# **DICE Embeddings**

Release 0.1.3.2

## **Caglar Demir**

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DICE Embeddings<sup>1</sup>: Hardware-agnostic Framework for Large-scale Knowledge Graph Embeddings:

### 1 Dicee Manual

**Version:** dicee 0.1.3.2

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

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

Contact: caglar.demir@upb.de

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

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

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

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

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

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

Why Hugging-face Gradio<sup>10</sup>? Deploy a pre-trained embedding model without writing a single line of code.

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

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

<sup>&</sup>lt;sup>3</sup> https://pandas.pydata.org/

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

<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 && \rightarrow 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
```

(continues on next page)

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

### where the data is in the following form

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

### A KGE model can also be trained from the command line

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

dicee automatically 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
dicee --dataset_dir "KGs/UMLS" --model Keci --eval_model "train_val_test"
# Evaluate Keci on Train set: Evaluate Keci on Train set
# {'H@1': 0.9518788343558282, 'H@3': 0.9988496932515337, 'H@10': 1.0, 'MRR': 0.
→9753123402351737}
# Evaluate Keci on Validation set: Evaluate Keci on Validation set
# {'H@1': 0.6932515337423313, 'H@3': 0.9041411042944786, 'H@10': 0.9754601226993865,
→ 'MRR': 0.8072362996241839}
# Evaluate Keci on Test set: Evaluate Keci on Test set
# {'H@1': 0.6951588502269289, 'H@3': 0.9039334341906202, 'H@10': 0.9750378214826021,
→ 'MRR': 0.8064032293278861}
# (2)
CUDA_VISIBLE_DEVICES=0,1 python dicee/scripts/run.py --trainer PL --dataset_dir "KGs/
→UMLS" --model Keci --eval_model "train_val_test"
# Evaluate Keci on Train set: Evaluate Keci on Train set
# {'H@1': 0.9518788343558282, 'H@3': 0.9988496932515337, 'H@10': 1.0, 'MRR': 0.
\hookrightarrow 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
# {'H01': 0.6951588502269289, 'H03': 0.9039334341906202, 'H010': 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

# {'H01': 0.9518788343558282, 'H03': 0.9988496932515337, 'H010': 1.0, 'MRR': 0.
→9753123402351737}

# Evaluate Keci on Validation set: Evaluate Keci on Validation set

# {'H01': 0.6932515337423313, 'H03': 0.9041411042944786, 'H010': 0.9754601226993865,
→'MRR': 0.8072499937521418}

# Evaluate Keci on Test set: Evaluate Keci on Test set

{'H01': 0.6951588502269289, 'H03': 0.9039334341906202, 'H010': 0.9750378214826021,
→'MRR': 0.8064032293278861}
```

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

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

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

where the data is in the following form

```
$ head -3 KGs/Family/train.txt
_:1 <a href="http://www.w3.org/1999/02/22-rdf-syntax-ns#type">http://www.w3.org/2002/07/owl</a>
_:1 <a href="http://www.w3.org/1999/02/22-rdf-syntax-ns#type">http://www.w3.org/1999/02/22-rdf-syntax-ns#type</a>
<a href="http://www.w3.org/2002/07/owl#0bjectProperty">http://www.w3.org/2002/07/owl#0bjectProperty</a>
<a href="http://www.benchmark.org/family#hasParent">http://www.w3.org/1999/02/22-rdf-syntax-ons#type</a> <a href="http://www.w3.org/2002/07/owl#0bjectProperty">http://www.w3.org/2002/07/owl#0bjectProperty</a>
<a href="http://www.w3.org/2002
```

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

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

For more, please refer to examples.

## 6 Creating an Embedding Vector Database

## 6.1 Learning Embeddings

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

### 6.2 Loading Embeddings into Qdrant Vector Database

### 6.3 Launching Webservice

```
diceeserve --path_model "CountryEmbeddings" --collection_name "dummy" --collection_

→location "localhost"
```

### **Retrieve and Search**

Get embedding of germany

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

Get most similar things to europe

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

## 7 Answering Complex Queries

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

(continues on next page)

```
pre_trained_kge = KGE(path=result['path_experiment_folder'])
# (3) Single-hop guery 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,
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/11

## 10 How to Deploy

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

### 11 Docker

To build the Docker image:

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

To test the Docker image:

```
docker run --rm -v ~/.local/share/dicee/KGs:/dicee/KGs dice-embeddings ./main.py --

--model AConEx --embedding_dim 16
```

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

## 12 Coverage Report

The coverage report is generated using coverage.py<sup>12</sup>:

```
Name
                                                                                                    Stmts
                                                                                                                   Miss Cover
                                                                                                                                             Missina
dicee/__init__.py
                                                                                                            7
                                                                                                                                100%
                                                                                                                         0
dicee/abstracts.py
                                                                                                        201
                                                                                                                       82
                                                                                                                                 59%
                                                                                                                                             104-105, _
→123, 146-147, 152, 165, 197, 240-254, 257-260, 263-266, 301, 314-317, 320-324, 364-

→375, 390-398, 413, 424-428, 555-575, 581-585, 589-591

dicee/callbacks.py
                                                                                                        245
                                                                                                                     102
                                                                                                                                  58%
                                                                                                                                             50-55, _
→67-73, 76, 88-93, 98-103, 106-109, 116-133, 138-142, 146-147, 276-280, 286-287, 305-
→311, 314, 319-320, 332-338, 344-353, 358-360, 405, 416-429, 433-468, 480-486
dicee/config.py
                                                                                                          93
                                                                                                                                  98%
                                                                                                                                             141-142
dicee/dataset_classes.py
                                                                                                        299
                                                                                                                       74
                                                                                                                                  75%
→87, 93, 99-106, 109, 112, 115-139, 195-201, 204, 207-209, 314, 325-328, 344, 410-
\Rightarrow411, 429, 528-536, 539, 543-557, 700-707, 710-714
                                                                                                        227
                                                                                                                       95
                                                                                                                                             101, 106,
dicee/eval_static_funcs.py
                                                                                                                                  58%
→ 111, 258-353, 360-411
dicee/evaluator.py
                                                                                                                       51
                                                                                                                                  81%
                                                                                                        262
                                                                                                                                             46. 51.
→56, 84, 89-90, 93, 109, 126, 137, 141, 146, 177-188, 195-206, 314, 344-367, 455, □
465, 482-487 482-487
dicee/executer.py
                                                                                                        113
                                                                                                                                  96%
                                                                                                                                             116, 258-
⇒259, 291
dicee/knowledge_graph.py
                                                                                                          65
                                                                                                                         3
                                                                                                                                  95%
                                                                                                                                             79, 110, _
\hookrightarrow 114
dicee/knowledge_graph_embeddings.py
                                                                                                         636
                                                                                                                     443
                                                                                                                                  30%
                                                                                                                                             27, 30-
→31, 39-52, 57-90, 93-127, 131-139, 170-184, 215-228, 254-274, 324-327, 330-333, 346,
→ 381-426, 484-486, 502-503, 509-517, 522-525, 528-533, 538, 547, 592-598, 630, 688-
→1053, 1084-1145, 1149-1177, 1200, 1227-1265
                                                                                                                         0
                                                                                                                                100%
dicee/models/__init__.py
dicee/models/base_model.py
                                                                                                        234
                                                                                                                       31
                                                                                                                                  87%
                                                                                                                                             54, 56, ...
→82, 88-103, 157, 190, 230, 236, 245, 248, 252, 259, 263, 265, 280, 288-289, 296-297,

→ 351, 354, 427, 439

dicee/models/clifford.py
                                                                                                         556
                                                                                                                     357
                                                                                                                                  36%
→68-117, 122-133, 156-168, 190-220, 235, 237, 241, 248-249, 276-280, 303-311, 325-
→327, 332-333, 364-384, 406, 413, 417-478, 495-499, 511, 514, 519, 524, 571-607, 625-
→631, 644, 647, 652, 657, 686-692, 705, 708, 713, 718, 728-737, 753-754, 774-845, □
→856-859, 884-909, 933-966, 1002-1006, 1019, 1029, 1032, 1037, 1042, 1047, 1051, □
→1055, 1064-1065, 1095, 1102, 1107, 1135-1139, 1167-1176, 1186-1194, 1212-1214, 1232-
→1234, 1250-1252
dicee/models/complex.py
                                                                                                         151
                                                                                                                                             86-109
dicee/models/dualE.py
                                                                                                          59
                                                                                                                       10
                                                                                                                                  83%
                                                                                                                                             93-102, _
→142-156
                                                                                                        262
                                                                                                                     221
                                                                                                                                  16%
dicee/models/function_space.py
                                                                                                                                             10-24, _
40-49, 53-70, 77-86, 89-98, 101-110, 114-126, 134-156, 159-165, 168-185, 188-185, 188-185, 188-185, 188-185, 188-185, 188-185, 188-185, 188-185, 188-185, 188-185, 188-185, 188-185, 188-185, 188-185, 188-185, 188-185, 188-185, 188-185, 188-185, 188-185, 188-185, 188-185, 188-185, 188-185, 188-185, 188-185, 188-185, 188-185, 188-185, 188-185, 188-185, 188-185, 188-185, 188-185, 188-185, 188-185, 188-185, 188-185, 188-185, 188-185, 188-185, 188-185, 188-185, 188-185, 188-185, 188-185, 188-185, 188-185, 188-185, 188-185, 188-185, 188-185, 188-185, 188-185, 188-185, 188-185, 188-185, 188-185, 188-185, 188-185, 188-185, 188-185, 188-185, 188-185, 188-185, 188-185, 188-185, 188-185, 188-185, 188-185, 188-185, 188-185, 188-185, 188-185, 188-185, 188-185, 188-185, 188-185, 188-185, 188-185, 188-185, 188-185, 188-185, 188-185, 188-185, 188-185, 188-185, 188-185, 188-185, 188-185, 188-185, 188-185, 188-185, 188-185, 188-185, 188-185, 188-185, 188-185, 188-185, 188-185, 188-185, 188-185, 188-185, 188-185, 188-185, 188-185, 188-185, 188-185, 188-185, 188-185, 188-185, 188-185, 188-185, 188-185, 188-185, 188-185, 188-185, 188-185, 188-185, 188-185, 188-185, 188-185, 188-185, 188-185, 188-185, 188-185, 188-185, 188-185, 188-185, 188-185, 188-185, 188-185, 188-185, 188-185, 188-185, 188-185, 188-185, 188-185, 188-185, 188-185, 188-185, 188-185, 188-185, 188-185, 188-185, 188-185, 188-185, 188-185, 188-185, 188-185, 188-185, 188-185, 188-185, 188-185, 188-185, 188-185, 188-185, 188-185, 188-185, 188-185, 188-185, 188-185, 188-185, 188-185, 188-185, 188-185, 188-185, 188-185, 188-185, 188-185, 188-185, 188-185, 188-185, 188-185, 188-185, 188-185, 188-185, 188-185, 188-185, 188-185, 188-185, 188-185, 188-185, 188-185, 188-185, 188-185, 188-185, 188-185, 188-185, 188-185, 188-185, 188-185, 188-185, 188-185, 188-185, 188-185, 188-185, 188-185, 188-185, 188-185, 188-185, 188-185, 188-185, 188-185, 188-185, 188-185, 188-185, 188-185, 188-185, 188-185, 188-185, 188-185, 188-185, 188-185, 188-185, 188-185, 188-185, 188-185, 188-185,
→194, 197-205, 208, 213-234, 243-246, 250-254, 258-267, 271-292, 301-307, 311-328, □
→332-335, 344-352, 355, 366-372, 392-406, 424-438, 443-453, 461-465, 474-478
                                                                                                                       83
dicee/models/octonion.py
                                                                                                        227
\Rightarrow320-329, 334-345, 348-370, 374-416, 426-474
dicee/models/pykeen_models.py
                                                                                                          50
                                                                                                                         5
                                                                                                                                  90%
                                                                                                                                             60-63, _
                                                                                                                                             7-21, 30-
dicee/models/quaternion.py
                                                                                                        192
                                                                                                                       69
                                                                                                                                  64%
⇒55, 68-72, 107, 185, 328-342, 345-364, 368-389, 399-426
dicee/models/real.py
                                                                                                                       12
                                                                                                                                             36-39, _
```

(continues on next page)

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

```
\leftrightarrow 66-69, 87, 103-106
dicee/models/static_funcs.py
                                                              10
                                                                            100%
dicee/models/transformers.py
                                                             236
                                                                     189
                                                                             20%
                                                                                   24-43,_
→46, 60-75, 84-102, 105-116, 123-125, 128, 134-151, 155-180, 186-190, 193-197, 203-
→207, 210-212, 229-256, 265-268, 271-276, 279-304, 310-315, 319-372, 376-398, 404-414
dicee/query_generator.py
                                                             374
                                                                     346
                                                                             7%
\hookrightarrow56, 62-65, 69-70, 78-92, 100-147, 155-188, 192-206, 212-269, 274-303, 307-443, 453-
\hookrightarrow472, 480-501, 508-512, 517, 522-528
dicee/read_preprocess_save_load_kg/__init__.py
                                                               3
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                                                                           100%
dicee/read_preprocess_save_load_kg/preprocess.py
                                                             256
                                                                      41
                                                                             84%
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\hookrightarrow78, 102-127, 133, 138-151, 184, 214, 388-389, 444
dicee/read_preprocess_save_load_kg/read_from_disk.py
                                                              36
                                                                      11
                                                                             69%
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\hookrightarrow40, 47, 55, 58-72
dicee/read_preprocess_save_load_kg/save_load_disk.py
                                                              45
                                                                      18
                                                                             60%
                                                                                   39-60
dicee/read_preprocess_save_load_kg/util.py
                                                             219
                                                                     126
                                                                             42%
                                                                                   65-67, _
→72-73, 91-97, 100-102, 107-109, 121, 134, 140-143, 148-156, 161-167, 172-177, 182-
→187, 199-220, 226-282, 286-290, 294-295, 299, 303-304, 334, 351, 356, 363-364
dicee/sanity_checkers.py
                                                              54
                                                                      23
                                                                            57%
                                                                                   8-12, 21-
⇒31, 46, 51, 58, 64-79, 85, 89, 96
dicee/static_funcs.py
                                                              418
                                                                     163
                                                                             61%
                                                                                   40, 50, ...
→56-61, 83, 105-106, 115, 138, 152, 157-159, 163-165, 167, 194-198, 246, 254, 263-
→268, 290-304, 316-336, 340-357, 362, 386-387, 392-393, 410-411, 413-414, 416-417, .
→419-420, 428, 446-450, 467-470, 474-479, 483-487, 491-492, 498-500, 526-527, 539-
\Rightarrow542, 547-550, 559-610, 615-627, 644-658, 661-669
dicee/static_funcs_training.py
                                                             123
                                                                      63
                                                                             49%
                                                                                   118-215, _
→223-224
dicee/static_preprocess_funcs.py
                                                              100
                                                                      44
                                                                             56%
                                                                                   17-25, _
\hookrightarrow 52, 56, 64, 67, 78, 91-115, 120-123, 128-131, 136-139
dicee/trainer/__init__.py
                                                               1
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                                                                           100%
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dicee/trainer/dice_trainer.py
                                                             126
                                                                      13
                                                                             90%
⇒91, 98, 103–108, 147
dicee/trainer/torch_trainer.py
                                                              79
                                                                             95%
                                                                                   31, 196, _
⇒207–208
dicee/trainer/torch_trainer_ddp.py
                                                             152
                                                                     128
                                                                             16%
                                                                                   13-14, _
\hookrightarrow43, 47-72, 83-112, 131-137, 140-149, 164-194, 204-217, 226-246, 251-260, 263-272,
⇒275-299, 302-309
TOTAL
                                                            6181
                                                                    2828
                                                                            54%
```

### 13 How to cite

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

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

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

(continues on next page)
```

```
# LitCOD
@inproceedings{demir2023litcqd,
 title={LitCQD: Multi-Hop Reasoning in Incomplete Knowledge Graphs with Numeric_
→Literals}.
 author={Demir, Caglar and Wiebesiek, Michel and Lu, Renzhong and Ngonga Ngomo, Axel-
→Cyrille and Heindorf, Stefan},
 booktitle={Joint European Conference on Machine Learning and Knowledge Discovery in_
→Databases},
 pages={617--633},
 year={2023},
  organization={Springer}
# DICE Embedding Framework
@article{demir2022hardware,
  title={Hardware-agnostic computation for large-scale knowledge graph embeddings},
  author={Demir, Caglar and Ngomo, Axel-Cyrille Ngonga},
  journal={Software Impacts},
  year={2022},
  publisher={Elsevier}
# KronE
@inproceedings{demir2022kronecker,
 title={Kronecker decomposition for knowledge graph embeddings},
  author={Demir, Caglar and Lienen, Julian and Ngonga Ngomo, Axel-Cyrille},
 booktitle={Proceedings of the 33rd ACM Conference on Hypertext and Social Media},
 pages=\{1--10\},
 year={2022}
# QMult, OMult, ConvQ, ConvO
@InProceedings{pmlr-v157-demir21a,
                   {Convolutional Hypercomplex Embeddings for Link Prediction},
 title =
                 {Demir, Caglar and Moussallem, Diego and Heindorf, Stefan and Ngonga-
→Ngomo, Axel-Cyrille},
                       {Proceedings of The 13th Asian Conference on Machine Learning},
  booktitle =
 pages =
                   {656--671},
                  {2021},
  year =
  editor =
                    {Balasubramanian, Vineeth N. and Tsang, Ivor},
  volume =
                    {157},
  series =
                    {Proceedings of Machine Learning Research},
                  \{17--19 \text{ Nov}\},
 month =
  publisher =
                 {PMLR},
                 {https://proceedings.mlr.press/v157/demir21a/demir21a.pdf},
 pdf =
 url =
                 {https://proceedings.mlr.press/v157/demir21a.html},
# ConEx
@inproceedings{demir2021convolutional,
title={Convolutional Complex Knowledge Graph Embeddings},
author={Caglar Demir and Axel-Cyrille Ngonga Ngomo},
booktitle={Eighteenth Extended Semantic Web Conference - Research Track},
year={2021},
url={https://openreview.net/forum?id=6T45-4TFqaX}}
# Shallom
@inproceedings{demir2021shallow,
 title={A shallow neural model for relation prediction},
  author={Demir, Caglar and Moussallem, Diego and Ngomo, Axel-Cyrille Ngonga},
  booktitle={2021 IEEE 15th International Conference on Semantic Computing (ICSC)},
                                                                          (continues on next page)
```

```
pages={179--182},
year={2021},
organization={IEEE}
```

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

### 14 dicee

### 14.1 Subpackages

dicee.models

**Submodules** 

dicee.models.base\_model

### **Classes**

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

### **Module Contents**

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

Bases: lightning.LightningModule

Base class for all neural network modules.

Your models should also subclass this class.

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

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

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

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

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

### **1** Note

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

### **Variables**

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

```
\label{eq:training_step_outputs} \textbf{training_step_outputs} \ = \ [] \label{eq:mem_of_model} \textbf{mem_of_model} \ () \ \to \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
```

(continues on next page)

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

### **1** Note

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

loss\_function(yhat\_batch: torch.FloatTensor, y\_batch: torch.FloatTensor)

### **Parameters**

- yhat\_batch
- y\_batch

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

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

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

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

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

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

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

```
\texttt{test\_dataloader}\,(\,)\,\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()

### 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.

### $\textbf{val\_dataloader} \; (\;) \; \to None$

An iterable or collection of iterables specifying validation samples.

For more information about multiple dataloaders, see this section.

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

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

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

### 1 Note

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

### 1 Note

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

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

An iterable or collection of iterables specifying prediction samples.

For more information about multiple dataloaders, see this section.

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

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

### 1 Note

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

### Returns

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

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

An iterable or collection of iterables specifying training samples.

For more information about multiple dataloaders, see this section.

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

For data processing use the following pattern:

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

However, the above are only necessary for distributed processing.

### **Marning**

do not assign state in prepare\_data

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

### 1 Note

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

### configure\_optimizers (parameters=None)

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

### Returns

Any of these 6 options.

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

The lr\_scheduler\_config is a dictionary which contains the scheduler and its associated configuration. The default configuration is shown below.

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

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

Metrics can be made available to monitor by simply logging it using self.log('metric\_to\_track', metric\_val) in your LightningModule.

### **1** Note

Some things to know:

- Lightning calls .backward() and .step() automatically in case of automatic optimization.
- If a learning rate scheduler is specified in configure\_optimizers() with key "interval" (default "epoch") in the scheduler configuration, Lightning will call the scheduler's . step() method automatically in case of automatic optimization.
- If you use 16-bit precision (precision=16), Lightning will automatically handle the optimizer.

- If you use torch.optim.LBFGS, Lightning handles the closure function automatically for you.
- If you use multiple optimizers, you will have to switch to 'manual optimization' mode and step them yourself.
- If you need to control how often the optimizer steps, override the optimizer\_step() hook.

class dicee.models.base\_model.BaseKGE (args: dict)

Bases: BaseKGELightning

Base class for all neural network modules.

Your models should also subclass this class.

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

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

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

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

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

### 1 Note

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

### **Variables**

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

### args

```
embedding_dim = None
num_entities = None
num_relations = None
num_tokens = None
learning_rate = None
apply_unit_norm = None
input_dropout_rate = None
```

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

```
· ordered_bpe_entities
     forward_triples (x: torch.LongTensor) \rightarrow torch.Tensor
             Parameters
     forward_k_vs_all(*args, **kwargs)
     forward_k_vs_sample(*args, **kwargs)
     get_triple_representation(idx_hrt)
     get_head_relation_representation(indexed_triple)
     get_sentence_representation (x: torch.LongTensor)
             Parameters
                 • (b(x shape)
                 • 3
                 • t)
     get_bpe_head_and_relation_representation (x: torch.LongTensor)
                → Tuple[torch.FloatTensor, torch.FloatTensor]
             Parameters
                x(B x 2 x T)
     get_embeddings() → Tuple[numpy.ndarray, numpy.ndarray]
class dicee.models.base_model.IdentityClass(args=None)
     Bases: torch.nn.Module
     Base class for all neural network modules.
```

Your models should also subclass this class.

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

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

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

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

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

### 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
__call__(x)
static forward(x)
```

### dicee.models.clifford

### **Classes**

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

### **Module Contents**

```
class dicee.models.clifford.CMult(args)
      Bases: dicee.models.base model.BaseKGE
      Cl_{(0,0)} => Real Numbers
      Cl_{-}(0,1) =>
             A multivector mathbf\{a\} = a_0 + a_1 e_1 A multivector mathbf\{b\} = b_0 + b_1 e_1
             multiplication is isomorphic to the product of two complex numbers
             mathbf{a} imes mathbf{b} = a_0 b_0 + a_0 b_1 e_1 + a_1 b_1 e_1 e_1
                  = (a_0 b_0 - a_1 b_1) + (a_0 b_1 + a_1 b_0) e_1
      Cl_{-}(2,0) =>
             A multivector mathbf\{a\} = a_0 + a_1 e_1 + a_2 e_2 + a_{12} e_1 e_2 A multivector mathbf\{b\} = b_0 + a_1 e_1 + a_2 e_2 + a_{12} e_1 e_2 A multivector mathbf\{b\} = b_0 + a_1 e_1 + a_2 e_2 + a_{12} e_1 e_2 A multivector mathbf\{b\} = b_0 e_1 + a_1 e_2 e_2 + a_2 e_3 e_4 A
             b_1 e_1 + b_2 e_2 + b_{12} e_1 e_2
             mathbf{a} imes mathbf{b} = a_0b_0 + a_0b_1 e_1 + a_0b_2 e_2 + a_0 b_1 e_1 e_2
                    • a_1 b_0 e_1 + a_1b_1 e_1_e1 ...
      C1 (0,2) \Rightarrow Quaternions
      name = 'CMult'
      entity_embeddings
      relation_embeddings
```

```
р
q
clifford_mul(x: torch.FloatTensor, y: torch.FloatTensor, p: int, q: int) \rightarrow tuple
          Clifford multiplication Cl_{p,q} (mathbb\{R\})
          ei ^2 = +1 for i =< i =< p ej ^2 = -1 for p < j =< p+q ei ej = -eje1 for i
     eq j
          x: torch.FloatTensor with (n,d) shape
          y: torch.FloatTensor with (n,d) shape
          p: a non-negative integer p \ge 0 q: a non-negative integer q \ge 0
score (head_ent_emb, rel_ent_emb, tail_ent_emb)
forward\_triples (x: torch.LongTensor) \rightarrow torch.FloatTensor
      Compute batch triple scores
      Parameter
```

```
x: torch.LongTensor with shape n by 3
```

rtype

torch.LongTensor with shape n

**forward\_k\_vs\_all** (x: torch.Tensor)  $\rightarrow$  torch.FloatTensor

Compute batch KvsAll triple scores

### **Parameter**

x: torch.LongTensor with shape n by 3

### rtvpe

torch.LongTensor with shape n

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

Bases: dicee.models.base model.BaseKGE

Base class for all neural network modules.

Your models should also subclass this class.

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

```
import torch.nn as nn
import torch.nn.functional as F
class Model (nn.Module):
    def __init__(self):
        super().__init__()
        self.conv1 = nn.Conv2d(1, 20, 5)
        self.conv2 = nn.Conv2d(20, 20, 5)
```

(continues on next page)

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

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

### 1 Note

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

### **Variables**

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

```
name = '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} = sather actions between along p bases For instance, let p e_1, e_2, e_3, we compute interactions between e_1 e_2, e_1 e_3, and e_2 e_3 This can be implemented with a nested two for loops
   results = [] for i in range(p - 1):
        for k in range(i + 1, p):
            results.append(hp[:, :, i] * rp[:, :, k] * rp[:, :, i])
        sigma_pp = torch.stack(results, dim=2) assert sigma_pp.shape == (b, r, int((p * (p - 1)) / 2))
```

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

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

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

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

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

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

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

results.append(hq[:, :, j] * rq[:, :, k] - hq[:, :, k] * rq[:, :, j])
```

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

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

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

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

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

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

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

### for j in range(q):

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

print(sigma\_pq.shape)

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

Multiplying a base vector with its scalar coefficient

### clifford\_multiplication (h0, hp, hq, r0, rp, rq)

Compute our CL multiplication

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

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

eq j

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

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

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

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

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

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

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

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

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

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

### **Parameter**

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

### returns

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

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

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

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

Kvsall training

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

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

 $\verb|forward_k_vs_sample|| (x: torch.LongTensor, target\_entity\_idx: torch.LongTensor)|$ 

 $\rightarrow$  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

### **Parameter**

### **Parameter**

Without learning dimension scaling

```
name = 'KeciBase'
requires_grad_for_interactions = False
class dicee.models.clifford.DeCaL(args)
```

Bases: dicee.models.base\_model.BaseKGE

Base class for all neural network modules.

Your models should also subclass this class.

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

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

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

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

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

### 1 Note

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

### **Variables**

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

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

### **Parameter**

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

### rtype

torch.FloatTensor with (n) shape

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

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

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

### compute\_sigmas\_single(list\_h\_emb, list\_r\_emb, list\_t\_emb)

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

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

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

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

### $forward_k\_vs\_all (x: torch.Tensor) \rightarrow torch.FloatTensor$

Kvsall training

- (1) Retrieve real-valued embedding vectors for heads and relations
- (2) Construct head entity and relation embeddings according to Cl\_{p,q, r}(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)

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

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):

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

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 i in range(q - 1):

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

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

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

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

compute\_sigma\_rr(hk, rk)

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

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

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)

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

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

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

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

print(sigma_pq.shape)

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

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

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

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

print(sigma_pq.shape)
```

### dicee.models.complex

### **Classes**

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

### **Module Contents**

```
class dicee.models.complex.ConEx (args)
    Bases: dicee.models.base_model.BaseKGE
    Convolutional ComplEx Knowledge Graph Embeddings
    name = 'ConEx'
    conv2d
    fc_num_input
    fc1
    norm_fc1
```

```
bn_conv2d
     feature_map_dropout
     residual_convolution (C_1: Tuple[torch.Tensor, torch.Tensor],
                  C_2: Tuple[torch.Tensor, torch.Tensor]) \rightarrow torch.FloatTensor
          Compute residual score of two complex-valued embeddings. :param C_1: a tuple of two pytorch tensors
          that corresponds complex-valued embeddings :param C_2: a tuple of two pytorch tensors that corresponds
          complex-valued embeddings :return:
     forward_k_vs_all(x: torch.Tensor) \rightarrow torch.FloatTensor
     forward\_triples (x: torch.Tensor) \rightarrow torch.FloatTensor
              Parameters
                  x
     forward_k_vs_sample (x: torch.Tensor, target_entity_idx: torch.Tensor)
class dicee.models.complex.AConEx (args)
     Bases: dicee.models.base model.BaseKGE
     Additive Convolutional ComplEx Knowledge Graph Embeddings
     name = 'AConEx'
     conv2d
     fc_num_input
     fc1
     norm fc1
     bn_conv2d
     feature_map_dropout
     residual_convolution (C_1: Tuple[torch.Tensor, torch.Tensor],
                  C_2: Tuple[torch.Tensor, torch.Tensor]) \rightarrow torch.FloatTensor
          Compute residual score of two complex-valued embeddings. :param C_1: a tuple of two pytorch tensors
          that corresponds complex-valued embeddings :param C_2: a tuple of two pytorch tensors that corresponds
          complex-valued embeddings :return:
     forward_k_vs_all(x: torch.Tensor) \rightarrow torch.FloatTensor
     forward_triples (x: torch.Tensor) \rightarrow torch.FloatTensor
              Parameters
                  ¥
     forward_k_vs_sample (x: torch.Tensor, target_entity_idx: torch.Tensor)
class dicee.models.complex.ComplEx (args)
     Bases: dicee.models.base model.BaseKGE
     Base class for all neural network modules.
```

Your models should also subclass this class.

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

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

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

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

Submodules assigned in this way will be registered, and will have their parameters converted too when you call  $t \circ ()$ , 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.

### **Parameters**

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

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

### dicee.models.dualE

### **Classes**

DualE	Dual	Quaternion	Knowledge	Graph	Embeddings
	(https:	://ojs.aaai.org/	/index.php/A/	AAI/artic	le/download/
	16850	)/16657)			

### **Module Contents**

```
class dicee.models.dualE.DualE(args)
      Bases: dicee.models.base_model.BaseKGE
      Dual Quaternion Knowledge Graph Embeddings (https://ojs.aaai.org/index.php/AAAI/article/download/16850/
      16657)
      name = 'DualE'
      entity_embeddings
      relation_embeddings
      num_ent
      kvsall_score (e_1_h, e_2_h, e_3_h, e_4_h, e_5_h, e_6_h, e_7_h, e_8_h, e_1_t, e_2_t, e_3_t, e_4_t,
                   e_5_t, e_6_t, e_7_t, e_8_t, r_1, r_2, r_3, r_4, r_5, r_6, r_7, r_8) \rightarrow \text{torch.tensor}
           KvsAll scoring function
           Input
           x: torch.LongTensor with (n, ) shape
           Output
           torch.FloatTensor with (n) shape
      \textbf{forward\_triples} \ (\textit{idx\_triple: torch.tensor}) \ \rightarrow \textbf{torch.tensor}) \ \rightarrow \textbf{torch.tensor}
           Negative Sampling forward pass:
           Input
           x: torch.LongTensor with (n, ) shape
           Output
           torch.FloatTensor with (n) shape
      forward_k_vs_all(x)
           KvsAll forward pass
```

### Input

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

### **Output**

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

### dicee.models.function\_space

### **Classes**

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

### **Module Contents**

```
class dicee.models.function_space.FMult (args)
    Bases: dicee.models.base_model.BaseKGE

    Learning Knowledge Neural Graphs
    name = 'FMult'
    entity_embeddings
    relation_embeddings
    k
    num_sample = 50
    gamma
    roots
    weights
    compute_func (weights: torch.FloatTensor, x) → torch.FloatTensor
    chain_func (weights, x: torch.FloatTensor)
```

```
forward\_triples(idx\_triple: torch.Tensor) \rightarrow torch.Tensor
             Parameters
class dicee.models.function_space.GFMult(args)
     Bases: dicee.models.base model.BaseKGE
     Learning Knowledge Neural Graphs
     name = 'GFMult'
     entity_embeddings
     relation_embeddings
     k
     num_sample = 250
     roots
     weights
     compute_func (weights: torch.FloatTensor, x) \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_{\text{layers}} = 3
     tuned_embedding_dim = False
     k
     n = 50
     score_func = 'compositional'
     discrete_points
     entity_embeddings
     relation_embeddings
    build_func(Vec)
    build_chain_funcs (list_Vec)
     compute\_func(W, b, x) \rightarrow torch.FloatTensor
```

```
function (list_W, list_b)
     trapezoid (list_W, list_b)
     forward_triples (idx\_triple: torch.Tensor) \rightarrow torch.Tensor
              Parameters
                  x
class dicee.models.function space.LFMult1(args)
     Bases: dicee.models.base_model.BaseKGE
     Embedding with trigonometric functions. We represent all entities and relations in the complex number space as:
     f(x) = sum_{k=0}^{k=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)
     vtp\_score(h, r, t)
class dicee.models.function_space.LFMult(args)
     Bases: dicee.models.base_model.BaseKGE
     Embedding with polynomial functions. We represent all entities and relations in the polynomial space as: f(x) =
     sum_{i=0}^{d-1} a_k x^{i\%d} and use the three differents scoring function as in the paper to evaluate the score.
     We also consider combining with Neural Networks.
     name = 'LFMult'
     entity_embeddings
     relation_embeddings
     degree
     m
     x_values
     forward_triples (idx_triple)
              Parameters
                  x
     construct_multi_coeff(x)
     poly_NN (x, coefh, coefr, coeft)
          Constructing a 2 layers NN to represent the embeddings. h = sigma(wh^T x + bh), r = sigma(wr^T x + br),
          t = sigma(wt^T x + bt)
```

```
linear (x, w, b)
```

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

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

```
tri_score (coeff_h, coeff_r, coeff_t)
```

this part implement the trilinear scoring techniques:

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

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

### $vtp\_score(h, r, t)$

this part implement the vector triple product scoring techniques:

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

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

### $comp_func(h, r, t)$

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

### polynomial (coeff, x, degree)

This function takes a matrix tensor of coefficients (coeff), a tensor vector of points x and range of integer [0,1,...d] and return a vector tensor (coeff $[0][0] + \text{coeff}[0][1]x + ... + \text{coeff}[0][d]x^d$ ,

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

```
pop(coeff, x, degree)
```

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

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

### dicee.models.octonion

### **Classes**

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

# **Functions**

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

### **Module Contents**

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

Base class for all neural network modules.

Your models should also subclass this class.

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

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

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

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

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

# **1** Note

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

# Variables

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

```
k_vs_all_score (bpe_head_ent_emb, bpe_rel_ent_emb, E)
```

```
forward_k_vs_all(x)
```

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

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

```
Bases: dicee.models.base model.BaseKGE
```

Base class for all neural network modules.

Your models should also subclass this class.

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

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

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

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

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

### 1 Note

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

# Variables

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

```
name = 'ConvO'
conv2d
fc_num_input
fc1
bn_conv2d
norm_fc1
feature_map_dropout
```

```
static octonion normalizer (emb_rel_e0, emb_rel_e1, emb_rel_e2, emb_rel_e3, emb_rel_e4,
                  emb_rel_e5, emb_rel_e6, emb_rel_e7)
     {\tt residual\_convolution}\,(O\_1,\,O\_2)
     forward_triples (x: torch.Tensor) \rightarrow torch.Tensor
               Parameters
                   x
     forward_k_vs_all (x: torch.Tensor)
           Given a head entity and a relation (h,r), we compute scores for all entities. [score(h,r,x)|x in Entities] =>
           [0.0,0.1,...,0.8], shape=> (1, |Entities|) Given a batch of head entities and relations => shape (size of batch,|
           Entities l)
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)
     {\tt 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)
dicee.models.pykeen_models
Classes
```

# PvkeenKGE

A class for using knowledge graph embedding models implemented in Pykeen

### **Module Contents**

```
class dicee.models.pykeen_models.PykeenKGE (args: dict)
     Bases: dicee.models.base_model.BaseKGE
     A class for using knowledge graph embedding models implemented in Pykeen
     Notes: Pykeen_DistMult: C Pykeen_ComplEx: Pykeen_QuatE: Pykeen_MuRE: Pykeen_CP: Pykeen_HolE: Py-
     keen HolE:
     model_kwargs
     name
     model
     loss history = []
     args
     entity_embeddings = None
     relation_embeddings = None
     forward_k_vs_all (x: torch.LongTensor)
           # => Explicit version by this we can apply bn and dropout
           # (1) Retrieve embeddings of heads and relations + apply Dropout & Normalization if given. h, r =
           self.get_head_relation_representation(x) \# (2) Reshape (1). if self.last_dim > 0:
               h = h.reshape(len(x), self.embedding\_dim, self.last\_dim) r = r.reshape(len(x), self.embedding\_dim,
               self.last dim)
           \# (3) Reshape all entities. if self.last_dim > 0:
               t = self.entity_embeddings.weight.reshape(self.num_entities, self.embedding_dim, self.last_dim)
           else:
               t = self.entity\_embeddings.weight
           # (4) Call the score_t from interactions to generate triple scores. return self.interaction.score_t(h=h, r=r,
           all_entities=t, slice_size=1)
     forward\_triples(x: torch.LongTensor) \rightarrow torch.FloatTensor
           # => Explicit version by this we can apply bn and dropout
           # (1) Retrieve embeddings of heads, relations and tails and apply Dropout & Normalization if given. h, r, t =
           self.get_triple_representation(x) \# (2) Reshape (1). if self.last_dim > 0:
               h = h.reshape(len(x), self.embedding dim, self.last dim) r = r.reshape(len(x), self.embedding dim,
               self.last_dim) t = t.reshape(len(x), self.embedding_dim, self.last_dim)
           # (3) Compute the triple score return self.interaction.score(h=h, r=r, t=t, slice_size=None, slice_dim=0)
     abstract forward_k_vs_sample (x: torch.LongTensor, target_entity_idx)
```

# dicee.models.quaternion

### **Classes**

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

### **Functions**

```
quaternion_mul_with_unit_norm(*, Q_1,
Q_2)
```

### **Module Contents**

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

class dicee.models.quaternion.QMult(args)

Bases: dicee.models.base model.BaseKGE

Base class for all neural network modules.

Your models should also subclass this class.

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

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

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

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

Submodules assigned in this way will be registered, and will have their parameters converted too when you call  $t \circ ()$ , 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**  $(b \circ o \circ 1)$  – 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*) → torch.FloatTensor

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

Absolute value of a quaternion

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

L2 norm of quaternion vector:

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

### **Parameters**

 $\mathbf{x}$  – The vector.

### Returns

The normalized vector.

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

# **Parameters**

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

forward\_k\_vs\_all(x)

# **Parameters**

x

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

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

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

```
\textbf{forward\_triples} \ (\textit{indexed\_triple: torch.Tensor}) \ \rightarrow \textbf{torch.Tensor}
```

### **Parameters**

x

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

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

#### dicee.models.real

### **Classes**

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

### **Module Contents**

1cecc7a77928ca8133fa24680a88d2f9-Paper.pdf

name = 'TransE'

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

```
margin = 4
      score (head_ent_emb, rel_ent_emb, tail_ent_emb)
      \textbf{forward\_k\_vs\_all} \ (\textit{x: torch.Tensor}) \ \rightarrow \text{torch.FloatTensor}
class dicee.models.real.Shallom(args)
      Bases: dicee.models.base_model.BaseKGE
      A shallow neural model for relation prediction (https://arxiv.org/abs/2101.09090)
      name = 'Shallom'
      shallom_width
      shallom
      \mathtt{get\_embeddings}() \rightarrow \mathsf{Tuple}[\mathsf{numpy}.\mathsf{ndarray}, \mathsf{None}]
      forward_k_vs_all (x) \rightarrow \text{torch.FloatTensor}
      forward_triples (x) \rightarrow \text{torch.FloatTensor}
               Parameters
               Returns
class dicee.models.real.Pyke(args)
      Bases: dicee.models.base_model.BaseKGE
      A Physical Embedding Model for Knowledge Graphs
      name = 'Pyke'
      dist_func
     margin = 1.0
      forward_triples (x: torch.LongTensor)
               Parameters
```

# dicee.models.static\_funcs

# **Functions**

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

### **Module Contents**

```
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

### **Classes**

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

### **Module Contents**

```
class dicee.models.transformers.BytE(*args, **kwargs)
Bases: dicee.models.base_model.BaseKGE
```

Base class for all neural network modules.

Your models should also subclass this class.

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

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

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

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

Submodules assigned in this way will be registered, and will have their parameters converted too when you call  $t \circ ()$ , 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.

```
name = 'BytE'
```

config

temperature = 0.5

topk = 2

transformer

lm\_head

weight

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

### **Parameters**

- yhat\_batch
- y\_batch

forward (x: torch.LongTensor)

### **Parameters**

 $\mathbf{x}$  (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 to nest them in a tree structure. You can assign the submodules as regular attributes:

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

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```

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

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

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

# 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.

```
c_attn
c_proj
attn_dropout
resid_dropout
n_head
n_embd
dropout
flash
forward(x)

class dicee.models.transformers.MLP(config)
Bases: torch.nn.Module
```

Base class for all neural network modules.

Your models should also subclass this class.

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

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

class Model(nn.Module):
    def __init__(self):
        super().__init__()
```

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```
self.conv1 = nn.Conv2d(1, 20, 5)
self.conv2 = nn.Conv2d(20, 20, 5)

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

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

# **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 to nest them in a tree structure. You can assign the submodules as regular attributes:

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

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

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

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

### 1 Note

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

### Variables

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

```
ln_1
  attn
  ln_2
  mlp
  forward(x)

class dicee.models.transformers.GPTConfig
  block_size: int = 1024
  vocab_size: int = 50304
  n_layer: int = 12
  n_head: int = 12
  n_embd: int = 768
  dropout: float = 0.0
  bias: bool = False

class dicee.models.transformers.GPT(config)
  Bases: torch.nn.Module
```

Base class for all neural network modules.

Your models should also subclass this class.

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

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

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

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

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



### 1 Note

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

### **Variables**

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

### config

transformer

lm\_head

weight

get\_num\_params (non\_embedding=True)

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

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

crop\_block\_size (block\_size)

classmethod from\_pretrained(model\_type, override\_args=None)

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

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

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

### **Classes**

BaseKGELightning	Base class for all neural network modules.
BaseKGE	Base class for all neural network modules.
IdentityClass	Base class for all neural network modules.
BaseKGE	Base class for all neural network modules.
DistMult	Embedding Entities and Relations for Learning and 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.

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Table 1 - continued from previous page

Table 1 Continues	a nom previous page
BaseKGE	Base class for all neural network modules.
IdentityClass	Base class for all neural network modules.
QMult	Base class for all neural network modules.
ConvQ	Convolutional Quaternion Knowledge Graph 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.
Conv0	Base class for all neural network modules.
AConv0	Additive Convolutional Octonion Knowledge Graph Em-
	beddings
Keci	Base class for all neural network modules.
KeciBase	Without learning dimension scaling
CMult	$Cl_{0,0} = Real Numbers$
DeCaL	Base class for all neural network modules.
BaseKGE	Base class for all neural network modules.
PykeenKGE	A class for using knowledge graph embedding models 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**

quaternion_mul(→ torch.Tensor,)	Tuple[torch.T	ensor,	Perform quaternion multiplication
<pre>quaternion_mul_with_uni Q_2)</pre>	t_norm(*,	Q_1,	
octonion_mul(*, O_1, O_2)			
octonion_mul_norm(*, O_1,	O_2)		

# **Package Contents**

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

Bases: lightning.LightningModule

Base class for all neural network modules.

Your models should also subclass this class.

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

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

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

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

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

# 1 Note

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

#### Variables

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

```
\begin{tabular}{ll} training\_step\_outputs = [] \\ mem\_of\_model() \rightarrow Dict \\ \end{tabular}
```

Size of model in MB and number of params

training\_step (batch, batch\_idx=None)

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

### **Parameters**

- batch The output of your data iterable, normally a DataLoader.
- batch\_idx The index of this batch.
- dataloader\_idx The index of the dataloader that produced this batch. (only if multiple dataloaders used)

### Returns

- Tensor The loss tensor
- dict A dictionary which can include any keys, but must include the key 'loss' in the case of automatic optimization.

• None - In automatic optimization, this will skip to the next batch (but is not supported for multi-GPU, TPU, or DeepSpeed). For manual optimization, this has no special meaning, as returning the loss is not required.

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

Example:

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

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

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

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

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

### 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 = []
```

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```
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])

# $\textbf{test\_dataloader} \; () \; \rightarrow None$

An iterable or collection of iterables specifying test samples.

For more information about multiple dataloaders, see this section.

For data processing use the following pattern:

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

However, the above are only necessary for distributed processing.

# **A** Warning

do not assign state in prepare\_data

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

# 1 Note

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

### **1** Note

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

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

An iterable or collection of iterables specifying validation samples.

For more information about multiple dataloaders, see this section.

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

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

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

# **1** Note

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

# **1** Note

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

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

An iterable or collection of iterables specifying prediction samples.

For more information about multiple dataloaders, see this section.

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

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

# 1 Note

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

### Returns

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

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

An iterable or collection of iterables specifying training samples.

For more information about multiple dataloaders, see this section.

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

For data processing use the following pattern:

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

However, the above are only necessary for distributed processing.



## **Marning**

do not assign state in prepare\_data

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



### 1 Note

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

### configure\_optimizers (parameters=None)

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

#### Returns

Any of these 6 options.

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

The lr\_scheduler\_config is a dictionary which contains the scheduler and its associated configuration. The default configuration is shown below.

```
lr_scheduler_config = {
    # REQUIRED: The scheduler instance
   "scheduler": lr_scheduler,
   # The unit of the scheduler's step size, could also be 'step'.
    # 'epoch' updates the scheduler on epoch end whereas 'step'
    # updates it after a optimizer update.
   "interval": "epoch",
    # How many epochs/steps should pass between calls to
    # `scheduler.step()`. 1 corresponds to updating the learning
    # rate after every epoch/step.
    "frequency": 1,
    # Metric to to monitor for schedulers like `ReduceLROnPlateau`
    "monitor": "val_loss",
    # If set to `True`, will enforce that the value specified 'monitor'
    # is available when the scheduler is updated, thus stopping
    # training if not found. If set to `False`, it will only produce a warning
```

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```
"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 . step() method automatically in case of automatic optimization.
- If you use 16-bit precision (precision=16), Lightning will automatically handle the optimizer.
- If you use torch.optim.LBFGS, Lightning handles the closure function automatically for you.
- If you use multiple optimizers, you will have to switch to 'manual optimization' mode and step them yourself.
- If you need to control how often the optimizer steps, override the optimizer\_step() hook.

class dicee.models.BaseKGE (args: dict)

Bases: BaseKGELightning

Base class for all neural network modules.

Your models should also subclass this class.

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

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

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

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

Submodules assigned in this way will be registered, and will have their parameters converted too when you call

to(), etc.

# **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
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
            \mathbf{x} (B \times 2 \times T)
forward_byte_pair_encoded_triple (x: Tuple[torch.LongTensor, torch.LongTensor])
    byte pair encoded neural link predictors
        Parameters
init_params_with_sanity_checking()
forward (x: torch.LongTensor | Tuple[torch.LongTensor, torch.LongTensor],
           y_idx: torch.LongTensor = None
        Parameters
            • x
            • y_idx
            • ordered_bpe_entities
forward_triples (x: torch.LongTensor) \rightarrow torch.Tensor
        Parameters
forward_k_vs_all (*args, **kwargs)
forward_k_vs_sample(*args, **kwargs)
get_triple_representation (idx_hrt)
get_head_relation_representation (indexed_triple)
get_sentence_representation (x: torch.LongTensor)
        Parameters
            • (b(x shape)
            • 3
            • t)
get_bpe_head_and_relation_representation (x: torch.LongTensor)
            → Tuple[torch.FloatTensor, torch.FloatTensor]
        Parameters
            x(B x 2 x T)
```

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

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

Bases: torch.nn.Module

Base class for all neural network modules.

Your models should also subclass this class.

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

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

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

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

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

### 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

```
__call__(x)
static forward(x)
```

class dicee.models.BaseKGE (args: dict)

Bases: BaseKGELightning

Base class for all neural network modules.

Your models should also subclass this class.

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

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

class Model(nn.Module):
    def __init__(self):
        super().__init__()
```

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```
self.conv1 = nn.Conv2d(1, 20, 5)
self.conv2 = nn.Conv2d(20, 20, 5)

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

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

# 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
                  \mathbf{x} (B \times 2 \times T)
     \texttt{get\_embeddings}() \rightarrow Tuple[numpy.ndarray, numpy.ndarray]
class dicee.models.DistMult (args)
     Bases: dicee.models.base model.BaseKGE
     Embedding Entities and Relations for Learning and Inference in Knowledge Bases https://arxiv.org/abs/1412.6575
     name = 'DistMult'
     k_vs_all_score (emb_h: torch.FloatTensor, emb_r: torch.FloatTensor, emb_E: torch.FloatTensor)
              Parameters
                  emb_h
                  • emb_r
                  • emb E
     forward_k_vs_all (x: torch.LongTensor)
     forward_k_vs_sample (x: torch.LongTensor, target_entity_idx: torch.LongTensor)
     score(h, r, t)
class dicee.models.TransE(args)
     Bases: dicee.models.base_model.BaseKGE
     Translating Embeddings for Modeling Multi-relational Data https://proceedings.neurips.cc/paper/2013/file/
     1cecc7a77928ca8133fa24680a88d2f9-Paper.pdf
     name = 'TransE'
     margin = 4
     score (head_ent_emb, rel_ent_emb, tail_ent_emb)
     forward_k_vs_all(x: torch.Tensor) \rightarrow torch.FloatTensor
class dicee.models.Shallom(args)
     Bases: dicee.models.base model.BaseKGE
     A shallow neural model for relation prediction (https://arxiv.org/abs/2101.09090)
     name = 'Shallom'
     shallom_width
     shallom
     get_embeddings() → Tuple[numpy.ndarray, None]
     forward_k_vs_all (x) \rightarrow \text{torch.FloatTensor}
```

Base class for all neural network modules.

Your models should also subclass this class.

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

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

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

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

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

### 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
          \mathbf{x} (B \times 2 \times 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)
     \texttt{get\_embeddings} \ () \ \to Tuple[numpy.ndarray, numpy.ndarray]
class dicee.models.ConEx (args)
     Bases: dicee.models.base_model.BaseKGE
     Convolutional ComplEx Knowledge Graph Embeddings
     name = 'ConEx'
     conv2d
     fc_num_input
     fc1
```

```
norm_fc1
     bn_conv2d
     feature_map_dropout
     residual_convolution (C_1: Tuple[torch.Tensor, torch.Tensor],
                  C_2: Tuple[torch.Tensor, torch.Tensor]) \rightarrow torch.FloatTensor
           Compute residual score of two complex-valued embeddings. :param C_1: a tuple of two pytorch tensors
           that corresponds complex-valued embeddings :param C_2: a tuple of two pytorch tensors that corresponds
           complex-valued embeddings :return:
     forward_k_vs_all(x: torch.Tensor) \rightarrow torch.FloatTensor
     \textbf{forward\_triples} \ (\textit{x: torch.Tensor}) \ \rightarrow \text{torch.FloatTensor}
               Parameters
     forward_k_vs_sample (x: torch.Tensor, target_entity_idx: torch.Tensor)
class dicee.models.AConEx(args)
     Bases: dicee.models.base_model.BaseKGE
     Additive Convolutional ComplEx Knowledge Graph Embeddings
     name = 'AConEx'
     conv2d
     fc_num_input
     fc1
     norm_fc1
     bn_conv2d
     feature_map_dropout
     residual_convolution (C_1: Tuple[torch.Tensor, torch.Tensor],
                  C_2: Tuple[torch.Tensor, torch.Tensor]) \rightarrow torch.FloatTensor
           Compute residual score of two complex-valued embeddings. :param C_1: a tuple of two pytorch tensors
           that corresponds complex-valued embeddings :param C_2: a tuple of two pytorch tensors that corresponds
           complex-valued embeddings :return:
     forward_k_vs_all (x: torch.Tensor) \rightarrow torch.FloatTensor
     forward\_triples (x: torch.Tensor) \rightarrow torch.FloatTensor
               Parameters
     forward_k_vs_sample (x: torch.Tensor, target_entity_idx: torch.Tensor)
class dicee.models.ComplEx (args)
     Bases: dicee.models.base model.BaseKGE
     Base class for all neural network modules.
```

Your models should also subclass this class.

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

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

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

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

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



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.

# **Parameters**

- emb\_h
- emb\_r
- emb E

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

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

→ Tuple[torch.Tensor, torch.Tensor, torch.Tensor, torch.Tensor]

Perform quaternion multiplication :param Q\_1: :param Q\_2: :return:

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

Bases: BaseKGELightning

Base class for all neural network modules.

Your models should also subclass this class.

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

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

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

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

Submodules assigned in this way will be registered, and will have their parameters converted too when you call  $t \circ ()$ , 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.IdentityClass(args=None)
```

Bases: torch.nn.Module

Base class for all neural network modules.

Your models should also subclass this class.

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

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

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

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

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

# **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
```

```
__call__(x)
```

static forward(x)

dicee.models.quaternion\_mul\_with\_unit\_norm(\*, Q\_1, Q\_2)

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

Bases: dicee.models.base\_model.BaseKGE

Base class for all neural network modules.

Your models should also subclass this class.

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

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

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

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

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

# 1 Note

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

#### Variables

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

```
\label{eq:power_product} \begin{split} & \texttt{name} \ = \ 'Q\texttt{Mult'} \\ & \texttt{explicit} \ = \ \texttt{True} \\ & \texttt{quaternion\_multiplication\_followed\_by\_inner\_product} \ (h, r, t) \end{split}
```

#### **Parameters**

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

### Returns

Triple scores.

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

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

Absolute value of a quaternion

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

L2 norm of quaternion vector:

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

### **Parameters**

 $\mathbf{x}$  – The vector.

### Returns

The normalized vector.

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

### **Parameters**

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

forward\_k\_vs\_all (x)

**Parameters** 

x

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

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

class dicee.models.ConvQ(args)

Bases: dicee.models.base\_model.BaseKGE

Convolutional Quaternion Knowledge Graph Embeddings

name = 'ConvQ'

entity\_embeddings

relation\_embeddings

conv2d

fc\_num\_input

fc1

bn\_conv1

bn\_conv2

feature\_map\_dropout

residual\_convolution  $(Q_1, Q_2)$ 

```
Parameters
                   x
     forward_k_vs_all (x: torch.Tensor)
          Given a head entity and a relation (h,r), we compute scores for all entities. [score(h,r,x)|x in Entities] =>
          [0.0,0.1,...,0.8], shape=> (1, |Entities|) Given a batch of head entities and relations => shape (size of batch,|
          Entities l)
class dicee.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 to nest them in a tree structure. You can assign the submodules
     as regular attributes:
      import torch.nn as nn
      import torch.nn.functional as F
```

**forward\_triples** (*indexed\_triple: torch.Tensor*) → torch.Tensor

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class Model (nn.Module):
 def \_\_init\_\_ (self):

(continued from previous page)

```
super().__init__()
self.conv1 = nn.Conv2d(1, 20, 5)
self.conv2 = nn.Conv2d(20, 20, 5)

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

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

# **1** Note

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

#### Variables

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

# args

```
embedding_dim = None
num_entities = None
num_relations = None
num_tokens = None
learning_rate = None
apply_unit_norm = None
input_dropout_rate = None
hidden_dropout_rate = None
optimizer_name = None
feature_map_dropout_rate = None
kernel_size = None
num_of_output_channels = None
weight_decay = None
loss
selected_optimizer = None
normalizer_class = None
normalize_head_entity_embeddings
normalize_relation_embeddings
```

```
normalize_tail_entity_embeddings
hidden_normalizer
param_init
input_dp_ent_real
input_dp_rel_real
hidden_dropout
loss_history = []
byte_pair_encoding
max_length_subword_tokens
block_size
forward_byte_pair_encoded_k_vs_all(x: torch.LongTensor)
        Parameters
           x(B x 2 x T)
forward_byte_pair_encoded_triple (x: Tuple[torch.LongTensor, torch.LongTensor])
    byte pair encoded neural link predictors
        Parameters
init_params_with_sanity_checking()
forward (x: torch.LongTensor | Tuple[torch.LongTensor, torch.LongTensor],
          y_idx: torch.LongTensor = None)
        Parameters
           • x
           • y_idx
           • ordered_bpe_entities
forward\_triples (x: torch.LongTensor) \rightarrow torch.Tensor
        Parameters
forward_k_vs_all (*args, **kwargs)
forward_k_vs_sample(*args, **kwargs)
get_triple_representation(idx_hrt)
get_head_relation_representation(indexed_triple)
get_sentence_representation (x: torch.LongTensor)
        Parameters
           • (b(x shape)
           • 3
```

```
• t)

get_bpe_head_and_relation_representation (x: torch.LongTensor)

→ Tuple[torch.FloatTensor, torch.FloatTensor]

Parameters

x (B x 2 x T)

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

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

Bases: torch.nn.Module

Base class for all neural network modules.

Your models should also subclass this class.

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

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

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

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

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

# **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
__call__(x)
static forward(x)

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

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

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

Base class for all neural network modules.

Your models should also subclass this class.

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

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

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

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

Submodules assigned in this way will be registered, and will have their parameters converted too when you call  $t \circ ()$ , 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.

forward\_k\_vs\_all(x)

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

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

Base class for all neural network modules.

Your models should also subclass this class.

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

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

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

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

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

# 1 Note

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

### **Variables**

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

```
name = 'ConvO'
conv2d
fc_num_input
fc1
bn conv2d
norm_fc1
feature map dropout
static octonion normalizer (emb_rel_e0, emb_rel_e1, emb_rel_e2, emb_rel_e3, emb_rel_e4,
            emb_rel_e5, emb_rel_e6, emb_rel_e7)
residual convolution (O 1, O 2)
forward_triples (x: torch. Tensor) \rightarrow torch. Tensor
         Parameters
             x
forward_k_vs_all (x: torch.Tensor)
     Given a head entity and a relation (h,r), we compute scores for all entities. [score(h,r,x)|x in Entities] =>
     [0.0,0.1,...,0.8], shape=> (1, |Entities|) Given a batch of head entities and relations => shape (size of batch,)
     Entities()
```

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

Bases: dicee.models.base\_model.BaseKGE

Additive Convolutional Octonion Knowledge Graph Embeddings

```
name = 'AConvO'
```

```
conv2d
     fc_num_input
     fc1
     bn_conv2d
     norm_fc1
     feature_map_dropout
     static octonion_normalizer(emb_rel_e0, emb_rel_e1, emb_rel_e2, emb_rel_e3, emb_rel_e4,
                 emb_rel_e5, emb_rel_e6, emb_rel_e7)
     residual\_convolution(O_1, O_2)
     forward_triples (x: torch.Tensor) \rightarrow torch.Tensor
              Parameters
     forward_k_vs_all (x: torch.Tensor)
          Given a head entity and a relation (h,r), we compute scores for all entities. [score(h,r,x)|x in Entities] =>
          [0.0,0.1,...,0.8], shape=> (1, |Entities|) Given a batch of head entities and relations => shape (size of batch,)
          Entities|)
class dicee.models.Keci(args)
```

2222 a1000;....0 a010;....001

Bases: dicee.models.base\_model.BaseKGE

Base class for all neural network modules.

Your models should also subclass this class.

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

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

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

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

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

### **1** Note

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

```
Variables
```

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

```
name = 'Keci'
p
q
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 (h0, hp, hq, r0, rp, rq)
```

Multiplying a base vector with its scalar coefficient

### clifford\_multiplication (h0, hp, hq, r0, rp, rq)

Compute our CL multiplication

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

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

eq j

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

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

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

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

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

#### **Parameter**

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

### returns

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

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

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

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

Kvsall training

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

```
forward_k_vs_sample (x: torch.LongTensor, target_entity_idx: torch.LongTensor)
                   → torch.FloatTensor
           Kvsall training
           (1) Retrieve real-valued embedding vectors for heads and relations mathbb\{R\}^d.
           (2) Construct head entity and relation embeddings according to Cl_{p,q}(\mathsf{mathbb}\{R\}^d) .
           (3) Perform Cl multiplication
           (4) Inner product of (3) and all entity embeddings
           Parameter
           x: torch.LongTensor with (n,2) shape
                   torch.FloatTensor with (n, |E|) shape
     score (h, r, t)
     forward\_triples (x: torch.Tensor) \rightarrow torch.FloatTensor
           Parameter
           x: torch.LongTensor with (n,3) shape
               rtype
                   torch.FloatTensor with (n) shape
class dicee.models.KeciBase(args)
     Bases: Keci
     Without learning dimension scaling
     name = 'KeciBase'
     requires_grad_for_interactions = False
class dicee.models.CMult (args)
     Bases: dicee.models.base_model.BaseKGE
     Cl(0,0) \Rightarrow Real Numbers
     Cl_{-}(0,1) =>
           A multivector mathbf\{a\} = a_0 + a_1 e_1 A multivector mathbf\{b\} = b_0 + b_1 e_1
           multiplication is isomorphic to the product of two complex numbers
           mathbf{a} imes mathbf{b} = a 0 b 0 + a 0b 1 e1 + a 1 b 1 e 1 e 1
               = (a_0 b_0 - a_1 b_1) + (a_0 b_1 + a_1 b_0) e_1
     Cl_{(2,0)} =>
           A multivector mathbf\{a\} = a_0 + a_1 e_1 + a_2 e_2 + a_4\{12\} e_1 e_2 A multivector mathbf\{b\} = b_0 +
           b_1 e_1 + b_2 e_2 + b_{12} e_1 e_2
           mathbf{a} imes mathbf{b} = a 0b 0 + a 0b 1 e 1 + a 0b 2e 2 + a 0 b 12 e 1 e 2
                 • a 1 b 0 e 1 + a 1b 1 e 1 e1 ..
     Cl_{(0,2)} => Quaternions
```

```
name = 'CMult'
     entity_embeddings
     relation_embeddings
     р
     q
     clifford_mul(x: torch.FloatTensor, y: torch.FloatTensor, p: int, q: int) \rightarrow tuple
               Clifford multiplication Cl_{p,q} (mathbb{R})
               ei ^2 = +1 for i =< i =< p ej ^2 = -1 for p < j =< p+q ei ej = -eje1 for i
           eq j
               x: torch.FloatTensor with (n,d) shape
               y: torch.FloatTensor with (n,d) shape
               p: a non-negative integer p \ge 0 q: a non-negative integer q \ge 0
     score (head_ent_emb, rel_ent_emb, tail_ent_emb)
     forward_triples (x: torch.LongTensor) \rightarrow torch.FloatTensor
           Compute batch triple scores
           Parameter
           x: torch.LongTensor with shape n by 3
               rtype
                   torch.LongTensor with shape n
     forward_k_vs_all(x: torch.Tensor) \rightarrow torch.FloatTensor
           Compute batch KvsAll triple scores
           Parameter
           x: torch.LongTensor with shape n by 3
               rtype
                   torch.LongTensor with shape n
class dicee.models.DeCaL(args)
     Bases: dicee.models.base_model.BaseKGE
     Base class for all neural network modules.
     Your models should also subclass this class.
```

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

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

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

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

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

### 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,

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

and return:

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

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

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

For same bases vectors interaction we have

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

For different base vector interactions, we have

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

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

Kvsall training

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

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

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

Multiplying a base vector with its scalar coefficient

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

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

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:

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

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 i in range(q - 1):

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

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

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

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

compute\_sigma\_rr(hk, rk)

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

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

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

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

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

for j in range(q):

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

print(sigma\_pq.shape)

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

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

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

for j in range(q):

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

print(sigma\_pq.shape)

class dicee.models.BaseKGE (args: dict)

Bases: BaseKGELightning

Base class for all neural network modules.

Your models should also subclass this class.

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

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

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

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

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

### 1 Note

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

### Variables

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

```
args
embedding_dim = None
num_entities = None
num_relations = None
num_tokens = None
learning_rate = None
apply_unit_norm = None
input_dropout_rate = None
hidden_dropout_rate = None
optimizer_name = None
feature_map_dropout_rate = None
kernel_size = None
num_of_output_channels = None
weight_decay = None
loss
selected_optimizer = None
normalizer_class = None
normalize_head_entity_embeddings
normalize_relation_embeddings
normalize_tail_entity_embeddings
hidden_normalizer
param_init
input_dp_ent_real
input_dp_rel_real
hidden_dropout
loss_history = []
byte_pair_encoding
max_length_subword_tokens
block_size
```

```
forward_byte_pair_encoded_k_vs_all (x: torch.LongTensor)
             Parameters
                 x(B x 2 x T)
     forward_byte_pair_encoded_triple (x: Tuple[torch.LongTensor, torch.LongTensor])
         byte pair encoded neural link predictors
             Parameters
     init_params_with_sanity_checking()
     forward (x: torch.LongTensor | Tuple[torch.LongTensor, torch.LongTensor],
                y_idx: torch.LongTensor = None
             Parameters
                 • x
                 • y_idx
                 · ordered_bpe_entities
     forward\_triples (x: torch.LongTensor) \rightarrow torch.Tensor
             Parameters
     forward_k_vs_all (*args, **kwargs)
     forward_k_vs_sample(*args, **kwargs)
     get_triple_representation(idx_hrt)
     get_head_relation_representation(indexed_triple)
     get_sentence_representation (x: torch.LongTensor)
             Parameters
                 • (b(x shape)
                 • 3
                 • t)
     get_bpe_head_and_relation_representation (x: torch.LongTensor)
                 → Tuple[torch.FloatTensor, torch.FloatTensor]
             Parameters
                 x(B x 2 x T)
     get_embeddings() → Tuple[numpy.ndarray, numpy.ndarray]
class dicee.models.PykeenKGE(args: dict)
     Bases: dicee.models.base_model.BaseKGE
     A class for using knowledge graph embedding models implemented in Pykeen
     Notes: Pykeen_DistMult: C Pykeen_ComplEx: Pykeen_QuatE: Pykeen_MuRE: Pykeen_CP: Pykeen_HolE: Py-
     keen_HolE:
```

```
model_kwargs
      name
      model
      loss_history = []
      args
      entity_embeddings = None
      relation_embeddings = None
      forward_k_vs_all (x: torch.LongTensor)
           # => Explicit version by this we can apply bn and dropout
           # (1) Retrieve embeddings of heads and relations + apply Dropout & Normalization if given. h, r =
           self.get_head_relation_representation(x) \# (2) Reshape (1). if self.last_dim > 0:
               h = h.reshape(len(x), self.embedding dim, self.last dim) r = r.reshape(len(x), self.embedding dim,
               self.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.models.BaseKGE (args: dict)
      Bases: BaseKGELightning
      Base class for all neural network modules.
```

Your models should also subclass this class.

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

```
import torch.nn as nn
import torch.nn.functional as F
class Model (nn.Module):
   def __init__(self):
```

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```
super().__init__()
self.conv1 = nn.Conv2d(1, 20, 5)
self.conv2 = nn.Conv2d(20, 20, 5)

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

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

# **1** Note

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

#### Variables

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

# args

```
embedding_dim = None
num_entities = None
num_relations = None
num_tokens = None
learning_rate = None
apply_unit_norm = None
input_dropout_rate = None
hidden_dropout_rate = None
optimizer_name = None
feature_map_dropout_rate = None
kernel_size = None
num_of_output_channels = None
weight_decay = None
loss
selected_optimizer = None
normalizer_class = None
normalize_head_entity_embeddings
normalize_relation_embeddings
```

```
normalize_tail_entity_embeddings
hidden_normalizer
param_init
input_dp_ent_real
input_dp_rel_real
hidden_dropout
loss_history = []
byte_pair_encoding
max_length_subword_tokens
block_size
forward_byte_pair_encoded_k_vs_all(x: torch.LongTensor)
        Parameters
           x(B x 2 x T)
forward_byte_pair_encoded_triple (x: Tuple[torch.LongTensor, torch.LongTensor])
    byte pair encoded neural link predictors
        Parameters
init_params_with_sanity_checking()
forward (x: torch.LongTensor | Tuple[torch.LongTensor, torch.LongTensor],
          y_idx: torch.LongTensor = None)
        Parameters
           • x
           • y_idx
           • ordered_bpe_entities
forward\_triples (x: torch.LongTensor) \rightarrow torch.Tensor
        Parameters
forward_k_vs_all (*args, **kwargs)
forward_k_vs_sample(*args, **kwargs)
get_triple_representation(idx_hrt)
get_head_relation_representation(indexed_triple)
get_sentence_representation (x: torch.LongTensor)
        Parameters
           • (b(x shape)
           • 3
```

```
• t)
     get_bpe_head_and_relation_representation (x: torch.LongTensor)
                 → Tuple[torch.FloatTensor, torch.FloatTensor]
             Parameters
                 x (B x 2 x T)
     \texttt{get\_embeddings}\:()\:\to 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
     k
     num_sample = 250
     roots
     weights
     compute\_func(weights: torch.FloatTensor, x) \rightarrow torch.FloatTensor
     chain_func (weights, x: torch.FloatTensor)
```

```
forward_triples (idx\_triple: torch.Tensor) \rightarrow torch.Tensor
             Parameters
class dicee.models.FMult2(args)
     Bases: dicee.models.base model.BaseKGE
     Learning Knowledge Neural Graphs
     name = 'FMult2'
     n_{ayers} = 3
     tuned_embedding_dim = False
     k
     n = 50
     score_func = 'compositional'
     discrete_points
     entity_embeddings
     relation embeddings
     build_func(Vec)
     build_chain_funcs (list_Vec)
     compute\_func(W, b, x) \rightarrow torch.FloatTensor
     function(list_W, list_b)
     trapezoid(list_W, list_b)
     forward\_triples(idx\_triple: torch.Tensor) \rightarrow torch.Tensor
             Parameters
class dicee.models.LFMult1(args)
     Bases: dicee.models.base_model.BaseKGE
     Embedding with trigonometric functions. We represent all entities and relations in the complex number space as:
     f(x) = sum_{k=0}^{k=0}^{k=d-1}wk e^{kix}, and use the three differents scoring function as in the paper to evaluate
     the score
     name = 'LFMult1'
     entity_embeddings
     relation_embeddings
     forward_triples (idx_triple)
             Parameters
                 x
```

```
vtp\_score(h, r, t)
class dicee.models.LFMult (args)
     Bases: dicee.models.base_model.BaseKGE
     Embedding with polynomial functions. We represent all entities and relations in the polynomial space as: f(x) =
     sum_{i=0}^{d-1} a_k x^{i\%d} and use the three differents scoring function as in the paper to evaluate the score.
     We also consider combining with Neural Networks.
     name = 'LFMult'
     entity_embeddings
     relation_embeddings
     degree
     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
```

 $tri_score(h, r, t)$ 

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

**kvsall\_score** (
$$e_1h$$
,  $e_2h$ ,  $e_3h$ ,  $e_4h$ ,  $e_5h$ ,  $e_6h$ ,  $e_7h$ ,  $e_8h$ ,  $e_1t$ ,  $e_2t$ ,  $e_3t$ ,  $e_4t$ ,  $e_5t$ ,  $e_6t$ ,  $e_7t$ ,  $e_8t$ ,  $e_1t$ ,  $e_2h$ ,  $e_3h$ ,  $e_4h$ ,  $e_5h$ ,  $e_6h$ ,  $e_7h$ ,  $e_8h$ ,  $e_7h$ ,  $e_7h$ ,  $e_8h$ ,  $e_7h$ 

KvsAll scoring function

### Input

x: torch.LongTensor with (n, ) shape

### **Output**

torch.FloatTensor with (n) shape

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

Negative Sampling forward pass:

# Input

x: torch.LongTensor with (n, ) shape

# **Output**

torch.FloatTensor with (n) shape

### $forward_k_vs_all(x)$

KvsAll forward pass

### Input

x: torch.LongTensor with (n, ) shape

# Output

torch.FloatTensor with (n) shape

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

Transpose function

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

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

### **Submodules**

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

# Classes

PreprocessKG

Preprocess the data in memory

# **Module Contents**

 $\verb|class| dicee.read_preprocess_save_load_kg.preprocess.PreprocessKG|(kg)|$ 

Preprocess the data in memory

kg

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

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

### **Parameter**

rtype

None

preprocess\_with\_byte\_pair\_encoding()

 ${\tt preprocess\_with\_byte\_pair\_encoding\_with\_padding\,(\,)} \, \to None$ 

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

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

- (1) Add recipriocal or noisy triples
- (2) Construct vocabulary
- (3) Index datasets

### **Parameter**

rtype

None

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

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

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

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

remove\_triples\_from\_train\_with\_condition()

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

kq

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

Read a knowledge graph from disk into memory

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

# **Parameter**

```
None

rtype
None

add_noisy_triples_into_training()
```

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

# 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**

```
apply_reciprical_or_noise(add_reciprical,
eval_model)
timeit(func)
read\_with\_polars(\rightarrow polars.DataFrame)
                                                     Load and Preprocess via Polars
read_with_pandas(data_path[, read_only_few, ...])
read_from_disk(data_path[, read_only_few, ...])
                                                     Read triples from triple store into pandas dataframe
read_from_triple_store([endpoint])
get_er_vocab(data[, file_path])
get_re_vocab(data[, file_path])
get_ee_vocab(data[, file_path])
create_constraints(triples[, file_path])
load_with_pandas(\rightarrow None)
                                                     Deserialize data
save_numpy_ndarray(*, data, file_path)
load_numpy_ndarray(*, file_path)
save_pickle(*, data[, file_path])
load_pickle(*[, file_path])
create recipriocal triples(x)
                                                     Add inverse triples into dask dataframe
index_triples_with_pandas(→
                                              pan-
das.core.frame.DataFrame)
\textit{dataset\_sanity\_checking}(\rightarrow None)
```

### **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. Crete constrainted entities based on the range of relations :param triples: :return: Tuple[dict, dict]

### **Parameters**

- train\_set pandas dataframe
- entity\_to\_idx a mapping from str to integer index
- relation\_to\_idx a mapping from str to integer index

entity to idx: dict, relation to idx: dict)  $\rightarrow$  pandas.core.frame.DataFrame

• num\_core - number of cores to be used

#### Returns

indexed triples, i.e., pandas dataframe

```
dicee.read_preprocess_save_load_kg.util.dataset_sanity_checking( train\_set: numpy.ndarray, num\_entities: int, num\_relations: int) \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**

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

```
class dicee.read_preprocess_save_load_kg.LoadSaveToDisk(kg)
     kg
     save()
     load()
class dicee.read_preprocess_save_load_kg.ReadFromDisk(kg)
     Read the data from disk into memory
     kg
     \mathtt{start}() \to \mathsf{None}
         Read a knowledge graph from disk into memory
         Data will be available at the train_set, test_set, valid_set attributes.
         Parameter
         None
             rtype
                None
     add_noisy_triples_into_training()
dicee.scripts
Submodules
dicee.scripts.index
Functions
 get_default_arguments()
 main()
Module Contents
dicee.scripts.index.get_default_arguments()
```

dicee.scripts.index.main()

# dicee.scripts.run

### **Functions**

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

### **Module Contents**

# dicee.scripts.serve

### **Attributes**

```
app
neural_searcher
```

# Classes

*NeuralSearcher* 

### **Functions**

```
get_default_arguments()
root()
search_embeddings(q)
retrieve_embeddings(q)
main()
```

### **Module Contents**

dicee.trainer

**Submodules** 

dicee.trainer.dice\_trainer

**Classes** 

DICE\_Trainer

DICE\_Trainer implement

### **Functions**

```
initialize_trainer(args, callbacks)

get_callbacks(args)
```

#### **Module Contents**

```
dicee.trainer.dice_trainer.initialize_trainer(args, callbacks)
dicee.trainer.dice_trainer.get_callbacks(args)
class dicee.trainer.dice_trainer.DICE_Trainer(args, is_continual_training, storage_path,
           evaluator=None)
     DICE_Trainer implement
          1- Pytorch Lightning trainer (https://pytorch-lightning.readthedocs.io/en/stable/common/trainer.html)
          2- Multi-GPU Trainer(https://pytorch.org/docs/stable/generated/torch.nn.parallel.DistributedDataParallel.
          html) 3- CPU Trainer
          args
          is_continual_training:bool
          storage_path:str
          evaluator:
          report:dict
     report
     args
     trainer = None
     is_continual_training
     storage_path
     evaluator
     form_of_labelling = None
     continual_start()
          (1) Initialize training.
          (2) Load model
          (3) Load trainer (3) Fit model
          Parameter
              returns
                  • model
                  • form_of_labelling (str)
     initialize\_trainer (callbacks: List) \rightarrow lightning. Trainer
          Initialize Trainer from input arguments
     initialize_or_load_model()
     initialize\_dataloader (dataset: torch.utils.data.Dataset) \rightarrow torch.utils.data.DataLoader
```

 $\verb|start| (knowledge\_graph: dicee.knowledge\_graph.KG)| \rightarrow \mathsf{Tuple}[dicee.models.base\_model.BaseKGE, \mathsf{str}]|$ 

Train selected model via the selected training strategy

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

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.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
```

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

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)

 $\textbf{extract\_input\_outputs\_set\_device} \ (\textit{batch: list}) \ \rightarrow \textbf{Tuple}$ 

Construct inputs and outputs from a batch of inputs with outputs From a batch of inputs and put

Arguments

# Return type

(tuple) mini-batch on select device

# dicee.trainer.torch\_trainer\_ddp

#### **Classes**

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

# **Functions**

print\_peak\_memory(prefix, device)

# **Module Contents**

```
dicee.trainer.torch_trainer_ddp.print_peak_memory (prefix, device)
class dicee.trainer.torch_trainer_ddp.TorchDDPTrainer(args, callbacks)
     Bases: dicee.abstracts.AbstractTrainer
          A Trainer based on torch.nn.parallel.DistributedDataParallel
          Arguments
     entity_idxs
         mapping.
     relation idxs
         mapping.
     form
     store
     label_smoothing_rate
         Using hard targets (0,1) drives weights to infinity. An outlier produces enormous gradients.
         Return type
             torch.utils.data.Dataset
     fit (*args, **kwargs)
         Train model
class dicee.trainer.torch_trainer_ddp.NodeTrainer(trainer, model: torch.nn.Module,
           train_dataset_loader: torch.utils.data.DataLoader, optimizer: torch.optim.Optimizer, callbacks,
           num_epochs: int)
     trainer
     local_rank
     global_rank
     model
     train_dataset_loader
     loss_func
     optimizer
     callbacks
     num_epochs
     loss_history = []
     extract_input_outputs (z: list)
```

#### **Classes**

DICE Trainer

DICE\_Trainer implement

# **Package Contents**

class dicee.trainer.DICE\_Trainer(args, is\_continual\_training, storage\_path, evaluator=None)

### **DICE\_Trainer implement**

- 1- Pytorch Lightning trainer (https://pytorch-lightning.readthedocs.io/en/stable/common/trainer.html)
- 2- Multi-GPU Trainer(https://pytorch.org/docs/stable/generated/torch.nn.parallel.DistributedDataParallel. html) 3- CPU Trainer

args

is\_continual\_training:bool

storage\_path:str

evaluator:

report:dict

report

args

trainer = None

```
is_continual_training
storage_path
evaluator
form_of_labelling = None
continual_start()
     (1) Initialize training.
     (2) Load model
     (3) Load trainer (3) Fit model
     Parameter
         returns

    model

              • form_of_labelling (str)
initialize_trainer (callbacks: List) → lightning.Trainer
     Initialize Trainer from input arguments
initialize_or_load_model()
initialize_dataloader (dataset: torch.utils.data.Dataset) → torch.utils.data.DataLoader
initialize_dataset (dataset: dicee.knowledge_graph.KG, form_of_labelling)
             \rightarrow torch.utils.data.Dataset
\verb|start| (knowledge\_graph: dicee.knowledge\_graph.KG)| \rightarrow \mathsf{Tuple}[dicee.models.base\_model.BaseKGE, \mathsf{str}]|
     Train selected model via the selected training strategy
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 Submodules

# dicee.abstracts

#### **Classes**

AbstractTrainer	Abstract class for Trainer class for knowledge graph embedding models
BaseInteractiveKGE	Abstract/base class for using knowledge graph embedding models interactively.
AbstractCallback	Abstract class for Callback class for knowledge graph embedding models
AbstractPPECallback	Abstract class for Callback class for knowledge graph embedding models

# **Module Contents**

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

Abstract class for Trainer class for knowledge graph embedding models

#### **Parameter**

```
args
    [str] ?
callbacks: list
    ?
attributes
callbacks
is_global_zero = True
strategy = None
on_fit_start(*args, **kwargs)
```

A function to call callbacks before the training starts.

#### **Parameter**

```
args
kwargs
rtype
None
on_fit_end(*args, **kwargs)
```

A function to call callbacks at the ned of the training.

```
Parameter
     args
     kwargs
         rtype
              None
on_train_epoch_end(*args, **kwargs)
     A function to call callbacks at the end of an epoch.
     Parameter
     args
     kwargs
         rtype
              None
on_train_batch_end(*args, **kwargs)
     A function to call callbacks at the end of each mini-batch during training.
     Parameter
     args
     kwargs
         rtype
              None
\verb|static save_checkpoint| (\mathit{full\_path: str}, \mathit{model}) \rightarrow None
     A static function to save a model into disk
     Parameter
     full_path: str
```

```
class dicee.abstracts.BaseInteractiveKGE (path: str = None, url: str = None, construct\_ensemble: bool = False, model\_name: <math>str = None,
```

apply\_semantic\_constraint: bool = False)

model:

**rtype**None

Abstract/base class for using knowledge graph embedding models interactively.

```
path_of_pretrained_model_dir
construct_ensemble: boolean
model_name: str apply_semantic_constraint : boolean
construct_ensemble
apply_semantic_constraint
configs
\texttt{get\_eval\_report}() \rightarrow \text{dict}
get_bpe_token_representation (str_entity_or_relation: List[str] | str)
             \rightarrow List[List[int]] \mid List[int]
         Parameters
              str_entity_or_relation(corresponds to a str or a list of strings
              to be tokenized via BPE and shaped.)
         Return type
              A list integer(s) or a list of lists containing integer(s)
\verb|get_padded_bpe_triple_representation| (triples: List[List[str]])| \rightarrow Tuple[List, List, List]
         Parameters
              triples
\verb"set_model_train_mode"() \to None
     Setting the model into training mode
     Parameter
\mathtt{set}\_\mathtt{model}\_\mathtt{eval}\_\mathtt{mode}\,(\,) \, \to None
     Setting the model into eval mode
     Parameter
property name
sample_entity(n:int) \rightarrow List[str]
sample\_relation(n:int) \rightarrow List[str]
is_seen (entity: str = None, relation: str = None) \rightarrow bool
save() \rightarrow None
get_entity_index (x: str)
get_relation_index (x: str)
```

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

```
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.
```

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

# dicee.analyse\_experiments

This script should be moved to dicee/scripts

# **Classes**

```
Experiment
```

## **Functions**

```
get_default_arguments()
analyse(args)
```

# **Module Contents**

```
dicee.analyse_experiments.get_default_arguments()
class dicee.analyse_experiments.Experiment
    model_name = []
    callbacks = []
    embedding_dim = []
    num_params = []
    num_epochs = []
    batch_size = []
    lr = []
    byte_pair_encoding = []
    aswa = []
```

```
path_dataset_folder = []
    full_storage_path = []
    pq = []
    train_mrr = []
    train_h1 = []
    train_h3 = []
    train_h10 = []
    val_mrr = []
    val_h1 = []
    val_h3 = []
    val_h10 = []
    test_mrr = []
    test_h1 = []
   test_h3 = []
    test_h10 = []
    runtime = []
    normalization = []
    scoring_technique = []
    save_experiment(x)
    to_df()
dicee.analyse_experiments.analyse(args)
```

# dicee.callbacks

# Classes

AccumulateEpochLossCallback	Abstract class for Callback class for knowledge graph embedding models
PrintCallback	Abstract class for Callback class for knowledge graph embedding models
KGESaveCallback	Abstract class for Callback class for knowledge graph embedding models
PseudoLabellingCallback	Abstract class for Callback class for knowledge graph embedding models
ASWA	Adaptive stochastic weight averaging
Eval	Abstract class for Callback class for knowledge graph embedding models
KronE	Abstract class for Callback class for knowledge graph embedding models
Perturb	A callback for a three-Level Perturbation

# **Functions**

estimate_q(eps)	estimate rate of convergence q from sequence esp
compute_convergence(seq, i)	

## **Module Contents**

```
Bases: dicee.abstracts.AbstractCallback

Abstract class for Callback class for knowledge graph embedding models

Parameter

path

on_fit_end(trainer, model) → None

Store epoch loss

Parameter

trainer:

model:

rtype
```

None

class dicee.callbacks.AccumulateEpochLossCallback (path: str)

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

Call at the end of each epoch during training.

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

model:

rtype

None

on\_train\_epoch\_end(\*args, \*\*kwargs)

Call at the end of each epoch during training.

```
Parameter
```

```
trainer:
          model:
              rtype
                 None
     on_fit_end(*args, **kwargs)
          Call at the end of the training.
          Parameter
          trainer:
          model:
              rtype
                  None
     on_epoch_end (model, trainer, **kwargs)
class dicee.callbacks.PseudoLabellingCallback(data_module, kg, batch_size)
     Bases: dicee.abstracts.AbstractCallback
     Abstract class for Callback class for knowledge graph embedding models
```

```
data_module
    kg
    num_of_epochs = 0
    unlabelled_size
    batch_size
    create_random_data()
    on_epoch_end (trainer, model)
dicee.callbacks.estimate_q(eps)
    estimate rate of convergence q from sequence esp
dicee.callbacks.compute_convergence(seq, i)
class dicee.callbacks.ASWA (num_epochs, path)
    Bases: dicee.abstracts.AbstractCallback
```

Adaptive stochastic weight averaging ASWE keeps track of the validation performance and update s the ensemble model accordingly.

path

```
num_epochs
     initial_eval_setting = None
     epoch_count = 0
     alphas = []
     val_aswa
     on_fit_end(trainer, model)
          Call at the end of the training.
          Parameter
          trainer:
          model:
              rtype
                  None
     \texttt{static compute\_mrr}(\textit{trainer}, model) \rightarrow \texttt{float}
     get_aswa_state_dict(model)
     decide (running_model_state_dict, ensemble_state_dict, val_running_model,
                 mrr\_updated\_ensemble\_model)
          Perform Hard Update, software or rejection
              Parameters
                  • running_model_state_dict
                  • ensemble_state_dict
                  • val_running_model
                  • mrr_updated_ensemble_model
     on_train_epoch_end (trainer, model)
          Call at the end of each epoch during training.
          Parameter
          trainer:
          model:
              rtype
                  None
class dicee.callbacks.Eval (path, epoch_ratio: int = None)
     Bases: dicee.abstracts.AbstractCallback
     Abstract class for Callback class for knowledge graph embedding models
```

```
path
reports = []
epoch_ratio
epoch_counter = 0
on_fit_start (trainer, model)
     Call at the beginning of the training.
     Parameter
     trainer:
     model:
         rtype
             None
on_fit_end(trainer, model)
     Call at the end of the training.
     Parameter
     trainer:
     model:
         rtype
             None
\verb"on_train_epoch_end" (\textit{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.
```

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

ratio

method

#### scaler

#### frequency

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

Called when the train batch begins.

#### dicee.config

#### **Classes**

Namespace

Simple object for storing attributes.

#### **Module Contents**

```
class dicee.config.Namespace(**kwargs)
```

Bases: argparse.Namespace

Simple object for storing attributes.

Implements equality by attribute names and values, and provides a simple string representation.

```
dataset_dir: str = None
```

The path of a folder containing train.txt, and/or valid.txt and/or test.txt

```
save_embeddings_as_csv: bool = False
```

Embeddings of entities and relations are stored into CSV files to facilitate easy usage.

```
storage_path: str = 'Experiments'
```

A directory named with time of execution under -storage\_path that contains related data about embeddings.

```
path_to_store_single_run: str = None
```

A single directory created that contains related data about embeddings.

```
path_single_kg = None
```

Path of a file corresponding to the input knowledge graph

```
sparql_endpoint = None
```

An endpoint of a triple store.

```
model: str = 'Keci'
```

KGE model

optim: str = 'Adam'

Optimizer

embedding\_dim: int = 64

Size of continuous vector representation of an entity/relation

num\_epochs: int = 150

Number of pass over the training data

batch\_size: int = 1024

Mini-batch size if it is None, an automatic batch finder technique applied

```
lr: float = 0.1
    Learning rate
add_noise_rate: float = None
    The ratio of added random triples into training dataset
qpus = None
    Number GPUs to be used during training
callbacks
    10}}
        Type
            Callbacks, e.g., {"PPE"
        Type
            { "last_percent_to_consider"
backend: str = 'pandas'
    Backend to read, process, and index input knowledge graph. pandas, polars and rdflib available
trainer: str = 'torchCPUTrainer'
    Trainer for knowledge graph embedding model
scoring_technique: str = 'KvsAll'
    Scoring technique for knowledge graph embedding models
neg_ratio: int = 0
    Negative ratio for a true triple in NegSample training_technique
weight_decay: float = 0.0
    Weight decay for all trainable params
normalization: str = 'None'
    LayerNorm, BatchNorm1d, or None
init_param: str = None
    xavier_normal or None
gradient_accumulation_steps: int = 0
    Not tested e
num_folds_for_cv: int = 0
    Number of folds for CV
eval_model: str = 'train_val_test'
    ["None", "train", "train_val", "train_val_test", "test"]
        Type
            Evaluate trained model choices
save_model_at_every_epoch: int = None
    Not tested
label_smoothing_rate: float = 0.0
num_core: int = 0
    Number of CPUs to be used in the mini-batch loading process
```

random\_seed: int = 0

Random Seed

sample\_triples\_ratio: float = None

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

read\_only\_few: int = None

Read only first few triples

pykeen\_model\_kwargs

Additional keyword arguments for pykeen models

kernel\_size: int = 3

Size of a square kernel in a convolution operation

num\_of\_output\_channels: int = 32

Number of slices in the generated feature map by convolution.

p: int = 0

P parameter of Clifford Embeddings

q: int = 1

Q parameter of Clifford Embeddings

input\_dropout\_rate: float = 0.0

Dropout rate on embeddings of input triples

hidden\_dropout\_rate: float = 0.0

Dropout rate on hidden representations of input triples

feature\_map\_dropout\_rate: float = 0.0

Dropout rate on a feature map generated by a convolution operation

byte\_pair\_encoding: bool = False

Byte pair encoding

**Type** 

WIP

adaptive\_swa: bool = False

Adaptive stochastic weight averaging

swa: bool = False

Stochastic weight averaging

block\_size: int = None

block size of LLM

continual\_learning = None

Path of a pretrained model size of LLM

\_\_iter\_\_()

## dicee.dataset classes

#### **Classes**

BPE_NegativeSamplingDataset	An abstract class representing a Dataset.
MultiLabelDataset	An abstract class representing a Dataset.
MultiClassClassificationDataset	Dataset for the 1vsALL training strategy
OnevsAllDataset	Dataset for the 1vsALL training strategy
KvsAll	Creates a dataset for KvsAll training by inheriting from
	torch.utils.data.Dataset.
AllvsAll	Creates a dataset for AllvsAll training by inheriting from
	torch.utils.data.Dataset.
KvsSampleDataset	KvsSample a Dataset:
NegSampleDataset	An abstract class representing a Dataset.
TriplePredictionDataset	Triple Dataset
CVDataModule	Create a Dataset for cross validation

#### **Functions**

reload_dataset(path, form_of_labelling,)	Reload the files from disk to construct the Pytorch dataset
$construct\_dataset( \rightarrow torch.utils.data.Dataset)$	

#### **Module Contents**

Reload the files from disk to construct the Pytorch dataset

dicee.dataset\_classes.construct\_dataset (\*, train\_set: numpy.ndarray | list, valid\_set=None, test\_set=None, ordered\_bpe\_entities=None, train\_target\_indices=None, target\_dim: int = None, entity\_to\_idx: dict, relation\_to\_idx: dict, form\_of\_labelling: str, scoring\_technique: str, neg\_ratio: int, label\_smoothing\_rate: float, byte\_pair\_encoding=None, block\_size: int = None)

→ torch.utils.data.Dataset

Bases: torch.utils.data.Dataset

An abstract class representing a Dataset.

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

# 1 Note

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

```
train_set
  ordered_bpe_entities
num_bpe_entities
neg_ratio
num_datapoints
  __len__()
  __getitem__(idx)
  collate_fn (batch_shaped_bpe_triples: List[Tuple[torch.Tensor, torch.Tensor]])
class dicee.dataset_classes.MultiLabelDataset (train_set: torch.LongTensor, train_indices_target: torch.LongTensor, target_dim: int, torch_ordered_shaped_bpe_entities: torch.LongTensor)
Bases: torch.utils.data.Dataset
An abstract class representing a Dataset.
```

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

#### 1 Note

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

```
train_set

train_indices_target

target_dim

num_datapoints

torch_ordered_shaped_bpe_entities

collate_fn = None

__len__()
__getitem__(idx)
```

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

Bases: torch.utils.data.Dataset

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

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

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



**TODO** 

### train\_set\_idx

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

#### entity idxs

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

## relation\_idxs

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

self: torch.utils.data.Dataset

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

train\_data = None
train\_target = None
label\_smoothing\_rate
collate\_fn = None
\_\_len\_\_()

 $\__getitem\__(idx)$ 

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

1 Note

```
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()
           ? array([0, 1, 2, 3, 4, 5, 6, 7, 8, 9])
     train_data = None
     train_target = None
     label_smoothing_rate
     collate_fn = None
     target_dim
     store
     __len__()
     \__getitem_{\_}(idx)
class dicee.dataset_classes.KvsSampleDataset (train_set: numpy.ndarray, num_entities,
            num_relations, neg_sample_ratio: int = None, label_smoothing_rate: float = 0.0)
     Bases: torch.utils.data.Dataset
           KvsSample a Dataset:
               D := \{(x,y)_i\}_i ^N, \text{ where }
                   . x:(h,r) is a unique h in E and a relation r in R and . y in [0,1]^{\{|E|\}} is a binary label.
     orall y_i = 1 s.t. (h r E_i) in KG
               At each mini-batch construction, we subsample(y), hence n
                   lnew_yl << IEI 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.
```

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

without 1s,

```
form
          store
          label_smoothing_rate
          torch.utils.data.Dataset
     train_data
     num_entities
     num_relations
     neg_sample_ratio
     label_smoothing_rate
     collate_fn = None
     store
     train_target
     __len__()
     \underline{\underline{getitem}}(idx)
class dicee.dataset_classes.NegSampleDataset (train_set: numpy.ndarray, num_entities: int,
           num\_relations: int, neg\_sample\_ratio: int = 1)
     Bases: torch.utils.data.Dataset
     An abstract class representing a Dataset.
```

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

# **1** Note

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

```
neg_sample_ratio
train_set
length
num_entities
num_relations
```

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

- 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.

be reloaded The dataloader you return will not unless you :paramset 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.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.

- 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:

# → See also

- move data to device()
- apply\_to\_collection()

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

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

# Warning

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

## Example:

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

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

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

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

#### Example:

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

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

This is called before requesting the dataloaders:

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

# dicee.eval\_static\_funcs

#### **Functions**

```
evaluate_link_prediction_performance(→
Dict)
evaluate_link_prediction_performance_w

evaluate_link_prediction_performance_w

evaluate_link_prediction_performance_w
...)
evaluate_lp_bpe_k_vs_all(model, triples[, er_vocab, ...])
```

#### **Module Contents**

```
dicee.eval_static_funcs.evaluate_link_prediction_performance( model: dicee.knowledge\_graph\_embeddings.KGE, triples, er\_vocab: Dict[Tuple, List], re\_vocab: Dict[Tuple, List]) <math>\rightarrow Dict
```

- model
- triples
- er\_vocab

```
re_vocab
```

```
dicee.eval_static_funcs.
```

evaluate\_link\_prediction\_performance\_with\_reciprocals (
model: dicee.knowledge\_graph\_embeddings.KGE, triples, er\_vocab: Dict[Tuple, List])

dicee.eval\_static\_funcs.

evaluate\_link\_prediction\_performance\_with\_bpe\_reciprocals (
model: dicee.knowledge\_graph\_embeddings.KGE, within\_entities: List[str], triples: List[List[str]],
er\_vocab: Dict[Tuple, List])

#### **Parameters**

- model
- triples
- within\_entities
- er\_vocab
- re\_vocab

## dicee.evaluator

# **Classes**

Evaluator

Evaluator class to evaluate KGE models in various downstream tasks

#### **Module Contents**

**class** dicee.evaluator.**Evaluator**(args, is continual training=None)

Evaluator class to evaluate KGE models in various downstream tasks

Arguments

re\_vocab = None
er\_vocab = None
ee\_vocab = None
func\_triple\_to\_bpe\_representation = None
is\_continual\_training

```
num_entities = None
num_relations = None
args
report
during_training = False
vocab\_preparation(dataset) \rightarrow None
     A function to wait future objects for the attributes of executor
         Return type
             None
eval (dataset: dicee.knowledge_graph.KG, trained_model, form_of_labelling, during_training=False)
             \rightarrow None
eval rank of head and tail entity (*, train set, valid set=None, test set=None,
            trained model)
eval_rank_of_head_and_tail_byte_pair_encoded_entity(*, train_set=None,
            valid set=None, test set=None, ordered bpe entities, trained model)
eval_with_byte(*, raw_train_set, raw_valid_set=None, raw_test_set=None, trained_model,
            form\_of\_labelling) \rightarrow None
     Evaluate model after reciprocal triples are added
eval_with_bpe_vs_all (*, raw_train_set, raw_valid_set=None, raw_test_set=None, trained_model,
            form\_of\_labelling) \rightarrow None
     Evaluate model after reciprocal triples are added
eval_with_vs_all (*, train_set, valid_set=None, test_set=None, trained_model, form_of_labelling)
             \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)
evaluate_lp_bpe_k_vs_all (model, triples: List[List[str]], info=None, form_of_labelling=None)
         Parameters
             • model
             • triples (List of lists)
             info

    form_of_labelling

evaluate_lp (model, triple_idx, info: str)
dummy_eval (trained_model, form_of_labelling: str)
eval_with_data(dataset, trained_model, triple_idx: numpy.ndarray, form_of_labelling: str)
```

### dicee.executer

### **Classes**

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

# **Module Contents**

```
class dicee.executer.Execute(args, continuous_training=False)
     A class for Training, Retraining and Evaluation a model.
      (1) Loading & Preprocessing & Serializing input data.
      (2) Training & Validation & Testing
      (3) Storing all necessary info
     is_continual_training
     trainer = None
     trained_model = None
     knowledge_graph = None
     report
     evaluator = None
     start_time = None
     read_or_load_kg()
     {\tt read\_preprocess\_index\_serialize\_data}\,(\,)\,\to None
          Read & Preprocess & Index & Serialize Input Data
          (1) Read or load the data from disk into memory.
          (2) Store the statistics of the data.
          Parameter
```

rtype None

 $\textbf{load\_indexed\_data}\,(\,)\,\to None$ 

Load the indexed data from disk into memory

### **Parameter**

# rtype

None

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

Save a knowledge graph embedding model

- (1) Send model to eval mode and cpu.
- (2) Store the memory footprint of the model.
- (3) Save the model into disk.
- (4) Update the stats of KG again?

### **Parameter**

# rtype

None

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

End training

- (1) Store trained model.
- (2) Report runtimes.
- (3) Eval model if required.

### **Parameter**

### rtype

A dict containing information about the training and/or evaluation

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

Report training related information in a report.json file

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

Start training

# (1) Loading the Data # (2) Create an evaluator object. # (3) Create a trainer object. # (4) Start the training

### **Parameter**

# rtype

A dict containing information about the training and/or evaluation

### class dicee.executer.ContinuousExecute(args)

Bases: Execute

A subclass of Execute Class for retraining

(1) Loading & Preprocessing & Serializing input data.

- (2) Training & Validation & Testing
- (3) Storing all necessary info

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

### previous\_args

### args

 $\textbf{continual\_start} \; (\,) \; \to dict$ 

**Start Continual Training** 

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

### **Parameter**

### rtype

A dict containing information about the training and/or evaluation

# dicee.knowledge\_graph

### **Classes**

KG Knowledge Graph

# **Module Contents**

```
num_relations = None
path_single_kg
path_for_deserialization
add_reciprical
eval_model
read_only_few
sample_triples_ratio
path_for_serialization
entity_to_idx
relation_to_idx
backend
training_technique
idx_entity_to_bpe_shaped
enc
num_tokens
num_bpe_entities = None
padding
dummy_id
max_length_subword_tokens = None
train_set_target = None
target_dim = None
train_target_indices = None
ordered_bpe_entities = None
property entities_str: List
property relations_str: List
func_triple_to_bpe_representation(triple: List[str])
```

# dicee.knowledge\_graph\_embeddings

### **Classes**

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

### **Module Contents**

```
class dicee.knowledge_graph_embeddings.KGE (path=None, url=None,
            construct ensemble=False, model name=None)
     Bases: dicee.abstracts.BaseInteractiveKGE
     Knowledge Graph Embedding Class for interactive usage of pre-trained models
     __str__()
           Return str(self).
     to (device: str) \rightarrow None
     get_transductive_entity_embeddings (indices: torch.LongTensor | List[str],
                  as_pytorch=False, as_numpy=False, as_list=True)
                   → torch.FloatTensor | numpy.ndarray | List[float]
     create_vector_database (collection_name: str, distance: str, location: str = 'localhost',
                  port: int = 6333)
     generate (h=", r=")
     eval_lp_performance (dataset=List[Tuple[str, str, str]], filtered=True)
     predict_missing_head_entity (relation: List[str] | str, tail_entity: List[str] | str, within=None)
                   \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)

→ 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  $\rightarrow$  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

```
 \begin{aligned} \textbf{predict} \ (*, h: List[str] \mid str = None, r: List[str] \mid str = None, t: List[str] \mid str = None, within=None, \\ logits=True) \ \to \text{torch.FloatTensor} \end{aligned}
```

# **Parameters**

- logits
- h

·r

• t

• within

Predict missing item in a given triple.

### **Parameter**

head\_entity: List[str]

String representation of selected entities.

relation: List[str]

String representation of selected relations.

tail\_entity: List[str]

String representation of selected entities.

k: int

Highest ranked k item.

# **Returns: Tuple**

Highest K scores and items

```
\label{eq:core}  \textbf{triple\_score} \ (h: List[str] \mid str = None, \, r: \, List[str] \mid str = None, \, t: \, List[str] \mid str = None, \, logits = False) \\ \rightarrow \text{torch.FloatTensor}
```

Predict triple score

# **Parameter**

head\_entity: List[str]

String representation of selected entities.

relation: List[str]

String representation of selected relations.

tail\_entity: List[str]

String representation of selected entities.

logits: bool

If logits is True, unnormalized score returned

# **Returns: Tuple**

```
pytorch tensor of triple score
t_norm (tens_1: torch. Tensor, tens_2: torch. Tensor, tnorm: str = 'min') \rightarrow torch. Tensor
tensor_t_norm (subquery\_scores: torch.FloatTensor, tnorm: str = 'min') \rightarrow torch.FloatTensor
     Compute T-norm over [0,1] ^{n imes d} where n denotes the number of hops and d denotes number of
     entities
t_conorm (tens_1: torch.Tensor, tens_2: torch.Tensor, tconorm: str = 'min') \rightarrow torch.Tensor
negnorm (tens 1: torch.Tensor, lambda: float, neg norm: str = 'standard') \rightarrow torch.Tensor
return multi hop query results (aggregated query for all entities, k: int, only scores)
single_hop_query_answering (query: tuple, only_scores: bool = True, k: int = None)
answer_multi_hop_query (query_type: str = None,
             query: Tuple[str | Tuple[str, str], Ellipsis] = None,
             queries: List[Tuple[str | Tuple[str, str], Ellipsis]] = None, tnorm: str = 'prod',
             neg_norm: str = 'standard', lambda_: float = 0.0, k: int = 10, only_scores=False)
              \rightarrow 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) | f(e,r,x) > confidence land (e,r,x)}
otin G

deploy (share: bool = False, top_k: int = 10)

train_triples (h: List[str], r: List[str], t: List[str], labels: List[float], iteration=2, optimizer=None)

train_k_vs_all (h, r, iteration=1, lr=0.001)
Train k vs all :param head_entity: :param relation: :param iteration: :param lr: :return:

train (kg, lr=0.1, epoch=10, batch_size=32, neg_sample_ratio=10, num_workers=1) → None
Retrained a pretrain model on an input KG via negative sampling.
```

# dicee.query\_generator

### **Classes**

QueryGenerator

### **Module Contents**

```
rel2id: Dict
ent_in: Dict
ent_out: Dict
query_name_to_struct
list2tuple (list_data)
tuple2list (x: List | Tuple) \rightarrow List | Tuple
     Convert a nested tuple to a nested list.
set_global_seed (seed: int)
     Set seed
construct_graph (paths: List[str]) → Tuple[Dict, Dict]
     Construct graph from triples Returns dicts with incoming and outgoing edges
fill_query (query_structure: List[str | List], ent_in: Dict, ent_out: Dict, answer: int) → bool
     Private method for fill_query logic.
achieve_answer (query: List[str | List], ent_in: Dict, ent_out: Dict) → set
     Private method for achieve_answer logic. @TODO: Document the code
write links(ent out, small ent out)
ground_queries (query_structure: List[str | List], ent_in: Dict, ent_out: Dict, small_ent_in: Dict,
            small_ent_out: Dict, gen_num: int, query_name: str)
     Generating queries and achieving answers
unmap (query_type, queries, tp_answers, fp_answers, fn_answers)
unmap_query (query_structure, query, id2ent, id2rel)
generate_queries (query_struct: List, gen_num: int, query_type: str)
     Passing incoming and outgoing edges to ground queries depending on mode [train valid or text] and getting
     queries and answers in return @ TODO: create a class for each single query struct
save_queries (query_type: str, gen_num: int, save_path: str)
abstract load_queries(path)
get_queries (query_type: str, gen_num: int)
static save queries and answers (path: str,
            data: List[Tuple[str, Tuple[collections.defaultdict]]]) \rightarrow None
     Save Queries into Disk
static load_queries_and_answers(path: str)
             → List[Tuple[str, Tuple[collections.defaultdict]]]
     Load Queries from Disk to Memory
```

# dicee.sanity\_checkers

### **Functions**

### **Module Contents**

```
dicee.sanity_checkers.is_sparql_endpoint_alive (sparql_endpoint: str = None)
dicee.sanity_checkers.validate_knowledge_graph (args)
    Validating the source of knowledge graph
dicee.sanity_checkers.sanity_checking_with_arguments (args)
```

# dicee.static\_funcs

# **Functions**

Add inverse triples into dask dataframe
Load weights and initialize pytorch module from namespace arguments
Construct Ensemble Of weights and initialize pytorch module from namespace arguments
Detect most efficient data type for a given triples
Store Pytorch model into disk
Store trained_model model and save embeddings into csv file.

continues on next page

Table 2 - continued from previous page

```
add\_noisy\_triples(\rightarrow pandas.DataFrame)
                                                     Add randomly constructed triples
read_or_load_kg(args, cls)
intialize model(\rightarrow Tuple[object, str])
load_json(\rightarrow dict)
                                                     Save it as CSV if memory allows.
save\_embeddings(\rightarrow None)
random_prediction(pre_trained_kge)
deploy_triple_prediction(pre_trained_kge,
str_subject, ...)
deploy_tail_entity_prediction(pre_trained_)
deploy_head_entity_prediction(pre_trained_)
deploy_relation_prediction(pre_trained_kge,
...)
vocab_to_parquet(vocab_to_idx, name, ...)
create experiment folder([folder name])
continual_training_setup_executor(→
                                                     storage_path:str A path leading to a parent directory,
None)
                                                     where a subdirectory containing KGE related data
exponential\_function(\rightarrow torch.FloatTensor)
load_numpy(\rightarrow numpy.ndarray)
evaluate(entity_to_idx,
                                                     # @TODO: CD: Renamed this function
                            scores,
                                      easy_answers,
hard_answers)
download_file(url[, destination_folder])
download\_files\_from\_url(\rightarrow None)
download\_pretrained\_model(\rightarrow str)
```

### **Module Contents**

```
dicee.static_funcs.create_recipriocal_triples(x)
    Add inverse triples into dask dataframe :param x: :return:
dicee.static_funcs.get_er_vocab(data, file_path: str = None)
dicee.static_funcs.get_re_vocab(data, file_path: str = None)
dicee.static_funcs.get_ee_vocab(data, file_path: str = None)
dicee.static_funcs.timeit(func)
dicee.static_funcs.save_pickle(*, data: object = None, file_path=str)
```

```
dicee.static_funcs.load_pickle(file_path=str)
dicee.static_funcs.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) \rightarrow Tuple[object, Tuple[dict, dict]]
     Load weights and initialize pytorch module from namespace arguments
dicee.static_funcs.load_model_ensemble(path_of_experiment_folder: str)
             → Tuple[dicee.models.base_model.BaseKGE, Tuple[pandas.DataFrame, pandas.DataFrame]]
     Construct Ensemble Of weights and initialize pytorch module from namespace arguments
       (1) Detect models under given path
      (2) Accumulate parameters of detected models
       (3) Normalize parameters
       (4) Insert (3) into model.
dicee.static_funcs.save_numpy_ndarray(*, data: numpy.ndarray, file_path: str)
dicee.static_funcs.numpy_data_type_changer(train_set: numpy.ndarray, num: int)
             \rightarrow numpy.ndarray
     Detect most efficient data type for a given triples :param train_set: :param num: :return:
dicee.static\_funcs.save\_checkpoint\_model(model, path: str) \rightarrow None
     Store Pytorch model into disk
dicee.static_funcs.store(trainer, trained_model, model_name: str = 'model',
            full\_storage\_path: str = None, save\_embeddings\_as\_csv=False) \rightarrow None
     Store trained_model model and save embeddings into csv file. :param trainer: an instance of trainer class :param
     full storage path: path to save parameters. :param model name: string representation of the name of the model.
     :param trained_model: an instance of BaseKGE see core.models.base_model . :param save_embeddings_as_csv:
     for easy access of embeddings. :return:
dicee.static_funcs.add_noisy_triples(train_set: pandas.DataFrame, add_noise_rate: float)
             \rightarrow pandas.DataFrame
     Add randomly constructed triples :param train_set: :param add_noise_rate: :return:
dicee.static_funcs.read_or_load_kg(args, cls)
dicee.static_funcs.intialize_model(args: dict, verbose=0) → 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,
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)
```

```
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
     storage_path:str A path leading to a parent directory, where a subdirectory containing KGE related data
     full_storage_path:str A path leading to a subdirectory containing KGE related data
dicee.static_funcs.exponential_function(x: numpy.ndarray, lam: float,
           ascending order=True) \rightarrow torch.FloatTensor
dicee.static_funcs.load_numpy(path) → numpy.ndarray
dicee.static_funcs.evaluate(entity_to_idx, scores, easy_answers, hard_answers)
     # @TODO: CD: Renamed this function Evaluate multi hop query answering on different query types
dicee.static_funcs.download_file (url, destination_folder='.')
dicee.static_funcs.download_files_from_url(base_url: str, destination_folder='.') \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-KvsAll")
```

dicee.static\_funcs.deploy\_relation\_prediction(pre\_trained\_kge, str\_subject, str\_object,

### dicee.static funcs training

### **Functions**

```
evaluate_lp(model, triple_idx, num_entities, Evaluate model in a standard link prediction task er_vocab, ...)
evaluate_bpe_lp(model, triple_idx, ...[, info])
efficient_zero_grad(model)
```

# **Module Contents**

```
dicee.static_funcs_training.evaluate_lp (model, triple_idx, num_entities, er_vocab: Dict[Tuple, List], re_vocab: Dict[Tuple, List], info='Eval Starts')
```

dicee.static\_funcs.download\_pretrained\_model(url: str)  $\rightarrow str$ 

Evaluate model in a standard link prediction task

for each triple the rank is computed by taking the mean of the filtered missing head entity rank and the filtered missing tail entity rank :param model: :param triple\_idx: :param info: :return:

# dicee.static\_preprocess\_funcs

### **Attributes**

```
enable_log
```

### **Functions**

### **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)
```

# 14.3 Attributes

version			

# 14.4 Classes

OM71	C1 (0.0) > D1 N
CMult	Cl_(0,0) => Real Numbers
Pyke	A Physical Embedding Model for Knowledge Graphs
DistMult	Embedding Entities and Relations for Learning and Infer-
	ence in Knowledge Bases
KeciBase	Without learning dimension scaling
Keci	Base class for all neural network modules.
TransE	Translating Embeddings for Modeling
DeCaL	Base class for all neural network modules.
DualE	Dual Quaternion Knowledge Graph Embeddings (https://ojs.aaai.org/index.php/AAAI/article/download/ 16850/16657)
ComplEx	Base class for all neural network modules.
AConEx	Additive Convolutional ComplEx Knowledge Graph Embeddings
AConv0	Additive Convolutional Octonion Knowledge Graph Embeddings
AConvQ	Additive Convolutional Quaternion Knowledge Graph Embeddings
ConvQ	Convolutional Quaternion Knowledge Graph Embeddings
ConvO	Base class for all neural network modules.
ConEx	Convolutional ComplEx Knowledge Graph Embeddings
QMult	Base class for all neural network modules.
OMult	Base class for all neural network modules.
Shallom	A shallow neural model for relation prediction (https://arxiv.org/abs/2101.09090)
LFMult	Embedding with polynomial functions. We represent all entities and relations in the polynomial space as:
PykeenKGE	A class for using knowledge graph embedding models implemented in Pykeen
BytE	Base class for all neural network modules.
BaseKGE	Base class for all neural network modules.
DICE_Trainer	DICE_Trainer implement
KGE	Knowledge Graph Embedding Class for interactive usage
	of pre-trained models
Execute	A class for Training, Retraining and Evaluation a model.
BPE_NegativeSamplingDataset	An abstract class representing a Dataset.

continues on next page

Table 3 - continued from previous page

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.
<i>KvsSampleDataset</i>	KvsSample a Dataset:
NegSampleDataset	An abstract class representing a Dataset.
TriplePredictionDataset	Triple Dataset
CVDataModule	Create a Dataset for cross validation
QueryGenerator	

# 14.5 Functions

create_recipriocal_triples(x)	Add inverse triples into dask dataframe
<pre>get_er_vocab(data[, file_path])</pre>	
<pre>get_re_vocab(data[, file_path])</pre>	
<pre>get_ee_vocab(data[, file_path])</pre>	
timeit(func)	
<pre>save_pickle(*[, data, file_path])</pre>	
load_pickle([file_path])	
<pre>select_model(args[, is_continual_training, stor- age_path])</pre>	
<pre>load_model(→ Tuple[object, Tuple[dict, dict]])</pre>	Load weights and initialize pytorch module from namespace arguments
<pre>load_model_ensemble()</pre>	Construct Ensemble Of weights and initialize pytorch module from namespace arguments
<pre>save_numpy_ndarray(*, data, file_path)</pre>	
$numpy\_data\_type\_changer(\rightarrow numpy.ndarray)$ $save\_checkpoint\_model(\rightarrow None)$	Detect most efficient data type for a given triples Store Pytorch model into disk
store(→ None)	Store trained_model model and save embeddings into csv file.
$add\_noisy\_triples(\rightarrow pandas.DataFrame)$	Add randomly constructed triples
read_or_load_kg(args, cls)	
$intialize\_model(\rightarrow Tuple[object, str])$	
$load_json(\rightarrow dict)$	
save_embeddings(→ None)	Save it as CSV if memory allows.

continues on next page

Table 4 - continued from previous page

```
random_prediction(pre_trained_kge)
deploy_triple_prediction(pre_trained_kge,
str subject, ...)
deploy_tail_entity_prediction(pre_trained_)
deploy_head_entity_prediction(pre_trained_)
deploy_relation_prediction(pre_trained_kge,
vocab_to_parquet(vocab_to_idx, name, ...)
create_experiment_folder([folder_name])
                                                    storage_path:str A path leading to a parent directory,
continual_training_setup_executor(→
                                                    where a subdirectory containing KGE related data
exponential\_function(\rightarrow torch.FloatTensor)
load_numpy(→ numpy.ndarray)
                                                    # @TODO: CD: Renamed this function
evaluate(entity to idx,
                                     easy answers,
hard answers)
download_file(url[, destination_folder])
download\_files\_from\_url(\rightarrow None)
download\_pretrained\_model(\rightarrow str)
mapping_from_first_two_cols_to_third(tra
timeit(func)
load_pickle([file_path])
reload_dataset(path, form_of_labelling, ...)
                                                    Reload the files from disk to construct the Pytorch dataset
construct\_dataset(\rightarrow torch.utils.data.Dataset)
```

# 14.6 Package Contents

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

Cl_(0,0) => Real Numbers

Cl_(0,1) =>
A multivector mathbf{a} = a_0 + a_1 e_1 A multivector mathbf{b} = b_0 + b_1 e_1
multiplication is isomorphic to the product of two complex numbers

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

```
C1 (2,0) =>
           A multivector mathbf\{a\} = a_0 + a_1 e_1 + a_2 e_2 + a_4\{12\} e_1 e_2 A multivector mathbf\{b\} = b_0 +
           b_1 e_1 + b_2 e_2 + b_{12} e_1 e_2
           mathbf{a} imes mathbf{b} = a_0b_0 + a_0b_1 e_1 + a_0b_2 e_2 + a_0 b_1 e_1 e_2
                 • a 1 b 0 e 1 + a 1b 1 e 1 e1...
     C1 (0,2) \Rightarrow Quaternions
     name = 'CMult'
     entity_embeddings
     relation_embeddings
     р
     q
     clifford_mul(x: torch.FloatTensor, y: torch.FloatTensor, p: int, q: int) \rightarrow tuple
               Clifford multiplication Cl_{p,q} (mathbb{R})
               ei ^2 = +1 for i =< i =< p ej ^2 = -1 for p < j =< p+q ei ej = -eje1 for i
           eq j
               x: torch.FloatTensor with (n,d) shape
               y: torch.FloatTensor with (n,d) shape
               p: a non-negative integer p \ge 0 q: a non-negative integer q \ge 0
     score (head_ent_emb, rel_ent_emb, tail_ent_emb)
     forward\_triples (x: torch.LongTensor) \rightarrow torch.FloatTensor
           Compute batch triple scores
           Parameter
           x: torch.LongTensor with shape n by 3
               rtvpe
                   torch.LongTensor with shape n
     forward_k_vs_all (x: torch.Tensor) \rightarrow torch.FloatTensor
           Compute batch KvsAll triple scores
           Parameter
           x: torch.LongTensor with shape n by 3
               rtype
                   torch.LongTensor with shape n
class dicee.Pyke(args)
     Bases: dicee.models.base_model.BaseKGE
     A Physical Embedding Model for Knowledge Graphs
```

```
name = 'Pyke'
     dist_func
     margin = 1.0
     forward_triples (x: torch.LongTensor)
             Parameters
class dicee.DistMult(args)
     Bases: dicee.models.base_model.BaseKGE
     Embedding Entities and Relations for Learning and Inference in Knowledge Bases https://arxiv.org/abs/1412.6575
     name = 'DistMult'
     k_vs_all_score (emb_h: torch.FloatTensor, emb_r: torch.FloatTensor, emb_E: torch.FloatTensor)
             Parameters
                 • emb h
                 • emb_r
                 • emb E
     forward_k_vs_all (x: torch.LongTensor)
     forward_k_vs_sample (x: torch.LongTensor, target_entity_idx: torch.LongTensor)
     score(h, r, t)
class dicee.KeciBase(args)
     Bases: Keci
     Without learning dimension scaling
     name = 'KeciBase'
     requires_grad_for_interactions = False
class dicee.Keci(args)
     Bases: dicee.models.base model.BaseKGE
     Base class for all neural network modules.
```

Your models should also subclass this class.

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

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

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

(continues on next page)

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

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

# 1 Note

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

### Variables

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

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

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

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

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

### for j in range(q):

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

print(sigma\_pq.shape)

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

Multiplying a base vector with its scalar coefficient

# clifford\_multiplication (h0, hp, hq, r0, rp, rq)

Compute our CL multiplication

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

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

eq j

$$\label{eq:hr} h\;r = sigma\_0 + sigma\_p + sigma\_q + sigma\_\{pp\} + sigma\_\{q\} + sigma\_\{pq\}\; where$$

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

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

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

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

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

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

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

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

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

### **Parameter**

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

### returns

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

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

**k** vs all score (bpe head ent emb, bpe rel ent emb, E)

```
forward_k_vs_all (x: torch.Tensor) \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}(\mathbf{mathbb}_{R}^{d}).
           (3) Perform Cl multiplication
           (4) Inner product of (3) and all entity embeddings
           forward_k_vs_with_explicit and this funcitons are identical Parameter — x: torch.LongTensor with
           (n,2) shape :rtype: torch.FloatTensor with (n, |E|) shape
      forward_k_vs_sample (x: torch.LongTensor, target_entity_idx: torch.LongTensor)
                   \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}(\mathbf{mathbb}_{R}^{d}).
           (3) Perform Cl multiplication
           (4) Inner product of (3) and all entity embeddings
           Parameter
           x: torch.LongTensor with (n,2) shape
                rtype
                    torch.FloatTensor with (n, |E|) shape
      score(h, r, t)
      forward_triples (x: torch.Tensor) \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: dicee.models.base\_model.BaseKGE

Base class for all neural network modules.

Your models should also subclass this class.

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

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

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

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

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

# **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))

compute\_sigmas\_single (list\_h\_emb, list\_r\_emb, list\_t\_emb)

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

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

and return:

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

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

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

For same bases vectors interaction we have

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

For different base vector interactions, we have

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

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

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):

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

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

**kvsall\_score** (*e\_1\_h*, *e\_2\_h*, *e\_3\_h*, *e\_4\_h*, *e\_5\_h*, *e\_6\_h*, *e\_7\_h*, *e\_8\_h*, *e\_1\_t*, *e\_2\_t*, *e\_3\_t*, *e\_4\_t*, *e\_5\_t*, *e\_6\_t*, *e\_7\_t*, *e\_8\_t*, *r\_1*, *r\_2*, *r\_3*, *r\_4*, *r\_5*, *r\_6*, *r\_7*, *r\_8*)  $\rightarrow$  torch.tensor

KvsAll scoring function

# Input

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

# **Output**

```
torch.FloatTensor with (n) shape
```

```
forward_triples (idx\_triple: torch.tensor) \rightarrow torch.tensor
```

Negative Sampling forward pass:

# Input

x: torch.LongTensor with (n, ) shape

# **Output**

torch.FloatTensor with (n) shape

```
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 to nest them in a tree structure. You can assign the submodules as regular attributes:

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

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

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

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

# 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
```

```
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],
```

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:

*C*\_2: *Tuple*[torch.Tensor, torch.Tensor])  $\rightarrow$  torch.FloatTensor

```
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()
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
     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<sub>()</sub>
class dicee.ConvQ(args)
     Bases: dicee.models.base_model.BaseKGE
     Convolutional Quaternion Knowledge Graph Embeddings
     name = 'ConvQ'
     entity_embeddings
     relation_embeddings
     conv2d
     fc_num_input
     fc1
     bn_conv1
     bn_conv2
     feature_map_dropout
     residual_convolution (Q_1, Q_2)
     forward\_triples (indexed_triple: torch.Tensor) \rightarrow torch.Tensor
               Parameters
                   x
     forward_k_vs_all (x: torch.Tensor)
          Given a head entity and a relation (h,r), we compute scores for all entities. [score(h,r,x)|x in Entities] =>
          [0.0,0.1,...,0.8], shape=> (1, |Entities|) Given a batch of head entities and relations => shape (size of batch,|
          Entities()
class dicee.ConvO(args: dict)
     Bases: dicee.models.base_model.BaseKGE
     Base class for all neural network modules.
     Your models should also subclass this class.
```

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

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

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

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

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

# 1 Note

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

### **Variables**

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

```
name = 'ConvO'
conv2d
fc_num_input
fc1
bn_conv2d
norm_fc1
feature_map_dropout
static octonion_normalizer(emb_rel_e0, emb_rel_e1, emb_rel_e2, emb_rel_e3, emb_rel_e4,
            emb_rel_e5, emb_rel_e6, emb_rel_e7)
residual_convolution (O_1, O_2)
forward\_triples(x: torch.Tensor) \rightarrow torch.Tensor
         Parameters
forward_k_vs_all (x: torch.Tensor)
     Given a head entity and a relation (h,r), we compute scores for all entities. [score(h,r,x)|x in Entities] =>
     [0.0,0.1,...,0.8], shape=> (1, |Entities|) Given a batch of head entities and relations => shape (size of batch,)
     Entities()
```

```
class dicee.ConEx(args)
```

Bases: dicee.models.base\_model.BaseKGE

Convolutional ComplEx Knowledge Graph Embeddings

```
name = 'ConEx'
     conv2d
     fc_num_input
     fc1
     norm_fc1
     bn_conv2d
     feature map dropout
     residual_convolution (C_1: Tuple[torch.Tensor, torch.Tensor],
                  C_2: Tuple[torch.Tensor, torch.Tensor]) \rightarrow torch.FloatTensor
          Compute residual score of two complex-valued embeddings. :param C_1: a tuple of two pytorch tensors
          that corresponds complex-valued embeddings :param C_2: a tuple of two pytorch tensors that corresponds
          complex-valued embeddings :return:
     forward_k_vs_all(x: torch.Tensor) \rightarrow torch.FloatTensor
     forward_triples (x: torch.Tensor) \rightarrow torch.FloatTensor
               Parameters
     forward_k_vs_sample (x: torch.Tensor, target_entity_idx: torch.Tensor)
class dicee.QMult(args)
     Bases: dicee.models.base model.BaseKGE
     Base class for all neural network modules.
```

Your models should also subclass this class.

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

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

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

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

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

## 1 Note

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

### Variables

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

name = 'QMult'

explicit = True

 $quaternion_multiplication_followed_by_inner_product(h, r, t)$ 

### **Parameters**

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

### **Returns**

Triple scores.

**static quaternion\_normalizer** (*x: torch.FloatTensor*) → torch.FloatTensor

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

Absolute value of a quaternion

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

L2 norm of quaternion vector:

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

### **Parameters**

 $\mathbf{x}$  – The vector.

### Returns

The normalized vector.

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

# **Parameters**

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

forward\_k\_vs\_all(x)

# **Parameters**

x

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

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

```
class dicee.OMult(args)
```

Bases: dicee.models.base\_model.BaseKGE

Base class for all neural network modules.

Your models should also subclass this class.

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

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

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

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

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

# 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 width
```

```
shallom
     get_embeddings() → Tuple[numpy.ndarray, None]
     forward_k_vs_all (x) \rightarrow \text{torch.FloatTensor}
     forward_triples (x) \rightarrow \text{torch.FloatTensor}
               Parameters
                   x
               Returns
class dicee.LFMult(args)
     Bases: dicee.models.base_model.BaseKGE
     Embedding with polynomial functions. We represent all entities and relations in the polynomial space as: f(x) =
     sum_{i=0}^{d-1} a_k x^{i\%d} and use the three differents scoring function as in the paper to evaluate the score.
     We also consider combining with Neural Networks.
     name = 'LFMult'
     entity_embeddings
     relation embeddings
     degree
     m
     x_values
     forward_triples (idx_triple)
               Parameters
                   x
     construct_multi_coeff(x)
     poly_NN(x, coefh, coefr, coeft)
           Constructing a 2 layers NN to represent the embeddings. h = sigma(wh^T x + bh), r = sigma(wr^T x + br),
           t = sigma(wt^T x + bt)
     linear(x, w, b)
     scalar_batch_NN(a, b, c)
           element wise multiplication between a,b and c: Inputs: a, b, c ====> torch.tensor of size batch_size x m x
           d Output: a tensor of size batch size x d
     tri_score (coeff_h, coeff_r, coeff_t)
           this part implement the trilinear scoring techniques:
           score(h,r,t) = int_{0}{1} h(x)r(x)t(x) dx = sum_{i,j,k} = 0}^{d-1} dfrac{a_i*b_j*c_k}{1+(i+j+k)%d}
            1. generate the range for i,j and k from [0 d-1]
           2. perform dfrac\{a_i*b_j*c_k\}\{1+(i+j+k)\%d\} in parallel for every batch
            3. take the sum over each batch
```

```
vtp\_score(h, r, t)
```

this part implement the vector triple product scoring techniques:

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

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

```
comp_func(h, r, t)
```

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

```
polynomial (coeff, x, degree)
```

This function takes a matrix tensor of coefficients (coeff), a tensor vector of points x and range of integer [0,1,...d] and return a vector tensor (coeff $[0][0] + \text{coeff}[0][1]x + ... + \text{coeff}[0][d]x^d$ ,

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

```
pop (coeff, x, degree)
```

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

```
and return a tensor (coeff[0][0] + coeff[0][1]x + ... + coeff[0][d]x^d, coeff[1][0] + coeff[1][1]x + ... + coeff[1][d]x^d)
```

```
class dicee.PykeenKGE (args: dict)
```

Bases: dicee.models.base\_model.BaseKGE

A class for using knowledge graph embedding models implemented in Pykeen

Notes: Pykeen\_DistMult: C Pykeen\_ComplEx: Pykeen\_QuatE: Pykeen\_MuRE: Pykeen\_CP: Pykeen\_HolE: Pykeen\_HolE: Pykeen\_HolE:

```
model_kwargs
```

name

model

loss\_history = []

args

entity\_embeddings = None

relation\_embeddings = None

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

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

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

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

# (3) Reshape all entities. if self.last\_dim > 0:

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

#### else:

 $t = self.entity\_embeddings.weight$ 

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

```
forward_triples (x: torch.LongTensor) \rightarrow torch.FloatTensor
```

- # => Explicit version by this we can apply bn and dropout
- # (1) Retrieve embeddings of heads, relations and tails and apply Dropout & Normalization if given. h, r, t = self.get\_triple\_representation(x) # (2) Reshape (1). if self.last\_dim > 0:

```
\label{eq:hammed} 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) \\ t = t.t. \\ t = t.
```

# (3) Compute the triple score return self.interaction.score(h=h, r=r, t=t, slice\_size=None, slice\_dim=0)

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

```
class dicee.BytE(*args, **kwargs)
```

Bases: dicee.models.base\_model.BaseKGE

Base class for all neural network modules.

Your models should also subclass this class.

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

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

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

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

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

# 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'

generate (idx, max\_new\_tokens, temperature=1.0, top\_k=None)

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

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

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

### **Parameters**

- batch The output of your data iterable, normally a DataLoader.
- batch\_idx The index of this batch.
- dataloader\_idx The index of the dataloader that produced this batch. (only if multiple dataloaders used)

#### Returns

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

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

#### Example:

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

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

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

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

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

# **1** Note

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

### class dicee.BaseKGE (args: dict)

Bases: BaseKGELightning

Base class for all neural network modules.

Your models should also subclass this class.

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

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

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

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

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

# 1 Note

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

# Variables

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

```
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
                  \mathbf{x} (B \times 2 \times T)
     \texttt{get\_embeddings} \ () \ \to Tuple[numpy.ndarray, numpy.ndarray]
dicee.create_recipriocal_triples(x)
     Add inverse triples into dask dataframe :param x: :return:
dicee.get_er_vocab (data, file_path: str = None)
dicee.get_re_vocab (data, file_path: str = None)
dicee.get_ee_vocab (data, file_path: str = None)
dicee.timeit(func)
dicee.save_pickle(*, data: object = None, file_path=str)
```

```
dicee.load_pickle(file_path=str)
dicee.select_model (args: dict, is_continual_training: bool = None, storage_path: str = None)
dicee.load_model(path_of_experiment_folder: str, model_name='model.pt', verbose=0)
             → Tuple[object, Tuple[dict, dict]]
     Load weights and initialize pytorch module from namespace arguments
dicee.load_model_ensemble(path_of_experiment_folder: str)
             → Tuple[dicee.models.base model.BaseKGE, Tuple[pandas.DataFrame, pandas.DataFrame]]
     Construct Ensemble Of weights and initialize pytorch module from namespace arguments
       (1) Detect models under given path
      (2) Accumulate parameters of detected models
       (3) Normalize parameters
       (4) Insert (3) into model.
dicee.save_numpy_ndarray(*, data: numpy.ndarray, file_path: str)
dicee.numpy_data_type_changer(train_set: numpy.ndarray, num: int) → numpy.ndarray
     Detect most efficient data type for a given triples :param train_set: :param num: :return:
dicee.save_checkpoint_model(model, path: str) → None
     Store Pytorch model into disk
dicee.store(trainer, trained_model, model_name: str = 'model', full_storage_path: str = None,
            save\_embeddings\_as\_csv=False) \rightarrow None
     Store trained_model model and save embeddings into csv file. :param trainer: an instance of trainer class :param
     full storage path: path to save parameters. :param model name: string representation of the name of the model.
     :param trained_model: an instance of BaseKGE see core.models.base_model . :param save_embeddings_as_csv:
     for easy access of embeddings. :return:
dicee.add_noisy_triples(train_set: pandas.DataFrame, add_noise_rate: float) \rightarrow pandas.DataFrame
     Add randomly constructed triples :param train_set: :param add_noise_rate: :return:
dicee.read_or_load_kg(args, cls)
dicee.intialize_model(args: dict, verbose=0) → Tuple[object, str]
dicee.load_json(p: str) \rightarrow dict
dicee.save_embeddings (embeddings: numpy.ndarray, indexes, path: str) \rightarrow None
     Save it as CSV if memory allows. :param embeddings: :param indexes: :param path: :return:
dicee.random_prediction(pre_trained_kge)
dicee.deploy_triple_prediction(pre_trained_kge, str_subject, str_predicate, str_object)
dicee.deploy_tail_entity_prediction(pre_trained_kge, str_subject, str_predicate, top_k)
dicee.deploy head entity prediction (pre_trained_kge, str_object, str_predicate, top_k)
dicee.deploy_relation_prediction(pre_trained_kge, str_subject, str_object, top_k)
dicee.vocab_to_parquet (vocab_to_idx, name, path_for_serialization, print_into)
dicee.create_experiment_folder(folder_name='Experiments')
```

```
dicee.continual_training_setup_executor(executor) \rightarrow None
     storage_path:str A path leading to a parent directory, where a subdirectory containing KGE related data
     full_storage_path:str A path leading to a subdirectory containing KGE related data
dicee.exponential_function(x: numpy.ndarray, lam: float, ascending_order=True)
             \rightarrow torch.FloatTensor
dicee.load_numpy(path) \rightarrow numpy.ndarray
dicee.evaluate(entity_to_idx, scores, easy_answers, hard_answers)
     # @TODO: CD: Renamed this function Evaluate multi hop query answering on different query types
dicee.download_file (url, destination_folder='.')
dicee.download_files_from_url(base\_url: str, destination\_folder='.') \rightarrow None
          Parameters
                • base_url
                                                 "https://files.dice-research.org/projects/DiceEmbeddings/
                  KINSHIP-Keci-dim128-epoch256-KvsAll")
                • destination folder(e.g. "KINSHIP-Keci-dim128-epoch256-KvsA11")
dicee.download_pretrained_model(url: str) \rightarrow str
class dicee.DICE_Trainer(args, is_continual_training, storage_path, evaluator=None)
     DICE_Trainer implement
          1- Pytorch Lightning trainer (https://pytorch-lightning.readthedocs.io/en/stable/common/trainer.html)
          2- Multi-GPU Trainer(https://pytorch.org/docs/stable/generated/torch.nn.parallel.DistributedDataParallel.
          html) 3- CPU Trainer
          args
          is_continual_training:bool
          storage path:str
          evaluator:
          report:dict
     report
     args
     trainer = None
     is_continual_training
     storage_path
     evaluator
     form_of_labelling = None
     continual_start()
           (1) Initialize training.
           (2) Load model
          (3) Load trainer (3) Fit model
```

#### **Parameter**

#### returns

- model
- form of labelling (str)

```
initialize_trainer (callbacks: List) → lightning.Trainer
```

Initialize Trainer from input arguments

```
initialize_or_load_model()
```

initialize\_dataloader (dataset: torch.utils.data.Dataset) → torch.utils.data.DataLoader

```
\verb|initialize_dataset|| \textit{dataset}: \textit{dicee.knowledge\_graph.KG}, \textit{form\_of\_labelling})|
```

→ torch.utils.data.Dataset

 $\textbf{start} \ (\textit{knowledge\_graph: dicee.knowledge\_graph.KG}) \ \rightarrow \textbf{Tuple}[\textit{dicee.models.base\_model.BaseKGE}, \textbf{str}]$ 

Train selected model via the selected training strategy

 $k\_fold\_cross\_validation$  (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
```

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

 $\rightarrow$  torch.FloatTensor | numpy.ndarray | List[float]

 $create\_vector\_database$  (collection\\_name: str, distance: str, location: str = 'localhost', port: int = 6333)

```
\mathtt{generate}\;(h=",\,r=")
```

```
eval_lp_performance (dataset=List[Tuple[str, str, str]], filtered=True)
predict_missing_head_entity (relation: List[str] | str, tail_entity: List[str] | str, within=None)
              \rightarrow Tuple
     Given a relation and a tail entity, return top k ranked head entity.
     argmax_{e} in E \} f(e,r,t), where r in R, t in E.
     Parameter
     relation: Union[List[str], str]
     String representation of selected relations.
     tail_entity: Union[List[str], str]
     String representation of selected entities.
     k: int
     Highest ranked k entities.
     Returns: Tuple
     Highest K scores and entities
predict_missing_relations (head_entity: List[str] | str, tail_entity: List[str] | str, within=None)
              \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 \rightarrow torch.FloatTensor
     Given a head entity and a relation, return top k ranked entities
```

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

# **Parameter**

```
head_entity: List[str]
```

String representation of selected entities.

```
tail_entity: List[str]
```

String representation of selected entities.

# **Returns: Tuple**

scores

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

# **Parameters**

- logits
- h
- r
- t
- within

Predict missing item in a given triple.

# **Parameter**

head\_entity: List[str]

String representation of selected entities.

relation: List[str]

String representation of selected relations.

tail\_entity: List[str]

String representation of selected entities.

k: int

Highest ranked k item.

# **Returns: Tuple**

```
Highest K scores and items
```

```
triple\_score (h: List[str] | str = None, r: List[str] | str = None, t: List[str] | str = None, logits=False) 

\rightarrow torch.FloatTensor

Predict triple score
```

#### **Parameter**

```
head_entity: List[str]
```

String representation of selected entities.

relation: List[str]

String representation of selected relations.

tail\_entity: List[str]

String representation of selected entities.

logits: bool

If logits is True, unnormalized score returned

# **Returns: Tuple**

pytorch tensor of triple score

```
t_norm(tens_1: torch.Tensor, tens_2: torch.Tensor, tnorm: str = 'min') \rightarrow torch.Tensor
```

 $tensor_t_norm$  (subquery\_scores: torch.FloatTensor, tnorm: str = 'min')  $\rightarrow$  torch.FloatTensor

Compute T-norm over [0,1] ^{n imes d} where n denotes the number of hops and d denotes number of entities

```
t_conorm(tens_1: torch.Tensor, tens_2: torch.Tensor, tconorm: str = 'min') \rightarrow torch.Tensor
```

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

return\_multi\_hop\_query\_results (aggregated\_query\_for\_all\_entities, k: int, only\_scores)

single\_hop\_query\_answering (query: tuple, only\_scores: bool = True, k: int = None)

```
answer_multi_hop_query (query_type: str = None,
```

```
query: Tuple[str | Tuple[str, str], Ellipsis] = None,
queries: List[Tuple[str | Tuple[str, str], Ellipsis]] = None, tnorm: str = 'prod',
neg_norm: str = 'standard', lambda_: float = 0.0, k: int = 10, only_scores=False)
→ List[Tuple[str, torch.Tensor]]
```

# @TODO: Refactoring is needed # @TODO: Score computation for each query type should be done in a static function

Find an answer set for EPFO queries including negation and disjunction

#### **Parameter**

```
query_type: str The type of the query, e.g., "2p".
            query: Union[str, Tuple[str, Tuple[str, str]]] The query itself, either a string or a nested tuple.
            queries: List of Tuple[Union[str, Tuple[str, str]], ...]
            tnorm: str The t-norm operator.
            neg_norm: str The negation norm.
            lambda_: float lambda parameter for sugeno and yager negation norms
            k: int The top-k substitutions for intermediate variables.
                 returns
                      • List[Tuple[str, torch.Tensor]]
                      • Entities and corresponding scores sorted in the descening order of scores
      find missing triples (confidence: float, entities: List[str] = None, relations: List[str] = None,
                    topk: int = 10, at_most: int = sys.maxsize) \rightarrow Set
                 Find missing triples
                 Iterative over a set of entities E and a set of relation R:
            orall e in E and orall r in R f(e,r,x)
                 Return (e,r,x)
            otin G and f(e,r,x) > confidence
                 confidence: float
                 A threshold for an output of a sigmoid function given a triple.
                 topk: int
                 Highest ranked k item to select triples with f(e,r,x) > confidence.
                 at_most: int
                 Stop after finding at_most missing triples
                 \{(e,r,x) \mid f(e,r,x) > \text{confidence land } (e,r,x)\}
            otin G
      deploy(share: bool = False, top_k: int = 10)
      train_triples (h: List[str], r: List[str], t: List[str], labels: List[float], iteration=2, optimizer=None)
      train_k_vs_all (h, r, iteration=1, lr=0.001)
            Train k vs all :param head_entity: :param relation: :param iteration: :param lr: :return:
      train (kg, lr=0.1, epoch=10, batch \ size=32, neg \ sample \ ratio=10, num \ workers=1) \rightarrow None
            Retrained a pretrain model on an input KG via negative sampling.
class dicee.Execute(args, continuous_training=False)
      A class for Training, Retraining and Evaluation a model.
       (1) Loading & Preprocessing & Serializing input data.
        (2) Training & Validation & Testing
```

(3) Storing all necessary info
args
is\_continual\_training
trainer = None
trained\_model = None
knowledge\_graph = None
report
evaluator = None
start\_time = None
read\_or\_load\_kg()
read\_preprocess\_index\_serialize\_data() → None
 Read & Preprocess & Index & Serialize Input Data

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

# **Parameter**

rtype

None

 $\textbf{load\_indexed\_data}\,(\,)\,\to None$ 

Load the indexed data from disk into memory

# **Parameter**

rtype

None

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

Save a knowledge graph embedding model

- (1) Send model to eval mode and cpu.
- (2) Store the memory footprint of the model.
- (3) Save the model into disk.
- (4) Update the stats of KG again?

#### **Parameter**

```
rtype
```

None

end (form of labelling: str)  $\rightarrow$  dict

End training

- (1) Store trained model.
- (2) Report runtimes.
- (3) Eval model if required.

#### **Parameter**

#### rtype

A dict containing information about the training and/or evaluation

```
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

```
dicee.mapping_from_first_two_cols_to_third(train_set_idx)
dicee.timeit(func)
```

```
dicee.load pickle(file path=str)
```

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

Reload the files from disk to construct the Pytorch dataset

```
dicee.construct_dataset (*, train_set: numpy.ndarray | list, valid_set=None, test_set=None, ordered_bpe_entities=None, train_target_indices=None, target_dim: int = None, entity_to_idx: dict, relation_to_idx: dict, form_of_labelling: str, scoring_technique: str, neg_ratio: int, label_smoothing_rate: float, byte_pair_encoding=None, block_size: int = None)

→ torch.utils.data.Dataset
```

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 <code>DataLoader</code>. Subclasses could also optionally implement <code>\_\_getitems\_\_</code>(), for speedup batched samples loading. This method accepts list of indices of samples of batch and returns list of samples.



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

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

Bases: torch.utils.data.Dataset

An abstract class representing a Dataset.

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

# **1** Note

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

```
train_set

train_indices_target

target_dim

num_datapoints

torch_ordered_shaped_bpe_entities

collate_fn = None

__len__()
__getitem__(idx)
```

```
block size: int = 8)
     Bases: torch.utils.data.Dataset
     Dataset for the 1vsALL training strategy
          Parameters
                • train_set_idx - Indexed triples for the training.
                • entity_idxs - mapping.
                • relation_idxs - mapping.
                • form - ?
                • num_workers - int for https://pytorch.org/docs/stable/data.html#torch.utils.data.
                  DataLoader
          Return type
              torch.utils.data.Dataset
     train_data
     block_size
     num_of_data_points
     collate_fn = None
     __len__()
     \__{getitem}_{\_}(idx)
class dicee.OnevsAllDataset (train_set_idx: numpy.ndarray, entity_idxs)
     Bases: torch.utils.data.Dataset
     Dataset for the 1vsALL training strategy
          Parameters
                • train_set_idx - Indexed triples for the training.
                • entity_idxs - mapping.
                • relation_idxs - mapping.
                • form - ?
                • num_workers - int for https://pytorch.org/docs/stable/data.html#torch.utils.data.
                  DataLoader
          Return type
              torch.utils.data.Dataset
     train_data
     target_dim
     collate_fn = None
     __len__()
     \underline{\underline{getitem}} (idx)
```

class dicee.MultiClassClassificationDataset (subword\_units: numpy.ndarray,

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



**TODO** 

# train\_set\_idx

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

#### entity idxs

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

# relation\_idxs

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

self: torch.utils.data.Dataset

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

train\_data = None

train\_target = None

label\_smoothing\_rate

collate\_fn = None

\_\_len\_\_() \_\_getitem\_\_(idx)

class dicee.AllvsAll (train\_set\_idx: numpy.ndarray, entity\_idxs, relation\_idxs,

*label\_smoothing\_rate=0.0*)

Bases: torch.utils.data.Dataset

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

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



Note

```
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()
           ? array([0, 1, 2, 3, 4, 5, 6, 7, 8, 9])
     train_data = None
     train_target = None
     label_smoothing_rate
     collate_fn = None
     target_dim
     store
     __len__()
     \__getitem_{\_}(idx)
class dicee. KvsSampleDataset (train_set: numpy.ndarray, num_entities, num_relations,
            neg_sample_ratio: int = None, label_smoothing_rate: float = 0.0)
     Bases: torch.utils.data.Dataset
           KvsSample a Dataset:
               D := \{(x,y)_i\}_i ^N, \text{ where }
                   . x:(h,r) is a unique h in E and a relation r in R and . y in [0,1]^{\{|E|\}} is a binary label.
     orall y_i = 1 s.t. (h r E_i) in KG
               At each mini-batch construction, we subsample(y), hence n
                   lnew_yl << IEI 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.
```

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

without 1s,

```
form
          store
          label smoothing rate
          torch.utils.data.Dataset
     train_data
     num_entities
     num_relations
     neg_sample_ratio
     label_smoothing_rate
     collate_fn = None
     store
     train_target
     __len__()
     \underline{\underline{}}getitem\underline{\underline{}} (idx)
class dicee. NegSampleDataset (train_set: numpy.ndarray, num_entities: int, num_relations: int,
            neg sample ratio: int = 1)
     Bases: torch.utils.data.Dataset
     An abstract class representing a Dataset.
```

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

# **1** Note

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

```
neg_sample_ratio
train_set
length
num_entities
num_relations
```

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

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

An iterable or collection of iterables specifying training samples.

For more information about multiple dataloaders, see this section.

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

For data processing use the following pattern:

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

However, the above are only necessary for distributed processing.

# 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.l1 = nn.Linear(28, data.num_classes)
```

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

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

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

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

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



# 1 Note

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

# **Parameters**

- batch A batch of data that needs to be transferred to a new device.
- **device** The target device as defined in PyTorch.

• dataloader\_idx - The index of the dataloader to which the batch belongs.

#### Returns

A reference to the data on the new device.

# Example:

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

### See also

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

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

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

# 🛕 Warning

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

# Example:

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

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

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

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

#### Example:

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

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

This is called before requesting the dataloaders:

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

```
train_path
val_path
test_path
gen_valid
gen_test
seed
max_ans_num = 1000000.0
mode
ent2id
rel2id: Dict
ent_in: Dict
ent_out: Dict
query_name_to_struct
list2tuple (list_data)
tuple2list (x: List \mid Tuple) \rightarrow List | Tuple
    Convert a nested tuple to a nested list.
```

```
set_global_seed (seed: int)
           Set seed
     construct_graph (paths: List[str]) → Tuple[Dict, Dict]
           Construct graph from triples Returns dicts with incoming and outgoing edges
     fill query (query structure: List[str | List], ent in: Dict, ent out: Dict, answer: int) \rightarrow bool
           Private method for fill_query logic.
     achieve\_answer (query: List[str | List], ent_in: Dict, ent_out: Dict) \rightarrow set
           Private method for achieve_answer logic. @TODO: Document the code
     write_links (ent_out, small_ent_out)
     ground_queries (query_structure: List[str | List], ent_in: Dict, ent_out: Dict, small_ent_in: Dict,
                  small_ent_out: Dict, gen_num: int, query_name: str)
           Generating queries and achieving answers
     unmap (query_type, queries, tp_answers, fp_answers, fn_answers)
     unmap_query (query_structure, query, id2ent, id2rel)
     generate_queries (query_struct: List, gen_num: int, query_type: str)
           Passing incoming and outgoing edges to ground queries depending on mode [train valid or text] and getting
           queries and answers in return @ TODO: create a class for each single query struct
     save_queries (query_type: str, gen_num: int, save_path: str)
     abstract load_queries(path)
     get_queries (query_type: str, gen_num: int)
     static save queries and answers (path: str,
                   data: List[Tuple[str, Tuple[collections.defaultdict]]]) \rightarrow None
           Save Queries into Disk
     static load queries and answers (path: str)
                   → List[Tuple[str, Tuple[collections.defaultdict]]]
           Load Queries from Disk to Memory
dicee.__version__ = '0.1.4'
```

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