# **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
                                                                    2
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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
                                                                         58%
                                                                                101, 106,
→ 111, 258-353, 360-411
dicee/evaluator.py
                                                           262
                                                                   51
                                                                         81%
                                                                                46, 51,_
→56, 84, 89-90, 93, 109, 126, 137, 141, 146, 177-188, 195-206, 314, 344-367, 455, □
→465, 482-487
dicee/executer.py
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                                                           113
⇒259, 291
dicee/knowledge_graph.py
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                                                                                79, 110, _
⇔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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                                                                         87%
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
                                                                         16%
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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
                                                           227
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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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                                                                    5
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dicee/models/quaternion.py
                                                                                7-21, 30-
                                                           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
                                                            10
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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
                                                               36
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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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                                                                      126
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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
                                                                            100%
                                                                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:)

```
# Keci
@inproceedings{demir2023clifford,
    title={Clifford Embeddings--A Generalized Approach for Embedding in Normed Algebras}

.,
    author={Demir, Caglar and Ngonga Ngomo, Axel-Cyrille},
    booktitle={Joint European Conference on Machine Learning and Knowledge Discovery in_
.Databases},
    pages={567--582},
    year={2023},
    organization={Springer}
}
# LitCQD
```

```
@inproceedings{demir2023litcqd,
 title={LitCQD: Multi-Hop Reasoning in Incomplete Knowledge Graphs with Numeric_
→Literals},
 author={Demir, Caglar and Wiebesiek, Michel and Lu, Renzhong and Ngonga Ngomo, Axel-
→Cyrille and Heindorf, Stefan},
 booktitle={Joint European Conference on Machine Learning and Knowledge Discovery in_
→Databases},
 pages={617--633},
 year={2023},
 organization={Springer}
# DICE Embedding Framework
@article{demir2022hardware,
 title={Hardware-agnostic computation for large-scale knowledge graph embeddings},
 author={Demir, Caglar and Ngomo, Axel-Cyrille Ngonga},
 journal={Software Impacts},
 year={2022},
 publisher={Elsevier}
# KronE
@inproceedings{demir2022kronecker,
 title={Kronecker decomposition for knowledge graph embeddings},
 author={Demir, Caglar and Lienen, Julian and Ngonga Ngomo, Axel-Cyrille},
 booktitle={Proceedings of the 33rd ACM Conference on Hypertext and Social Media},
 pages={1--10},
 year={2022}
# QMult, OMult, ConvQ, ConvO
@InProceedings{pmlr-v157-demir21a,
                   {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
global_rank = 0

local_rank = 0

strategy = None
```

```
on_fit_start(*args, **kwargs)
     A function to call callbacks before the training starts.
     Parameter
     args
     kwargs
          rtype
               None
on_fit_end(*args, **kwargs)
     A function to call callbacks at the ned of the training.
     Parameter
     args
     kwargs
          rtype
               None
on_train_epoch_end(*args, **kwargs)
     A function to call callbacks at the end of an epoch.
     Parameter
     args
     kwargs
          rtype
              None
on_train_batch_end(*args, **kwargs)
     A function to call callbacks at the end of each mini-batch during training.
     Parameter
     args
     kwargs
          rtype
              None
\mathtt{static}\ \mathtt{save\_checkpoint}\ (\mathit{full\_path}: \mathit{str}, \mathit{model}) \ 	o \ \mathsf{None}
     A static function to save a model into disk
     Parameter
     full_path: str
     model:
          rtype
              None
```

```
class dicee.abstracts.BaseInteractiveKGE (path: str = None, url: str = None,
             construct\_ensemble: bool = False, model\_name: str = None,
             apply_semantic_constraint: bool = False)
      Abstract/base class for using knowledge graph embedding models interactively.
      Parameter
      path_of_pretrained_model_dir
           [str] ?
      construct_ensemble: boolean
      model_name: str apply_semantic_constraint : boolean
      construct_ensemble = False
      apply_semantic_constraint = False
      configs
      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]}
                    str_entity_or_relation (corresponds to a str or a list of strings to
                    be tokenized via BPE and shaped.)
                Return type
                    A list integer(s) or a list of lists containing integer(s)
      get_padded_bpe_triple_representation (triples: List[List[str]]) \rightarrow Tuple[List, List, List]
                Parameters
                    triples
      \mathtt{set\_model\_train\_mode}() \rightarrow None
           Setting the model into training mode
           Parameter
      \verb"set_model_eval_mode"() \to None
           Setting the model into eval mode
           Parameter
      property name
      sample\_entity(n:int) \rightarrow List[str]
      sample\_relation(n:int) \rightarrow List[str]
      is\_seen(entity: str = None, relation: str = None) \rightarrow bool
      save() \rightarrow None
      get_entity_index(x: str)
```

```
get_relation_index (x: str)
      index_triple (head_entity: List[str], relation: List[str], tail_entity: List[str])
                   → Tuple[torch.LongTensor, torch.LongTensor, torch.LongTensor]
           Index Triple
           Parameter
           head_entity: List[str]
           String representation of selected entities.
           relation: List[str]
           String representation of selected relations.
           tail_entity: List[str]
           String representation of selected entities.
           Returns: Tuple
           pytorch tensor of triple score
      add_new_entity_embeddings (entity_name: str = None, embeddings: torch.FloatTensor = None)
      get_entity_embeddings (items: List[str])
           Return embedding of an entity given its string representation
           Parameter
           items:
               entities
      get_relation_embeddings (items: List[str])
           Return embedding of a relation given its string representation
           Parameter
           items:
               relations
      construct_input_and_output (head_entity: List[str], relation: List[str], tail_entity: List[str], labels)
           Construct a data point :param head_entity: :param relation: :param tail_entity: :param labels: :return:
      parameters()
class dicee.abstracts.AbstractCallback
      Bases: abc.ABC, lightning.pytorch.callbacks.Callback
      Abstract class for Callback class for knowledge graph embedding models
      Parameter
      on_init_start(*args, **kwargs)
```

```
Parameter
     trainer:
     model:
         rtype
             None
on_init_end(*args, **kwargs)
     Call at the beginning of the training.
     Parameter
     trainer:
     model:
         rtype
             None
\verb"on_fit_start" (\textit{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
```

# dicee.analyse\_experiments

 $store\_ensemble (param\_ensemble) \rightarrow None$ 

This script should be moved to dicee/scripts Example: python dicee/analyse\_experiments.py -dir Experiments -features "model" "trainMRR" "testMRR"

### **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**

```
\begin{tabular}{ll} \textbf{class} & \texttt{dicee.callbacks.AccumulateEpochLossCallback} & (\textit{path: str}) \\ \textbf{Bases:} & \textit{dicee.abstracts.AbstractCallback} \\ \end{tabular}
```

Abstract class for Callback class for knowledge graph embedding models

```
Parameter
```

```
path
      on\_fit\_end(\mathit{trainer}, \mathit{model}) \rightarrow 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: 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 = -1
     on_fit_end(trainer, model)
          Call at the end of the training.
          Parameter
          trainer:
          model:
              rtype
                  None
     static compute\_mrr(trainer, model) \rightarrow float
     get_aswa_state_dict(model)
     {\tt 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 = None
```

```
epoch_counter = 0
     on_fit_start(trainer, model)
          Call at the beginning of the training.
          Parameter
          trainer:
          model:
              rtype
                  None
     on_fit_end(trainer, model)
          Call at the end of the training.
          Parameter
          trainer:
          model:
              rtype
                  None
     on_train_epoch_end(trainer, model)
          Call at the end of each epoch during training.
          Parameter
          trainer:
          model:
              rtype
                  None
     on_train_batch_end(*args, **kwargs)
          Call at the end of each mini-batch during the training.
          Parameter
          trainer:
          model:
              rtype
                  None
class dicee.callbacks.KronE
     Bases: dicee.abstracts.AbstractCallback
```

Abstract class for Callback class for knowledge graph embedding models

#### **Parameter**

```
f = None
     static batch_kronecker_product(a, b)
           Kronecker product of matrices a and b with leading batch dimensions. Batch dimensions are broadcast. The
           number of them mush :type a: torch.Tensor :type b: torch.Tensor :rtype: torch.Tensor
     get_kronecker_triple_representation(indexed_triple: torch.LongTensor)
           Get kronecker embeddings
     on_fit_start (trainer, model)
           Call at the beginning of the training.
           Parameter
           trainer:
           model:
               rtype
                   None
class dicee.callbacks.Perturb (level: str = 'input', ratio: float = 0.0, method: str = None,
            scaler: float = None, frequency=None)
     Bases: dicee.abstracts.AbstractCallback
     A callback for a three-Level Perturbation
     Input Perturbation: During training an input x is perturbed by randomly replacing its element. In the context of
     knowledge graph embedding models, x can denote a triple, a tuple of an entity and a relation, or a tuple of two
```

entities. A perturbation means that a component of x is randomly replaced by an entity or a relation.

Parameter Perturbation:

```
Output Perturbation:

level = 'input'

ratio = 0.0

method = None

scaler = None

frequency = None

on_train_batch_start (trainer, model, batch, batch_idx)

Called when the train batch begins.
```

# dicee.config

# **Classes**

Namespace

Simple object for storing attributes.

### **Module Contents**

```
class dicee.config.Namespace(**kwargs)
     Bases: argparse.Namespace
     Simple object for storing attributes.
     Implements equality by attribute names and values, and provides a simple string representation.
     dataset_dir: str = None
          The path of a folder containing train.txt, and/or valid.txt and/or test.txt
     save_embeddings_as_csv: bool = False
          Embeddings of entities and relations are stored into CSV files to facilitate easy usage.
     storage_path: str = 'Experiments'
          A directory named with time of execution under -storage_path that contains related data about embeddings.
     path_to_store_single_run: str = None
          A single directory created that contains related data about embeddings.
     path_single_kg = None
          Path of a file corresponding to the input knowledge graph
     sparql_endpoint = None
          An endpoint of a triple store.
     model: str = 'Keci'
          KGE model
     optim: str = 'Adam'
          Optimizer
     embedding_dim: int = 64
          Size of continuous vector representation of an entity/relation
     num_epochs: int = 150
          Number of pass over the training data
     batch_size: int = 1024
          Mini-batch size if it is None, an automatic batch finder technique applied
     lr: float = 0.1
          Learning rate
     add_noise_rate: float = None
          The ratio of added random triples into training dataset
     gpus = None
          Number GPUs to be used during training
     callbacks
          10}}
               Type
                   Callbacks, e.g., {"PPE"
               Type
                   { "last_percent_to_consider"
```

```
backend: str = 'pandas'
    Backend to read, process, and index input knowledge graph. pandas, polars and rdflib available
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"]
            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
auto_batch_finding = False
     A flag for using auto batch finding
__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 em-
	beddings, 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

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.

```
• 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 = 8
num_of_data_points
collate_fn = None
__len__()
__getitem__(idx)
```

class dicee.dataset\_classes.OnevsAllDataset(train\_set\_idx: numpy.ndarray, entity\_idxs)

Bases: torch.utils.data.Dataset

Dataset for the 1vsALL training strategy

#### **Parameters**

- train\_set\_idx Indexed triples for the training.
- entity\_idxs mapping.
- relation\_idxs mapping.
- form ?
- num\_workers int for https://pytorch.org/docs/stable/data.html#torch.utils.data.
   DataLoader

## Return type

torch.utils.data.Dataset

```
train_data
target_dim
collate_fn = None
__len__()
__getitem__(idx)
```

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.



**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()
```

```
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 AllysAll training by inheriting from torch.utils.data.Dataset.

Let D denote a dataset for AllvsAll training and be defined as D:=  $\{(x,y)_i\}_i$  ^N, where x: (h,r) is a possible unique tuple of an entity h in E and a relation r in R. Hence  $N = |E| \times |R|$  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 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.dataset\_classes.OnevsSample ( $train\_set$ : numpy.ndarray,  $num\_entities$ ,  $num\_relations$ , neg sample ratio: int = None, label smoothing rate: <math>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 = None
label_smoothing_rate
collate_fn = None
__len__()
    Returns the number of sam
```

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

 $\begin{tabular}{ll} {\tt classe} & \tt dicee.dataset\_classes. {\tt KvsSampleDataset} ({\it train\_set\_idx: numpy.ndarray, entity\_idxs, relation\_idxs, form, store=None, neg\_ratio=None, label\_smoothing\_rate: float = 0.0) \end{tabular}$ 

Bases: torch.utils.data.Dataset

# **KvsSample a Dataset:**

### $D := \{(x,y)_i\}_i ^N$ , where

. x:(h,r) is a unique h in E and a relation r in R and . y in  $[0,1]^{\{|E|\}}$  is a binary label.

```
orall y_i = 1 s.t. (h r E_i) in KG
               At each mini-batch construction, we subsample(y), hence n
                    | new_y| << |E| new_y contains all 1's if sum(y)< neg_sample ratio new_y contains
           train_set_idx
               Indexed triples for the training.
           entity idxs
               mapping.
           relation_idxs
               mapping.
           form
           store
           label_smoothing_rate
           torch.utils.data.Dataset
      train_data = None
      train_target = None
      neg ratio = None
      num entities
      label_smoothing_rate
      collate fn = None
      max_num_of_classes
      __len__()
      \underline{\phantom{a}}getitem\underline{\phantom{a}} (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.



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__()
```

- num\_relations relation to index mapping.
- batch\_size int
- form ?
- num\_workers int for https://pytorch.org/docs/stable/data.html#torch.utils.data.
   DataLoader

# Return type

?

```
train_set_idx
num_entities
num_relations
neg_sample_ratio
batch_size
num_workers
```

 $\verb|train_dataloader|()| \rightarrow torch.utils.data.DataLoader|$ 

An iterable or collection of iterables specifying training samples.

For more information about multiple dataloaders, see this section.

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

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_
    →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_i

evaluate_link_prediction_performance_with_i
...)
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 = None
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)
             \rightarrow None
eval_rank_of_head_and_tail_entity(*, train_set, valid_set=None, test_set=None, trained_model)
eval_rank_of_head_and_tail_byte_pair_encoded_entity(*, train_set=None, valid_set=None,
             test_set=None, ordered_bpe_entities, trained_model)
eval_with_byte (*, raw_train_set, raw_valid_set=None, raw_test_set=None, trained_model,
            form of labelling) \rightarrow None
     Evaluate model after reciprocal triples are added
eval with bpe vs all (*, raw train set, raw valid set=None, raw test set=None, trained model,
            form\_of\_labelling) \rightarrow None
     Evaluate model after reciprocal triples are added
eval_with_vs_all (*, train_set, valid_set=None, test_set=None, trained_model, form_of_labelling)
     Evaluate model after reciprocal triples are added
evaluate_lp_k_vs_all (model, triple_idx, info=None, form_of_labelling=None)
     Filtered link prediction evaluation. :param model: :param triple_idx: test triples :param info: :param
     form_of_labelling: :return:
evaluate_lp_with_byte (model, triples: List[List[str]], info=None)
evaluate_lp_bpe_k_vs_all (model, triples: List[List[str]], info=None, form_of_labelling=None)
         Parameters
              • model
              • triples (List of lists)
              • info
              • form_of_labelling
evaluate_lp (model, triple_idx, info: str)
dummy_eval (trained_model, form_of_labelling: str)
eval_with_data(dataset, trained_model, triple_idx: numpy.ndarray, form_of_labelling: str)
```

# dicee.executer

# **Classes**

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

# **Module Contents**

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

A class for Training, Retraining and Evaluation a model.

- (1) Loading & Preprocessing & Serializing input data.
- (2) Training & Validation & Testing
- (3) Storing all necessary info

```
args
```

```
is_continual_training = False
trainer = None
trained_model = None
knowledge_graph = None
report
evaluator = None
start_time = None
setup_executor() → 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

# $write\_report() \rightarrow None$

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

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.

 ${\tt continual\_start}\,()\,\to dict$ 

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

```
class dicee.knowledge_graph.KG(dataset_dir: str = None, byte_pair_encoding: bool = False,
           padding: bool = False, add_noise_rate: float = None, sparql_endpoint: str = None,
           path\_single\_kg: str = None, path\_for\_deserialization: str = None, add\_reciprocal: bool = None,
           eval_model: str = None, read_only_few: int = None, sample_triples_ratio: float = None,
           path_for_serialization: str = None, entity_to_idx=None, relation_to_idx=None, backend=None,
           training\_technique: str = None, separator: str = None)
     Knowledge Graph
     dataset_dir = None
     sparql_endpoint = None
     path_single_kg = None
     byte_pair_encoding = False
     ordered_shaped_bpe_tokens = None
     add_noise_rate = None
     num_entities = None
     num_relations = None
     path_for_deserialization = None
     add reciprocal = None
     eval_model = None
     read_only_few = None
     sample_triples_ratio = None
     path_for_serialization = None
     entity_to_idx = None
     relation_to_idx = None
     backend = 'pandas'
     training_technique = None
     idx_entity_to_bpe_shaped
     enc
     num_tokens
     num_bpe_entities = None
     padding = False
     dummy_id
     max_length_subword_tokens = None
     train_set_target = None
```

```
target_dim = None

train_target_indices = None

ordered_bpe_entities = None

separator = None

description_of_input = None

describe() \rightarrow 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

```
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

```
\label{eq:predict_missing_tail_entity} $$ (head\_entity: List[str] \mid str, relation: List[str] \mid str, \\ within: List[str] = None) \to 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
- t
- within

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

```
\label{eq:core}  \textbf{triple\_score} \ (h: List[str] \mid str = None, \, r: \, List[str] \mid str = None, \, t: \, List[str] \mid str = None, \, logits = False) \\ \rightarrow \text{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.
          topk: int
          Highest ranked k item to select triples with f(e,r,x) > confidence.
          at most: int
          Stop after finding at_most missing triples
          \{(e,r,x) \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.adopt

#### **Classes**

ADOPT Base class for all optimizers.	
--------------------------------------	--

# **Functions**

adopt(params,	grads,	exp_avgs,	exp_avg_sqs,	Functional API that performs ADOPT algorithm compu-
state_steps)				tation.

# **Module Contents**

```
class dicee.models.adopt.ADOPT (params: torch.optim.optimizer.ParamsT,
             lr: float | torch. Tensor = 0.001, betas: Tuple float, float | = (0.9, 0.9999), eps: float = 1e-06,
             clip_lambda: Callable[[int], float] | None = lambda step: ..., weight_decay: float = 0.0,
             decouple: bool = False, *, foreach: bool | None = None, maximize: bool = False,
             capturable: bool = False, differentiable: bool = False, fused: bool | None = None)
      Bases: torch.optim.optimizer.Optimizer
```

Base class for all optimizers.



# Warning

Parameters need to be specified as collections that have a deterministic ordering that is consistent between runs. Examples of objects that don't satisfy those properties are sets and iterators over values of dictionaries.

#### **Parameters**

- params (*iterable*) an iterable of torch. Tensors or dicts. Specifies what Tensors should be optimized.
- **defaults** (dict): a dict containing default values of optimization options (used when a parameter group doesn't specify them).

#### clip\_lambda

```
__setstate__(state)
step(closure=None)
```

Perform a single optimization step.

#### **Parameters**

closure (Callable, optional) - A closure that reevaluates the model and returns the
loss.

```
dicee.models.adopt (params: List[torch.Tensor], grads: List[torch.Tensor],
exp_avgs: List[torch.Tensor], exp_avg_sqs: List[torch.Tensor], state_steps: List[torch.Tensor],
foreach: bool | None = None, capturable: bool = False, differentiable: bool = False,
fused: bool | None = None, grad_scale: torch.Tensor | None = None,
found_inf: torch.Tensor | None = None, has_complex: bool = False, *, beta1: float, beta2: float,
lr: float | torch.Tensor, clip_lambda: Callable[[int], float] | None, weight_decay: float,
decouple: bool, eps: float, maximize: bool)
```

Functional API that performs ADOPT algorithm computation.

# 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 them to be nested in a tree structure. You can assign the sub-modules 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)
```

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```
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 also have their parameters converted 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} \textbf{ = []} \label{eq:mem_of_model()} \rightarrow \text{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])

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

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.

# Warning

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 reloaded :paramdataloader you return will not be unless you ref: `~lightning.pytorch.trainer.trainer.Trainer.reload\_dataloaders\_every\_n\_epochs` 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.

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

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 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.

# **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 them to be nested in a tree structure. You can assign the sub-modules 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 also have their parameters converted 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
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)
                  \rightarrow Tuple[torch.FloatTensor, torch.FloatTensor]
              Parameters
                  x (B x 2 x T)
     \mathtt{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 them to be nested in a tree structure. You can assign the sub-modules 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 also have their parameters converted 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 = None
_call__(x)
static forward(x)
```

# dicee.models.clifford

# **Classes**

Keci	Base class for all neural network modules.
CKeci	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 them to be nested in a tree structure. You can assign the sub-modules 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 also have their parameters converted 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.

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_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.clifford.CKeci(args)
      Bases: Keci
      Without learning dimension scaling
      name = 'CKeci'
```

# 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 them to be nested in a tree structure. You can assign the sub-modules 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 also have their parameters converted 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

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

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

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.

 $compute\_sigma\_rr(hk, rk)$ 

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

 $\texttt{compute\_sigma\_pq}\,(\,^*\!,\,hp,\,hq,\,rp,\,rq)$ 

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

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

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

for j in range(q):

$$sigma_pq[:,:,i,j] = hp[:,:,i] * rq[:,:,j] - hq[:,:,j] * rp[:,:,i]$$

print(sigma\_pq.shape)

compute\_sigma\_qr(\*, hq, hk, rq, rk)

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

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

for j in range(q):

$$sigma\_pq[:,:,i,j] = hp[:,:,i] * rq[:,:,j] - hq[:,:,j] * rp[:,:,i]$$

print(sigma\_pq.shape)

# dicee.models.complex

# **Classes**

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

### **Module Contents**

class dicee.models.complex.ConEx(args)

Bases: dicee.models.base\_model.BaseKGE

Convolutional ComplEx Knowledge Graph Embeddings

name = 'ConEx'

```
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:
      \texttt{forward\_k\_vs\_all} \ (\textit{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)
```

conv2d

```
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 them to be nested in a tree structure. You can assign the sub-modules 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 also have their parameters converted 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**  $(b \circ \circ 1)$  – 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.dualE

#### **Classes**

DualE	Dual	Quaternion	Knowledge	Graph	Embeddings
		://ojs.aaai.org //16657)	/index.php/A	AAI/artic	le/download/

```
class dicee.models.dualE.DualE(args)
                         Bases: \ \textit{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 = None
                        {\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
                         \textbf{forward\_triples} \ (\textit{idx\_triple: torch.tensor}) \ \rightarrow \textbf{torch.tensor}) \ \rightarrow \textbf{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

```
\mathbf{T}(x: torch.tensor) \rightarrow torch.tensor
Transpose function
Input: Tensor with shape (nxm) Output: Tensor with shape (mxn)
```

# dicee.models.ensemble

# **Classes**

EnsembleKGE

```
class dicee.models.ensemble.EnsembleKGE (seed_model=None, pretrained_models: List = None)
     name
     train_mode = True
     named_children()
     property example_input_array
     parameters()
     modules()
     __iter__()
     __len__()
     eval()
     to (device)
     mem_of_model()
     __call__(x_batch)
     step()
     get_embeddings()
     __str__()
```

# 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:

```
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 them to be nested in a tree structure. You can assign the sub-modules 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 also have their parameters converted 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.

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 them to be nested in a tree structure. You can assign the sub-modules as regular attributes:

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

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

(continued from previous page)

```
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 also have their parameters converted 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 Entities] =>
```

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 im-
	plemented 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 them to be nested in a tree structure. You can assign the sub-modules 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 also have their parameters converted 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**  $(b \circ \circ 1)$  – 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/
     1cecc7a77928ca8133fa24680a88d2f9-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 them to be nested in a tree structure. You can assign the sub-modules 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 also have their parameters converted 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.models.transformers.LayerNorm(ndim, bias)
```

Bases: torch.nn.Module

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

weight

bias

forward(input)

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

Bases: torch.nn.Module

Base class for all neural network modules.

Your models should also subclass this class.

Modules can also contain other Modules, allowing them to be nested in a tree structure. You can assign the sub-modules 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 also have their parameters converted 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 = True
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 them to be nested in a tree structure. You can assign the sub-modules 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 also have their parameters converted 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 them to be nested in a tree structure. You can assign the sub-modules 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)
```

(continued from previous page)

```
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 also have their parameters converted 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.

```
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 them to be nested in a tree structure. You can assign the sub-modules as regular attributes:

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

class Model (nn.Module):
```

(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 also have their parameters converted 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.

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**

Base class for all optimizers.
Base class for all neural network modules.
Base class for all neural network modules.
Base class for all neural network modules.
Base class for all neural network modules.
Embedding Entities and Relations for Learning and Inference in Knowledge Bases

Table 1 - continued from previous page

	r - continued from previous page
TransE	Translating Embeddings for Modeling
Shallom	A shallow neural model for relation prediction (https:
	//arxiv.org/abs/2101.09090)
Pyke	A Physical Embedding Model for Knowledge Graphs
BaseKGE	Base class for all neural network modules.
ConEx	Convolutional ComplEx Knowledge Graph Embeddings
AConEx	Additive Convolutional ComplEx Knowledge Graph Embeddings
ComplEx	Base class for all neural network modules.
BaseKGE	Base class for all neural network modules.
IdentityClass	Base class for all neural network modules.
QMult	Base class for all neural network modules.
ConvQ	Convolutional Quaternion Knowledge Graph Embeddings
AConvQ	Additive Convolutional Quaternion Knowledge Graph Embeddings
BaseKGE	Base class for all neural network modules.
IdentityClass	Base class for all neural network modules.
OMult	Base class for all neural network modules.
ConvO	Base class for all neural network modules.
AConv0	Additive Convolutional Octonion Knowledge Graph Embeddings
Keci	Base class for all neural network modules.
CKeci	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.ADOPT (params: torch.optim.optimizer.ParamsT, lr: float | torch.Tensor = 0.001,
             betas: Tuple[float, float] = (0.9, 0.9999), eps: float = 1e-06,
             clip_lambda: Callable[[int], float] \ None = lambda step: ..., weight_decay: float = 0.0,
             decouple: bool = False, *, foreach: bool | None = None, maximize: bool = False,
             capturable: bool = False, differentiable: bool = False, fused: bool | None = None)
      Bases: torch.optim.optimizer.Optimizer
```

Base class for all optimizers.

# Warning

Parameters need to be specified as collections that have a deterministic ordering that is consistent between runs. Examples of objects that don't satisfy those properties are sets and iterators over values of dictionaries.

#### **Parameters**

- params (iterable) an iterable of torch. Tensor s or dict s. Specifies what Tensors should be optimized.
- defaults (dict): a dict containing default values of optimization options (used when a parameter group doesn't specify them).

```
clip_lambda
__setstate__(state)
step(closure=None)
     Perform a single optimization step.
```

# **Parameters**

closure (Callable, optional) - A closure that reevaluates the model and returns the loss.

```
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 them to be nested 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 also have their parameters converted 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**  $(b \circ o 1)$  – Boolean represents whether this module is in training or evaluation mode.

```
training_step_outputs = []
mem\_of\_model() \rightarrow 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)
```

(continued from previous page)

```
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.

# **A** Warning

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.

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

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 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.

dataloader will not be reloaded unless you set :paramref: "~lightning.pytorch.trainer.trainer.Trainer.reload\_dataloaders\_every\_n\_epochs" to a positive integer.

For data processing use the following pattern:

- download in prepare\_data()
- process and split in setup()

However, the above are only necessary for distributed processing.

# Warning

do not assign state in prepare\_data

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

# **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 them to be nested in a tree structure. You can assign the sub-modules 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 also have their parameters converted 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

```
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
```

```
forward (x: torch.LongTensor | Tuple[torch.LongTensor, torch.LongTensor],
                 y idx: torch.LongTensor = None)
              Parameters
                  • x
                  y_idx
                  • ordered_bpe_entities
     \texttt{forward\_triples} \ (x: torch.LongTensor) \ \to 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.IdentityClass(args=None)
     Bases: torch.nn.Module
     Base class for all neural network modules.
     Your models should also subclass this class.
     modules as regular attributes:
```

init\_params\_with\_sanity\_checking()

Modules can also contain other Modules, allowing them to be nested in a tree structure. You can assign the sub-

```
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)
```

(continued from previous page)

```
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 also have their parameters converted 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 = None
__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 them to be nested in a tree structure. You can assign the sub-modules 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 also have their parameters converted 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.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
     \texttt{get\_embeddings}\,() \, \to Tuple[numpy.ndarray,\,None]
     \mathbf{forward\_k\_vs\_all}\;(x)\;\to \mathrm{torch.FloatTensor}
     forward_triples (x) \rightarrow \text{torch.FloatTensor}
               Parameters
               Returns
class dicee.models.Pyke(args)
     Bases: dicee.models.base_model.BaseKGE
     A Physical Embedding Model for Knowledge Graphs
     name = 'Pyke'
     dist_func
     margin = 1.0
```

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

## **Parameters**

x

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

Bases: BaseKGELightning

Base class for all neural network modules.

Your models should also subclass this class.

Modules can also contain other Modules, allowing them to be nested in a tree structure. You can assign the sub-modules 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 also have their parameters converted 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
\verb"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.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
                  x
```

```
forward_k_vs_sample (x: torch.Tensor, target_entity_idx: torch.Tensor)
class dicee.models.AConEx(args)
     Bases: dicee.models.base_model.BaseKGE
     Additive Convolutional ComplEx Knowledge Graph Embeddings
     name = 'AConEx'
     conv2d
     fc_num_input
     fc1
     norm_fc1
     bn_conv2d
     feature_map_dropout
     residual_convolution (C_1: Tuple[torch.Tensor, torch.Tensor],
                  C_2: Tuple[torch.Tensor, torch.Tensor]) \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 (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 them to be nested in a tree structure. You can assign the sub-
     modules as regular attributes:
      import torch.nn as nn
      import torch.nn.functional as F
```

```
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 also have their parameters converted 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.

forward k vs all (x: torch.LongTensor)  $\rightarrow$  torch.FloatTensor

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

```
\verb|dicee.models.quaternion_mul| (*, Q\_1, Q\_2)
```

→ Tuple[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 them to be nested in a tree structure. You can assign the sub-modules 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 also have their parameters converted 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.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 them to be nested in a tree structure. You can assign the sub-modules 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 also have their parameters converted 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 = None
__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 them to be nested in a tree structure. You can assign the sub-modules as regular attributes:

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

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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 also have their parameters converted 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**  $(b \circ o 1)$  – 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.
- $\mathbf{r}$  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
      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 \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.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)
      \textbf{forward\_triples} \ (\textit{indexed\_triple: torch.Tensor}) \ \rightarrow \textbf{torch.Tensor}) \ \rightarrow \textbf{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
     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()
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 them to be nested in a tree structure. You can assign the sub-modules 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 also have their parameters converted 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)
\mathtt{get\_embeddings}() \rightarrow \mathsf{Tuple}[\mathsf{numpy}.\mathsf{ndarray}, \mathsf{numpy}.\mathsf{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 them to be nested in a tree structure. You can assign the sub-modules 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 also have their parameters converted 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 = None
__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 them to be nested in a tree structure. You can assign the sub-modules as regular attributes:

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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 also have their parameters converted 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.

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 them to be nested in a tree structure. You can assign the sub-modules 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)
```

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```
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 also have their parameters converted when you call to (), etc.

# 1 Note

conv2d

fc\_num\_input

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 = '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()
class dicee.models.AConvO(args: dict)
     Bases: dicee.models.base_model.BaseKGE
     Additive Convolutional Octonion Knowledge Graph Embeddings
     name = 'AConvO'
```

```
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)

 ${\tt residual\_convolution}\,(O\_1,\,O\_2)$ 

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

## **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.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 them to be nested in a tree structure. You can assign the sub-modules 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 also have their parameters converted 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'
р
q
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.
{\tt compute\_sigma\_qq}\,(hq,rq)
     Compute sigma_{qq} = sum_{j=1}^{p+q-1} sum_{k=j+1}^{p+q} (h_j r_k - h_k r_j) e_j e_k sigma_{q}
     captures the interactions between along q bases For instance, let q e_1, e_2, e_3, we compute interactions
     between e_1 e_2, e_1 e_3, and e_2 e_3 This can be implemented with a nested two for loops
          results = [] for j in range(q - 1):
              for k in range(j + 1, q):
                 results.append(hq[:,:,j]*rq[:,:,k] - hq[:,:,k]*rq[:,:,j]) \\
          sigma_qq = torch.stack(results, dim=2) assert sigma_qq.shape == (b, r, int((q * (q - 1)) / 2))
     Yet, this computation would be quite inefficient. Instead, we compute interactions along all p, e.g., e1e1,
     e1e2, e1e3,
          e2e1, e2e2, e2e3, e3e1, e3e2, e3e3
     Then select the triangular matrix without diagonals: e1e2, e1e3, e2e3.
compute_sigma_pq(*, hp, hq, rp, rq)
     sum_{i=1}^{p} sum_{j=p+1}^{p+q} (h_i r_j - h_j r_i) e_i e_j
     results = [] sigma_pq = torch.zeros(b, r, p, q) for i in range(p):
          for j in range(q):
              sigma_pq[:, :, i, j] = hp[:, :, i] * rq[:, :, j] - hq[:, :, j] * rp[:, :, i]
     print(sigma_pq.shape)
apply_coefficients(hp, hq, rp, rq)
     Multiplying a base vector with its scalar coefficient
```

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

Compute our CL multiplication

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

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

eq j

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

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

 $\rightarrow$  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. 

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
```

#### rtvpe

torch.FloatTensor with (n) shape

```
class dicee.models.CKeci(args)
     Bases: Keci
```

Without learning dimension scaling

```
name = 'CKeci'
```

requires\_grad\_for\_interactions = False

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

```
Bases: \ \textit{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 them to be nested in a tree structure. You can assign the sub-modules 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)
```

(continues on next page)

```
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 also have their parameters converted 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**  $(b \circ o 1)$  – Boolean represents whether this module is in training or evaluation mode.

name = 'DeCaL'

entity\_embeddings

relation\_embeddings

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) —> 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,

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

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

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

For different base vector interactions, we have

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

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

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:

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

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):

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

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

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):

```
\begin{aligned} & \textbf{for j in range(q):} \\ & \text{sigma\_pq[:,:,i,j] = hp[:,:,i] * rq[:,:,j] - hq[:,:,j] * rp[:,:,i]} \\ & print(sigma\_pq.shape) \\ & \textbf{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 \\ & \text{results = [] sigma\_pq = torch.zeros(b, r, p, q) for i in range(p):} \\ & \textbf{for j in range(q):} \\ & \text{sigma\_pq[:,:,i,j] = hp[:,:,i] * rq[:,:,j] - hq[:,:,j] * rp[:,:,i]} \\ & \text{print(sigma\_pq.shape)} \\ & \textbf{class dicee.models.BaseKGE}(\textit{args: dict}) \\ & \text{Bases: } \textit{BaseKGELightning} \end{aligned}
```

Base class for all neural network modules.

Your models should also subclass this class.

Modules can also contain other Modules, allowing them to be nested in a tree structure. You can assign the sub-modules 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 also have their parameters converted 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
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,  $r = self.get_head_relation_representation(x) # (2) Reshape (1). if <math>self.last_dim > 0$ :
  - $h = h.reshape(len(x), self.embedding\_dim, self.last\_dim) r = r.reshape(len(x), self.embedding\_dim, self.last\_dim)$
- # (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:
  - $$\label{eq:hamma} \begin{split} &h = h.reshape(len(x), self.embedding\_dim, self.last\_dim) \ r = r.reshape(len(x), self.embedding\_dim, self.last\_dim) \end{split}$$
      $self.last\_dim) \ t = t.reshape(len(x), self.embedding\_dim, self.last\_dim) \end{split}$
- # (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 them to be nested in a tree structure. You can assign the sub-modules 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 also have their parameters converted 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)
{\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]
```

```
class dicee.models.FMult(args)
     Bases: dicee.models.base_model.BaseKGE
     Learning Knowledge Neural Graphs
     name = 'FMult'
     entity_embeddings
     relation_embeddings
     k
     num_sample = 50
     gamma
     roots
     weights
     compute\_func(weights: torch.FloatTensor, x) \rightarrow torch.FloatTensor
     chain_func (weights, x: torch.FloatTensor)
     forward\_triples(idx\_triple: torch.Tensor) \rightarrow torch.Tensor
              Parameters
                  x
class dicee.models.GFMult(args)
     Bases: dicee.models.base_model.BaseKGE
     Learning Knowledge Neural Graphs
     name = 'GFMult'
     entity_embeddings
     relation embeddings
     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_{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 \text{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=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
     tri_score(h, r, t)
     \mathtt{vtp\_score}\left(h,r,t\right)
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
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_i*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} h(x)r(x)t(x) dx = sum_{i,j,k} = 0}^{d-1} dfrac_{a_i}c_j*b_k
     b_i*c_j*a_k{(1+(i+j)%d)(1+k)}
       1. generate the range for i,j and k from [0 d-1]
       2. Compute the first and second terms of the sum
       3. Multiply with then denominator and take the sum
       4. take the sum over each batch
comp\_func(h, r, t)
     this part implement the function composition scoring techniques: i.e. score = <hor, t>
polynomial (coeff, x, degree)
     This function takes a matrix tensor of coefficients (coeff), a tensor vector of points x and range of integer
     [0,1,...d] and return a vector tensor (coeff[0][0] + coeff[0][1]x +...+ coeff[0][d]x^d,
```

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

```
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 = None
      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 \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
```

pop(coeff, x, degree)

```
\mathbf{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**

```
class dicee.query_generator.QueryGenerator(train_path, val_path: str, test_path: str,
            ent2id: Dict = None, rel2id: Dict = None, seed: int = 1, gen_valid: bool = False,
            gen\_test: bool = True)
     train_path
     val_path
     test_path
     gen_valid = False
     gen_test = True
     seed = 1
     max_ans_num = 1000000.0
     mode
     ent2id = None
     rel2id: Dict = None
     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) \rightarrow 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**

None

```
class dicee.read_preprocess_save_load_kg.preprocess.PreprocessKG (kg) Preprocess the data in memory kg start () \rightarrow N one Preprocess train, valid and test datasets stored in knowledge graph instance Parameter rtype
```

```
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
sequential\_vocabulary\_construction() \rightarrow None
     (1) Read input data into memory
     (2) Remove triples with a condition
     (3) Serialize vocabularies in a pandas dataframe where
              => the index is integer and => a single column is string (e.g. URI)
```

# dicee.read\_preprocess\_save\_load\_kg.read\_from\_disk

# **Classes**

ReadFromDisk

Read the data from disk into memory

## **Module Contents**

# $dicee.read\_preprocess\_save\_load\_kg.save\_load\_disk$

# Classes

LoadSaveToDisk

# **Module Contents**

```
class dicee.read_preprocess_save_load_kg.save_load_disk.LoadSaveToDisk(kg)
    kg
    save()
    load()
```

dicee.read\_preprocess\_save\_load\_kg.util

## **Functions**

polars_dataframe_indexer(→ polars.DataFrame)	Replaces 'subject', 'relation', and 'object' columns in the input Polars DataFrame with their corresponding index values
<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) \\ \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)
```

(1) Add reciprocal triples (2) Add noisy triples

```
dicee.read_preprocess_save_load_kg.util.timeit(func)
dicee.read_preprocess_save_load_kg.util.read_with_polars(data_path,
```

read\_only\_few: int = None, sample\_triples\_ratio: float = None, separator: str = None)  $\rightarrow polars.DataFrame$ 

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_kg.util.get_er_vocab(data, file_path: str = None)
```

```
dicee.read_preprocess_save_load_kg.util.get_re_vocab(data, file_path: str = None)
```

```
dicee.read_preprocess_save_load_kg.util.get_ee_vocab(data, file_path: str = None)
```

```
dicee.read_preprocess_save_load_kg.util.create_constraints(triples, file_path: str = None)
```

- (1) Extract domains and ranges of relations
- (2) Store a mapping from relations to entities that are outside of the domain and range. Crete constrainted entities based on the range of relations :param triples: :return: Tuple[dict, dict]

```
dicee.read_preprocess_save_load_kg.util.load_with_pandas(self) \rightarrow None
```

Deserialize data

#### **Classes**

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

# **Package Contents**

(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

(2) Construct vocabulary
```

# **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\_serve

\$ docker pull qdrant/qdrant && docker run -p 6333:6333 -p 6334:6334 -v \$(pwd)/qdrant\_storage:/qdrant/storage:z qdrant/qdrant \$ dicee\_vector\_db -index -serve -path CountryEmbeddings -collection "countries\_vdb"

# **Attributes**

```
app
neural_searcher
```

# **Classes**

NeuralSearcher		
StringListRequest	Usage docs: models/	https://docs.pydantic.dev/2.10/concepts/

### **Functions**

```
get_default_arguments()
index(args)

root()
search_embeddings(q)

retrieve_embeddings(q)
search_embeddings_batch(request)
serve(args)

main()
```

### **Module Contents**

```
dicee.scripts.index_serve.get_default_arguments()
dicee.scripts.index_serve.index(args)
dicee.scripts.index_serve.app
dicee.scripts.index_serve.neural_searcher = None
class dicee.scripts.index_serve.NeuralSearcher(args)
     collection name
     entity to idx = None
     qdrant_client
     topk = 5
     retrieve_embedding (entity: str = None, entities: List[str] = None) \rightarrow List
     search (entity: str)
async dicee.scripts.index_serve.root()
async dicee.scripts.index_serve.search_embeddings(q: str)
async dicee.scripts.index_serve.retrieve_embeddings(q: str)
class dicee.scripts.index_serve.StringListRequest(/, **data: Any)
     Bases: pydantic.BaseModel
     Usage docs: https://docs.pydantic.dev/2.10/concepts/models/
     A base class for creating Pydantic models.
     __class_vars__
          The names of the class variables defined on the model.
     __private_attributes__
          Metadata about the private attributes of the model.
     __signature__
          The synthesized __init__ [Signature][inspect.Signature] of the model.
     __pydantic_complete__
          Whether model building is completed, or if there are still undefined fields.
     __pydantic_core_schema__
          The core schema of the model.
     __pydantic_custom_init__
          Whether the model has a custom __init__ function.
     __pydantic_decorators__
          Metadata containing the decorators defined on the model. This replaces Model._validators_ and
          Model.__root_validators__ from Pydantic V1.
```

```
__pydantic_generic_metadata__
          Metadata for generic models; contains data used for a similar purpose to __args__, __origin__, __parame-
          ters in typing-module generics. May eventually be replaced by these.
      __pydantic_parent_namespace__
          Parent namespace of the model, used for automatic rebuilding of models.
     __pydantic_post_init__
          The name of the post-init method for the model, if defined.
      __pydantic_root_model__
          Whether the model is a [RootModel][pydantic.root_model.RootModel].
     __pydantic_serializer__
          The pydantic-core SchemaSerializer used to dump instances of the model.
     __pydantic_validator__
          The pydantic-core Schema Validator used to validate instances of the model.
     __pydantic_fields__
          A dictionary of field names and their corresponding [FieldInfo][pydantic.fields.FieldInfo] objects.
     __pydantic_computed_fields__
               dictionary
                            of
                                 computed
                                             field
                                                     names
                                                              and
                                                                     their
                                                                            corresponding
                                                                                             [ComputedField-
          Info][pydantic.fields.ComputedFieldInfo] objects.
     __pydantic_extra__
          A dictionary containing extra values, if [extra][pydantic.config.ConfigDict.extra] is set to 'allow'.
      __pydantic_fields_set__
          The names of fields explicitly set during instantiation.
     __pydantic_private__
          Values of private attributes set on the model instance.
     queries: List[str]
     reducer: str | None = None
async dicee.scripts.index_serve.search_embeddings_batch (request: StringListRequest)
dicee.scripts.index_serve.serve(args)
dicee.scripts.index_serve.main()
```

# dicee.scripts.run

# **Functions**

```
get_default_arguments([description])
Extends pytorch_lightning Trainer's arguments with ours
main()
```

# **Module Contents**

# dicee.static\_funcs

# **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>	
get_ee_vocab(data[, file_path])	
timeit(func)	
<pre>save_pickle(*[, data, file_path])</pre>	
load_pickle([file_path])	
<pre>load_term_mapping([file_path])</pre>	
<pre>select_model(args[, is_continual_training, stor- age_path])</pre>	
$load_model(\rightarrow Tuple[object, Tuple[dict, dict]])$	Load weights and initialize pytorch module from namespace arguments
load_model_ensemble()	Construct Ensemble Of weights and initialize pytorch module from namespace arguments
<pre>save_numpy_ndarray(*, data, file_path)</pre>	
numpy_data_type_changer(→ numpy.ndarray)	Detect most efficient data type for a given triples
$save\_checkpoint\_model(\rightarrow None)$ $store(\rightarrow None)$	Store Pytorch model into disk
add_noisy_triples(→ pandas.DataFrame)	Add randomly constructed triples
read_or_load_kg(args, cls)	
$intialize\_model(\rightarrow Tuple[object, str])$	
load_json(→ dict)	
$save\_embeddings(\rightarrow None)$	Save it as CSV if memory allows.
random_prediction(pre_trained_kge)	
<pre>deploy_triple_prediction(pre_trained_kge, str_subject,)</pre>	
<pre>deploy_tail_entity_prediction(pre_trained_kge,)</pre>	
	continues on next page

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Table 2 - continued from previous page

```
deploy_head_entity_prediction(pre_trained_kge,
deploy_relation_prediction(pre_trained_kge,
...)
 vocab_to_parquet(vocab_to_idx, name, ...)
create_experiment_folder([folder_name])
continual_training_setup_executor(→ None)
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)
write_csv_from_model_parallel(path)
                                                     Create
 from_pretrained_model_write_embeddings_into
None)
```

#### **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)
```

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(trained_model, model_name: str = 'model', full_storage_path: str = None, save\_embeddings\_as\_csv=False) \rightarrow None
```

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\_tail\_entity\_prediction( $pre\_trained\_kge$ ,  $str\_subject$ ,  $str\_predicate$ ,  $top\_k$ )

 $\label{local_discrete_discrete} \verb|discrete_static_funcs.deploy_head_entity_prediction|| (pre\_trained\_kge, str\_object, str\_predicate, top\_k)|$ 

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

 $\label{local_discrete_discrete} \begin{tabular}{ll} \tt discrete_static_funcs.exponential\_function (\it{x: numpy.ndarray, lam: float, ascending\_order=True)} \\ \to torch. Float Tensor \end{tabular}$ 

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='.') 	o 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-KvsA11")

```
dicee.static_funcs.download_pretrained_model(url: str) \rightarrow str
```

dicee.static\_funcs.write\_csv\_from\_model\_parallel(path: str)

Create

 $\texttt{dicee.static\_funcs.from\_pretrained\_model\_write\_embeddings\_into\_csv} \ (\textit{path: str}) \rightarrow None$ 

# dicee.static\_funcs\_training

#### **Functions**

```
make\_iterable\_verbose(\rightarrow Iterable)
evaluate\_lp([model, triple\_idx, num\_entities, ...])
evaluate\_bpe\_lp(model, triple\_idx, ...[, info])
efficient\_zero\_grad(model)
```

## **Module Contents**

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

```
dicee.static_funcs_training.evaluate_lp (model=None, triple_idx=None, num_entities=None, er_vocab: Dict[Tuple, List] = None, re_vocab: Dict[Tuple, List] = None, info='Eval Starts', batch_size=128, chunk_size=1000)
```

dicee.static\_funcs\_training.efficient\_zero\_grad(model)

# dicee.static\_preprocess\_funcs

#### **Attributes**

enable\_log

### **Functions**

```
timeit(func)
preprocesses\_input\_args(args) \qquad Sanity Checking in input arguments
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)
```

#### **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**

DICE\_Trainer implement

### **Functions**

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

### **Module Contents**

```
dicee.trainer.dice_trainer.load_term_mapping(file_path=str)
dicee.trainer.dice_trainer.initialize_trainer(args, callbacks)
            \rightarrow dicee.trainer.torch_trainer.Torch_trainer.Torch_trainer.ddp.arallelism.TensorParallel \(\) dicee.trainer.torch_trainer_ddp.
dicee.trainer.dice_trainer.get_callbacks(args)
class dicee.trainer.dice_trainer.DICE_Trainer(args, is_continual_training: bool, 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 = None
     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)

→ lightning.Trainer | dicee.trainer.model\_parallelism.TensorParallel | dicee.trainer.torch\_trainer.TorchTrainer | dicee.trainer.TorchTrainer | dicee.trainer.torch\_trainer.TorchTrainer | dicee.trainer.torch\_trainer.TorchTrainer | dicee.trainer.torch\_trai

```
initialize_or_load_model()
```

 $init\_dataloader$  (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.

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

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**

TensorParallel Abstract class for Knowledge graph embedding models

### **Functions**

```
extract_input_outputs(z[, device])

find_good_batch_size(train_loader,

tp_ensemble_model)

forward_backward_update_loss(→ float)
```

### **Module Contents**

## dicee.trainer.torch\_trainer

### Classes

TorchTrainer	TorchTrainer for using single GPU or multi CPUs on a
	single node

### **Module Contents**

```
class dicee.trainer.torch_trainer.TorchTrainer(args, callbacks)

Bases: dicee.abstracts.AbstractTrainer

TorchTrainer for using single GPU or multi CPUs on a single node

Arguments

callbacks: list of Abstract callback instances

loss_function = None
```

```
optimizer = None
model = None
train_dataloaders = None
training_step = None
process
fit (*args, train\_dataloaders, **kwargs) \rightarrow None
           Training starts
           Arguments
      kwargs:Tuple
           empty dictionary
           Return type
                batch loss (float)
\textbf{forward\_backward\_update} \ (x\_\textit{batch: torch.Tensor}, \ y\_\textit{batch: torch.Tensor}) \ \to \ \text{torch.Tensor}) \ \to \ \text{torch.Tensor})
           Compute forward, loss, backward, and parameter update
           Arguments
           Return type
                batch loss (float)
\textbf{extract\_input\_outputs\_set\_device} \ (\textit{batch: list}) \ \rightarrow \textbf{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
```

### **Classes**

DICE\_Trainer

DICE\_Trainer implement

# **Package Contents**

class dicee.trainer.DICE\_Trainer(args, is\_continual\_training: bool, 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 = None

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)

→ lightning.Trainer | dicee.trainer.model\_parallelism.TensorParallel | dicee.trainer.torch\_trainer.TorchTrainer | dicee.trainer.TorchTrainer | dicee.trainer.torch\_trainer.TorchTrainer | dicee.trainer.torch\_trainer.TorchTrainer | dicee.trainer.torch\_trai

### initialize\_or\_load\_model()

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

 $\verb"init_dataset" () \rightarrow torch.utils.data.Dataset"$ 

 $\verb|start| (knowledge\_graph: dicee.knowledge\_graph.KG \mid numpy.memmap)|$ 

→ 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

# 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
CKeci	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.

continues on next page

Table 3 - continued from previous page

	continued from previous page
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 Embeddings
AConvQ	Additive Convolutional Quaternion Knowledge Graph Embeddings
ConvQ	Convolutional Quaternion Knowledge Graph Embeddings
ConvO	Base class for all neural network modules.
ConEx	Convolutional ComplEx Knowledge Graph Embeddings
QMult	Base class for all neural network modules.
OMult	Base class for all neural network modules.
Shallom	A shallow neural model for relation prediction (https:
SHATTOM	//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 im-
	plemented in Pykeen
BytE	Base class for all neural network modules.
BaseKGE	Base class for all neural network modules.
EnsembleKGE	
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	2

# 14.4 Functions

create_recipriocal_triples(x)	Add inverse triples into dask dataframe
	continues on next page

Table 4 - 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)
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)
```

continues on next page

Table 4 - continued from previous page

```
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)
                                                      Create
write_csv_from_model_parallel(path)
 from_pretrained_model_write_embeddings_int
 None)
 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'
     \verb+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.CKeci(args)
Bases: Keci
Without learning dimension scaling
name = 'CKeci'
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 them to be nested in a tree structure. You can assign the sub-modules 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 also have their parameters converted 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 = 'Keci'
p
q
```

```
requires_grad_for_interactions = True
compute\_sigma\_pp(hp, rp)
          Compute sigma_{pp} = sum_{i=1}^{p-1} sum_{k=i+1}^p (h_i r_k - h_k r_i) e_i e_k
          sigma_{pp} captures the interactions between along p bases For instance, let p e_1, e_2, e_3, we compute
          interactions between e 1 e 2, e 1 e 3, and e 2 e 3 This can be implemented with a nested two for loops
                  results = [] for i in range(p - 1):
                          for k in range(i + 1, p):
                               results.append(hp[:, :, i] * rp[:, :, k] - hp[:, :, k] * rp[:, :, i])
                  sigma_pp = torch.stack(results, dim=2) assert sigma_pp.shape == (b, r, int((p * (p - 1)) / 2))
          Yet, this computation would be quite inefficient. Instead, we compute interactions along all p, e.g., e1e1,
          e1e2, e1e3,
                  e2e1, e2e2, e2e3, e3e1, e3e2, e3e3
          Then select the triangular matrix without diagonals: e1e2, e1e3, e2e3.
compute\_sigma\_qq(hq, rq)
          Compute sigma_{qq} = sum_{j=1}^{p+q-1} sum_{k=j+1}^{p+q} (h_j r_k - h_k r_j) e_j e_k sigma_{q}
          captures the interactions between along q bases For instance, let q e 1, e 2, e 3, we compute interactions
          between e 1 e 2, e 1 e 3, and e 2 e 3 This can be implemented with a nested two for loops
                  results = [] for j in range(q - 1):
                          for k in range(j + 1, q):
                               results.append(hq[:,:,j]*rq[:,:,k]-hq[:,:,k]*rq[:,:,j])\\
                  sigma_qq = torch.stack(results, dim=2) assert sigma_qq.shape == (b, r, int((q * (q - 1)) / 2))
          Yet, this computation would be quite inefficient. Instead, we compute interactions along all p, e.g., e1e1,
          e1e2, e1e3,
                  e2e1, e2e2, e2e3, e3e1, e3e2, e3e3
          Then select the triangular matrix without diagonals: e1e2, e1e3, e2e3.
compute_sigma_pq(*, hp, hq, rp, rq)
          sum_{i=1}^{p} sum_{j=p+1}^{p+q} (h_i r_j - h_j r_i) e_i e_j
          results = [] sigma_pq = torch.zeros(b, r, p, q) for i in range(p):
                  for j in range(q):
                          sigma_pq[:, :, i, j] = hp[:, :, i] * rq[:, :, j] - hq[:, :, j] * rp[:, :, i]
          print(sigma_pq.shape)
apply_coefficients(hp, hq, rp, rq)
          Multiplying a base vector with its scalar coefficient
clifford_multiplication (h0, hp, hq, r0, rp, rq)
          Compute our CL multiplication
                  h = h_0 + sum_{i=1}^p h_i e_i + sum_{j=p+1}^p 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)  $sigma_q = sum_{j=p+1}^{q} (h_0 r_j + h_j r_0) e_j$
- (4)  $sigma_{pp} = sum_{i=1}^{p-1} sum_{k=i+1}^p (h_i r_k h_k r_i) e_i e_k$
- (5)  $sigma_{qq} = sum_{j=1}^{p+q-1} sum_{k=j+1}^{p+q} (h_j r_k h_k r_j) e_j e_k$
- (6)  $sigma_{pq} = sum_{i=1}^{p} sum_{j=p+1}^{p+q} (h_i r_j h_j r_i) e_i e_j$

construct\_cl\_multivector (x: torch.FloatTensor, r: int, p: int, q: int)

→ tuple[torch.FloatTensor, torch.FloatTensor, torch.FloatTensor]

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

#### **Parameter**

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

# returns

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

forward\_k\_vs\_with\_explicit(x: torch.Tensor)

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

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

**Kvsall** training

- (1) Retrieve real-valued embedding vectors for heads and relations  $\operatorname{mathbb}\{R\}^d$ .
- (2) Construct head entity and relation embeddings according to  $Cl_{p,q}(\mathbf{mathbb}_{R}^{d})$ .
- (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  \begin{aligned} &\text{target\_entity\_idx: torch.LongTensor with (n, k) shape k denotes the selected number of examples.} \\ & &\textbf{rtype} \\ & & & & & & & & & & & & & & & \\ & & & & & & & & & & & & & \\ & & & & & & & & & & & & \\ & & & & & & & & & & & & \\ & & & & & & & & & & & \\ & & & & & & & & & & & \\ & & & & & & & & & & & \\ & & & & & & & & & & \\ & & & & & & & & & & \\ & & & & & & & & & & \\ & & & & & & & & & & \\ & & & & & & & & & & \\ & & & & & & & & & \\ & & & & & & & & & \\ & & & & & & & & & \\ & & & & & & & & & \\ & & & & & & & & \\ & & & & & & & & \\ & & & & & & & & \\ & & & & & & & & \\ & & & & & & & & \\ & & & & & & & \\ & & & & & & & \\ & & & & & & & \\ & & & & & & & \\ & & & & & & & \\ & & & & & & & \\ & & & & & & & \\ & & & & & & & \\ & & & & & & & \\ & & & & & & & \\ & & & & & & & \\ & & & & & & & \\ & & & & & & & \\ & & & & & & & \\ & & & & & & & \\ & & & & & & \\ & & & & & & \\ & & & & & & \\ & & & & & & \\ & & & & & & \\ & & & & & & \\ & & & & & \\ & & & & & & \\ & & & & & & \\ & & & & & & \\ & & & & & & \\ & & & & & & \\ & & & & & \\ & & & & & \\ & & & & & \\ & & & & & \\ & & & & & \\ & & & & & \\ & & & & & \\ & & & & \\ & & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & \\ & & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & &
```

#### **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 them to be nested in a tree structure. You can assign the sub-modules 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 also have their parameters converted 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 = '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,

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

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

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

For different base vector interactions, we have

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

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

Kvsall training

- (1) Retrieve real-valued embedding vectors for heads and relations
- (2) Construct head entity and relation embeddings according to  $Cl_{p,q, r}(\text{mathbb}\{R\}^d)$ .
- (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

 $\verb"apply_coefficients" (h0, hp, hq, hk, r0, rp, rq, rk)$ 

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} $$ \sum_{p=1}^{p} \sup_{i=1}^{p-1}\sum_{i'=i+1}^{p} (x_iy_{i'}-x_{i'}) $$
```

sigma\_{pp} captures the interactions between along p bases For instance, let p e\_1, e\_2, e\_3, we compute interactions between e\_1 e\_2, e\_1 e\_3, and e\_2 e\_3 This can be implemented with a nested two for loops

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

```
for k in range(i + 1, p):
```

```
results.append(hp[:, :, i] * rp[:, :, k] - hp[:, :, k] * rp[:, :, i])
```

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

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

```
e2e1, e2e2, e2e3, e3e1, e3e2, e3e3
```

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

 $compute\_sigma\_qq(hq, rq)$ 

Compute

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

sigma\_{q} captures the interactions between along q bases For instance, let q e\_1, e\_2, e\_3, we compute interactions between e\_1 e\_2, e\_1 e\_3, and e\_2 e\_3 This can be implemented with a nested two for loops

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

# for k in range(j + 1, q):

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

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

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

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)

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

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

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 = None
                    \texttt{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\_6\_h, e\_7\_h, e\_8\_h, e\_1\_t, e\_2\_t, e\_3\_t, e\_4\_t, e\_4\_t, e\_6\_h, e\_7\_h, e\_8\_h, e\_1\_t, e\_6\_t, e\_6\_h, e\_7\_h, e\_8\_h, e\_1\_t, e\_8\_t, e\_8
                                                                 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
                    \textbf{forward\_triples} \ (\textit{idx\_triple: torch.tensor}) \ \rightarrow \textbf{torch.tensor}) \ \rightarrow \textbf{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)
```

```
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 them to be nested in a tree structure. You can assign the sub-modules 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 also have their parameters converted 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.

## **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)
```

 $Bases: \ \textit{dicee.models.base\_model.BaseKGE}$ 

Additive Convolutional ComplEx Knowledge Graph Embeddings

```
name = 'AConEx'
     conv2d
     fc_num_input
     fc1
     norm_fc1
     bn_conv2d
     feature_map_dropout
     {\tt 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.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)
     {\tt residual\_convolution}\,(O\_1,\,O\_2)
     forward\_triples(x: torch.Tensor) \rightarrow torch.Tensor
               Parameters
                   x
```

```
Given a head entity and a relation (h,r), we compute scores for all entities. [score(h,r,x)|x in Entities] =>
          [0.0,0.1,...,0.8], shape=> (1, |Entities|) Given a batch of head entities and relations => shape (size of batch,)
          Entities()
class dicee.AConvQ(args)
     Bases: dicee.models.base_model.BaseKGE
     Additive Convolutional Quaternion Knowledge Graph Embeddings
     name = 'AConvQ'
     entity_embeddings
     relation_embeddings
     conv2d
     fc_num_input
     fc1
     bn_conv1
     bn_conv2
     feature_map_dropout
     residual_convolution (Q_1, Q_2)
     forward\_triples (indexed_triple: torch.Tensor) \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.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
```

forward\_k\_vs\_all (x: torch.Tensor)

```
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] => [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 them to be nested in a tree structure. You can assign the sub-modules 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 also have their parameters converted 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 = '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.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 them to be nested in a tree structure. You can assign the sub-modules 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 also have their parameters converted 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.

```
\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.

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

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.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 them to be nested in a tree structure. You can assign the sub-modules 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 also have their parameters converted 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 = '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)
     \verb+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
     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.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

#### 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.embedding\_dim) \\ r = r.reshap
                                      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 them to be nested 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)
```

(continues on next page)

```
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 also have their parameters converted 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 them to be nested in a tree structure. You can assign the sub-modules 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 also have their parameters converted 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.EnsembleKGE (seed_model=None, pretrained_models: List = None)
     name
     train_mode = True
     named_children()
     property example_input_array
     parameters()
     modules()
     __iter__()
     __len__()
     eval()
     to (device)
     mem_of_model()
     __call__(x_batch)
     step()
     get_embeddings()
     __str__()
dicee.create_recipriocal_triples(x)
     Add inverse triples into dask dataframe :param x: :return:
dicee.get_er_vocab(data, file_path: str = None)
dicee.get_re_vocab(data, file_path: str = None)
dicee.get_ee_vocab (data, file_path: str = None)
dicee.timeit(func)
dicee.save_pickle(*, data: object = None, file_path=str)
```

```
dicee.load_pickle(file_path=str)
dicee.load_term_mapping(file_path=str)
dicee.select_model(args: dict, is_continual_training: bool = None, storage_path: str = None)
dicee.load_model(path_of_experiment_folder: str, model_name='model.pt', verbose=0)
             → Tuple[object, Tuple[dict, dict]]
     Load weights and initialize pytorch module from namespace arguments
dicee.load_model_ensemble(path_of_experiment_folder: str)
             → Tuple[dicee.models.base_model.BaseKGE, Tuple[pandas.DataFrame, pandas.DataFrame]]
     Construct Ensemble Of weights and initialize pytorch module from namespace arguments
       (1) Detect models under given path
       (2) Accumulate parameters of detected models
       (3) Normalize parameters
       (4) Insert (3) into model.
dicee.save_numpy_ndarray(*, data: numpy.ndarray, file_path: str)
dicee.numpy_data_type_changer(train\_set: numpy.ndarray, num: int) \rightarrow 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(trained_model, model_name: str = 'model', full_storage_path: str = None,
            save\_embeddings\_as\_csv=False) \rightarrow None
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) \rightarrow 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')
dicee.continual_training_setup_executor(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
                                                   "https://files.dice-research.org/projects/DiceEmbeddings/
                   KINSHIP-Keci-dim128-epoch256-KvsAll")
                 • destination_folder(e.g. "KINSHIP-Keci-dim128-epoch256-KvsAll")
dicee.download_pretrained_model(url: str) \rightarrow str
dicee.write_csv_from_model_parallel(path: str)
     Create
\texttt{dicee.from\_pretrained\_model\_write\_embeddings\_into\_csv}(\textit{path: str}) \rightarrow \texttt{None}
class dicee.DICE_Trainer(args, is_continual_training: bool, 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 = None
     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)

→ lightning.Trainer | dicee.trainer.model\_parallelism.TensorParallel | dicee.trainer.torch\_trainer.TorchTrainer | dicee.trainer.TorchTrainer | dicee.trainer.torch\_trainer.TorchTrainer | dicee.trainer.torch\_trainer.TorchTrainer | dicee.trainer.torch\_trai

```
initialize_or_load_model()
```

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

init\_dataset() → 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.

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

Perform K-fold Cross-Validation

- 1. Obtain K train and test splits.
- 2. For each split,
  - 2.1 initialize trainer and model 2.2. Train model with configuration provided in args. 2.3. Compute the mean reciprocal rank (MRR) score of the model on the test respective split.
- 3. Report the mean and average MRR.

## **Parameters**

- self
- dataset

### Returns

model

class dicee.KGE (path=None, url=None, construct\_ensemble=False, model\_name=None)

Bases: dicee.abstracts.BaseInteractiveKGE

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

```
__str__()
```

to (device: str)  $\rightarrow$  None

 $\begin{tabular}{ll} \tt get\_transductive\_entity\_embeddings (\it indices: torch.LongTensor \mid List[str], as\_pytorch=False, \\ as\_numpy=False, as\_list=True) \rightarrow {\tt torch.FloatTensor \mid numpy.ndarray \mid List[float]} \\ \end{tabular}$ 

 $create\_vector\_database$  (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
predict_missing_relations (head_entity: List[str] | str, tail_entity: List[str] | str, within=None)
     Given a head entity and a tail entity, return top k ranked relations.
     argmax_{r in R} f(h,r,t), where h, t in E.
     Parameter
     head_entity: List[str]
     String representation of selected entities.
     tail_entity: List[str]
     String representation of selected entities.
     k: int
     Highest ranked k entities.
     Returns: Tuple
     Highest K scores and entities
predict_missing_tail_entity (head_entity: List[str] | str, relation: List[str] | str,
              within: List[str] = None \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 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

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.
                topk: int
                Highest ranked k item to select triples with f(e,r,x) > confidence.
                at_most: int
                Stop after finding at_most missing triples
                \{(e,r,x) \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 = False
      trainer = None
      trained_model = None
      knowledge_graph = None
      report
      evaluator = None
```

start\_time = None

```
setup\_executor() \rightarrow 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
      {\tt write\_report}\,()\,\to 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
dicee.mapping_from_first_two_cols_to_third(train_set_idx)
dicee.timeit(func)
dicee.load_term_mapping(file_path=str)
dicee.reload_dataset (path: str, form_of_labelling, scoring_technique, neg_ratio, label_smoothing_rate)
      Reload the files from disk to construct the Pytorch dataset
dicee.construct_dataset(*, train_set: numpy.ndarray| list, valid_set=None, test_set=None,
             ordered_bpe_entities=None, train_target_indices=None, target_dim: int = None, entity_to_idx: dict,
             relation to idx: dict, form of labelling: str, scoring technique: str, neg ratio: int,
             label_smoothing_rate: float, byte_pair_encoding=None, block_size: int = None)
```

→ torch.utils.data.Dataset

```
class dicee.BPE NegativeSamplingDataset (train set: torch.LongTensor,
            ordered_shaped_bpe_entities: torch.LongTensor, neg_ratio: int)
```

Bases: torch.utils.data.Dataset

An abstract class representing a Dataset.

All datasets that represent a map from keys to data samples should subclass it. All subclasses should overwrite \_\_getitem\_\_(), supporting fetching a data sample for a given key. Subclasses could also optionally overwrite \_\_len\_\_(), which is expected to return the size of the dataset by many Sampler implementations and the default options of DataLoader. Subclasses could also optionally implement \_\_qetitems\_\_(), 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.

```
train_set
ordered_bpe_entities
num_bpe_entities
neg_ratio
num_datapoints
__len__()
\__getitem\__(idx)
collate_fn (batch_shaped_bpe_triples: List[Tuple[torch.Tensor, torch.Tensor]])
```

class dicee.MultiLabelDataset (train\_set: torch.LongTensor, train\_indices\_target: torch.LongTensor, target\_dim: int, torch\_ordered\_shaped\_bpe\_entities: torch.LongTensor)

Bases: torch.utils.data.Dataset

An abstract class representing a Dataset.

All datasets that represent a map from keys to data samples should subclass it. All subclasses should overwrite \_\_getitem\_\_(), supporting fetching a data sample for a given key. Subclasses could also optionally overwrite \_len\_\_ (), which is expected to return the size of the dataset by many Sampler implementations and the default options of DataLoader. Subclasses could also optionally implement \_\_getitems\_\_(), for speedup batched samples loading. This method accepts list of indices of samples of batch and returns list of samples.

## 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.

```
train_set
train_indices_target
target_dim
```

```
num_datapoints
     torch_ordered_shaped_bpe_entities
     collate_fn = None
     __len__()
     \__getitem__(idx)
class dicee.MultiClassClassificationDataset (subword_units: numpy.ndarray, block_size: int = 8)
     Bases: torch.utils.data.Dataset
     Dataset for the 1vsALL training strategy
          Parameters
                • train_set_idx - Indexed triples for the training.
                • entity_idxs - mapping.
                • relation_idxs - mapping.
                • form - ?
                                                https://pytorch.org/docs/stable/data.html#torch.utils.data.
                • num_workers -
                                      int
                                          for
                  DataLoader
          Return type
              torch.utils.data.Dataset
     train_data
     block_size = 8
     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 - ?
                • num_workers - int for https://pytorch.org/docs/stable/data.html#torch.utils.data.
                  DataLoader
```

## Return type

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.



1 Note

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
```

```
train_data = None
train_target = None
label_smoothing_rate
collate_fn = None
target_dim
__len__()
\__{\texttt{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 = None
label_smoothing_rate
```

Returns the number of samples in the dataset.

 $\__{getitem}_{\_}(idx)$ 

\_\_len\_\_()

collate\_fn = None

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
```

 $\__getitem\__(idx)$ 

```
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, \text{ 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 = None
     num_entities
     label_smoothing_rate
     collate_fn = None
     max_num_of_classes
     __len__()
```

```
class dicee. NegSampleDataset (train_set: numpy.ndarray, num_entities: int, num_relations: int,
             neg\_sample\_ratio: int = 1)
```

Bases: torch.utils.data.Dataset

An abstract class representing a Dataset.

All datasets that represent a map from keys to data samples should subclass it. All subclasses should overwrite \_\_getitem\_\_(), supporting fetching a data sample for a given key. Subclasses could also optionally overwrite \_\_len\_\_(), which is expected to return the size of the dataset by many Sampler implementations and the default options of DataLoader. Subclasses could also optionally implement \_\_getitems\_\_(), for speedup batched samples loading. This method accepts list of indices of samples of batch and returns list of samples.

## **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__()
      \__{\texttt{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) \mid i \mid i \mid 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__()
     \__{\texttt{getitem}} (idx)
     collate_fn (batch: List[torch.Tensor])
class dicee. CVDataModule (train_set_idx: numpy.ndarray, num_entities, num_relations, neg_sample_ratio,
            batch_size, num_workers)
     Bases: pytorch_lightning.LightningDataModule
     Create a Dataset for cross validation
          Parameters
                • train_set_idx - Indexed triples for the training.
                • num_entities - entity to index mapping.
                • num_relations - relation to index mapping.
                • batch_size - int
                • form - ?
                                           for https://pytorch.org/docs/stable/data.html#torch.utils.data.
                • num_workers - int
                  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.

will dataloader return not be reloaded unless :paramyou 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.

```
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.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, ...).



This hook should only transfer the data and not modify it, nor should it move the data to any other device than the one passed in as argument (unless you know what you are doing). To check the current state of execution of this hook you can use self.trainer.training/testing/validating/predicting so that you can add different logic as per your requirement.

#### **Parameters**

- batch A batch of data that needs to be transferred to a new device.
- **device** The target device as defined in PyTorch.
- dataloader\_idx The index of the dataloader to which the batch belongs.

#### Returns

A reference to the data on the new device.

## Example:

```
def transfer_batch_to_device(self, batch, device, dataloader_idx):
    if isinstance(batch, CustomBatch):
        # move all tensors in your custom data structure to the device
        batch.samples = batch.samples.to(device)
        batch.targets = batch.targets.to(device)
    elif dataloader_idx == 0:
        # skip device transfer for the first dataloader or anything you wish
        pass
    else:
        batch = super().transfer_batch_to_device(batch, device, dataloader_
    →idx)
    return batch
```

## → See also

- move\_data\_to\_device()
- apply\_to\_collection()

```
prepare_data(*args, **kwargs)
```

Use this to download and prepare data. Downloading and saving data with multiple processes (distributed settings) will result in corrupted data. Lightning ensures this method is called only within a single process, so you can safely add your downloading logic within.

## **Marning**

DO NOT set state to the model (use setup instead) since this is NOT called on every device

## Example:

```
def prepare_data(self):
    # good
    download_data()
    tokenize()
    etc()

# bad
self.split = data_split
self.some_state = some_other_state()
```

In a distributed environment, prepare\_data can be called in two ways (using prepare\_data\_per\_node)

- 1. Once per node. This is the default and is only called on LOCAL\_RANK=0.
- 2. Once in total. Only called on GLOBAL\_RANK=0.

## Example:

```
# DEFAULT
# called once per node on LOCAL_RANK=0 of that node
class LitDataModule(LightningDataModule):
    def __init__(self):
        super().__init__()
        self.prepare_data_per_node = True

# call on GLOBAL_RANK=0 (great for shared file systems)
class LitDataModule(LightningDataModule):
    def __init__(self):
        super().__init__()
        self.prepare_data_per_node = False
```

This is called before requesting the dataloaders:

```
model.prepare_data()
initialize_distributed()
model.setup(stage)
model.train_dataloader()
model.val_dataloader()
model.test_dataloader()
model.predict_dataloader()
```

class dicee.QueryGenerator(train\_path, val\_path: str, test\_path: str, ent2id: Dict = None, rel2id: Dict = None, seed: int = 1, gen\_valid: bool = False, gen\_test: bool = True)

```
train_path
val_path
test_path
gen_valid = False
gen_test = True
seed = 1
max_ans_num = 1000000.0
mode
ent2id = None
rel2id: Dict = None
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 \mid List], ent\_in: Dict, ent\_out: Dict) \rightarrow 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)
```

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