $\textbf{forward\_k\_vs\_all} \ (x: torch.Tensor) \ \rightarrow \text{torch.FloatTensor}$ 

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 functions 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)  $\rightarrow$  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)

 $forward\_triples(x: torch.Tensor) \rightarrow torch.FloatTensor$ 

### **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.

# 1 Note

As per the example above, an \_\_init\_\_() call to the parent class must be made before assignment on the child.

#### **Variables**

**training**  $(b \circ o 1)$  – Boolean represents whether this module is in training or evaluation mode.

```
name = 'DeCaL'
```

entity\_embeddings

relation\_embeddings

р

q

r

re

 $forward\_triples(x: torch.Tensor) \rightarrow torch.FloatTensor$ 

#### **Parameter**

x: torch.LongTensor with (n, ) shape

#### rtype

torch.FloatTensor with (n) shape

 $cl\_pqr(a: torch.tensor) \rightarrow torch.tensor$ 

Input: tensor(batch\_size, emb\_dim)  $\longrightarrow$  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_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_i + h_i r_0 t_i) s4 = \sum_{i=p+q+1}^{p+q+r} (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_i + h_i r_0 t_i) s4 = \sum_{i=p+q+1}^{p+q+r} (h_0 r_i t_i + h_i r_0 t_i) s4 = \sum_{i=p+q+1}^{p+q+r} (h_0 r_i t_i + h_i r_0 t_i) s4 = \sum_{i=p+q+1}^{p+q+r} (h_0 r_i t_i + h_i r_0 t_i) s4 = \sum_{i=p+q+1}^{p+q+r} (h_0 r_i t_i + h_i r_0 t_i) s4 = \sum_{i=p+q+1}^{p+q+r} (h_0 r_i t_i + h_i r_0 t_i) s4 = \sum_{i=p+q+1}^{p+q+r} (h_0 r_i t_i + h_i r_0 t_i) s4 = \sum_{i=p+q+1}^{p+q+r} (h_0 r_i t_i + h_i r_0 t_i) s4 = \sum_{i=p+q+1}^{p+q+r} (h_0 r_i t_i + h_i r_0 t_i) s4 = \sum_{i=p+q+1}^{p+q+r} (h_0 r_i t_i + h_i r_0 t_i) s4 = \sum_{i=p+q+1}^{p+q+r} (h_0 r_i t_i + h_i r_0 t_i) s4 = \sum_{i=p+q+1}^{p+q+r} (h_0 r_i t_i + h_i r_0 t_i) s4 = \sum_{i=p+q+1}^{p+q+r} (h_0 r_i t_i + h_i r_0 t_i) s4 = \sum_{i=p+q+1}^{p+q+r} (h_0 r_i t_i + h_i r_0 t_i) s4 = \sum_{i=p+q+1}^{p+q+r} (h_0 r_i t_i + h_i r_0 t_i) s4 = \sum_{i=p+q+1}^{p+q+r} (h_0 r_i t_i + h_i r_0 t_i) s4 = \sum_{i=p+q+1}^{p+q+r} (h_0 r_i t_i + h_i r_0 t_i) s4 = \sum_{i=p+q+1}^{p+q+r} (h_0 r_i t_i + h_i r_0 t_i) s4 = \sum_{i=p+q+r}^{p+q+r} (h_0 r_i t_i + h_i r_0 t_i) s4 = \sum_{i=p+q+r}^{p+q+r} (h_0 r_i t_i + h_i r_0 t_i) s4 = \sum_{i=p+q+r}^{p+q+r} (h_0 r_i t_i + h_i r_0 t_i) s4 = \sum_{i=p+q+r}^{p+q+r} (h_0 r_i t_i + h_i r_0 t_i) s4 = \sum_{i=p+q+r}^{p+q+r} (h_0 r_i t_i + h_i r_0 t_i) s4 = \sum_{i=p+q+r}^{p+q+r} (h_0 r_i t_i + h_i r_0 t_i) s4 = \sum_{i=p+q+r}^{p+q+r} (h_0 r_i t_i + h_i r_0 t_i) s4 = \sum_{i=p+q+r}^{p+q+r} (h_0 r_i t_i + h_i r_0 t_i) s4 = \sum_{i=p+q+r}^{p+q+r} (h_0 r_i t_i + h_i r_0 t_i) s4 = \sum_{i=p+q+r}^{p+q+r} (h_0 r_i t_i + h_i r_0 t_i) s4 = \sum_{i=p+q+r}^{p+q+r} (h_0 r_i t_i + h_i r_0 t_i) s4 = \sum_{i=p+q+r}^{p+q+r} (h_0 r_i t_i + h_i r_0 t_i) s4 = \sum_{i=p+q+r}^{p+q+r} (h_0 r_i t_i + h_i r_0 t_i) s4 = \sum_{i=p+q+r}^{p+q+r}$$

and return:

$$sigma_0t = \sigma_0 \cdot t_0 = s0 + s1 - s2s3, s4ands5$$

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

For different base vector interactions, we have

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

 $forward_k_vs_all(x: torch.Tensor) \rightarrow torch.FloatTensor$ 

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\_{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,

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

 $\texttt{compute\_sigma\_qq}\,(hq,rq)$ 

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):

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

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

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)

 $\texttt{compute\_sigma\_pr} \ (*, hp, hk, rp, rk)$ 

Compute

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

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)

 $\texttt{compute\_sigma\_qr} \ (*, hq, hk, rq, rk)$ 

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

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
                    {\tt 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\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e_4\_t,e_4\_t,e_4\_t,e_4\_t,e_4\_t,e_4\_t,e_4\_t,e_4\_t,e_4\_t,e_4\_t,e_4\_t,e_4\_t,e_4\_t,e_4\_t,e_4\_t,e_4\_t,e_4\_t,e_4\_t,e_4\_t,e_4\_t,e_4\_t,e_4\_t,e_4\_t,e_4\_t,e_4\_t,e_4\_t,e_4\_
                                                                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) \rightarrow \text{torch.tensor}
                                      KvsAll scoring function
                                       Input
                                      x: torch.LongTensor with (n, ) shape
                                       Output
                                      torch.FloatTensor with (n) shape
                    forward_triples (idx\_triple: torch.tensor) \rightarrow torch.tensor
                                       Negative Sampling forward pass:
                                       Input
                                      x: torch.LongTensor with (n, ) shape
                                       Output
                                       torch.FloatTensor with (n) shape
                    {\tt forward\_k\_vs\_all}\;(\mathcal{X})
                                      KvsAll forward pass
                                       Input
                                       x: torch.LongTensor with (n, ) shape
                                       Output
                                       torch.FloatTensor with (n) shape
                    T (x: torch.tensor) \rightarrow 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.



As per the example above, an \_\_init\_\_() call to the parent class must be made before assignment on the child.

#### **Variables**

fc\_num\_input

**training**  $(b \circ o 1)$  – 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) \rightarrow 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
```

```
fc1
     norm_fc1
     bn_conv2d
     feature_map_dropout
     residual_convolution (C_1: Tuple[torch.Tensor, torch.Tensor],
                   C_2: Tuple[torch.Tensor, torch.Tensor]) \rightarrow 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:
     \texttt{forward\_k\_vs\_all} \ (\textit{x: torch.Tensor}) \ \rightarrow \text{torch.FloatTensor}
     forward_triples (x: torch.Tensor) \rightarrow torch.FloatTensor
               Parameters
     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) \rightarrow torch.Tensor
               Parameters
     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 l)
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
     {\tt residual\_convolution}\,(Q\_1,\,Q\_2)
     forward\_triples (indexed\_triple: torch.Tensor) \rightarrow 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 l)
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
     {\tt residual\_convolution}\,(Q\_I,\,Q\_2)
     forward\_triples(indexed\_triple: torch.Tensor) \rightarrow 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.

# 1 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) \rightarrow 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 l)
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]) \rightarrow 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) \rightarrow torch.FloatTensor
     forward\_triples(x: torch.Tensor) \rightarrow torch.FloatTensor
               Parameters
     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):
                                                                                             (continues on next page)
```

(continued from previous page)

```
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.

# 1 Note

As per the example above, an <u>\_\_init\_\_</u>() 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.

```
\label{eq:power_product} $$ name = 'QMult'$ $$ 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.

 $static quaternion\_normalizer(x: torch.FloatTensor) \rightarrow torch.FloatTensor$ 

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:

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

### **Parameters**

 $\mathbf{x}$  – The vector.

#### Returns

The normalized vector.

 $k\_vs\_all\_score$  (bpe\_head\_ent\_emb, bpe\_rel\_ent\_emb, E)

### **Parameters**

- bpe\_head\_ent\_emb
- bpe\_rel\_ent\_emb
- E

 ${\tt forward\_k\_vs\_all}\;(\mathcal{X})$ 

#### **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.

# **1** Note

As per the example above, an \_\_init\_\_() call to the parent class must be made before assignment on the child.

#### **Variables**

**training**  $(b \circ \circ 1)$  – 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 \text{ 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
     \mathtt{get\_embeddings}() \rightarrow Tuple[numpy.ndarray, None]
     \mathbf{forward\_k\_vs\_all}\;(x)\;\to torch.FloatTensor
     forward_triples (x) \rightarrow \text{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
     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

### $\mathtt{vtp\_score}(h, r, t)$

this part implement the vector triple product scoring techniques:

```
score(h,r,t) = int_{0}{1} \quad h(x)r(x)t(x) \quad dx = sum_{i,j,k} = 0^{d-1} \quad 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 $[0][0] + \text{coeff}[0][1]x + ... + \text{coeff}[0][d]x^d$ ,

$$coeff[1][0] + coeff[1][1]x + ... + coeff[1][d]x^d$$

```
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: 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.embeddin
                                      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) \rightarrow 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__()
        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.



### 1 Note

As per the example above, an \_\_init\_\_() call to the parent class must be made before assignment on the child.

#### Variables

name = 'BytE'

**training**  $(b \circ o 1)$  – Boolean represents whether this module is in training or evaluation mode.

```
config
temperature = 0.5
topk = 2
transformer
lm_head
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()
```

#### 1 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.

# 1 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
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) \rightarrow torch.Tensor
        Parameters
forward_k_vs_all(*args, **kwargs)
forward_k_vs_sample(*args, **kwargs)
get_triple_representation(idx_hrt)
{\tt 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)
\texttt{dicee.numpy\_data\_type\_changer} (\textit{train\_set: numpy.ndarray}, \textit{num: int}) \rightarrow \texttt{numpy.ndarray}
     Detect most efficient data type for a given triples :param train_set: :param num: :return:
dicee.save_checkpoint_model(model, path: str) \rightarrow 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) \rightarrow 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) \rightarrow 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) \rightarrow dict
dicee.save_embeddings(embeddings: numpy.ndarray, indexes, path: str) \rightarrow 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')
\texttt{dicee.continual\_training\_setup\_executor}(\textit{executor}) \rightarrow None
dicee.exponential_function (x: numpy.ndarray, lam: float, ascending\_order=True) \rightarrow torch.FloatTensor
dicee.load_numpy(path) \rightarrow 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='.') \rightarrow 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")

 ${\tt dicee.download\_pretrained\_model}\,(\mathit{url}:\mathit{str})\,\to \mathit{str}$ 

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 (knowledge_graph)
                   (1) Initialize training.
                   (2) Load model
                 (3) Load trainer (3) Fit model
                 Parameter
                                returns

    model

                                               • form_of_labelling (str)
initialize_trainer(callbacks: List)
                                             \rightarrow lightning. Trainer \mid \textit{dicee.trainer.model\_parallelism.MP} \mid \textit{dicee.trainer.torch\_trainer.TorchTrainer} \mid \textit{dicee.trainer.torch\_trainer} \mid \textit{dicee.trainer.torch\_trainer.torch\_trainer.torch\_trainer.torch\_trainer.torch\_trainer.torch\_trainer.torch\_trainer.torch\_trainer.torch\_trainer.torch\_trainer.torch\_trainer.torch\_trainer.torch\_trainer.torch\_trainer.torch\_trainer.torch\_trainer.torch\_trainer.torch\_trainer.torch\_trainer.torch\_trainer.torch\_trainer.torch\_trainer.torch\_trainer.torch\_trainer.torch\_trainer.torch\_trainer.torch\_trainer.torch\_trainer.torch\_trainer.torch\_trainer.torch\_trainer.torch\_trainer.torch\_trainer.torch\_trainer.torch\_trainer.torch\_trainer.torch\_trainer.torch\_trainer.torch\_trainer.torch\_trainer.torch\_trainer.torch\_trainer.torch\_trainer.torch\_trainer.torch\_trainer.torch\_trainer.torch\_trainer.torch\_trainer.torch\_trainer.torch\_trainer.torch\_trainer.torch\_trainer.torch\_trainer.torch\_trainer.torch\_trainer.torch\_trainer.torch\_trainer.torch\_trainer.torch\_trainer.torch\_trainer.torch\_trainer.torch\_trainer.torch\_trainer.torch\_trainer.torch\_trainer.torch\_trainer.torch\_trainer.torch\_trainer.torch\_trainer.torch\_trainer.torch\_trainer.torch\_trainer.torch\_trainer.torch\_trainer.torch\_trainer.torch\_trainer.torch\_trainer.torch\_trainer.torch\_trainer.torch\_trainer.torch\_trainer.torch\_trainer.torch\_trainer.torch\_trainer.torch\_trainer.torch\_trainer.torch\_trainer.torch\_trainer.torch\_trainer.torch\_trainer.torch\_trainer.torch\_trainer.torch\_trainer.torch\_trainer.torch\_trainer.torch\_trainer.torch\_trainer.torch\_trainer.torch\_trainer.torch\_trainer.torch\_trainer.torch\_trainer.torch\_trainer.torch\_trainer.torch\_trainer.torch\_trainer.torch\_trainer.torch\_trainer.torch\_trainer.torch\_trainer.torch\_trainer.torch\_trainer.torch\_trainer.torch\_trainer.torch\_trainer.torch\_traine
                 Initialize Trainer from input arguments
initialize_or_load_model()
\verb|init_dataloader| (\textit{dataset: torch.utils.data.Dataset})| \rightarrow torch.utils.data.DataLoader|
\verb"init_dataset"() \rightarrow torch.utils.data.Dataset"
start (knowledge_graph: dicee.knowledge_graph.KG | numpy.memmap)
                                             → Tuple[dicee.models.base_model.BaseKGE, str]
                 Start the training
                   (1) Initialize Trainer
                   (2) Initialize or load a pretrained KGE model
                 in DDP setup, we need to load the memory map of already read/index KG.
```

```
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

#### **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
```

```
\label{limitsing_relations} \begin{split} &\texttt{predict\_missing\_relations} \ (\textit{head\_entity: List[str]} \mid \textit{str, tail\_entity: List[str]} \mid \textit{str, within=None}) \\ &\rightarrow \mathsf{Tuple} \end{split}
```

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

```
{\tt predict\_missing\_tail\_entity} \ (\textit{head\_entity: List[str]} \ | \ \textit{str, relation: List[str]} \ | \ \textit{str
```

*within:* List[str] = None  $\rightarrow$  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) <math>\rightarrow torch. Float Tensor
```

# **Parameters**

- logits
- h
- r
- +
- within

```
predict_topk(*, h: str \mid List[str] = None, r: str \mid List[str] = None, t: str \mid 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
 \texttt{triple\_score} \ (h: List[str] \mid str = None, \, r: \, List[str] \mid str = None, \, t: \, List[str] \mid str = None, \, logits = False) 
               \rightarrow 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') \rightarrow torch.Tensor
tensor_t_norm(subquery\_scores: torch.FloatTensor, tnorm: str = 'min') \rightarrow 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') \rightarrow torch.Tensor
```

 $negnorm(tens\_1: torch.Tensor, lambda\_: float, neg\_norm: str = 'standard') \rightarrow torch.Tensor$ 

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) \rightarrow 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.
          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) \mid f(e,r,x) > \text{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,  $batch\_size=32$ ,  $neg\_sample\_ratio=10$ ,  $num\_workers=1$ )  $\rightarrow$  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

 $\mathtt{setup\_executor}() \to \mathsf{None}$ 

# ${\tt dept\_read\_preprocess\_index\_serialize\_data}\,()\,\to None$

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

### ${\tt save\_trained\_model}\,()\,\to None$

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)  $\rightarrow$  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

```
\textbf{write\_report}\,()\,\to None
```

Report training related information in a report json file

 $start() \rightarrow dict$ 

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

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.

# **1** 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 <code>\_\_getitem\_\_()</code>, supporting fetching a data sample for a given key. Subclasses could also optionally overwrite <code>\_\_len\_\_()</code>, which is expected to return the size of the dataset by many <code>Sampler</code> implementations and the default options of <code>DataLoader</code>. Subclasses could also optionally implement <code>\_\_getitems\_\_()</code>, 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 mapstyle 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)
```

```
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__()
     \__{\texttt{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 - ?
                                          for https://pytorch.org/docs/stable/data.html#torch.utils.data.
                • num_workers - int
                  DataLoader
          Return type
              torch.utils.data.Dataset
     train_data
     target_dim
     collate_fn = None
     __len__()
     \__getitem__(idx)
```

class dicee.MultiClassClassificationDataset (subword\_units: numpy.ndarray, block\_size: int = 8)

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



## 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)
```

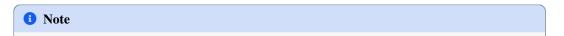
class dicee. AllvsAll (train\_set\_idx: numpy.ndarray, entity\_idxs, relation\_idxs, label\_smoothing\_rate=0.0)

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:=  $\{(x,y)_i\}_i^n N$ , where x: (h,r) is a possible unique tuple of an entity h in E and a relation r in R. Hence  $N = |E| \times |R| y$ : 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



AllysAll extends KysAll 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
__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.

```
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</pre>
           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
     max_num_of_classes
     __len__()
     \__{\texttt{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
```

**Return type** 

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.



DataLoader by default constructs an index sampler that yields integral indices. To make it work with a mapstyle 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, \text{ 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__()
      \underline{\phantom{a}}getitem\underline{\phantom{a}} (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: \verb"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 - ?
                                                    https://pytorch.org/docs/stable/data.html#torch.utils.data.
                 • num_workers -
                                               for
                                         int
                   DataLoader
           Return type
      train_set_idx
      num_entities
      num_relations
      neg_sample_ratio
      batch_size
      num_workers
      train\_dataloader() \rightarrow torch.utils.data.DataLoader
           An iterable or collection of iterables specifying training samples.
           For more information about multiple dataloaders, see this section.
                  dataloader
                                you
                                       return
                                                 will
                                                        not
                                                               be
                                                                     reloaded
                                                                                 unless
                                                                                           you
                                                                                                         :param-
           ref: ~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()

# **1** 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.11 = None

def prepare_data(self):
        download_data()
        tokenize()

# don't do this
        self.something = else

def setup(self, stage):
        data = load_data(...)
        self.11 = 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, ...).



## **1** 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
   else:
        batch = super().transfer_batch_to_device(batch, device, dataloader_
\rightarrowidx)
    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()
```

```
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) \rightarrow List | Tuple
           Convert a nested tuple to a nested list.
      set_global_seed(seed: int)
           Set seed
      construct\_graph(paths: List[str]) \rightarrow 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) \rightarrow 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]]])
                    \rightarrow 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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