# **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 0.2.0

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

Publisher and maintainer: Caglar Demir<sup>2</sup>

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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>&</sup>lt;sup>1</sup> https://github.com/dice-group/dice-embeddings

<sup>&</sup>lt;sup>2</sup> https://github.com/Demirrr

<sup>3</sup> https://pandas.pydata.org/

<sup>4</sup> https://pytorch.org/

<sup>&</sup>lt;sup>5</sup> https://huggingface.co/

<sup>6</sup> https://pandas.pydata.org/

<sup>&</sup>lt;sup>7</sup> https://pytorch.org/

<sup>8</sup> https://pytorch.org/

<sup>9</sup> https://www.pytorchlightning.ai/

<sup>10</sup> 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
```

(continues on next page)

```
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/ <b>init</b> .py	7	0	100%	
dicee/abstracts.py	338	115	66%	112-113,_
			(con	tinues on next page)

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

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

```
→131, 154-155, 160, 173, 197, 240-254, 290, 303-306, 309-313, 353-364, 379-387, 402, □
→413-417, 427-428, 434-436, 442-445, 448-453, 576-596, 602-606, 610-612, 631, 658-696
dicee/callbacks.py
                                                            248
                                                                   103
                                                                          58%
                                                                                 50-55, _
\hookrightarrow 67-73, 76, 88-93, 98-103, 106-109, 116-133, 138-142, 146-147, 247, 281-285, 291-292,
→ 310-316, 319, 324-325, 337-343, 349-358, 363-365, 410, 421-434, 438-473, 485-491
dicee/config.py
                                                             97
                                                                     2
                                                                          98%
                                                                                 146-147
dicee/dataset_classes.py
                                                            430
                                                                   146
                                                                          66%
                                                                                 16, 44, _
→57, 89-98, 104, 111-118, 121, 124, 127-151, 207-213, 216, 219-221, 324, 335-338, □
→354, 420-421, 439, 562-581, 583, 587-599, 606-615, 618, 622-636, 780-787, 790-794, □
\hookrightarrow 845, 866-878, 902-915, 937, 941-954, 964-967, 973, 985, 987, 989, 1012-1022
                                                                          61%
dicee/eval_static_funcs.py
                                                            256
                                                                   100
                                                                                 104, 109,

→ 114, 261-356, 363-414, 442, 465-468

                                                                    48
                                                                          82%
dicee/evaluator.py
                                                            267
                                                                                 48, 53, ...
→58, 77, 82-83, 86, 102, 119, 130, 134, 139, 173-184, 191-202, 310, 340-358, 452, □
→462, 480-485
dicee/executer.py
                                                            134
                                                                    16
                                                                          88%
                                                                                 53-57, _
\hookrightarrow166-176, 235-236, 283
dicee/knowledge_graph.py
                                                             82
                                                                    10
                                                                          88%
                                                                                 84, 94-
\hookrightarrow 95, 124, 128, 132-134, 137-138, 140
dicee/knowledge_graph_embeddings.py
                                                            654
                                                                   415
                                                                          37%

→29, 37-50, 55-88, 91-125, 129-137, 171, 173-229, 261, 265, 276-277, 301-303, 311,

→339-362, 493, 497-519, 523-547, 580, 656, 665, 710-716, 748, 806-1171, 1202-1263, □
→1267–1295, 1326, 1332
dicee/models/__init__.py
                                                              9
                                                                         100%
                                                                     0
dicee/models/adopt.py
                                                            187
                                                                   172
                                                                           8%
                                                                                 50-86, _
\hookrightarrow 99-110, 129-185, 195-242, 266-322, 346-448, 484-517
dicee/models/base_model.py
                                                            240
                                                                    35
                                                                          85%
→64, 66, 92, 99-116, 171, 204, 244, 250, 259, 262, 266, 273, 277, 279, 294, 307-308, □
→362, 365, 438, 450
                                                            470
dicee/models/clifford.py
                                                                   278
                                                                          41%
                                                                                 10, 12, _
→16, 24-25, 52-56, 79-87, 101-103, 108-109, 140-160, 184, 191, 195-256, 273-277, 289,

→ 292, 297, 302, 346-361, 377-444, 464-470, 483, 486, 491, 496, 525-531, 544, 547,

→552, 557, 567-576, 592-593, 613-685, 696-699, 724-749, 773-806, 842-846, 859, 869, □
→872, 877, 882, 887, 891, 895, 904-905, 935, 942, 947, 975-979, 1007-1016, 1026-1034,
\rightarrow 1052-1054, 1072-1074, 1090-1092
dicee/models/complex.py
                                                            162
                                                                    25
                                                                          85%
                                                                                 86-109, _
⇔273−287
dicee/models/dualE.py
                                                             59
                                                                    10
                                                                          83%
                                                                                 93-102, _
→142-156
dicee/models/ensemble.py
                                                             89
                                                                    67
                                                                          25%
                                                                                 7-29, 31,

→ 34, 37, 40, 43, 46, 49, 52-54, 56-58, 64-68, 71-90, 93-94, 97-112, 131

dicee/models/function_space.py
                                                            262
                                                                   221
→27-36, 39-48, 52-69, 76-87, 90-99, 102-111, 115-127, 135-157, 160-166, 169-186, 189-
→195, 198-206, 209, 214-235, 244-247, 251-255, 259-268, 272-293, 302-308, 312-329, □
→333-336, 345-353, 356, 367-373, 393-407, 425-439, 444-454, 462-466, 475-479
dicee/models/literal.py
                                                             33
                                                                     1
                                                                          97%
dicee/models/octonion.py
                                                            227
                                                                          63%
                                                                    83
                                                                                 21-44,_
\Rightarrow320-329, 334-345, 348-370, 374-416, 426-474
dicee/models/pykeen_models.py
                                                                     5
                                                                          91%
                                                                                 77-80, _
                                                             55
→135
dicee/models/quaternion.py
                                                            192
                                                                    69
                                                                           64%
                                                                                 7-21, 30-
⇒55, 68-72, 107, 185, 328-342, 345-364, 368-389, 399-426
```

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```
dicee/models/real.py
                                                               61
                                                                       12
                                                                             80%
                                                                                    37-42,_
→70-73, 91, 107-110
                                                                            100%
dicee/models/static_funcs.py
                                                               10
                                                                        0
                                                              234
                                                                             19%
dicee/models/transformers.py
                                                                      189
                                                                                    20-39,
→42, 56-71, 80-98, 101-112, 119-121, 124, 130-147, 151-176, 182-186, 189-193, 199-
→203, 206-208, 225-252, 261-264, 267-272, 275-300, 306-311, 315-368, 372-394, 400-410
dicee/query_generator.py
                                                              374
                                                                      346
                                                                              7%
                                                                                    17-51,_
→55, 61-64, 68-69, 77-91, 99-146, 154-187, 191-205, 211-268, 273-302, 306-442, 452-
\hookrightarrow471, 479-502, 509-513, 518, 523-529
dicee/read_preprocess_save_load_kg/__init__.py
                                                                            100%
                                                                       40
dicee/read_preprocess_save_load_kg/preprocess.py
                                                              243
                                                                             84%
                                                                                    33, 39, ...
\rightarrow76, 100-125, 131, 136-149, 175, 205, 380-381
dicee/read_preprocess_save_load_kg/read_from_disk.py
                                                                             69%
                                                                                    34, 38-
                                                               36
                                                                      11
\leftrightarrow 40, 47, 55, 58-72
dicee/read_preprocess_save_load_kg/save_load_disk.py
                                                                       21
                                                                             60%
                                                                                    29-30, _
                                                               53
⇒38, 47-68
dicee/read_preprocess_save_load_kg/util.py
                                                              236
                                                                      125
                                                                             47%
                                                                                    159, 173-
→175, 179-180, 198-204, 207-209, 214-216, 230, 244-247, 252-260, 265-271, 276-281, □
→286-291, 303-324, 330-386, 390-394, 398-399, 403, 407-408, 436, 441, 448-449
dicee/sanity_checkers.py
                                                               47
                                                                      19
                                                                             60%
                                                                                    8-12, 21-
\hookrightarrow 31, 46, 51, 58, 69-79
dicee/static_funcs.py
                                                              483
                                                                      194
                                                                             60%
                                                                                    42, 52, _
→58-63, 85, 92-96, 109-119, 129-131, 136, 143, 167, 172, 184, 190, 198, 202, 229-233,

→ 295, 303-309, 320-330, 341-361, 389, 413-414, 419-420, 437-438, 440-441, 443-444, 

→452, 470-474, 491-494, 498-503, 507-511, 515-516, 522-524, 539-553, 558-561, 566-
\hookrightarrow 569, 578-629, 634-646, 663-680, 683-691, 695-713, 724
dicee/static_funcs_training.py
                                                              155
                                                                       66
                                                                             57%
                                                                                    7-10, _
⇔222-319, 327-328
dicee/static_preprocess_funcs.py
                                                               98
                                                                       43
                                                                             56%
                                                                                    17-25, _
\hookrightarrow 50, 57, 59, 70, 83-107, 112-115, 120-123, 128-131
                                                                        0
                                                                            100%
dicee/trainer/__init__.py
                                                                                    22, 30-
dicee/trainer/dice_trainer.py
                                                              151
                                                                       18
                                                                             88%
\Rightarrow31, 33-35, 97, 104, 109-114, 152, 237, 280-283
dicee/trainer/model_parallelism.py
                                                               99
                                                                       87
                                                                             12%
                                                                                    10-25, _
\hookrightarrow 30-116, 121-132, 136, 141-197
                                                                                    31, 102, _
dicee/trainer/torch_trainer.py
                                                               77
                                                                        6
                                                                             92%
→168, 179-181
dicee/trainer/torch_trainer_ddp.py
                                                               89
                                                                       71
                                                                             20%
                                                                                    11-14, _
\hookrightarrow 43, 47-67, 78-94, 113-122, 126-136, 151-158, 168-191
TOTAL
                                                             6948
                                                                    3169
                                                                             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}

...
(continues on next page)
```

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

(continues on next page)

```
@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.
InteractiveQueryDecomposition	
AbstractCallback	Abstract class for Callback class for knowledge graph embedding models
AbstractPPECallback	Abstract class for Callback class for knowledge graph embedding models
BaseInteractiveTrainKGE	Abstract/base class for training knowledge graph embedding models interactively.

# **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
```

```
static save_checkpoint (full\_path: str, model) \rightarrow None
            A static function to save a model into disk
            Parameter
           full_path: str
            model:
                rtype
                     None
class dicee.abstracts.BaseInteractiveKGE (path: str = None, url: str = None,
             construct\_ensemble: bool = False, model\_name: str = None,
             apply_semantic_constraint: bool = False)
      Abstract/base class for using knowledge graph embedding models interactively.
      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
      \texttt{get\_eval\_report}() \rightarrow dict
      \texttt{get\_bpe\_token\_representation} (\textit{str\_entity\_or\_relation: List[str]} \mid \textit{str}) \rightarrow \texttt{List[List[int]]} \mid \texttt{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)
      \verb|get_padded_bpe_triple_representation| (\textit{triples: List[List[str]]}) \rightarrow Tuple[List, List, List]
                Parameters
                    triples
      {\tt set\_model\_train\_mode}\:(\:)\:\to 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])
              \rightarrow 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.InteractiveQueryDecomposition
     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
class dicee.abstracts.AbstractCallback
     Bases: abc.ABC, lightning.pytorch.callbacks.Callback
     Abstract class for Callback class for knowledge graph embedding models
     Parameter
     on_init_start(*args, **kwargs)
           Parameter
           trainer:
           model:
               rtype
                   None
     on_init_end(*args, **kwargs)
           Call at the beginning of the training.
           Parameter
           trainer:
           model:
               rtype
                   None
     on_fit_start (trainer, model)
           Call at the beginning of the training.
           Parameter
           trainer:
           model:
               rtype
                   None
     on_train_epoch_end(trainer, model)
           Call at the end of each epoch during training.
```

```
Parameter
          trainer:
          model:
              rtype
                  None
     on_train_batch_end(*args, **kwargs)
          Call at the end of each mini-batch during the training.
          Parameter
          trainer:
          model:
              rtype
                  None
     on_fit_end(*args, **kwargs)
          Call at the end of the training.
          Parameter
          trainer:
          model:
              rtype
                  None
class dicee.abstracts.AbstractPPECallback (num_epochs, path, epoch_to_start,
            last_percent_to_consider)
     Bases: AbstractCallback
     Abstract class for Callback class for knowledge graph embedding models
     Parameter
     num_epochs
     path
     sample_counter = 0
     epoch_count = 0
     alphas = None
     on_fit_start (trainer, model)
          Call at the beginning of the training.
          Parameter
          trainer:
```

model:

#### rtvpe

None

on\_fit\_end(trainer, model)

Call at the end of the training.

#### **Parameter**

trainer:

model:

rtype

None

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

#### class dicee.abstracts.BaseInteractiveTrainKGE

Abstract/base class for training knowledge graph embedding models interactively. This class provides methods for re-training KGE models and also Literal Embedding model.

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.

train\_literals (train\_file\_path: str = None, num\_epochs: int = 100, lit\_lr: float = 0.001, lit\_normalization\_type: str = 'z-norm', batch\_size: int = 1024, sampling\_ratio: float = None, random\_seed=1, loader\_backend: str = 'pandas', freeze\_entity\_embeddings: bool = True, gate\_residual: bool = True, device: str = None, suffle\_data: bool = True)

Trains the Literal Embeddings model using literal data.

#### **Parameters**

- train\_file\_path (str) Path to the training data file.
- num\_epochs (int) Number of training epochs.
- lit\_lr (float) Learning rate for the literal model.
- norm type (str) Normalization type to use ('z-norm', 'min-max', or None).
- batch\_size (int) Batch size for training.
- sampling\_ratio (float) Ratio of training triples to use.
- loader\_backend (str) Backend for loading the dataset ('pandas' or 'rdflib').
- **freeze\_entity\_embeddings** (bool) If True, freeze the entity embeddings during training.
- gate\_residual (bool) If True, use gate residual connections in the model.
- device (str) Device to use for training ('cuda' or 'cpu'). If None, will use available GPU or CPU.
- **suffle\_data** (bool) If True, shuffle the dataset before training.

# dicee.analyse experiments

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**

```
class dicee.callbacks.AccumulateEpochLossCallback(path: str)
     Bases: dicee.abstracts.AbstractCallback
     Abstract class for Callback class for knowledge graph embedding models
     Parameter
     path
     on_fit_end(trainer, model) \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
     on_fit_start (trainer, pl_module)
          Call at the beginning of the training.
          Parameter
          trainer:
          model:
              rtype
                  None
     on_fit_end(trainer, pl_module)
          Call at the end of the training.
          Parameter
          trainer:
          model:
              rtype
                  None
     on_train_batch_end(*args, **kwargs)
          Call at the end of each mini-batch during the training.
```

```
Parameter
          trainer:
          model:
              rtype
                  None
     on_train_epoch_end(*args, **kwargs)
          Call at the end of each epoch during training.
          Parameter
          trainer:
          model:
              rtype
                  None
class dicee.callbacks.KGESaveCallback (every_x_epoch: int, max_epochs: int, path: str)
     Bases: dicee.abstracts.AbstractCallback
     Abstract class for Callback class for knowledge graph embedding models
     Parameter
     every_x_epoch
     max_epochs
     epoch_counter = 0
     path
     on_train_batch_end(*args, **kwargs)
          Call at the end of each mini-batch during the training.
          Parameter
          trainer:
          model:
              rtype
                  None
     on_fit_start (trainer, pl_module)
          Call at the beginning of the training.
          Parameter
          trainer:
          model:
              rtype
                  None
```

```
on_train_epoch_end(*args, **kwargs)
          Call at the end of each epoch during training.
          Parameter
          trainer:
          model:
              rtype
                  None
     on_fit_end(*args, **kwargs)
          Call at the end of the training.
          Parameter
          trainer:
          model:
              rtype
                  None
     on_epoch_end (model, trainer, **kwargs)
class dicee.callbacks.PseudoLabellingCallback (data_module, kg, batch_size)
     Bases: \ \textit{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
     \verb|static compute_mrr|(trainer, model)| \rightarrow \verb|float|
     {\tt get\_aswa\_state\_dict} \ (model)
     decide (running_model_state_dict, ensemble_state_dict, val_running_model,
                 mrr_updated_ensemble_model)
          Perform Hard Update, software or rejection
              Parameters
                   • running_model_state_dict
                   • ensemble_state_dict
                   • val_running_model
                   • mrr_updated_ensemble_model
     on_train_epoch_end(trainer, model)
          Call at the end of each epoch during training.
          Parameter
          trainer:
          model:
              rtype
                  None
class dicee.callbacks.Eval (path, epoch_ratio: int = None)
     Bases: dicee.abstracts.AbstractCallback
```

Abstract class for Callback class for knowledge graph embedding models

# **Parameter**

```
path
reports = []
epoch_ratio = 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

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"]
        Type
            Evaluate trained model choices
save_model_at_every_epoch: int = None
    Not tested
label_smoothing_rate: float = 0.0
num_core: int = 0
    Number of CPUs to be used in the mini-batch loading process
random_seed: int = 0
    Random Seed
sample_triples_ratio: float = None
```

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

```
read_only_few: int = None
    Read only first few triples
pykeen_model_kwargs
     Additional keyword arguments for pykeen models
kernel size: int = 3
    Size of a square kernel in a convolution operation
num_of_output_channels: int = 32
    Number of slices in the generated feature map by convolution.
p: int = 0
    P parameter of Clifford Embeddings
q: int = 1
     Q parameter of Clifford Embeddings
input_dropout_rate: float = 0.0
     Dropout rate on embeddings of input triples
hidden_dropout_rate: float = 0.0
     Dropout rate on hidden representations of input triples
feature_map_dropout_rate: float = 0.0
     Dropout rate on a feature map generated by a convolution operation
byte_pair_encoding: bool = False
     Byte pair encoding
         Type
            WIP
adaptive_swa: bool = False
     Adaptive stochastic weight averaging
swa: bool = False
     Stochastic weight averaging
block_size: int = None
    block size of LLM
continual_learning = None
     Path of a pretrained model size of LLM
auto_batch_finding = False
```

dicee.dataset\_classes

\_\_iter\_\_()

A flag for using auto batch finding

#### **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
LiteralDataset	Dataset for loading and processing literal data for training Literal Embedding model.

#### **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

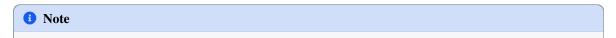
dicee.dataset\_classes.construct\_dataset (\*, train\_set: numpy.ndarray | list, valid\_set=None, test\_set=None, ordered\_bpe\_entities=None, train\_target\_indices=None, target\_dim: int = None, entity\_to\_idx: dict, relation\_to\_idx: dict, form\_of\_labelling: str, scoring\_technique: str, neg\_ratio: 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
```

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)
```

An abstract class representing a Dataset.

```
subword_units: numpy.ndarray, block_size: int = 8)
     Bases: torch.utils.data.Dataset
     Dataset for the 1vsALL training strategy
          Parameters
                • train_set_idx - Indexed triples for the training.
                • entity_idxs - mapping.
                • relation_idxs - mapping.
                • form - ?
                • num_workers - int for
                                                https://pytorch.org/docs/stable/data.html#torch.utils.data.
                  DataLoader
          Return type
              torch.utils.data.Dataset
     train_data
     block_size = 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)
```

class dicee.dataset\_classes.MultiClassClassificationDataset(

class dicee.dataset\_classes. KvsAll (train\_set\_idx: numpy.ndarray, entity\_idxs, relation\_idxs, form, store=None, label\_smoothing\_rate: float = 0.0)

Bases: torch.utils.data.Dataset

#### Creates a dataset for KvsAll training by inheriting from torch.utils.data.Dataset.

Let D denote a dataset for KvsAll training and be defined as D:=  $\{(x,y)_i\}_i$  ^N, where x: (h,r) is an unique tuple of an entity h in E and a relation r in R that has been seed in the input graph. y: denotes a multi-label vector in  $[0,1]^{\{E\}}$  is a binary label.

orall  $y_i = 1$  s.t. (h r  $E_i$ ) in KG



### 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])
```

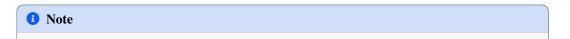
```
train_data = None
train_target = None
label_smoothing_rate
collate_fn = None
__len__()
__getitem__(idx)
```

Bases: torch.utils.data.Dataset

# Creates a dataset for AllvsAll training by inheriting from torch.utils.data.Dataset.

Let D denote a dataset for AllvsAll training and be defined as D:=  $\{(x,y)_i\}_i^n$ , where x: (h,r) is a possible unique tuple of an entity h in E and a relation r in R. Hence  $N = |E| \times |R|$  y: denotes a multi-label vector in  $[0,1]^{\{|E|\}}$  is a binary label.

orall y\_i =1 s.t. (h r E\_i) in KG



AllysAll extends KysAll via none existing (h,r). Hence, it adds data points that are labelled without 1s,

only with 0s.

#### train\_set\_idx

[numpy.ndarray] n by 3 array representing n triples

### entity\_idxs

[dictonary] string representation of an entity to its integer id

# relation\_idxs

[dictonary] string representation of a relation to its integer id

self: torch.utils.data.Dataset

```
>>> a = AllvsAll()
>>> a
? array([0, 1, 2, 3, 4, 5, 6, 7, 8, 9])
```

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

class dicee.dataset\_classes.OnevsSample ( $train\_set$ : numpy.ndarray,  $num\_entities$ ,  $num\_relations$ ,  $neg\_sample\_ratio$ : int = None,  $label\_smoothing\_rate$ : float = 0.0)

Bases: torch.utils.data.Dataset

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

#### **Parameters**

- train\_set (np.ndarray) A numpy array containing triples of knowledge graph data. Each triple consists of (head\_entity, relation, tail\_entity).
- num\_entities (int) The number of unique entities in the knowledge graph.
- num\_relations (int) The number of unique relations in the knowledge graph.
- neg\_sample\_ratio (int, optional) The number of negative samples to be generated per positive sample. Must be a positive integer and less than num\_entities.
- label\_smoothing\_rate (float, optional) A label smoothing rate to apply to the positive and negative labels. Defaults to 0.0.

# train\_data

The input data converted into a PyTorch tensor.

#### **Type**

torch.Tensor

```
num_entities
```

Number of entities in the dataset.

```
Type
```

int

### num\_relations

Number of relations in the dataset.

```
Type
```

int

# neg\_sample\_ratio

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

Type

int

### label\_smoothing\_rate

The smoothing factor applied to the labels.

**Type** 

torch.Tensor

### collate\_fn

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

### **Type**

function, optional

train\_data

num\_entities

num\_relations

neg\_sample\_ratio = None

label\_smoothing\_rate

collate\_fn = None

\_\_len\_\_()

Returns the number of samples in the dataset.

 $\__getitem__(idx)$ 

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

#### Parameters

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

#### **Returns**

# A tuple consisting of:

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

```
Return type
                 tuple
class dicee.dataset_classes.KvsSampleDataset (train_set_idx: numpy.ndarray, entity_idxs,
           relation_idxs, form, store=None, neg_ratio=None, label_smoothing_rate: float = 0.0)
     Bases: torch.utils.data.Dataset
          KvsSample a Dataset:
              D := \{(x,y)_i\}_i ^N, where
                 . x:(h,r) is a unique h in E and a relation r in R and . y in [0,1]^{\{|E|\}} is a binary label.
     orall y_i = 1 s.t. (h r E_i) in KG
              At each mini-batch construction, we subsample(y), hence n
                 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__()
     \__{\texttt{getitem}} (idx)
class dicee.dataset_classes.NegSampleDataset (train_set: numpy.ndarray, num_entities: int,
           num_relations: int, neg_sample_ratio: int = 1)
```

Bases: torch.utils.data.Dataset
An abstract class representing a Dataset.

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



DataLoader by default constructs an index sampler that yields integral indices. To make it work with a mapstyle dataset with non-integral indices/keys, a custom sampler must be provided.

```
neg_sample_ratio
      train_set
      length
      num_entities
      num relations
      __len__()
      getitem (idx)
class dicee.dataset_classes.TriplePredictionDataset (train_set: numpy.ndarray,
             num entities: int, num relations: int, neg sample ratio: int = 1, label smoothing rate: float = 0.0)
      Bases: torch.utils.data.Dataset
           Triple Dataset
                D := \{(x)_i\}_i \ ^N, \text{ where }
                    . x:(h,r,t) in KG is a unique h in E and a relation r in R and . collact_fn => Generates
                    negative triples
                collect_fn:
      orall (h,r,t) in G obtain, create negative triples \{(h,r,x),(r,t),(h,m,t)\}
                y:labels are represented in torch.float16
           train_set_idx
                Indexed triples for the training.
           entity idxs
                mapping.
           relation_idxs
                mapping.
           form
           store
           label_smoothing_rate
           collate_fn: batch:List[torch.IntTensor] Returns ——- torch.utils.data.Dataset
```

```
label_smoothing_rate
     neg_sample_ratio
     train_set
     length
     num_entities
     num_relations
     __len__()
     \__getitem__(idx)
     collate_fn (batch: List[torch.Tensor])
class dicee.dataset_classes.CVDataModule(train_set_idx: numpy.ndarray, num_entities,
            num_relations, neg_sample_ratio, batch_size, num_workers)
     Bases: pytorch_lightning.LightningDataModule
     Create a Dataset for cross validation
          Parameters
                • train_set_idx - Indexed triples for the training.
                • num_entities — entity to index mapping.
                • num_relations - relation to index mapping.
                • batch size - int
                 • form - ?
                                                 https://pytorch.org/docs/stable/data.html#torch.utils.data.
                • num_workers -
                                       int
                                            for
                  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.
                 dataloader
                              you
                                     return
                                              will
                                                     not
                                                           be
                                                                 reloaded
                                                                             unless
                                                                                      you
                                                                                                   :param-
          ref: ~pytorch_lightning.trainer.trainer.Trainer.reload_dataloaders_every_n_epochs to a positive
          integer.
          For data processing use the following pattern:
```

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

However, the above are only necessary for distributed processing.

# **▲** Warning

do not assign state in prepare\_data

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

# **1** Note

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

```
setup(*args, **kwargs)
```

Called at the beginning of fit (train + validate), validate, test, or predict. This is a good hook when you need to build models dynamically or adjust something about them. This hook is called on every process when using DDP.

#### **Parameters**

```
stage - either 'fit', 'validate', 'test', or 'predict'
```

Example:

```
class LitModel(...):
    def __init__(self):
        self.11 = None

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

# don't do this
        self.something = else

def setup(self, stage):
        data = load_data(...)
        self.11 = nn.Linear(28, data.num_classes)
```

# transfer\_batch\_to\_device(\*args, \*\*kwargs)

Override this hook if your DataLoader returns tensors wrapped in a custom data structure.

The data types listed below (and any arbitrary nesting of them) are supported out of the box:

- torch. Tensor or anything that implements .to(...)
- list
- dict

• tuple

For anything else, you need to define how the data is moved to the target device (CPU, GPU, TPU, ...).



## **1** Note

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

#### **Parameters**

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

#### Returns

A reference to the data on the new device.

## Example:

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

# See also

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

#### prepare\_data(\*args, \*\*kwargs)

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



# Warning

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

## Example:

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

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

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

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

## Example:

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

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

This is called before requesting the dataloaders:

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

Bases: torch.utils.data.Dataset

Dataset for loading and processing literal data for training Literal Embedding model. This dataset handles the loading, normalization, and preparation of triples for training a literal embedding model.

Extends torch.utils.data.Dataset for supporting PyTorch dataloaders.

## train\_file\_path

Path to the training data file.

```
Type str
```

```
normalization
```

Type of normalization to apply ('z-norm', 'min-max', or None).

**Type** 

str

## normalization\_params

Parameters used for normalization.

**Type** 

dict

## sampling\_ratio

Fraction of the training set to use for ablations.

**Type** 

float

## entity\_to\_idx

Mapping of entities to their indices.

**Type** 

dict

## num\_entities

Total number of entities.

Type

int

# data\_property\_to\_idx

Mapping of data properties to their indices.

**Type** 

dict

## num\_data\_properties

Total number of data properties.

**Type** 

int

## loader\_backend

Backend to use for loading data ('pandas' or 'rdflib').

**Type** 

str

train\_file\_path

loader\_backend = 'pandas'

normalization\_type = 'z-norm'

normalization\_params

sampling\_ratio = None

entity\_to\_idx = None

num\_entities

Loads and validates the literal data file. :param file\_path: Path to the literal data file. :type file\_path: str

#### Returns

DataFrame containing the loaded and validated data.

## Return type

pd.DataFrame

static denormalize(preds\_norm, attributes, normalization\_params) → numpy.ndarray

Denormalizes the predictions based on the normalization type.

Args: preds\_norm (np.ndarray): Normalized predictions to be denormalized. attributes (list): List of attributes corresponding to the predictions. normalization\_params (dict): Dictionary containing normalization parameters for each attribute.

#### **Returns**

Denormalized predictions.

## **Return type**

np.ndarray

## dicee.eval static funcs

#### **Functions**

```
evaluate_link_prediction_performance(→
Dict)
evaluate_link_prediction_performance_with_.

evaluate_link_prediction_performance_with_j

evaluate_link_prediction_performance_with_j
...)
evaluate_lp_bpe_k_vs_all(model, triples[, er_vocab, ...])
evaluate_literal_prediction(kge_model[, ...]) Evaluates the trained literal prediction model on a test file.
```

#### **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.eval\_static\_funcs.evaluate\_literal\_prediction(
   kge\_model: dicee.knowledge\_graph\_embeddings.KGE, eval\_file\_path: str = None,
   store\_lit\_preds: bool = True, eval\_literals: bool = True, loader\_backend: str = 'pandas',
   return\_attr\_error\_metrics: bool = False)

Evaluates the trained literal prediction model on a test file.

#### **Parameters**

- eval\_file\_path (str) Path to the evaluation file.
- store\_lit\_preds (bool) If True, stores the predictions in a CSV file.
- eval\_literals (bool) If True, evaluates the literal predictions and prints error metrics.
- loader\_backend (str) Backend for loading the dataset ('pandas' or 'rdflib').

#### Returns

DataFrame containing error metrics for each attribute if return\_attr\_error\_metrics is True.

## Return type

pd.DataFrame

#### Raises

- RuntimeError If the kGE model does not have a trained literal model.
- AssertionError If the kGE model is not an instance of KGE or if the test set has no valid
  entities or attributes.

#### dicee.evaluator

## Classes

Evaluator	Evaluator class to evaluate KGE models in various down-
	stream 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
     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)
                  \rightarrow None
          Evaluate model after reciprocal triples are added
     evaluate_lp_k_vs_all (model, triple_idx, info=None, form_of_labelling=None)
          Filtered link prediction evaluation. :param model: :param triple_idx: test triples :param info: :param
          form_of_labelling: :return:
     evaluate_lp_with_byte (model, triples: List[List[str]], info=None)
```

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
save_trained_model() → None
```

Save a knowledge graph embedding model

- (1) Send model to eval mode and cpu.
- (2) Store the memory footprint of the model.

- (3) Save the model into disk.
- (4) Update the stats of KG again?

#### **Parameter**

## rtype

None

end  $(form\_of\_labelling: str) \rightarrow dict$ 

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.

 $continual\_start() \rightarrow dict$ 

Start Continual Training

- (1) Initialize training.
- (2) Start continual training.
- (3) Save trained model.

## **Parameter**

#### rtype

A dict containing information about the training and/or evaluation

## dicee.knowledge graph

## **Classes**

KG

## Knowledge Graph

#### **Module Contents**

```
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
\mathtt{describe}() \to None
property entities_str: List
property relations_str: List
exists(h: str, r: str, t: str)
__iter__()
__len__()
func_triple_to_bpe_representation(triple: List[str])
```

# dicee.knowledge\_graph\_embeddings

## **Classes**

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

## **Module Contents**

```
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, batch\_size=2, topk=1, return\_indices=False)  $\rightarrow$  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, batch\_size=2, topk=1, return\_indices=False)  $\rightarrow$  Tuple

Given a head entity and a tail entity, return top k ranked relations.

 $argmax_{r} in R$  f(h,r,t), where h, t in E.

## Parameter

head\_entity: List[str]

String representation of selected entities.

tail\_entity: List[str]

String representation of selected entities.

k: int

Highest ranked k entities.

# **Returns: Tuple**

Highest K scores and entities

```
predict_missing_tail_entity (head_entity: List[str] | str, relation: List[str] | str, within: List[str] = None, batch_size=2, topk=1, return_indices=False) \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.

#### Returns

- If you query a single (h, r, ?) or (?, r, t) or (h, ?, t), returns List[(item, score)]
- If you query a batch of B, returns List of B such lists.

$$\label{eq:core} \begin{split} \texttt{triple\_score} \ (h: List[str] \mid str = None, \, r: \, List[str] \mid str = None, \, t: \, List[str] \mid str = None, \, logits = False) \\ &\rightarrow \mathsf{torch.FloatTensor} \end{split}$$

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
```

```
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
\texttt{deploy}(\textit{share: bool} = \textit{False, top\_k: int} = 10)
\texttt{predict\_literals}(\textit{entity: List[str]} \mid \textit{str} = \textit{None, attribute: List[str]} \mid \textit{str} = \textit{None, denormalize\_preds: bool} = \textit{True}) \rightarrow \text{numpy.ndarray}
```

Predicts literal values for given entities and attributes.

#### **Parameters**

- entity (Union[List[str], str]) Entity or list of entities to predict literals for.
- attribute (Union[List[str], str]) Attribute or list of attributes to predict literals for.
- denormalize\_preds (bool) If True, denormalizes the predictions.

#### Returns

Predictions for the given entities and attributes.

## **Return type**

numpy ndarray

## 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. 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

```
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.

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

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

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

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

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

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

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

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

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

Compute sigma\_ $\{qq\}$  = sum\_ $\{j=1\}^{p+q-1}$  sum\_ $\{k=j+1\}^{p+q}$  (h\_j r\_k - h\_k r\_j) e\_j e\_k sigma\_ $\{q\}$  captures the interactions between along q bases For instance, let q e\_1, e\_2, e\_3, we compute interactions between e\_1 e\_2, e\_1 e\_3, and e\_2 e\_3 This can be implemented with a nested two for loops

```
results = [] for j in range(q - 1):
                             for k in range(j + 1, q):
                                  results.append(hq[:, :, j] * rq[:, :, k] - hq[:, :, k] * rq[:, :, j])
                    sigma_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_{i=1}^p r_i e_i + sum_{i=1}^n p_i e_j r = r_0 + sum_{i=1}^n p_i e_i + sum_{i=1}^n p_i e_j r = r_0 + sum_{i=1}^n p_i e_j r = 
                    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) s5 = \sum_{i=p+q+1}^{p+q+r} (h_0 r_i t_i + h_i r_0 t_i) s6 = \sum_{i=p+q+1}^{p+q+r} (h_0 r_i t_i + h_i r_0 t_i) s6 = \sum_{i=p+q+1}^{p+q+r} (h_0 r_i t_i + h_i r_0 t_i) s6 = \sum_{i=p+q+1}^{p+q+r} (h_0 r_i t_i + h_i r_0 t_i) s6 = \sum_{i=p+q+1}^{p+q+r} (h_0 r_i t_i + h_i r_0 t_i) s6 = \sum_{i=p+q+1}^{p+q+r} (h_0 r_i t_i + h_i r_0 t_i) s6 = \sum_{i=p+q+1}^{p+q+r} (h_0 r_i t_i + h_i r_0 t_i) s6 = \sum_{i=p+q+1}^{p+q+r} (h_0 r_i t_i + h_i r_0 t_i) s6 = \sum_{i=p+q+1}^{p+q+r} (h_0 r_i t_i + h_i r_0 t_i) s6 = \sum_{i=p+q+1}^{p+q+r} (h_0 r_i t_i + h_i r_0 t_i) s6 = \sum_{i=p+q+1}^{p+q+r} (h_0 r_i t_i + h_i r_0 t_i) s6 = \sum_{i=p+q+1}^{p+q+r} (h_0 r_i t_i + h_i r_0 t_i) s6 = \sum_{i=p+q+1}^{p+q+r} (h_0 r_i t_i + h_i r_0 t_i) s6 = \sum_{i=p+q+1}^{p+q+r} (h_0 r_i t_i + h_i r_0 t_i) s6 = \sum_{i=p+q+1}^{p+q+r} (h_0 r_i t_i + h_i r_0 t_i) s6 = \sum_{i=p+q+1}^{p+q+r} (h_0 r_i t_i + h_i r_0 t_i) s6 = \sum_{i=p+q+1}^{p+q+r} (h_0 r_i t_i + h_i r_0 t_i) s6 = \sum_{i=p+q+1}^{p+q+r} (h_0 r_i t_i + h_i r_0 t_i) s6 = \sum_{i=p+q+r}^{p+q+r} (h_0 r_i t_i + h_i r_0 t_i) s6 = \sum_{i=p+q+r}^{p+q+r} (h_0 r_i t_i + h_i r_0 t_i) s6 = \sum_{i=p+q+r}^{p+q+r} (h_0 r_i t_i + h_i r_0 t_i) s6 = \sum_{i=p+q+r}^{p+q+r} (h_0 r_i t_i + h_i r_0 t_i) s6 = \sum_{i=p+q+r}^{p+q+r} (h_0 r_i t_i + h_i r_0 t_i) s6 = \sum_{i=p+q+r}^{p+q+r} (h_0 r_i t_i + h_i r_0 t_i) s6 = \sum_{i=p+q+r}^{p+q+r} (h_0 r_i t_i + h_i r_0 t_i) s6 = \sum_{i=p+q+r}^{p+q+r} (h_0 r_i t_i + h_i r_0 t_i) s6 = \sum_{i=p+q+r}^{p+q+r} (h_0 r_i t_i + h_i r_0 t_i) s6 = \sum_{i=p+q+r}^{p+q+r} (h_0 r_i t_i + h_i r_0 t_i) s6 = \sum_{i=p+q+r}^{p+q+r} (h_0 r_i t_i + h_i r_0 t_i) s6 = \sum_{i=p+q+r}^{p+q+r} (h_0 r_i t_i + h_i r_0 t_i) s6 = \sum_{i=p+q+r}^{$$

and return:

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

compute\_sigmas\_multivect(list\_h\_emb, list\_r\_emb)

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

For same bases vectors interaction we have

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

For different base vector interactions, we have

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

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

Kvsall training

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

forward\_k\_vs\_with\_explicit and this funcitons are identical Parameter — x: torch.LongTensor with (n, ) shape :rtype: torch.FloatTensor with (n, |E|) shape

apply\_coefficients(h0, hp, hq, hk, r0, rp, rq, rk)

Multiplying a base vector with its scalar coefficient

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

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

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

#### **Parameter**

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

#### returns

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

 $compute\_sigma\_pp(hp, rp)$ 

Compute .. math:

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

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

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

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

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

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

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

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

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

Compute

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

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

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

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

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

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

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

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

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

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

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'

```
conv2d
     fc_num_input
     fc1
     norm_fc1
     bn_conv2d
     feature_map_dropout
     residual_convolution(C_1: Tuple[torch.Tensor, torch.Tensor],
                  C 2: Tuple[torch, Tensor, torch, Tensor]) \rightarrow torch.FloatTensor
           Compute residual score of two complex-valued embeddings. :param C_1: a tuple of two pytorch tensors
           that corresponds complex-valued embeddings :param C_2: a tuple of two pytorch tensors that corresponds
           complex-valued embeddings :return:
     forward_k_vs_all(x: torch.Tensor) \rightarrow torch.FloatTensor
     forward\_triples(x: torch.Tensor) \rightarrow torch.FloatTensor
               Parameters
     forward_k_vs_sample (x: torch.Tensor, target_entity_idx: torch.Tensor)
class dicee.models.complex.AConEx(args)
     Bases: dicee.models.base_model.BaseKGE
     Additive Convolutional ComplEx Knowledge Graph Embeddings
     name = 'AConEx'
     conv2d
     fc_num_input
     fc1
     norm_fc1
     bn_conv2d
     feature_map_dropout
     residual convolution (C 1: Tuple[torch.Tensor, torch.Tensor],
                  C 2: Tuple[torch.Tensor, torch.Tensor]) \rightarrow torch.FloatTensor
           Compute residual score of two complex-valued embeddings. :param C_1: a tuple of two pytorch tensors
           that corresponds complex-valued embeddings :param C_2: a tuple of two pytorch tensors that corresponds
           complex-valued embeddings :return:
     forward_k_vs_all(x: torch.Tensor) \rightarrow torch.FloatTensor
     forward\_triples(x: torch.Tensor) \rightarrow torch.FloatTensor
               Parameters
     forward_k_vs_sample (x: torch.Tensor, target_entity_idx: torch.Tensor)
```

```
class dicee.models.complex.Complex(args)
Bases: dicee.models.base_model.BaseKGE
```

Base class for all neural network modules.

Your models should also subclass this class.

Modules can also contain other Modules, allowing 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**  $(b \circ \circ 1)$  – 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)

## dicee.models.dualE

## **Classes**

DualE	Dual	Quaternion	Knowledge	Graph	Embeddings
		://ojs.aaai.org/ )/16657)	/index.php/AA	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

```
torch.FloatTensor with (n) shape

T (x: torch.tensor) → torch.tensor

Transpose function

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

## dicee.models.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.literal

### **Classes**

LiteralEmbeddings

A model for learning and predicting numerical literals using pre-trained KGE.

# **Module Contents**

```
class dicee.models.literal.LiteralEmbeddings (num\_of\_data\_properties: int, embedding\_dims: int, entity_embeddings: torch.tensor, dropout: float = 0.3, gate_residual=True, freeze_entity_embeddings=True)
```

Bases: torch.nn.Module

A model for learning and predicting numerical literals using pre-trained KGE.

## num\_of\_data\_properties

Number of data properties (attributes).

Type int

# embedding\_dims

Dimension of the embeddings.

Type int

# entity\_embeddings

Pre-trained entity embeddings.

**Type** 

torch.tensor

```
dropout
    Dropout rate for regularization.
        Type
            float
gate_residual
    Whether to use gated residual connections.
         Type
            bool
freeze_entity_embeddings
     Whether to freeze the entity embeddings during training.
         Type
            bool
embedding_dim
num_of_data_properties
hidden_dim
gate_residual = True
freeze_entity_embeddings = True
entity_embeddings
data_property_embeddings
fc
fc_out
dropout
gated_residual_proj
layer_norm
forward(entity_idx, attr_idx)
        Parameters
             • entity_idx (Tensor) - Entity indices (batch).
             • attr_idx (Tensor) - Attribute (Data property) indices (batch).
        Returns
            scalar predictions.
        Return type
            Tensor
```

property device

## dicee.models.octonion

### **Classes**

OMult	Base class for all neural network modules.
Conv0	Base class for all neural network modules.
AConv0	Additive Convolutional Octonion Knowledge Graph Embeddings
	ocuangs

## **Functions**

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

## **Module Contents**

```
dicee.models.octonion.octonion_mul(*, O_1, O_2)
dicee.models.octonion.octonion_mul_norm(*, O_1, O_2)
class dicee.models.octonion.OMult(args)
    Bases: dicee.models.base_model.BaseKGE
```

Base class for all neural network modules.

Your models should also subclass this class.

Modules can also contain other Modules, allowing 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.

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__()
        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 = '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.octonion.AConvO(args: dict)
     Bases: dicee.models.base model.BaseKGE
     Additive Convolutional Octonion Knowledge Graph Embeddings
     name = 'AConvO'
     conv2d
     fc_num_input
     fc1
     bn_conv2d
     norm_fc1
     feature_map_dropout
     static octonion_normalizer(emb_rel_e0, emb_rel_e1, emb_rel_e2, emb_rel_e3, emb_rel_e4,
                  emb_rel_e5, emb_rel_e6, emb_rel_e7)
     residual_convolution (O_1, O_2)
     forward_triples (x: torch.Tensor) \rightarrow torch.Tensor
               Parameters
                   x
     forward_k_vs_all (x: torch.Tensor)
           Given a head entity and a relation (h,r), we compute scores for all entities. [score(h,r,x)|x in Entities] =>
           [0.0,0.1,...,0.8], shape=> (1, |Entities|) Given a batch of head entities and relations => shape (size of batch,|
           Entities l)
```

# 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: Py-
     keen_HolE: Pykeen_TransD: Pykeen_TransE: Pykeen_TransF: Pykeen_TransH: Pykeen_TransR:
     model_kwargs
     name
     model
     loss_history = []
     args
     entity_embeddings = None
     relation embeddings = None
     forward_k_vs_all (x: torch.LongTensor)
           # => Explicit version by this we can apply bn and dropout
           # (1) Retrieve embeddings of heads and relations + apply Dropout & Normalization if given. h, r =
           self.get head relation representation(x) # (2) Reshape (1). if self.last dim > 0:
               h = h.reshape(len(x), self.embedding_dim, self.last_dim) r = r.reshape(len(x), self.embedding_dim,
               self.last dim)
           \# (3) Reshape all entities. if self.last dim > 0:
               t = self.entity embeddings.weight.reshape(self.num entities, self.embedding dim, self.last dim)
           else:
               t = self.entity_embeddings.weight
           # (4) Call the score_t from interactions to generate triple scores. return self.interaction.score_t(h=h, r=r,
           all_entities=t, slice_size=1)
     forward\_triples (x: torch.LongTensor) \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 =
```

 $h = h.reshape(len(x), self.embedding\_dim, self.last\_dim) r = r.reshape(len(x), self.embedding\_dim, self.embeddin$ 

 $self.get\_triple\_representation(x) \# (2) Reshape (1). if <math>self.last\_dim > 0$ :

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 <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.

name = 'QMult'

explicit = True

 $quaternion_multiplication_followed_by_inner_product(h, r, t)$ 

#### **Parameters**

- h shape: (\*batch\_dims, dim) The head representations.
- **r** shape: (\*batch\_dims, dim) The head representations.
- t shape: (\*batch\_dims, dim) The tail representations.

## **Returns**

Triple scores.

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

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

Absolute value of a quaternion

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

L2 norm of quaternion vector:

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

# **Parameters**

 $\mathbf{x}$  – The vector.

## Returns

The normalized vector.

 $\verb+k_vs_all_score+ (bpe\_head\_ent\_emb, bpe\_rel\_ent\_emb, E)$ 

# **Parameters**

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

 $forward_k_vs_all(x)$ 

## **Parameters**

x

```
[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] =>
          [0.0,0.1,...,0.8], shape=> (1, |Entities|) Given a batch of head entities and relations => shape (size of batch,|
          Entities()
class dicee.models.quaternion.AConvQ(args)
     Bases: dicee.models.base_model.BaseKGE
     Additive Convolutional Quaternion Knowledge Graph Embeddings
     name = 'AConvQ'
     entity_embeddings
     relation_embeddings
     conv2d
     fc_num_input
     fc1
     bn_conv1
     bn_conv2
```

Completed. Given a head entity and a relation (h,r), we compute scores for all possible triples, i.e.,

forward\_k\_vs\_sample (x, target\_entity\_idx)

```
\label{lem:convolution} \begin{picture}(Q_1,Q_2) \\ \begin{picture}(Q_1,Q_
```

## **Parameters**

x

```
forward_k_vs_all (x: torch.Tensor)
```

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

## dicee.models.real

### **Classes**

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

## **Module Contents**

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

Bases: dicee.models.base\_model.BaseKGE

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

```
name = 'DistMult'
```

 $\verb+k_vs_all_score+ (emb_h: torch.FloatTensor, emb_r: torch.FloatTensor, emb_E: torch.FloatTensor)$ 

## **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.models.real.TransE(args)

Bases: dicee.models.base\_model.BaseKGE

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

```
name = 'TransE'
     margin = 4
     score (head_ent_emb, rel_ent_emb, tail_ent_emb)
     forward_k_vs_all(x: torch.Tensor) \rightarrow 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
                   x
               Returns
class dicee.models.real.Pyke(args)
     Bases: dicee.models.base_model.BaseKGE
     A Physical Embedding Model for Knowledge Graphs
     name = 'Pyke'
     dist_func
     margin = 1.0
     forward_triples (x: torch.LongTensor)
               Parameters
```

# dicee.models.static\_funcs

# **Functions**

```
quaternion\_mul( \rightarrow Tuple[torch.Tensor, torch.Tensor, Perform quaternion multiplication ...)
```

```
\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**

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

```
name = 'BytE'
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**

```
\mathbf{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):
```

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```
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.

```
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)
```

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

```
c_fc
gelu
c_proj
dropout
forward(x)
class dicee.models.transformers.Block(config)
Bases: torch.nn.Module
```

Base class for all neural network modules.

Your models should also subclass this class.

Modules can also contain other Modules, allowing 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.

```
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):
    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.

#### 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.

```
forward(idx, targets=None)
crop_block_size(block_size)
classmethod from_pretrained(model_type, override_args=None)
```

configure\_optimizers (weight\_decay, learning\_rate, betas, device\_type)

estimate\_mfu(fwdbwd\_per\_iter, dt)

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

## **Classes**

ADOPT	Base class for all optimizers.
BaseKGELightning	Base class for all neural network modules.
BaseKGE	Base class for all neural network modules.
IdentityClass	Base class for all neural network modules.
BaseKGE	Base class for all neural network modules.
DistMult	Embedding Entities and Relations for Learning and Infer-
	ence in Knowledge Bases
TransE	Translating Embeddings for Modeling
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 Em-
	beddings
ComplEx	Base class for all neural network modules.
BaseKGE	Base class for all neural network modules.
IdentityClass	Base class for all neural network modules.

continues on next page

Table 1 - continued from previous page

QMult	Base class for all neural network modules.
ConvQ	Convolutional Quaternion Knowledge Graph Embed-
	dings
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 Em-
	beddings
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 im-
	plemented 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**

**Bases.** Colon.opcim.opcimilol.op

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 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

```
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 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()
```

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

loss function(yhat batch: torch.FloatTensor, y batch: torch.FloatTensor)

### **Parameters**

- yhat\_batch
- y\_batch

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

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

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

```
class MyLightningModule(L.LightningModule):
   def __init__(self):
        super().__init__()
        self.training_step_outputs = []
   def training_step(self):
        loss = ...
        self.training_step_outputs.append(loss)
        return loss
   def on_train_epoch_end(self):
        # do something with all training_step outputs, for example:
        epoch_mean = torch.stack(self.training_step_outputs).mean()
        self.log("training_epoch_mean", epoch_mean)
        # free up the memory
        self.training_step_outputs.clear()
```

test\_epoch\_end(outputs: List[Any])

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

An iterable or collection of iterables specifying test samples.

For more information about multiple dataloaders, see this section.

For data processing use the following pattern:

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

However, the above are only necessary for distributed processing.

# Warning

do not assign state in prepare\_data

• test()

- prepare\_data()
- setup()

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

# 1 Note

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

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

An iterable or collection of iterables specifying validation samples.

For more information about multiple dataloaders, see this section.

The dataloader you return will not be reloaded unless you set **:param-ref:** "lightning.pytorch.trainer.trainer.Trainer.reload\_dataloaders\_every\_n\_epochs" to a positive integer.

It's recommended that all data downloads and preparation happen in prepare\_data().

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

# 1 Note

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

# 1 Note

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

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

An iterable or collection of iterables specifying prediction samples.

For more information about multiple dataloaders, see this section.

It's recommended that all data downloads and preparation happen in prepare\_data().

- predict()
- prepare\_data()
- setup()

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

#### Returns

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

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

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

#### args

```
embedding_dim = None
num_entities = None
num_relations = None
num_tokens = None
learning_rate = None
apply_unit_norm = None
input_dropout_rate = None
hidden_dropout_rate = None
optimizer_name = None
feature_map_dropout_rate = None
```

```
kernel_size = None
num_of_output_channels = None
weight_decay = None
loss
selected_optimizer = None
normalizer_class = None
normalize_head_entity_embeddings
normalize_relation_embeddings
normalize_tail_entity_embeddings
hidden_normalizer
param_init
input_dp_ent_real
input_dp_rel_real
hidden_dropout
loss_history = []
byte_pair_encoding
max_length_subword_tokens
block_size
forward_byte_pair_encoded_k_vs_all (x: torch.LongTensor)
        Parameters
           x (B x 2 x T)
forward_byte_pair_encoded_triple (x: Tuple[torch.LongTensor, torch.LongTensor])
    byte pair encoded neural link predictors
        Parameters
init_params_with_sanity_checking()
forward(x: torch.LongTensor | Tuple[torch.LongTensor, torch.LongTensor],
          y_idx: torch.LongTensor = None
        Parameters
            • x
            • y_idx
            • ordered_bpe_entities
```

```
forward\_triples(x: torch.LongTensor) \rightarrow torch.Tensor
              Parameters
                  x
     forward_k_vs_all(*args, **kwargs)
     forward_k_vs_sample(*args, **kwargs)
     get_triple_representation(idx_hrt)
     get_head_relation_representation(indexed_triple)
     get_sentence_representation (x: torch.LongTensor)
              Parameters
                  • (b (x shape)
                  • 3
                  • t)
     get_bpe_head_and_relation_representation(x: torch.LongTensor)
                  → Tuple[torch.FloatTensor, torch.FloatTensor]
              Parameters
                  x (B x 2 x T)
     \mathtt{get\_embeddings}() \rightarrow Tuple[numpy.ndarray, numpy.ndarray]
class dicee.models.IdentityClass(args=None)
     Bases: torch.nn.Module
```

Base class for all neural network modules.

Your models should also subclass this class.

Modules can also contain other Modules, allowing 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.

```
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**  $(b \circ o 1)$  – 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.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)
     \mathtt{score}\left(h,r,t\right)
class dicee.models.TransE(args)
     Bases: dicee.models.base_model.BaseKGE
     Translating Embeddings for Modeling Multi-relational Data https://proceedings.neurips.cc/paper/2013/file/
     1cecc7a77928ca8133fa24680a88d2f9-Paper.pdf
     name = 'TransE'
     margin = 4
     score (head_ent_emb, rel_ent_emb, tail_ent_emb)
     forward_k_vs_all(x: torch.Tensor) \rightarrow torch.FloatTensor
class dicee.models.Shallom(args)
     Bases: dicee.models.base model.BaseKGE
     A shallow neural model for relation prediction (https://arxiv.org/abs/2101.09090)
     name = 'Shallom'
     shallom
     get_embeddings() → Tuple[numpy.ndarray, None]
     forward_k_vs_all (x) \rightarrow \text{torch.FloatTensor}
     forward\_triples(x) \rightarrow torch.FloatTensor
               Parameters
                  x
               Returns
class dicee.models.Pyke(args)
     Bases: dicee.models.base model.BaseKGE
     A Physical Embedding Model for Knowledge Graphs
     name = 'Pyke'
     dist_func
     margin = 1.0
     forward_triples (x: torch.LongTensor)
               Parameters
                   x
class dicee.models.BaseKGE (args: dict)
     Bases: BaseKGELightning
     Base class for all neural network modules.
```

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

Your models should also subclass this class.

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

class Model(nn.Module):
    def __init__(self) -> None:
        super().__init__()
        self.conv1 = nn.Conv2d(1, 20, 5)
        self.conv2 = nn.Conv2d(20, 20, 5)

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

Submodules assigned in this way will be registered, and will 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.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:

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

```
name = 'ComplEx'
     static score (head_ent_emb: torch.FloatTensor, rel_ent_emb: torch.FloatTensor,
                 tail ent emb: torch.FloatTensor)
     static k_vs_all_score (emb_h: torch.FloatTensor, emb_r: torch.FloatTensor,
                 emb E: torch.FloatTensor)
              Parameters
                   • emb h
                   • emb_r
                   • emb E
     forward_k_vs_all(x: torch.LongTensor) \rightarrow torch.FloatTensor
     forward_k_vs_sample (x: torch.LongTensor, target_entity_idx: torch.LongTensor)
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 <u>\_\_init\_\_()</u> call to the parent class must be made before assignment on the child.

#### Variables

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

```
args
embedding_dim = None
num_entities = None
num_relations = None
num_tokens = None
learning_rate = None
apply_unit_norm = None
input_dropout_rate = None
hidden_dropout_rate = None
optimizer_name = None
feature_map_dropout_rate = None
kernel_size = None
num_of_output_channels = None
weight_decay = None
loss
selected_optimizer = None
normalizer_class = None
normalize_head_entity_embeddings
normalize_relation_embeddings
normalize_tail_entity_embeddings
hidden_normalizer
param_init
input_dp_ent_real
input_dp_rel_real
hidden_dropout
loss_history = []
byte_pair_encoding
max_length_subword_tokens
block_size
forward_byte_pair_encoded_k_vs_all (x: torch.LongTensor)
       Parameters
          x (B x 2 x T)
```

```
forward_byte_pair_encoded_triple(x: Tuple[torch.LongTensor, torch.LongTensor])
          byte pair encoded neural link predictors
              Parameters
     init_params_with_sanity_checking()
     forward(x: torch.LongTensor | Tuple[torch.LongTensor, torch.LongTensor],
                 y idx: torch.LongTensor = None
              Parameters
                  • x
                  • y_idx
                  • ordered_bpe_entities
     forward_triples (x: torch.LongTensor) \rightarrow torch.Tensor
              Parameters
     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.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**  $(b \circ \circ 1)$  – 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

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.

name = 'OMult'

explicit = True

 $quaternion_multiplication_followed_by_inner_product(h, r, t)$ 

#### **Parameters**

- h shape: (\*batch\_dims, dim) The head representations.
- **r** shape: (\*batch dims, dim) The head representations.
- t shape: (\*batch dims, dim) The tail representations.

#### **Returns**

Triple scores.

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

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

Absolute value of a quaternion

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

L2 norm of quaternion vector:

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

## **Parameters**

 $\mathbf{x}$  – The vector.

### Returns

The normalized vector.

score (head\_ent\_emb: torch.FloatTensor, rel\_ent\_emb: torch.FloatTensor, tail ent emb: torch.FloatTensor)

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

#### **Parameters**

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

```
forward_k_vs_all(x)
               Parameters
                  x
     forward_k_vs_sample (x, target_entity_idx)
          Completed. Given a head entity and a relation (h,r), we compute scores for all possible triples, i.e.,
          [score(h,r,x)|x \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
     {\tt residual\_convolution}\,(Q\_1,\,Q\_2)
     forward_triples (indexed_triple: torch.Tensor) → torch.Tensor
               Parameters
                  x
     forward_k_vs_all (x: torch.Tensor)
          Given a head entity and a relation (h,r), we compute scores for all entities. [score(h,r,x)|x in Entities] =>
          [0.0,0.1,...,0.8], shape=> (1, |Entities|) Given a batch of head entities and relations => shape (size of batch,|
          Entities()
class dicee.models.AConvQ(args)
     Bases: dicee.models.base_model.BaseKGE
     Additive Convolutional Quaternion Knowledge Graph Embeddings
     name = 'AConvQ'
     entity_embeddings
     relation_embeddings
     conv2d
     fc_num_input
     fc1
```

```
bn_conv1
bn_conv2
feature_map_dropout
residual_convolution (Q_1, Q_2)
forward\_triples (indexed\_triple: torch.Tensor) \rightarrow torch.Tensor
```

### **Parameters**

```
forward_k_vs_all (x: torch.Tensor)
```

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

class dicee.models.BaseKGE (args: dict)

Bases: BaseKGELightning

Base class for all neural network modules.

Your models should also subclass this class.

Modules can also contain other Modules, allowing 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 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.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.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:

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

class Model (nn.Module):
    def __init__ (self) -> None:
        super().__init__()
        self.conv1 = nn.Conv2d(1, 20, 5)
        self.conv2 = nn.Conv2d(20, 20, 5)

def forward(self, x):
```

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```
x = F.relu(self.conv1(x))
return F.relu(self.conv2(x))
```

Submodules assigned in this way will be registered, and will 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** (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.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**

name = 'ConvO'

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

```
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.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)
```

```
\begin{tabular}{ll} {\bf residual\_convolution} & (O\_1,O\_2) \\ {\bf forward\_triples} & (x:torch.Tensor) & \rightarrow {\bf torch}.{\bf Tensor} \\ {\bf Parameters} & {\bf x} \\ \end{tabular}
```

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|)

```
\verb"class" dicee.models.Keci" (args)
```

```
Bases: dicee.models.base_model.BaseKGE
```

Base class for all neural network modules.

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

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 = 'Keci'
p
q
r
requires_grad_for_interactions = True
```

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

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

- (2)  $sigma_p = sum_{i=1}^p (h_0 r_i + h_i r_0) e_i$
- (3)  $sigma_q = sum_{j=p+1}^{p+q} (h_0 r_j + h_j r_0) e_j$
- (4)  $sigma_{pp} = sum_{i=1}^{p-1} sum_{k=i+1}^p (h_i r_k h_k r_i) e_i e_k$
- (5)  $sigma_{qq} = sum_{j=1}^{p+q-1} sum_{k=j+1}^{p+q} (h_j r_k h_k r_j) e_j e_k$
- (6)  $sigma_{pq} = sum_{i=1}^{p} sum_{j=p+1}^{p+q} (h_i r_j h_j r_i) e_i e_j$

construct cl multivector(x: torch.FloatTensor, r: int, p: int, q: int)

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

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

### **Parameter**

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

#### returns

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

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

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

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

Kvsall training

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

forward\_k\_vs\_with\_explicit and this functions are identical Parameter — x: torch.LongTensor with (n,2) shape :rtype: torch.FloatTensor with (n,|E|) shape

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

 $\rightarrow$  tuple[torch.FloatTensor, torch.FloatTensor, torch.FloatTensor]

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

### **Parameter**

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

### returns

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

 $forward_k\_vs\_sample$  (x: torch.LongTensor, target\_entity\_idx: torch.LongTensor)  $\rightarrow$  torch.FloatTensor

#### **Parameter**

```
x: torch.LongTensor with (n,2) shape
          target_entity_idx: torch.LongTensor with (n, k) shape k denotes the selected number of examples.
               rtype
                   torch.FloatTensor with (n, k) shape
     score(h, r, t)
     forward\_triples(x: torch.Tensor) \rightarrow torch.FloatTensor
          Parameter
          x: torch.LongTensor with (n,3) shape
               rtype
                   torch.FloatTensor with (n) shape
class dicee.models.CKeci(args)
     Bases: Keci
     Without learning dimension scaling
     name = 'CKeci'
     requires_grad_for_interactions = False
class dicee.models.DeCaL(args)
     Bases: dicee.models.base_model.BaseKGE
```

Base class for all neural network modules.

Your models should also subclass this class.

Modules can also contain other Modules, allowing 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 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

\_

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))

 $\verb|compute_sigmas_single| (\textit{list}\_h\_\textit{emb}, \textit{list}\_r\_\textit{emb}, \textit{list}\_t\_\textit{emb})|$ 

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

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

For different base vector interactions, we have

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

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

Kvsall training

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

forward\_k\_vs\_with\_explicit and this funcitons are identical Parameter — x: torch.LongTensor with (n, ) shape :rtype: torch.FloatTensor with (n, |E|) shape

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

Multiplying a base vector with its scalar coefficient

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

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

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

### **Parameter**

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

#### returns

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

 $compute\_sigma\_pp(hp, rp)$ 

Compute .. math:

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

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

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

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

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

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

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

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

Compute

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

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

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

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

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

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

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

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

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

compute\_sigma\_pq(\*, hp, hq, rp, rq)

Compute

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

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

### for j in range(q):

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

print(sigma\_pq.shape)

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

Compute

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

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

#### for j in range(q):

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

print(sigma\_pq.shape)

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

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

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

# for j in range(q):

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

print(sigma\_pq.shape)

```
class dicee.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
                                             x
             forward_k_vs_all(*args, **kwargs)
             forward_k_vs_sample(*args, **kwargs)
             get_triple_representation (idx_hrt)
             get_head_relation_representation(indexed_triple)
             get_sentence_representation(x: torch.LongTensor)
                                    Parameters
                                              • (b (x shape)
                                              • 3
                                              • t)
             get_bpe_head_and_relation_representation(x: torch.LongTensor)
                                             → Tuple[torch.FloatTensor, torch.FloatTensor]
                                    Parameters
                                             x (B x 2 x T)
             get_embeddings() → Tuple[numpy.ndarray, numpy.ndarray]
class dicee.models.PykeenKGE(args: dict)
             Bases: dicee.models.base_model.BaseKGE
             A class for using knowledge graph embedding models implemented in Pykeen
             Notes: Pykeen_DistMult: C Pykeen_ComplEx: Pykeen_QuatE: Pykeen_MuRE: Pykeen_CP: Pykeen_HolE: Py-
             keen_HolE: Pykeen_TransD: Pykeen_TransE: Pykeen_TransF: Pykeen_TransH: Pykeen_TransR:
             model kwargs
             name
             model
             loss_history = []
             args
             entity_embeddings = None
             relation_embeddings = None
             forward_k_vs_all (x: torch.LongTensor)
                         # => Explicit version by this we can apply bn and dropout
                          # (1) Retrieve embeddings of heads and relations + apply Dropout & Normalization if given. h, r =
                          self.get_head_relation_representation(x) \# (2) Reshape (1). if self.last_dim > 0:
                                    h = h.reshape(len(x), self.embedding\_dim, self.last\_dim) r = r.reshape(len(x), self.embedding\_dim, self.embeddin
                                    self.last_dim)
                          \# (3) Reshape all entities. if self.last dim > 0:
```

t = self.entity\_embeddings.weight.reshape(self.num\_entities, self.embedding\_dim, self.last\_dim)

else:

t = self.entity\_embeddings.weight

# (4) Call the score\_t from interactions to generate triple scores. return self.interaction.score\_t(h=h, r=r, all\_entities=t, slice\_size=1)

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

- # => Explicit version by this we can apply bn and dropout
- # (1) Retrieve embeddings of heads, relations and tails and apply Dropout & Normalization if given. h, r, t = self.get\_triple\_representation(x) # (2) Reshape (1). if self.last\_dim > 0:
  - $$\label{eq:hammon} \begin{split} &h = h.reshape(len(x), self.embedding\_dim, self.last\_dim) \ r = r.reshape(len(x), self.embedding\_dim, self.last\_dim) \end{split}$$
      $\ & t = t.reshape(len(x), self.embedding\_dim, self.last\_dim) \end{split}$
- # (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)
     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.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
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
      \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 \text{torch.Tensor}
                Parameters
class dicee.models.FMult2(args)
      Bases: dicee.models.base_model.BaseKGE
      Learning Knowledge Neural Graphs
      name = 'FMult2'
      n_{\text{layers}} = 3
      n = 50
      score_func = 'compositional'
      discrete_points
```

```
entity_embeddings
     relation_embeddings
     build_func(Vec)
     build_chain_funcs (list_Vec)
     compute_func (W, b, x) \rightarrow \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=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}(h, r, t)
class dicee.models.LFMult(args)
     Bases: dicee.models.base_model.BaseKGE
     Embedding with polynomial functions. We represent all entities and relations in the polynomial space as: f(x) =
     sum \{i=0\}^{d-1} a k x^{i} and use the three differents scoring function as in the paper to evaluate the score.
     We also consider combining with Neural Networks.
     name = 'LFMult'
     entity_embeddings
     relation_embeddings
     degree
     x_values
```

forward\_triples (idx\_triple)

### **Parameters**

x

construct\_multi\_coeff(X)

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

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

linear(x, w, b)

### $scalar_batch_NN(a, b, c)$

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

tri\_score (coeff\_h, coeff\_r, coeff\_t)

this part implement the trilinear scoring techniques:

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

- 1. generate the range for i, j and k from [0 d-1]
- 2. perform  $dfrac\{a_i*b_j*c_k\}\{1+(i+j+k)\%d\}$  in parallel for every batch
- 3. take the sum over each batch

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

this part implement the vector triple product scoring techniques:

```
score(h,r,t) = int_{0}{1} 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] $x + ... + coeff[0][d]x^d$ ,

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

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
{\tt forward\_k\_vs\_all}\;(\mathcal{X})
     KvsAll forward pass
     Input
     x: torch.LongTensor with (n, ) shape
     Output
     torch.FloatTensor with (n) shape
T (x: torch.tensor) \rightarrow torch.tensor
     Transpose function
     Input: Tensor with shape (nxm) Output: Tensor with shape (mxn)
```

# dicee.query\_generator

## **Classes**

QueryGenerator

### **Module Contents**

```
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)
```

```
passing incoming and outgoing edges to ground queries depending on mode [train valid or text] and getting queries and answers in return @ TODO: create a class for each single query struct

save_queries (query_type: str, gen_num: int, save_path: str)

abstract load_queries (path)

get_queries (query_type: str, gen_num: int)

static save_queries_and_answers (path: str, data: List[Tuple[str, Tuple[collections.defaultdict]]])

→ None

Save Queries into Disk

static load_queries_and_answers (path: str) → List[Tuple[str, Tuple[collections.defaultdict]]]]

Load Queries from Disk to Memory

dicee.read_preprocess_save_load_kg

Submodules

dicee.read_preprocess_save_load_kg.preprocess

Classes
```

PreprocessKG

Preprocess the data in memory

### **Module Contents**

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

Preprocess the data in memory

kg

start() → None

Preprocess train, valid and test datasets stored in knowledge graph instance

Parameter

rtype

None

preprocess_with_byte_pair_encoding()

preprocess_with_byte_pair_encoding_with_padding() → None

preprocess_with_pandas() → None

Preprocess train, valid and test datasets stored in knowledge graph instance with pandas

(1) Add recipriocal or noisy triples
```

(3) Index datasets

#### **Parameter**

rtype

None

```
{\tt preprocess\_with\_polars}\,()\,\to None
```

 $\verb"sequential_vocabulary_construction"\ () \ \to None$ 

- (1) Read input data into memory
- (2) Remove triples with a condition
- (3) Serialize vocabularies in a pandas dataframe where

=> the index is integer and => a single column is string (e.g. URI)

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

#### **Classes**

ReadFromDisk

Read the data from disk into memory

#### **Module Contents**

```
\verb|class| dicee.read_preprocess_save_load_kg.read_from_disk.ReadFromDisk| (kg)
```

Read the data from disk into memory

kg

 $\mathtt{start}() \to None$ 

Read a knowledge graph from disk into memory

Data will be available at the train\_set, test\_set, valid\_set attributes.

## **Parameter**

None

rtype

None

add\_noisy\_triples\_into\_training()

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

#### **Classes**

LoadSaveToDisk

# **Module Contents**

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

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

# **Functions**

polars_dataframe_indexer(→ polars.DataFrame)	Replaces 'subject', 'relation', and 'object' columns in the input Polars DataFrame with their corresponding index values
<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(→ polars.DataFrame)	Load and Preprocess via Polars
<pre>read_with_pandas(data_path[, read_only_few,])</pre>	
$read\_from\_disk(\rightarrow Tuple[polars.DataFrame, pan-$	
das.DataFrame])	
<pre>read_from_triple_store([endpoint])</pre>	Read triples from triple store into pandas dataframe
<pre>get_er_vocab(data[, file_path])</pre>	
<pre>get_re_vocab(data[, file_path])</pre>	
<pre>get_ee_vocab(data[, file_path])</pre>	
<pre>create_constraints(triples[, file_path])</pre>	
$load_with_pandas(\rightarrow None)$	Deserialize data
<pre>save_numpy_ndarray(*, data, file_path)</pre>	
<pre>load_numpy_ndarray(*, file_path)</pre>	
<pre>save_pickle(*, data[, file_path])</pre>	
load_pickle(*[, file_path])	
create_recipriocal_triples(x)	Add inverse triples into dask dataframe
$dataset\_sanity\_checking(\rightarrow None)$	

#### **Module Contents**

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

This function processes the DataFrame in three main steps: 1. Replace the 'relation' values with the corresponding index from *idx\_relation*. 2. Replace the 'subject' values with the corresponding index from *idx\_entity*. 3. Replace the 'object' values with the corresponding index from *idx\_entity*.

#### **Parameters:**

## df\_polars

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

#### idx entity

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

#### idx relation

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

#### **Returns:**

#### polars.DataFrame

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

#### **Example Usage:**

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

## Steps:

- 1. Join the input DataFrame *df\_polars* on the 'relation' column with *idx\_relation* to replace the relations with their indices.
- 2. Join on 'subject' to replace it with the corresponding entity index using a left join on idx\_entity.
- 3. Join on 'object' to replace it with the corresponding entity index using a left join on idx\_entity.

4. Select only the 'subject', 'relation', and 'object' columns to return the final result.

```
dicee.read_preprocess_save_load_kg.util.pandas_dataframe_indexer( df_pandas: pandas.DataFrame, idx_entity: pandas.DataFrame, idx_relation: pandas.DataFrame) <math>\rightarrow pandas.DataFrame
```

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

#### **Parameters:**

#### df pandas

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

## idx\_entity

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

#### idx\_relation

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

#### **Returns:**

#### pd.DataFrame

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

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

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

Load and Preprocess via Polars

```
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]

```
\verb|dicee.read_preprocess_save_load_kg.util.load_with_pandas| (self) \rightarrow None
     Deserialize data
dicee.read_preprocess_save_load_kg.util.save_numpy_ndarray(*, data: numpy.ndarray,
           file_path: str)
dicee.read_preprocess_save_load_kg.util.load_numpy_ndarray(*, file_path: str)
dicee.read_preprocess_save_load_kg.util.save_pickle(*, data: object, file_path=str)
dicee.read_preprocess_save_load_kq.util.load_pickle(*, file path=str)
dicee.read_preprocess_save_load_kg.util.create_recipriocal_triples(X)
     Add inverse triples into dask dataframe :param x: :return:
dicee.read_preprocess_save_load_kg.util.dataset_sanity_checking(
           train\_set: numpy.ndarray, num\_entities: int, num\_relations: int) \rightarrow None
          Parameters
                train_set
                num_entities
               • num_relations
          Returns
```

#### **Classes**

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

## **Package Contents**

```
Preprocess train, valid and test datasets stored in knowledge graph instance with pandas
           (1) Add recipriocal or noisy triples
           (2) Construct vocabulary
           (3) Index datasets
           Parameter
               rtype
                   None
     {\tt preprocess\_with\_polars}\, () \, \to None
     \verb|sequential_vocabulary_construction|()| \to None
           (1) Read input data into memory
           (2) Remove triples with a condition
           (3) Serialize vocabularies in a pandas dataframe where
                   => the index is integer and => a single column is string (e.g. URI)
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
     \mathtt{start}() \to 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
```

 $preprocess\_with\_pandas() \rightarrow None$ 

#### **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	!!! abstract "Usage Documentation"

#### **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: {\tt pydantic.BaseModel}
     !!! abstract "Usage Documentation"
         [Models](../concepts/models.md)
     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.
     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
                                                                their
                                                                        corresponding
                                                                                        [ComputedField-
                                                names
                                                         and
     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.scripts.run.get_default_arguments(description=None)
     Extends pytorch_lightning Trainer's arguments with ours
dicee.scripts.run.main()
```

## dicee.static\_funcs

## **Functions**

```
Add inverse triples into dask dataframe
create_recipriocal_triples(x)
get_er_vocab(data[, file_path])
get_re_vocab(data[, file_path])
get_ee_vocab(data[, file_path])
timeit(func)
save_pickle(*[, data, file_path])
load_pickle([file_path])
load_term_mapping([file_path])
select_model(args[,
                        is_continual_training,
                                               stor-
age path])
                                                      Load weights and initialize pytorch module from names-
load_model(→ Tuple[object, Tuple[dict, dict]])
                                                      pace arguments
load_model_ensemble(...)
                                                      Construct Ensemble Of weights and initialize pytorch
                                                      module from namespace arguments
save_numpy_ndarray(*, data, file_path)
                                                      Detect most efficient data type for a given triples
numpy_data_type_changer(→ numpy.ndarray)
```

continues on next page

Table 2 - continued from previous page

```
save\_checkpoint\_model(\rightarrow None)
                                                        Store Pytorch model into disk
store(\rightarrow None)
                                                        Add randomly constructed triples
add\_noisy\_triples(\rightarrow pandas.DataFrame)
read_or_load_kg(args, cls)
intialize\_model(\rightarrow Tuple[object, str])
load_json(\rightarrow dict)
                                                        Save it as CSV if memory allows.
save\_embeddings(\rightarrow None)
random_prediction(pre_trained_kge)
deploy_triple_prediction(pre_trained_kge,
str_subject, ...)
deploy_tail_entity_prediction(pre_trained_kge,
deploy_head_entity_prediction(pre_trained_kge,
deploy_relation_prediction(pre_trained_kge,
vocab_to_parquet(vocab_to_idx, name, ...)
create_experiment_folder([folder_name])
continual\_training\_setup\_executor(\rightarrow None)
exponential\_function(\rightarrow torch.FloatTensor)
load_numpy(→ 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_int
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)
dicee.static_funcs.numpy_data_type_changer(train_set: numpy.ndarray, num: int)
             \rightarrow numpy.ndarray
     Detect most efficient data type for a given triples :param train_set: :param num: :return:
dicee.static_funcs.save_checkpoint_model(model, path: str) \rightarrow None
     Store Pytorch model into disk
dicee.static_funcs.store(trained model, model name: str = 'model', full storage path: str = None,
            save\_embeddings\_as\_csv=False) \rightarrow None
dicee.static_funcs.add_noisy_triples(train_set: pandas.DataFrame, add_noise_rate: float)
             \rightarrow pandas.DataFrame
     Add randomly constructed triples :param train_set: :param add_noise_rate: :return:
dicee.static_funcs.read_or_load_kg(args, cls)
dicee.static_funcs.intialize model(args: dict, verbose=0) \rightarrow Tuple[object, str]
dicee.static_funcs.load_json(p: str) \rightarrow dict
dicee.static_funcs.save_embeddings (embeddings: numpy.ndarray, indexes, path: str) \rightarrow None
     Save it as CSV if memory allows. :param embeddings: :param indexes: :param path: :return:
dicee.static_funcs.random_prediction(pre_trained_kge)
dicee.static_funcs.deploy_triple_prediction(pre_trained_kge, str_subject, str_predicate,
            str_object)
dicee.static_funcs.deploy_tail_entity_prediction(pre_trained_kge, str_subject, str_predicate,
            top_k)
```

```
dicee.static_funcs.deploy_head_entity_prediction(pre_trained_kge, str_object, str_predicate,
           top_k)
dicee.static_funcs.deploy_relation_prediction(pre_trained_kge, str_subject, str_object, top_k)
dicee.static_funcs.vocab_to_parquet(vocab_to_idx, name, path_for_serialization, print_into)
dicee.static_funcs.create_experiment_folder(folder_name='Experiments')
dicee.static_funcs.continual_training_setup_executor(executor) \rightarrow None
dicee.static_funcs.exponential function (x: numpy.ndarray, lam: float, ascending order=True)
            → torch.FloatTensor
dicee.static_funcs.load_numpy(path) \rightarrow numpy.ndarray
dicee.static_funcs.evaluate(entity_to_idx, scores, easy_answers, hard_answers)
     # @TODO: CD: Renamed this function Evaluate multi hop query answering on different query types
dicee.static_funcs.download_file(url, destination_folder='.')
dicee.static_funcs.download_files_from_url(base\_url: str, destination\_folder='.') \rightarrow None
          Parameters
                                                "https://files.dice-research.org/projects/DiceEmbeddings/
                • base_url
                                (e.g.
                  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
dicee.static_funcs.from_pretrained_model_write_embeddings_into_csv(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\_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.TorchTrainer | dicee.trainer.model_parallelism.TensorParallel | dicee.trainer.torch_trainer_ddp
\verb|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.torch_trainer.TorchTrainer | dicee.trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_traine
             Initialize Trainer from input arguments
initialize_or_load_model()
init_dataloader (dataset: torch.utils.data.Dataset) → torch.utils.data.DataLoader
init_dataset() → torch.utils.data.Dataset
start (knowledge_graph: dicee.knowledge_graph.KG | numpy.memmap)
                                  → Tuple[dicee.models.base_model.BaseKGE, str]
             Start the training
              (1) Initialize Trainer
              (2) Initialize or load a pretrained KGE model
             in DDP setup, we need to load the memory map of already read/index KG.
k\_fold\_cross\_validation(dataset) \rightarrow Tuple[dicee.models.base\_model.BaseKGE, str]
             Perform K-fold Cross-Validation
                 1. Obtain K train and test splits.
                 2. For each split,
                                  2.1 initialize trainer and model 2.2. Train model with configuration provided in args. 2.3. Compute
                                  the mean reciprocal rank (MRR) score of the model on the test respective split.
                 3. Report the mean and average MRR.
                        Parameters

    self

                                   • dataset
```

Returns model

## dicee.trainer.model\_parallelism

#### **Classes**

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

#### **Functions**

```
extract_input_outputs(z[, device])

find_good_batch_size(train_loader,

tp_ensemble_model)

forward_backward_update_loss(→ float)
```

#### **Module Contents**

```
args
[str] ?

callbacks: list
?

fit (*args, **kwargs)
Train model
```

## dicee.trainer.torch\_trainer

# Classes

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

## **Module Contents**

```
class dicee.trainer.torch_trainer.TorchTrainer(args, callbacks)
     Bases: dicee.abstracts.AbstractTrainer
           TorchTrainer for using single GPU or multi CPUs on a single node
           Arguments
     callbacks: list of Abstract callback instances
     loss_function = None
     optimizer = None
     model = None
     train_dataloaders = None
     training_step = None
     process
     fit (*args, train\_dataloaders, **kwargs) \rightarrow None
               Training starts
               Arguments
           kwargs:Tuple
               empty dictionary
               Return type
                   batch loss (float)
     forward\_backward\_update(x\_batch: torch.Tensor, y\_batch: torch.Tensor) \rightarrow torch.Tensor
               Compute forward, loss, backward, and parameter update
               Arguments
               Return type
                   batch loss (float)
     \verb|extract_input_outputs_set_device| (\textit{batch: list}) \rightarrow Tuple
               Construct inputs and outputs from a batch of inputs with outputs From a batch of inputs and put
               Arguments
               Return type
                   (tuple) mini-batch on select device
```

## dicee.trainer.torch\_trainer\_ddp

#### **Classes**

```
TorchDDPTrainer A Trainer based on torch.nn.parallel.DistributedDataParallel
NodeTrainer
```

#### **Functions**

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

#### **Module Contents**

```
dicee.trainer.torch_trainer_ddp.make_iterable_verbose(iterable_object, verbose,
            desc='Default', position=None, leave=True) \rightarrow Iterable
class dicee.trainer.torch_trainer_ddp.TorchDDPTrainer(args, callbacks)
     Bases: dicee.abstracts.AbstractTrainer
          A Trainer based on torch.nn.parallel.DistributedDataParallel
          Arguments
     entity_idxs
          mapping.
     relation_idxs
          mapping.
     form
     store
     label_smoothing_rate
          Using hard targets (0,1) drives weights to infinity. An outlier produces enormous gradients.
          Return type
              torch.utils.data.Dataset
     fit (*args, **kwargs)
          Train model
class dicee.trainer.torch_trainer_ddp.NodeTrainer(trainer, model: torch.nn.Module,
            train_dataset_loader: torch.utils.data.DataLoader, callbacks, num_epochs: int)
     trainer
     local_rank
     global_rank
```

```
optimizer

train_dataset_loader

loss_func

callbacks

model

num_epochs

loss_history = []

ctx

scaler

extract_input_outputs(z: list)

train()

Training loop for DDP
```

#### **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.torch_trainer.TorchTrainer | dicee.trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_traine
                Initialize Trainer from input arguments
initialize_or_load_model()
\verb"init_dataloader" (dataset: torch.utils.data.Dataset") 	o 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

## 14.2 Attributes

\_version\_\_

# 14.3 Classes

A Physical Embedding Model for Knowledge Graphs
Embedding Entities and Relations for Learning and Infer-
ence in Knowledge Bases
Without learning dimension scaling
Base class for all neural network modules.
Translating Embeddings for Modeling
Base class for all neural network modules.
Dual Quaternion Knowledge Graph Embeddings
(https://ojs.aaai.org/index.php/AAAI/article/download/ 16850/16657)
Base class for all neural network modules.
Additive Convolutional ComplEx Knowledge Graph Embeddings
Additive Convolutional Octonion Knowledge Graph Em-
beddings
Additive Convolutional Quaternion Knowledge Graph
Embeddings
Convolutional Quaternion Knowledge Graph Embed-
dings
Base class for all neural network modules.
Convolutional ComplEx Knowledge Graph Embeddings
Base class for all neural network modules.
Base class for all neural network modules.
A shallow neural model for relation prediction (https://arxiv.org/abs/2101.09090)
Embedding with polynomial functions. We represent all entities and relations in the polynomial space as:
A class for using knowledge graph embedding models implemented in Pykeen
Base class for all neural network modules.
Base class for all neural network modules.
DICE_Trainer implement
Knowledge Graph Embedding Class for interactive usage of pre-trained models
An abstract class representing a Dataset.
An abstract class representing a Dataset.
Dataset for the 1vsALL training strategy
Dataset for the 1vsALL training strategy
Creates a dataset for KvsAll training by inheriting from torch.utils.data.Dataset.
Creates a dataset for AllvsAll training by inheriting from torch.utils.data.Dataset.
A custom PyTorch Dataset class for knowledge graph embeddings, which includes
KvsSample a Dataset:
An abstract class representing a Dataset.
Triple Dataset
Create a Dataset for cross validation
continues on next page

continues on next page

Table 3 - continued from previous page

LiteralDataset	Dataset for loading and processing literal data for training Literal Embedding model.
QueryGenerator	

# 14.4 Functions

create_recipriocal_triples(x)	Add inverse triples into dask dataframe
get_er_vocab(data[, file_path])	That inverse triples into another antiferror
<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>	rg.
numpy_data_type_changer(→ numpy.ndarray) save_checkpoint_model(→ None)	Detect most efficient data type for a given triples Store Pytorch model into disk
store(→ None)	
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)	
deploy_triple_prediction(pre_trained_kge,	
<pre>str_subject,) deploy_tail_entity_prediction(pre_trained_kge,</pre>	
)	
deploy_head_entity_prediction(pre_trained_kge,	
)	

continues on next page

Table 4 - continued from previous page

```
deploy_relation_prediction(pre_trained_kge,
...)
vocab_to_parquet(vocab_to_idx, name, ...)
create_experiment_folder([folder_name])
continual\_training\_setup\_executor(\rightarrow None)
exponential\_function( \rightarrow torch.FloatTensor)
load_numpy(→ numpy.ndarray)
                                                       # @TODO: CD: Renamed this function
evaluate(entity_to_idx,
                            scores,
                                       easy_answers,
hard_answers)
download_file(url[, destination_folder])
download\_files\_from\_url(\rightarrow None)
download\_pretrained\_model(\rightarrow str)
write_csv_from_model_parallel(path)
                                                       Create
from_pretrained_model_write_embeddings_int
{\it mapping\_from\_first\_two\_cols\_to\_third} (train\_se
timeit(func)
load_term_mapping([file_path])
                                                       Reload the files from disk to construct the Pytorch dataset
reload_dataset(path, form_of_labelling, ...)
construct_dataset(→ torch.utils.data.Dataset)
```

# 14.5 Package Contents

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

```
name = 'Keci'
p
q
r
requires_grad_for_interactions = True
compute\_sigma\_pp(hp, rp)
     Compute sigma_{pp} = sum_{i=1}^{p-1} sum_{k=i+1}^p (h_i r_k - h_k r_i) e_i e_k
     sigma_{pp} captures the interactions between along p bases For instance, let p e_1, e_2, e_3, we compute
     interactions between e_1 e_2, e_1 e_3, and e_2 e_3 This can be implemented with a nested two for loops
          results = [] for i in range(p - 1):
              for k in range(i + 1, p):
                results.append(hp[:,:,i]*rp[:,:,k] - hp[:,:,k]*rp[:,:,i]) \\
          sigma_pp = torch.stack(results, dim=2) assert sigma_pp.shape == (b, r, int((p * (p - 1)) / 2))
     Yet, this computation would be quite inefficient. Instead, we compute interactions along all p, e.g., e1e1,
     e1e2, e1e3,
          e2e1, e2e2, e2e3, e3e1, e3e2, e3e3
     Then select the triangular matrix without diagonals: e1e2, e1e3, e2e3.
compute\_sigma\_qq(hq, rq)
     Compute sigma_{qq} = sum_{j=1}^{p+q-1} sum_{k=j+1}^{p+q} (h_j r_k - h_k r_j) e_j e_k sigma_{q}
     captures the interactions between along q bases For instance, let q e_1, e_2, e_3, we compute interactions
     between e_1 e_2, e_1 e_3, and e_2 e_3 This can be implemented with a nested two for loops
          results = [] for j in range(q - 1):
              for k in range(j + 1, q):
                 results.append(hq[:, :, j] * rq[:, :, k] - hq[:, :, k] * rq[:, :, j])
          sigma 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

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

- (1)  $sigma_0 = h_0 r_0 + sum_{i=1}^p (h_0 r_i) e_i sum_{j=p+1}^{p+q} (h_j r_j) e_j$
- (2)  $sigma_p = sum_{i=1}^p (h_0 r_i + h_i r_0) e_i$
- (3)  $sigma_q = sum_{j=p+1}^{p+q} (h_0 r_j + h_j r_0) e_j$
- (4)  $sigma_{pp} = sum_{i=1}^{p-1} sum_{k=i+1}^p (h_i r_k h_k r_i) e_i e_k$
- (5)  $sigma_{qq} = sum_{j=1}^{p+q-1} sum_{k=j+1}^{p+q} (h_j r_k h_k r_j) e_j e_k$
- (6)  $sigma_{pq} = sum_{i=1}^{p} sum_{j=p+1}^{p+q} (h_i r_j h_j r_i) e_i e_j$

 ${\tt construct\_cl\_multivector}$  (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)

 $\verb+k_vs_all_score+ (bpe\_head\_ent\_emb, bpe\_rel\_ent\_emb, E)$ 

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

Kvsall training

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

 $\textbf{forward\_k\_vs\_sample} \ (x: torch.LongTensor, target\_entity\_idx: torch.LongTensor) \ \rightarrow \\ \textbf{torch.FloatTensor}$ 

#### **Parameter**

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

target\_entity\_idx: torch.LongTensor with (n, k) shape k denotes the selected number of examples.

#### rtvpe

torch.FloatTensor with (n, k) shape

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

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

#### **Parameter**

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

#### rtype

torch.FloatTensor with (n) shape

class dicee.TransE(args)

Bases: dicee.models.base\_model.BaseKGE

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

```
name = 'TransE'
margin = 4
score(head_ent_emb, rel_ent_emb, tail_ent_emb)
```

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

class dicee.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):
```

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

```
name = 'DeCaL'
entity_embeddings
relation_embeddings
p
q
r
re
forward_triples(x: torch.Tensor) → torch.FloatTensor
```

## **Parameter**

x: torch.LongTensor with (n, ) shape

#### rtype

torch.FloatTensor with (n) shape

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

Input: tensor(batch\_size, emb\_dim)  $\longrightarrow$  output: tensor with 1+p+q+r components with size (batch\_size, emb\_dim/(1+p+q+r)) each.

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

 $\verb|compute_sigmas_single| (\textit{list}\_h\_\textit{emb}, \textit{list}\_r\_\textit{emb}, \textit{list}\_t\_\textit{emb})$ 

here we compute all the sums with no others vectors interaction taken with the scalar product with t, that is,

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

and return:

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

compute\_sigmas\_multivect (list\_h\_emb, list\_r\_emb)

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

For same bases vectors interaction we have

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

For different base vector interactions, we have

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

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

**Kvsall** training

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

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

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):

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

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

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

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

Compute

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

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

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

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

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

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

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

compute sigma rr(hk, rk)

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

compute\_sigma\_pq(\*, hp, hq, rp, rq)

Compute

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

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

#### for j in range(q):

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

print(sigma\_pq.shape)

compute\_sigma\_pr(\*, hp, hk, rp, rk)

Compute

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

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

for j in range(q):

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

print(sigma\_pq.shape)

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

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

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

for j in range(q):

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

print(sigma\_pq.shape)

class dicee.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** ( $e_1h, e_2h, e_3h, e_4h, e_5h, e_6h, e_7h, e_8h, e_1t, e_2t, e_3t, e_4t, e_5t, e_6t, e_7t, e_8t, r_1, r_2, r_3, r_4, r_5, r_6, r_7, r_8) o$ torch.tensor

KvsAll scoring function

#### Input

x: torch.LongTensor with (n, ) shape

## **Output**

torch.FloatTensor with (n) shape

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

Negative Sampling forward pass:

#### Input

x: torch.LongTensor with (n, ) shape

## **Output**

torch.FloatTensor with (n) shape

```
forward_k_vs_all(x)
```

KvsAll forward pass

## Input

x: torch.LongTensor with (n, ) shape

# **Output**

torch.FloatTensor with (n) shape

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

Transpose function

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

```
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

 $\textbf{training} \ (\textit{bool}) - Boolean \ represents \ whether \ this \ module \ is \ in \ training \ or \ evaluation \ mode.$ 

```
name = 'ComplEx'
```

```
static score (head_ent_emb: torch.FloatTensor, rel_ent_emb: torch.FloatTensor,
                  tail_ent_emb: torch.FloatTensor)
     static k_vs_all_score (emb_h: torch.FloatTensor, emb_r: torch.FloatTensor,
                  emb E: torch.FloatTensor)
               Parameters
                   • emb h
                   • emb_r
                   • emb E
     forward_k_vs_all(x: torch.LongTensor) \rightarrow torch.FloatTensor
     forward_k_vs_sample (x: torch.LongTensor, target_entity_idx: torch.LongTensor)
class dicee.AConEx(args)
     Bases: dicee.models.base_model.BaseKGE
     Additive Convolutional ComplEx Knowledge Graph Embeddings
     name = 'AConEx'
     conv2d
     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.AConvO(args: dict)
     Bases: dicee.models.base_model.BaseKGE
     Additive Convolutional Octonion Knowledge Graph Embeddings
     name = 'AConvO'
     conv2d
     fc_num_input
```

```
fc1
     bn_conv2d
     norm_fc1
     feature_map_dropout
     static octonion_normalizer(emb_rel_e0, emb_rel_e1, emb_rel_e2, emb_rel_e3, emb_rel_e4,
                  emb_rel_e5, emb_rel_e6, emb_rel_e7)
     residual\_convolution(O\_1, O\_2)
     forward\_triples(x: torch.Tensor) \rightarrow torch.Tensor
               Parameters
     forward_k_vs_all (x: torch.Tensor)
           Given a head entity and a relation (h,r), we compute scores for all entities. [score(h,r,x)|x in Entities] =>
           [0.0,0.1,...,0.8], shape=> (1, |Entities|) Given a batch of head entities and relations => shape (size of batch,|
           Entities l)
class dicee.AConvQ(args)
     Bases: dicee.models.base model.BaseKGE
     Additive Convolutional Quaternion Knowledge Graph Embeddings
     name = 'AConvQ'
     entity_embeddings
     relation_embeddings
     conv2d
     fc_num_input
     fc1
     bn_conv1
     bn_conv2
     feature_map_dropout
     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
     feature_map_dropout
     {\tt residual\_convolution}\,(Q\_I,\,Q\_2)
     forward\_triples (indexed\_triple: torch.Tensor) \rightarrow torch.Tensor
               Parameters
     forward_k_vs_all (x: torch.Tensor)
           Given a head entity and a relation (h,r), we compute scores for all entities. [score(h,r,x)|x in Entities] =>
           [0.0,0.1,...,0.8], shape=> (1, |Entities|) Given a batch of head entities and relations => shape (size of batch,|
           Entities()
class dicee.ConvO(args: dict)
     Bases: dicee.models.base_model.BaseKGE
```

Base class for all neural network modules.

buse class for an hearth 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**

feature\_map\_dropout

```
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
     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
```

```
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:

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.

### 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: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.

#### $\mathtt{static}\ \mathtt{quaternion\_normalizer}\ (x:\ torch.FloatTensor) \ o \ torch.FloatTensor$

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

Absolute value of a quaternion

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

L2 norm of quaternion vector:

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

#### **Parameters**

 $\mathbf{x}$  – The vector.

#### Returns

The normalized vector.

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

#### **Parameters**

- bpe\_head\_ent\_emb
- bpe rel ent emb
- E

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

#### **Parameters**

x

forward\_k\_vs\_sample (x, target\_entity\_idx)

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

class dicee.OMult(args)

Bases: dicee.models.base\_model.BaseKGE

Base class for all neural network modules.

Your models should also subclass this class.

Modules can also contain other Modules, allowing 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.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() \rightarrow Tuple[numpy.ndarray, None]
forward_k_vs_all(x) \rightarrow torch.FloatTensor
forward_triples(x) \rightarrow 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
     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}{-1}
           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\_TransD: Pykeen\_TransE: Pykeen\_TransF: Pykeen\_TransH: Pykeen\_TransR:

```
model_kwargs
```

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)

```
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 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 = 'BytE'
config
temperature = 0.5
topk = 2
transformer
```

#### 1m head

loss\_function(yhat\_batch, y\_batch)

#### **Parameters**

- · yhat batch
- y\_batch

forward (x: torch.LongTensor)

#### **Parameters**

```
\mathbf{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
```

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(continued from previous page)

```
# 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
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.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:
\texttt{dicee.save\_checkpoint\_model} \ (\textit{model}, \textit{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
                                                   "https://files.dice-research.org/projects/DiceEmbeddings/

    base_url

                                  (e.g.
                   KINSHIP-Keci-dim128-epoch256-KvsAll")
                 • destination_folder (e.g. "KINSHIP-Keci-dim128-epoch256-KvsA11")
dicee.download\_pretrained\_model(\mathit{url:str}) \rightarrow str
dicee.write_csv_from_model_parallel(path: str)
dicee.from_pretrained_model_write_embeddings_into_csv(path:str) \rightarrow 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)
                                     \rightarrow lightning.Trainer | dicee.trainer.model_parallelism.TensorParallel | dicee.trainer.torch_trainer.TorchTrainer | dicee.trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_train
              Initialize Trainer from input arguments
initialize_or_load_model()
init\_dataloader (dataset: torch.utils.data.Dataset) \rightarrow torch.utils.data.DataLoader
init_dataset() \rightarrow torch.utils.data.Dataset
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

```
class dicee.KGE (path=None, url=None, construct ensemble=False, model name=None)
```

Bases: dicee.abstracts.BaseInteractiveKGE, dicee.abstracts.

InteractiveQueryDecomposition, dicee.abstracts.BaseInteractiveTrainKGE

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)

 $\label{limitsing_head_entity} $$predict_missing_head_entity$ (relation: List[str] \mid str, tail\_entity$: List[str] \mid str, within=None, \\ batch\_size=2, topk=1, return\_indices=False) $\to $$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, batch_size=2, topk=1, return_indices=False) \rightarrow Tuple
```

Given a head entity and a tail entity, return top k ranked relations.

```
argmax_{r in R} f(h,r,t), where h, t in E.
```

#### **Parameter**

head\_entity: List[str]

String representation of selected entities.

tail\_entity: List[str]

String representation of selected entities.

k: int

Highest ranked k entities.

### **Returns: Tuple**

Highest K scores and entities

```
predict_missing_tail_entity (head_entity: List[str] | str, relation: List[str] | str, within: List[str] = None, batch_size=2, topk=1, return_indices=False) \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.

#### **Returns**

- If you query a single (h, r, ?) or (?, r, t) or (h, ?, t), returns List[(item, score)]
- If you query a batch of B, returns List of B such lists.

```
\label{eq:core} \begin{split} \texttt{triple\_score} \; (h: List[str] \mid str = None, \, r: \, List[str] \mid str = None, \, logits = False) \\ &\rightarrow \mathsf{torch}. \\ \mathsf{FloatTensor} \end{split}
```

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

```
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, 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

dicee.load\_term\_mapping(file\_path=str)

Reload the files from disk to construct the Pytorch dataset

```
• 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)
      predict literals (entity: List[str] | str = None, attribute: List[str] | str = None,
                    denormalize\_preds: bool = True) \rightarrow numpy.ndarray
            Predicts literal values for given entities and attributes.
                 Parameters
                     • entity (Union[List[str], str]) - Entity or list of entities to predict literals for.
                     • attribute (Union[List[str], str]) - Attribute or list of attributes to predict literals
                       for.
                     • denormalize_preds (bool) - If True, denormalizes the predictions.
                 Returns
                     Predictions for the given entities and attributes.
                 Return type
                     numpy ndarray
dicee.mapping_from_first_two_cols_to_third(train_set_idx)
dicee.timeit(func)
```

dicee.reload\_dataset(path: str, form\_of\_labelling, scoring\_technique, neg\_ratio, label\_smoothing\_rate)

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
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]])
```

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 - ?
                • 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.OnevsAllDataset (train_set_idx: numpy.ndarray, entity_idxs)
     Bases: torch.utils.data.Dataset
     Dataset for the 1vsALL training strategy
          Parameters
                • train_set_idx - Indexed triples for the training.
                • entity_idxs - mapping.
                • relation_idxs - mapping.
                • form - ?
```

num\_workers – int for https://pytorch.org/docs/stable/data.html#torch.utils.data.
 DataLoader

#### Return type

torch.utils.data.Dataset

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

class dicee.KvsAll(train\_set\_idx: numpy.ndarray, entity\_idxs, relation\_idxs, form, store=None,

 $label\_smoothing\_rate: float = 0.0)$ 

Bases: torch.utils.data.Dataset

### Creates a dataset for KvsAll training by inheriting from torch.utils.data.Dataset.

Let D denote a dataset for KvsAll training and be defined as D:=  $\{(x,y)_i\}_i$  ^N, where x: (h,r) is an unique tuple of an entity h in E and a relation r in R that has been seed in the input graph. y: denotes a multi-label vector in  $[0,1]^{\{E\}}$  is a binary label.

orall y\_i =1 s.t. (h r E\_i) in KG



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

Let D denote a dataset for AllvsAll training and be defined as D:=  $\{(x,y) \mid i \mid i \land N, \text{ where } x: (h,r) \text{ is a possible} \}$ 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

[dictonary] string representation of an entity to its integer id

#### relation\_idxs

[dictonary] string representation of a relation to its integer id

self: torch.utils.data.Dataset

```
>>> a = AllvsAll()
>>> a
? array([0, 1, 2, 3, 4, 5, 6, 7, 8, 9])
```

```
train_data = None
train_target = None
label_smoothing_rate
collate_fn = None
target_dim
__len__()
\__{getitem}_{(idx)}
```

class dicee.OnevsSample(train\_set: numpy.ndarray, num\_entities, num\_relations,

 $neg\_sample\_ratio: int = None, label\_smoothing\_rate: float = 0.0)$ 

Bases: torch.utils.data.Dataset

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

### **Parameters**

- train set (np.ndarray) A numpy array containing triples of knowledge graph data. Each triple consists of (head\_entity, relation, tail\_entity).
- num entities (int) The number of unique entities in the knowledge graph.

- num\_relations (int) The number of unique relations in the knowledge graph.
- neg\_sample\_ratio (int, optional) The number of negative samples to be generated per positive sample. Must be a positive integer and less than num\_entities.
- label\_smoothing\_rate (float, optional) A label smoothing rate to apply to the positive and negative labels. Defaults to 0.0.

### train\_data

The input data converted into a PyTorch tensor.

```
Type
```

torch.Tensor

#### num\_entities

Number of entities in the dataset.

**Type** 

int

#### num\_relations

Number of relations in the dataset.

**Type** 

int

#### neg\_sample\_ratio

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

Type

int

#### label\_smoothing\_rate

The smoothing factor applied to the labels.

**Type** 

torch.Tensor

#### collate\_fn

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

Type

function, optional

train\_data

num\_entities

num\_relations

neg\_sample\_ratio = None

label\_smoothing\_rate

collate\_fn = None

\_\_len\_\_()

Returns the number of samples in the dataset.

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

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

#### **Parameters**

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

#### Returns

### A tuple consisting of:

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

#### Return type

tuple

### **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
```

|new\_y| << |E| new\_y contains all 1's if sum(y)< neg\_sample ratio new\_y contains</pre>

#### train\_set\_idx

Indexed triples for the training.

### entity\_idxs

mapping.

### relation\_idxs

mapping.

form

?

store

label\_smoothing\_rate

?

torch.utils.data.Dataset

```
train_data = None
train_target = None
```

neg\_ratio = None

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__()
       \underline{\phantom{a}}getitem\underline{\phantom{a}} (idx)
class dicee. TriplePredictionDataset (train_set: numpy.ndarray, num_entities: int, num_relations: int,
              neg\_sample\_ratio: int = 1, label\_smoothing\_rate: float = 0.0)
      Bases: torch.utils.data.Dataset
            Triple Dataset
                 D := \{(x)_i\}_i \ ^N, \text{ where }
                      . x:(h,r, t) in KG is a unique h in E and a relation r in R and . collact fn => Generates
                     negative triples
                 collect_fn:
      orall (h,r,t) in G obtain, create negative triples \{(h,r,x),(r,t),(h,m,t)\}
                 y:labels are represented in torch.float16
```

```
train_set_idx
               Indexed triples for the training.
          entity_idxs
              mapping.
          relation_idxs
              mapping.
          form
          store
          label_smoothing_rate
          collate_fn: batch:List[torch.IntTensor] Returns ——- torch.utils.data.Dataset
     label_smoothing_rate
     neg_sample_ratio
     train_set
     length
     num_entities
     num_relations
     __len__()
     \__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: \verb"pytorch_lightning.LightningDataModule" \\
     Create a Dataset for cross validation
          Parameters
                 • train_set_idx - Indexed triples for the training.
                 • num_entities – entity to index mapping.
                 • num_relations - relation to index mapping.
                 • batch_size - int
                 • form - ?
                 • num_workers - int for https://pytorch.org/docs/stable/data.html#torch.utils.data.
                   DataLoader
          Return type
     train_set_idx
```

```
num_entities
num_relations
neg_sample_ratio
batch_size
num_workers
```

train\_dataloader() → torch.utils.data.DataLoader

An iterable or collection of iterables specifying training samples.

For more information about multiple dataloaders, see this section.

The dataloader you return will not be reloaded unless you set :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.11 = None
```

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

# don't do this
    self.something = else

def setup(self, stage):
    data = load_data(...)
    self.l1 = nn.Linear(28, data.num_classes)
```

### transfer\_batch\_to\_device(\*args, \*\*kwargs)

Override this hook if your DataLoader returns tensors wrapped in a custom data structure.

The data types listed below (and any arbitrary nesting of them) are supported out of the box:

- torch. Tensor or anything that implements .to(...)
- list
- dict
- tuple

For anything else, you need to define how the data is moved to the target device (CPU, GPU, TPU, ...).

### **1** Note

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

#### **Parameters**

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

#### Returns

A reference to the data on the new device.

#### Example:

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

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```
→idx)
return batch
```

```
• See also
• move_data_to_device()
• apply_to_collection()
```

### prepare\_data(\*args, \*\*kwargs)

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

# **▲** Warning

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

#### Example:

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

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

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

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

#### Example:

```
# DEFAULT
# called once per node on LOCAL_RANK=0 of that node

class LitDataModule(LightningDataModule):
    def __init__(self):
        super().__init__()
        self.prepare_data_per_node = True

# call on GLOBAL_RANK=0 (great for shared file systems)

class LitDataModule(LightningDataModule):
    def __init__(self):
        super().__init__()
        self.prepare_data_per_node = False
```

This is called before requesting the dataloaders:

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

```
class dicee.LiteralDataset (file\_path: str, ent\_idx: dict = None, normalization\_type: str = 'z-norm', sampling\_ratio: float = None, loader\_backend: str = 'pandas')
```

Bases: torch.utils.data.Dataset

Dataset for loading and processing literal data for training Literal Embedding model. This dataset handles the loading, normalization, and preparation of triples for training a literal embedding model.

Extends torch.utils.data.Dataset for supporting PyTorch dataloaders.

#### train\_file\_path

Path to the training data file.

**Type** 

str

#### normalization

Type of normalization to apply ('z-norm', 'min-max', or None).

**Type** 

str

#### normalization\_params

Parameters used for normalization.

**Type** 

dict

#### sampling\_ratio

Fraction of the training set to use for ablations.

**Type** 

float

### entity\_to\_idx

Mapping of entities to their indices.

**Type** 

dict

#### num\_entities

Total number of entities.

Type

int

## data\_property\_to\_idx

Mapping of data properties to their indices.

Type

dict

```
num_data_properties
           Total number of data properties.
               Type
                   int
     loader_backend
           Backend to use for loading data ('pandas' or 'rdflib').
               Type
                   str
     train_file_path
     loader_backend = 'pandas'
     normalization_type = 'z-norm'
     normalization_params
     sampling_ratio = None
     entity_to_idx = None
     num_entities
     __getitem__(index)
     __len__()
     static load_and_validate_literal_data (file_path: str = None, loader_backend: str = 'pandas')
                   \rightarrow pandas.DataFrame
           Loads and validates the literal data file. :param file_path: Path to the literal data file. :type file_path: str
                   DataFrame containing the loaded and validated data.
               Return type
                   pd.DataFrame
     static denormalize (preds_norm, attributes, normalization_params) → numpy.ndarray
           Denormalizes the predictions based on the normalization type.
           Args: preds_norm (np.ndarray): Normalized predictions to be denormalized. attributes (list): List of at-
           tributes corresponding to the predictions, normalization params (dict): Dictionary containing normalization
           parameters for each attribute.
               Returns
                   Denormalized predictions.
               Return type
                   np.ndarray
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 | List], ent_in: Dict, ent_out: Dict) → set
     Private method for achieve_answer logic. @TODO: Document the code
write_links(ent_out, small_ent_out)
ground_queries (query_structure: List[str | List], ent_in: Dict, ent_out: Dict, small_ent_in: Dict,
             small_ent_out: Dict, gen_num: int, query_name: str)
     Generating queries and achieving answers
unmap (query_type, queries, tp_answers, fp_answers, fn_answers)
unmap_query (query_structure, query, id2ent, id2rel)
generate_queries (query_struct: List, gen_num: int, query_type: str)
     Passing incoming and outgoing edges to ground queries depending on mode [train valid or text] and getting
     queries and answers in return @ TODO: create a class for each single query struct
save_queries (query_type: str, gen_num: int, save_path: str)
abstract load_queries(path)
get_queries (query_type: str, gen_num: int)
static save_queries_and_answers (path: str, data: List[Tuple[str, Tuple[collections.defaultdict]]])
              \rightarrow None
     Save Queries into Disk
```

```
\mbox{\bf static load\_queries\_and\_answers}\ (path:str) \ \rightarrow \mbox{List[Tuple[str, Tuple[collections.defaultdict]]]} \\ \mbox{Load Queries from Disk to Memory}
```

dicee.\_\_version\_\_ = '0.1.5'

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