DICE Embeddings

Release 0.1.3.2

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Contents:

1	Dicee Manual	2
2	Installation 2.1 Installation from Source	3 3
3	Download Knowledge Graphs	3
4	Knowledge Graph Embedding Models	3
5	How to Train	3
6	Creating an Embedding Vector Database 6.1 Learning Embeddings	5 5 6 6
7	Answering Complex Queries	6
8	Predicting Missing Links	8
9	Downloading Pretrained Models	8
10	How to Deploy	8
11	Docker	8
12	Coverage Report	9
13	How to cite	10
14	14.2 Submodules	

DICE Embeddings¹: 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 Demir²

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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. Pandas³ & Co. to use parallelism at preprocessing a large knowledge graph,
- 2. PyTorch⁴ & Co. to learn knowledge graph embeddings via multi-CPUs, GPUs, TPUs or computing cluster, and
- 3. **Huggingface**⁵ to ease the deployment of pre-trained models.

Why Pandas⁶ & 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 PyTorch⁷ & 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 PyTorch⁸ & PytorchLightning⁹. 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 Gradio¹⁰? Deploy a pre-trained embedding model without writing a single line of code.

¹ https://github.com/dice-group/dice-embeddings

² https://github.com/Demirrr

³ https://pandas.pydata.org/

⁴ https://pytorch.org/

⁵ https://huggingface.co/

⁶ https://pandas.pydata.org/

⁷ https://pytorch.org/

⁸ https://pytorch.org/

⁹ https://www.pytorchlightning.ai/

¹⁰ https://huggingface.co/gradio

2 Installation

2.1 Installation from Source

```
git clone https://github.com/dice-group/dice-embeddings.git conda create -n dice python=3.10.13 --no-default-packages && conda activate dice && \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
```

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

12 Coverage Report

The coverage report is generated using coverage.py¹²:

```
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
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                                                                                                                                             79, 110, _
\hookrightarrow 114
dicee/knowledge_graph_embeddings.py
                                                                                                         636
                                                                                                                     443
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                                                                                                                                             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, _
```

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¹² 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
                                                                       0
                                                                           100%
dicee/read_preprocess_save_load_kg/preprocess.py
                                                             256
                                                                      41
                                                                             84%
                                                                                   34, 40, _
\hookrightarrow78, 102-127, 133, 138-151, 184, 214, 388-389, 444
dicee/read_preprocess_save_load_kg/read_from_disk.py
                                                              36
                                                                      11
                                                                             69%
                                                                                   33, 38-
\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
                                                                       0
                                                                           100%
                                                                                   27-32, _
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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```

(continued from previous page)

```
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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(continued from previous page)

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

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

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

continues on next page

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):
```

(continues on next page)

(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)
     \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)

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

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

Arguments

Return type

(tuple) mini-batch on select device

dicee.trainer.torch_trainer_ddp

Classes

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

Functions

```
print_peak_memory(prefix, device)

make_iterable_verbose(→ Iterable)
```

Module Contents

```
dicee.trainer.torch_trainer_ddp.print_peak_memory(prefix, device)
dicee.trainer.torch_trainer_ddp.make_iterable_verbose(iterable_object, verbose,
           desc='Default', position=None, leave=True) \rightarrow Iterable
class dicee.trainer.torch_trainer_ddp.TorchDDPTrainer(args, callbacks)
     Bases: dicee.abstracts.AbstractTrainer
          A Trainer based on torch.nn.parallel.DistributedDataParallel
          Arguments
     entity_idxs
          mapping.
     relation_idxs
         mapping.
     form
     store
     label_smoothing_rate
          Using hard targets (0,1) drives weights to infinity. An outlier produces enormous gradients.
          Return type
              torch.utils.data.Dataset
     fit (*args, **kwargs)
          Train model
class dicee.trainer.torch_trainer_ddp.NodeTrainer(trainer, model: torch.nn.Module,
           train_dataset_loader: torch.utils.data.DataLoader, 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)
     train()
         Training loop for DDP
class dicee.trainer.torch_trainer_ddp.DDPTrainer (model: torch.nn.Module,
           train_dataset_loader: torch.utils.data.DataLoader, optimizer: torch.optim.Optimizer, gpu_id: int,
           callbacks, num_epochs)
     gpu_id
     model
     train_dataset_loader
     loss_func
     optimizer
     callbacks
     num_epochs
     loss_history = []
     extract_input_outputs (z: list)
     train()
```

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) \rightarrow 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
start(knowledge\_graph: dicee.knowledge\_graph.KG) \rightarrow Tuple[dicee.models.base\_model.BaseKGE, 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.__main__

dicee.abstracts

Classes

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

Module Contents

class dicee.abstracts.AbstractTrainer(args, callbacks)

Abstract class for Trainer class for knowledge graph embedding models

Parameter

```
args
    [str] ?

callbacks: list
    ?

attributes

callbacks

is_global_zero = True

strategy = None

on_fit_start(*args, **kwargs)
```

A function to call callbacks before the training starts.

```
Parameter
```

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

```
Parameter
```

```
full_path: str
           model:
               rtype
                   None
class dicee.abstracts.BaseInteractiveKGE (path: str = None, url: str = None,
            construct ensemble: bool = False, model name: str = None,
            apply_semantic_constraint: bool = False)
     Abstract/base class for using knowledge graph embedding models interactively.
     Parameter
     path_of_pretrained_model_dir
          [str]?
     construct_ensemble: boolean
     model_name: str apply_semantic_constraint : boolean
     construct_ensemble
     apply_semantic_constraint
     configs
     \texttt{get\_eval\_report}\;(\,)\;\to dict
     get_bpe_token_representation (str_entity_or_relation: List[str] | str)
                   \rightarrow List[List[int]] | List[int]
               Parameters
                   str_entity_or_relation(corresponds to a str or a list of strings
                   to be tokenized via BPE and shaped.)
               Return type
                   A list integer(s) or a list of lists containing integer(s)
     \verb|get_padded_bpe_triple_representation| (\textit{triples: List[List[str]]})| \rightarrow \text{Tuple}[List, List, List]
               Parameters
                   triples
     \verb"set_model_train_mode"() \to None
```

Setting the model into training mode

Parameter

```
\verb"set_model_eval_mode" () \to None
     Setting the model into eval mode
     Parameter
property name
sample_entity(n:int) \rightarrow List[str]
sample\_relation(n: int) \rightarrow List[str]
is_seen (entity: str = None, relation: str = None) \rightarrow bool
save() \rightarrow None
get_entity_index (x: str)
get_relation_index (x: str)
index_triple (head_entity: List[str], relation: List[str], tail_entity: List[str])
              → 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
```

```
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
     Parameter
     on_init_start(*args, **kwargs)
          Parameter
          trainer:
          model:
              rtype
                  None
     on_init_end(*args, **kwargs)
          Call at the beginning of the training.
          Parameter
          trainer:
          model:
              rtvpe
                  None
     on_fit_start (trainer, model)
          Call at the beginning of the training.
```

Parameter

```
Parameter
          trainer:
          model:
              rtype
                  None
     on_train_epoch_end (trainer, model)
          Call at the end of each epoch during training.
          Parameter
          trainer:
          model:
              rtype
                  None
     on_train_batch_end(*args, **kwargs)
          Call at the end of each mini-batch during the training.
          Parameter
          trainer:
          model:
              rtype
                  None
     on_fit_end(*args, **kwargs)
          Call at the end of the training.
          Parameter
          trainer:
          model:
              rtype
                  None
class dicee.abstracts.AbstractPPECallback (num_epochs, path, epoch_to_start,
            last_percent_to_consider)
     Bases: AbstractCallback
```

Abstract class for Callback class for knowledge graph embedding models

Parameter

```
num_epochs
path
sample_counter = 0
epoch_count = 0
alphas = None
on_fit_start (trainer, model)
    Call at the beginning of the training.
    Parameter
    trainer:
    model:
        rtype
            None
on_fit_end(trainer, model)
    Call at the end of the training.
    Parameter
    trainer:
    model:
        rtype
            None
store\_ensemble (param\_ensemble) \rightarrow None
```

dicee.analyse_experiments

This script should be moved to dicee/scripts

Classes

Experiment

Functions

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

Module Contents

```
dicee.analyse_experiments.get_default_arguments()
class dicee.analyse_experiments.Experiment
    model_name = []
    callbacks = []
    embedding_dim = []
    num_params = []
    num_epochs = []
    batch_size = []
    lr = []
    byte_pair_encoding = []
    aswa = []
    path_dataset_folder = []
    full_storage_path = []
    pq = []
    train_mrr = []
    train_h1 = []
    train_h3 = []
    train_h10 = []
    val_mrr = []
    val_h1 = []
    val_h3 = []
    val_h10 = []
    test_mrr = []
    test_h1 = []
```

```
test_h3 = []
test_h10 = []
runtime = []
normalization = []
scoring_technique = []
save_experiment(x)
to_df()
dicee.analyse_experiments.analyse(args)
```

dicee.callbacks

Classes

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

Functions

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

Module Contents

```
class dicee.callbacks.AccumulateEpochLossCallback(path: str)
     Bases: dicee.abstracts.AbstractCallback
     Abstract class for Callback class for knowledge graph embedding models
     Parameter
     path
     on\_fit\_end(\mathit{trainer}, \mathit{model}) \rightarrow None
          Store epoch loss
          Parameter
          trainer:
          model:
              rtype
                  None
class dicee.callbacks.PrintCallback
     Bases: dicee.abstracts.AbstractCallback
     Abstract class for Callback class for knowledge graph embedding models
     Parameter
     start_time
     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.

```
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
```

Parameter

Abstract class for Callback class for knowledge graph embedding models

```
Parameter
```

```
data_module
     kg
     num_of_epochs = 0
     unlabelled_size
     batch_size
     create_random_data()
     on_epoch_end (trainer, model)
dicee.callbacks.estimate_q(eps)
     estimate rate of convergence q from sequence esp
dicee.callbacks.compute_convergence (seq, i)
class dicee.callbacks.ASWA (num_epochs, path)
     Bases: dicee.abstracts.AbstractCallback
     Adaptive stochastic weight averaging ASWE keeps track of the validation performance and update s the ensemble
     model accordingly.
     path
     num_epochs
     initial_eval_setting = None
     epoch_count = 0
     alphas = []
     val_aswa
     on_fit_end(trainer, model)
          Call at the end of the training.
          Parameter
          trainer:
          model:
             rtype
                 None
     \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
     Parameter
     path
     reports = []
     epoch_ratio
     epoch_counter = 0
     on_fit_start (trainer, model)
          Call at the beginning of the training.
          Parameter
          trainer:
          model:
             rtype
                 None
     on_fit_end(trainer, model)
          Call at the end of the training.
```

```
Parameter
```

```
trainer:
          model:
              rtype
                  None
     \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.
          Parameter
          trainer:
          model:
              rtype
                  None
class dicee.callbacks.KronE
     Bases: dicee.abstracts.AbstractCallback
     Abstract class for Callback class for knowledge graph embedding models
     Parameter
     f = None
     static batch_kronecker_product(a, b)
          Kronecker product of matrices a and b with leading batch dimensions. Batch dimensions are broadcast. The
```

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

```
\verb|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.

```
A directory named with time of execution under -storage_path that contains related data about embeddings.
path_to_store_single_run: str = None
    A single directory created that contains related data about embeddings.
path_single_kg = None
    Path of a file corresponding to the input knowledge graph
sparql_endpoint = None
    An endpoint of a triple store.
model: str = 'Keci'
    KGE model
optim: str = 'Adam'
    Optimizer
embedding_dim: int = 64
    Size of continuous vector representation of an entity/relation
num_epochs: int = 150
    Number of pass over the training data
batch_size: int = 1024
    Mini-batch size if it is None, an automatic batch finder technique applied
lr: float = 0.1
    Learning rate
add_noise_rate: float = None
    The ratio of added random triples into training dataset
gpus = None
    Number GPUs to be used during training
callbacks
    10}}
        Type
            Callbacks, e.g., {"PPE"
        Type
            { "last_percent_to_consider"
backend: str = 'pandas'
    Backend to read, process, and index input knowledge graph. pandas, polars and rdflib available
trainer: str = 'torchCPUTrainer'
    Trainer for knowledge graph embedding model
scoring_technique: str = 'KvsAll'
    Scoring technique for knowledge graph embedding models
neg ratio: int = 0
    Negative ratio for a true triple in NegSample training_technique
weight_decay: float = 0.0
    Weight decay for all trainable params
```

storage_path: str = 'Experiments'

```
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

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

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

An abstract class representing a Dataset.

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

Parameters

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

```
train_set
     train_indices_target
     target_dim
     num_datapoints
     torch_ordered_shaped_bpe_entities
     collate_fn = None
     __len__()
     \__getitem\__(idx)
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
```

```
• 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

```
i Note
TODO
```

train_set_idx

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

entity_idxs

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

relation_idxs

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

self: torch.utils.data.Dataset

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

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

```
collate_fn = None
__len__()
\__getitem_{\_}(idx)
```

class dicee.dataset_classes.AllvsAll (train_set_idx: numpy.ndarray, entity_idxs, relation_idxs, label_smoothing_rate=0.0)

Bases: torch.utils.data.Dataset

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

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

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



1 Note

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

only with 0s.

train set idx

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

entity_idxs

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

relation_idxs

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

self: torch.utils.data.Dataset

```
>>> a = AllvsAll()
? 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
                  | new_y| << |E| new_y contains all 1's if sum(y)< neg_sample ratio new_y contains
          train_set_idx
              Indexed triples for the training.
          entity_idxs
              mapping.
          relation_idxs
              mapping.
          form
          store
          label_smoothing_rate
          torch.utils.data.Dataset
     train_data
     num_entities
     num_relations
     neg_sample_ratio
     label_smoothing_rate
     collate_fn = None
     store
     train_target
     __len__()
     \__{getitem}_{\_}(idx)
class dicee.dataset_classes.NegSampleDataset (train_set: numpy.ndarray, num_entities: int,
            num_relations: int, neg_sample_ratio: int = 1)
     Bases: torch.utils.data.Dataset
     An abstract class representing a Dataset.
```

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



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__()
     \__getitem\__(idx)
     collate_fn (batch: List[torch.Tensor])
class dicee.dataset_classes.CVDataModule(train_set_idx: numpy.ndarray, num_entities,
           num_relations, neg_sample_ratio, batch_size, num_workers)
     Bases: pytorch_lightning.LightningDataModule
     Create a Dataset for cross validation
          Parameters
                • train_set_idx - Indexed triples for the training.
                • num_entities - entity to index mapping.
                • num_relations - relation to index mapping.
                • batch_size - int
                • form - ?
                • num_workers - int for https://pytorch.org/docs/stable/data.html#torch.utils.data.
                 DataLoader
          Return type
     train_set_idx
     num_entities
     num_relations
     neg_sample_ratio
     batch_size
     num_workers
     train_dataloader() → torch.utils.data.DataLoader
          An iterable or collection of iterables specifying training samples.
          For more information about multiple dataloaders, see this section.
                dataloader
                             you
                                   return
                                            will
                                                   not
                                                         be
                                                               reloaded
                                                                         unless
                                                                                  you
                                                                                               :param-
          ref: ~pytorch_lightning.trainer.trainer.Trainer.reload_dataloaders_every_n_epochs to a positive
          integer.
          For data processing use the following pattern:
```

- download in prepare_data()
- process and split in setup ()

However, the above are only necessary for distributed processing.

▲ Warning

do not assign state in prepare_data

- fit()
- prepare_data()
- setup()

1 Note

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

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

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

Parameters

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

Example:

```
class LitModel(...):
    def __init__(self):
        self.l1 = None

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

# don't do this
        self.something = else

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

transfer_batch_to_device(*args, **kwargs)

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

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

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

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



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

- **bat.ch** 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_
\hookrightarrow idx)
    return batch
```

See also

- move_data_to_device()
- apply_to_collection()

prepare_data(*args, **kwargs)

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



🛕 Warning

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

Example:

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

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

In a distributed environment, prepare_data can be called in two ways (using prepare_data_per_node)

- 1. Once per node. This is the default and is only called on LOCAL_RANK=0.
- 2. Once in total. Only called on GLOBAL_RANK=0.

Example:

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

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

This is called before requesting the dataloaders:

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

dicee.eval static funcs

Functions

```
evaluate_link_prediction_performance(→
Dict)
evaluate_link_prediction_performance_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
```

Parameters

- model
- triples
- er_vocab
- re_vocab

dicee.eval_static_funcs.

evaluate_link_prediction_performance_with_reciprocals (
model: dicee.knowledge_graph_embeddings.KGE, triples, er_vocab: Dict[Tuple, List])

dicee.eval_static_funcs.

evaluate_link_prediction_performance_with_bpe_reciprocals (
model: dicee.knowledge_graph_embeddings.KGE, within_entities: List[str], triples: List[List[str]],
er_vocab: Dict[Tuple, List])

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(\mathit{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)
```

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

Evaluate model after reciprocal triples are added

 $\begin{tabular}{ll} \textbf{eval_with_bpe_vs_all} (*, raw_train_set, raw_valid_set=None, raw_test_set=None, trained_model, \\ form_of_labelling) \rightarrow None \\ \end{tabular}$

Evaluate model after reciprocal triples are added

Evaluate model after reciprocal triples are added

evaluate_lp_k_vs_all (model, triple_idx, info=None, form_of_labelling=None)

Filtered link prediction evaluation. :param model: :param triple_idx: test triples :param info: :param form_of_labelling: :return:

evaluate_lp_with_byte (model, triples: List[List[str]], info=None)

evaluate_lp_bpe_k_vs_all (model, triples: List[List[str]], info=None, form_of_labelling=None)

Parameters

- model
- triples (List of lists)
- info
- form_of_labelling

evaluate_lp (model, triple_idx, info: str)

dummy_eval (trained_model, form_of_labelling: str)

eval_with_data (dataset, trained_model, triple_idx: numpy.ndarray, form_of_labelling: str)

dicee.executer

Classes

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

Module Contents

class dicee.executer.**Execute** (args, continuous training=False)

A class for Training, Retraining and Evaluation a model.

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

args

```
is_continual_training
trainer = None
trained_model = None
knowledge_graph = None
report
evaluator = None
start_time = None
read_or_load_kg()
read_preprocess_index_serialize_data() → None
    Read & Preprocess & Index & Serialize Input Data
```

(1) Read or load the data from disk into memory.

(2) Store the statistics of the data.

Parameter

rtype

None

$load_indexed_data() \rightarrow None$

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

 $continual_start() \rightarrow dict$

Start Continual Training

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

Parameter

rtype

A dict containing information about the training and/or evaluation

dicee.knowledge_graph

Classes

KG Knowledge Graph

Module Contents

relation_to_idx

```
class dicee.knowledge_graph.KG(dataset_dir: str = None, byte_pair_encoding: bool = False,
           padding: bool = False, add_noise_rate: float = None, sparql_endpoint: str = None,
           path\_single\_kg: str = None, path\_for\_deserialization: str = None, add\_reciprical: bool = None,
           eval_model: str = None, read_only_few: int = None, sample_triples_ratio: float = None,
           path_for_serialization: str = None, entity_to_idx=None, relation_to_idx=None, backend=None,
           training\_technique: str = None)
     Knowledge Graph
     dataset_dir
     byte_pair_encoding
     ordered_shaped_bpe_tokens = None
     sparql_endpoint
     add_noise_rate
     num_entities = None
     num_relations = None
     path_single_kg
     path_for_deserialization
     add_reciprical
     eval_model
     read_only_few
     sample_triples_ratio
     path_for_serialization
     entity_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

$$\label{eq:continuous_list} \begin{split} \mathbf{predict_missing_head_entity} \; (\textit{relation: List[str]} \; | \; \textit{str, tail_entity: List[str]} \; | \; \textit{str, within=None}) \\ &\rightarrow \mathsf{Tuple} \end{split}$$

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

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

Parameter

relation: Union[List[str], str]

String representation of selected relations.

tail_entity: Union[List[str], str]

String representation of selected entities.

k: int

Highest ranked k entities.

Returns: Tuple

Highest K scores and entities

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

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

Parameter

head_entity: List[str]

String representation of selected entities.

tail_entity: List[str]

String representation of selected entities.

k: int

Highest ranked k entities.

Returns: Tuple

```
Highest K scores and entities
```

```
\label{eq:predict_missing_tail_entity} \begin{split} &\texttt{predict\_missing\_tail\_entity} \ (\textit{head\_entity: List[str]} \mid \textit{str}, \textit{relation: List[str]} \mid \textit{str}, \\ &\textit{within: List[str]} = \textit{None}) \ \rightarrow \texttt{torch.FloatTensor} \end{split}
```

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

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

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
```

```
\label{eq:core} \begin{split} \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} \\ & \text{Predict triple score} \end{split}
```

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 \mid Tuple[str, str], Ellipsis] = None,
queries: List[Tuple[str \mid Tuple[str, str], Ellipsis]] = None, tnorm: <math>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, Str]]] The query itself, either a string or a nested tuple.
     queries: List of Tuple[Union[str, Tuple[str, str]], ...]
     tnorm: str The t-norm operator.
     neg_norm: str The negation norm.
     lambda_: float lambda parameter for sugeno and yager negation norms
     k: int The top-k substitutions for intermediate variables.
          returns
               • List[Tuple[str, torch.Tensor]]
               • Entities and corresponding scores sorted in the descening order of scores
find_missing_triples (confidence: float, entities: List[str] = None, relations: List[str] = None,
              topk: int = 10, at_most: int = sys.maxsize) \rightarrow Set
          Find missing triples
          Iterative over a set of entities E and a set of relation R:
     orall e in E and orall r in R f(e,r,x)
          Return (e,r,x)
     otin G and f(e,r,x) > confidence
          confidence: float
          A threshold for an output of a sigmoid function given a triple.
          topk: int
          Highest ranked k item to select triples with f(e,r,x) > \text{confidence}.
          at most: int
          Stop after finding at_most missing triples
          \{(e,r,x) \mid f(e,r,x) > \text{confidence land } (e,r,x)\}
     otin G
deploy (share: bool = False, top_k: int = 10)
train_triples (h: List[str], r: List[str], t: List[str], labels: List[float], iteration=2, optimizer=None)
train_k_vs_all (h, r, iteration=1, lr=0.001)
     Train k vs all :param head_entity: :param relation: :param iteration: :param lr: :return:
train (kg, lr=0.1, epoch=10, batch\_size=32, neg\_sample\_ratio=10, num\_workers=1) \rightarrow None
     Retrained a pretrain model on an input KG via negative sampling.
```

dicee.query_generator

Classes

QueryGenerator

Module Contents

```
class dicee.query_generator.QueryGenerator(train_path, val_path: str, test_path: str,
            ent2id: Dict = None, rel2id: Dict = None, seed: int = 1, gen_valid: bool = False,
            gen\_test: bool = True)
     train_path
     val path
     test_path
     gen_valid
     gen_test
     seed
     max_ans_num = 1000000.0
     mode
     ent2id
     rel2id: Dict
     ent_in: Dict
     ent_out: Dict
     query_name_to_struct
     list2tuple (list_data)
     tuple2list (x: List | Tuple) \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) → 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

<pre>create_recipriocal_triples(x) get_er_vocab(data[, file_path])</pre>	Add inverse triples into dask dataframe
<pre>get_re_vocab(data[, file_path])</pre>	
get_ee_vocab(data[, file_path])	
timeit(func)	
<pre>save_pickle(*[, data, file_path])</pre>	
load_pickle([file_path])	
<pre>select_model(args[, is_continual_training, stor- age_path])</pre>	
<pre>load_mode1(→ Tuple[object, Tuple[dict, dict]])</pre>	Load weights and initialize pytorch module from namespace arguments
load_model_ensemble()	Construct Ensemble Of weights and initialize pytorch module from namespace arguments
<pre>save_numpy_ndarray(*, data, file_path)</pre>	
$numpy_data_type_changer(\rightarrow numpy.ndarray)$ $save_checkpoint_model(\rightarrow None)$	Detect most efficient data type for a given triples Store Pytorch model into disk
$store(\rightarrow None)$	Store trained_model model and save embeddings into csv file.
a del made a trade la contra Desa Desa Erroma)	
add_noisy_triples(→ pandas.DataFrame) read_or_load_kg(args, cls)	Add randomly constructed triples
$intialize_model(\rightarrow Tuple[object, str])$	
$load_json(\rightarrow dict)$	
$save_embeddings(\rightarrow None)$	Save it as CSV if memory allows.
random_prediction(pre_trained_kge)	, , , , , , , , , , , , , , , , , , ,
<pre>deploy_triple_prediction(pre_trained_kge, str_subject,)</pre>	
<pre>deploy_tail_entity_prediction(pre_trained)</pre>	
<pre>deploy_head_entity_prediction(pre_trained)</pre>	
<pre>deploy_relation_prediction(pre_trained_kge,)</pre>	
<pre>vocab_to_parquet(vocab_to_idx, name,)</pre>	
<pre>create_experiment_folder([folder_name])</pre>	

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Table 2 - continued from previous page

```
      continual_training_setup_executor(→
      storage_path:str A path leading to a parent directory, where a subdirectory containing KGE related data

      exponential_function(→ torch.FloatTensor)
      load_numpy(→ numpy.ndarray)

      evaluate(entity_to_idx, scores, easy_answers, hard_answers)
      # @TODO: CD: Renamed this function

      download_file(url[, destination_folder])
      download_files_from_url(→ None)

      download_pretrained_model(→ str)
```

Module Contents

```
dicee.static_funcs.create_recipriocal_triples(x)
     Add inverse triples into dask dataframe :param x: :return:
dicee.static_funcs.get_er_vocab(data, file_path: str = None)
dicee.static_funcs.get_re_vocab(data, file_path: str = None)
dicee.static_funcs.get_ee_vocab(data, file_path: str = None)
dicee.static funcs.timeit(func)
dicee.static_funcs.save_pickle(*, data: object = None, file_path=str)
dicee.static_funcs.load_pickle(file_path=str)
dicee.static_funcs.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,
           str object)
dicee.static_funcs.deploy_tail_entity_prediction(pre_trained_kge, str_subject,
           str_predicate, top_k)
dicee.static_funcs.deploy_head_entity_prediction(pre_trained_kge, str_object,
           str_predicate, top_k)
dicee.static_funcs.deploy_relation_prediction(pre_trained_kge, str_subject, str_object,
           top_k)
dicee.static_funcs.vocab_to_parquet(vocab_to_idx, name, path_for_serialization, print_into)
dicee.static_funcs.create_experiment_folder(folder_name='Experiments')
dicee.static funcs.continual training setup executor (executor) \rightarrow None
     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($base_url: str, destination_folder='.') <math>\rightarrow$ None

Parameters

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

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

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

Evaluate model in a standard link prediction task

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

dicee.static_funcs_training.efficient_zero_grad(model)

dicee.static preprocess funcs

Attributes

enable_log

Functions

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

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:

14.3 Attributes

__version__

14.4 Classes

CMult	$Cl_{-}(0,0) \Rightarrow Real Numbers$
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
AConvO	Additive Convolutional Octonion Knowledge Graph Embeddings
AConvQ	Additive Convolutional Quaternion Knowledge Graph Embeddings
ConvQ	Convolutional Quaternion Knowledge Graph Embeddings
ConvO	Base class for all neural network modules.
ConEx	Convolutional ComplEx Knowledge Graph Embeddings
QMult	Base class for all neural network modules.
OMult	Base class for all neural network modules.
Shallom	A shallow neural model for relation prediction (https://arxiv.org/abs/2101.09090)
LFMult	Embedding with polynomial functions. We represent all entities and relations in the polynomial space as:
PykeenKGE	A class for using knowledge graph embedding models implemented in Pykeen
BytE	Base class for all neural network modules.
BaseKGE	Base class for all neural network modules.
DICE_Trainer	DICE_Trainer implement
KGE	Knowledge Graph Embedding Class for interactive usage of pre-trained models
Execute	A class for Training, Retraining and Evaluation a model.
BPE_NegativeSamplingDataset	An abstract class representing a Dataset.
MultiLabelDataset	An abstract class representing a Dataset.
MultiClassClassificationDataset	Dataset for the 1vsALL training strategy
OnevsAllDataset	Dataset for the 1vsALL training strategy
KvsAll	Creates a dataset for KvsAll training by inheriting from torch.utils.data.Dataset.
AllvsAll	Creates a dataset for AllvsAll training by inheriting from torch.utils.data.Dataset.
	KvsSample a Dataset:
<i>KvsSampleDataset</i>	Kyssample a Dataset.
KvsSampleDataset NegSampleDataset	An abstract class representing a Dataset.
	<u>*</u>

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QueryGenerator

14.5 Functions

```
Add inverse triples into dask dataframe
create_recipriocal_triples(x)
get_er_vocab(data[, file_path])
get_re_vocab(data[, file_path])
get_ee_vocab(data[, file_path])
 timeit(func)
save_pickle(*[, data, file_path])
load_pickle([file_path])
select_model(args[, is_continual_training,
age_path])
load_model(→ Tuple[object, Tuple[dict, dict]])
                                                       Load weights and initialize pytorch module from names-
                                                       pace arguments
load_model_ensemble(...)
                                                       Construct Ensemble Of weights and initialize pytorch
                                                       module from namespace arguments
save_numpy_ndarray(*, data, file_path)
numpy_data_type_changer(\rightarrow numpy.ndarray)
                                                       Detect most efficient data type for a given triples
save\_checkpoint\_model(\rightarrow None)
                                                       Store Pytorch model into disk
store(\rightarrow None)
                                                       Store trained_model model and save embeddings into csv
                                                       file.
                                                       Add randomly constructed triples
add\_noisy\_triples(\rightarrow pandas.DataFrame)
 read_or_load_kg(args, cls)
intialize\_model(\rightarrow Tuple[object, str])
load_{json}(\rightarrow dict)
save\_embeddings(\rightarrow None)
                                                       Save it as CSV if memory allows.
 random_prediction(pre_trained_kge)
deploy_triple_prediction(pre_trained_kge,
str_subject, ...)
deploy_tail_entity_prediction(pre_trained_)
deploy_head_entity_prediction(pre_trained_)
...)
deploy_relation_prediction(pre_trained_kge,
```

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Table 4 - continued from previous page

```
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)
                                                     # @TODO: CD: Renamed this function
evaluate(entity_to_idx,
                            scores,
                                      easy_answers,
hard_answers)
download_file(url[, destination_folder])
download\_files\_from\_url(\rightarrow None)
download\_pretrained\_model(\rightarrow str)
mapping_from_first_two_cols_to_third(tra
timeit(func)
load_pickle([file_path])
                                                      Reload the files from disk to construct the Pytorch dataset
reload_dataset(path, form_of_labelling, ...)
 construct_dataset(→ torch.utils.data.Dataset)
```

14.6 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

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 + b_1 e_1 + b_2 e_2 + b_{12} e_1 e_2

mathbf{a} imes mathbf{b} = a_0 b_0 + a_0 b_1 e_1 + a_0 b_2 e_2 + a_0 b_1 2 e_1 e_2

• a_1 b_0 e_1 + a_1 b_1 e_1 e_1 ..

Cl_(0,2) => Quaternions

name = 'CMult'
```

```
entity_embeddings
     relation_embeddings
     p
     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.Pyke(args)
     Bases: dicee.models.base_model.BaseKGE
     A Physical Embedding Model for Knowledge Graphs
     name = 'Pyke'
     dist_func
     margin = 1.0
     forward_triples (x: torch.LongTensor)
               Parameters
                   x
```

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

Your models should also subclass this class.

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

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

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

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.

$\verb|compute_sigma_qq| (hq, rq)$

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

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

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

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

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

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

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

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

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

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

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

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

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

eq j

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

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

construct_cl_multivector(x: torch.FloatTensor, r: int, p: int, q: int)

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

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

Parameter

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

returns

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

forward_k_vs_with_explicit(x: torch.Tensor)

 $k_vs_all_score$ (bpe_head_ent_emb, bpe_rel_ent_emb, E)

 $\textbf{forward_k_vs_all} \ (\textit{x: torch.Tensor}) \ \rightarrow \ torch.FloatTensor$

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

```
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 $Cl_{p,q}(mathbb\{R\}^d)$.
- (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.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)
```

Base class for all neural network modules.

Bases: dicee.models.base model.BaseKGE

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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(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.

```
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) s4 = \sum_{i=p+q+1}^{p+q+r} (h_0 r_i t_i + h_i r_0 t_i) s4 = \sum_{i=p+q+1}^{p+q+r} (h_0 r_i t_i + h_i r_0 t_i) s4 = \sum_{i=p+q+1}^{p+q+r} (h_0 r_i t_i + h_i r_0 t_i) s4 = \sum_{i=p+q+1}^{p+q+r} (h_0 r_i t_i + h_i r_0 t_i) s4 = \sum_{i=p+q+1}^{p+q+r} (h_0 r_i t_i + h_i r_0 t_i) s4 = \sum_{i=p+q+1}^{p+q+r} (h_0 r_i t_i + h_i r_0 t_i) s4 = \sum_{i=p+q+1}^{p+q+r} (h_0 r_i t_i + h_i r_0 t_i) s4 = \sum_{i=p+q+1}^{p+q+r} (h_0 r_i t_i + h_i r_0 t_i) s4 = \sum_{i=p+q+1}^{p+q+r} (h_0 r_i t_i + h_i r_0 t_i) s4 = \sum_{i=p+q+1}^{p+q+r} (h_0 r_i t_i + h_i r_0 t_i) s4 = \sum_{i=p+q+1}^{p+q+r} (h_0 r_i t_i + h_i r_0 t_i) s4 = \sum_{i=p+q+1}^{p+q+r} (h_0 r_i t_i + h_i r_0 t_i) s4 = \sum_{i=p+q+1}^{p+q+r} (h_0 r_i t_i + h_i r_0 t_i) s4 = \sum_{i=p+q+1}^{p+q+r} (h_0 r_i t_i + h_i r_0 t_i) s4 = \sum_{i=p+q+1}^{p+q+r} (h_0 r_i t_i + h_i r_0 t_i) s4 = \sum_{i=p+q+1}^{p+q+r} (h_0 r_i t_i + h_i r_0 t_i) s4 = \sum_{i=p+q+1}^{p+q+r} (h_0 r_i t_i + h_i r_0 t_i) s4 = \sum_{i=p+q+r}^{p+q+r} (h_0 r_i t_i + h_i r_0 t_i) s4 = \sum_{i=p+q+r}^{p+q+r} (h_0 r_i t_i + h_i r_0 t_i) s4 = \sum_{i=p+q+r}^{p+q+r} (h_0 r_i t_i + h_i r_0 t_i) s4 = \sum_{i=p+q+r}^{p+q+r} (h_0 r_i t_i + h_i r_0 t_i) s4 = \sum_{i=p+q+r}^{p+q+r} (h_0 r_i t_i + h_i r_0 t_i) s4 = \sum_{i=p+q+r}^{p+q+r} (h_0 r_i t_i + h_i r_0 t_i) s4 = \sum_{i=p+q+r}^{p+q+r} (h_0 r_i t_i + h_i r_0 t_i) s4 = \sum_{i=p+q+r}^{p+q+r} (h_0 r_i t_i + h_i r_0 t_i) s4 = \sum_{i=p+q+r}^{p+q+r} (h_0 r_i t_i + h_i r_0 t_i) s4 = \sum_{i=p+q+r}^{p+q+r} (h_0 r_i t_i + h_i r_0 t_i) s4 = \sum_{i=p+q+r}^{p+q+r} (h_0 r_i t_i + h_i r_0 t_i) s4 = \sum_{i=p+q+r}^{p+q+r} (h_0 r_i t_i + h_i r_0 t_i) s4 = \sum_{i=p+q+r}^{p+q+$$

and return:

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

compute_sigmas_multivect(list_h_emb, list_r_emb)

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

For same bases vectors interaction we have

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

For different base vector interactions, we have

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

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

Kvsall training

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

forward_k_vs_with_explicit and this funcitons are identical Parameter — x: torch.LongTensor with (n,) shape :rtype: torch.FloatTensor with (n, |E|) shape

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

Multiplying a base vector with its scalar coefficient

construct_cl_multivector(x: torch.FloatTensor, re: int, p: int, q: int, r: int)

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

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:

$$sigma_{p,p}^* = \sum_{i=1}^{p-1}\sum_{i'=i+1}^{p} (x_{i'}-x_{i'}-x_{i'}y_{i})$$

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):

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

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

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

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

$compute_sigma_qq(hq, rq)$

Compute

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

sigma_{q} captures the interactions between along q bases For instance, let q e_1, e_2, e_3, we compute interactions between e_1 e_2, e_1 e_3, and e_2 e_3 This can be implemented with a nested two for loops

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

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

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

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

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

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

compute_sigma_rr (hk, rk)

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

 $\texttt{compute_sigma_pq} (*, hp, hq, rp, rq)$

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.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_1h , e_2h , e_1h , e_2h , e_1h , e_2h , e_1h , e_1h , e_2h , e_1h

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)

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 = '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],
                 C_2: Tuple[torch.Tensor, torch.Tensor]) \rightarrow torch.FloatTensor
          Compute residual score of two complex-valued embeddings. :param C_1: a tuple of two pytorch tensors
          that corresponds complex-valued embeddings :param C_2: a tuple of two pytorch tensors that corresponds
          complex-valued embeddings :return:
     forward_k_vs_all (x: torch.Tensor) \rightarrow torch.FloatTensor
     forward\_triples (x: torch.Tensor) \rightarrow torch.FloatTensor
              Parameters
     forward_k_vs_sample (x: torch.Tensor, target_entity_idx: torch.Tensor)
class dicee.AConvO(args: dict)
     Bases: dicee.models.base_model.BaseKGE
     Additive Convolutional Octonion Knowledge Graph Embeddings
     name = 'AConvO'
```

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

```
class dicee.ConvQ(args)
     Bases: dicee.models.base_model.BaseKGE
     Convolutional Quaternion Knowledge Graph Embeddings
     name = 'ConvQ'
     entity_embeddings
     relation_embeddings
     conv2d
     fc_num_input
     fc1
     bn conv1
     bn_conv2
     feature_map_dropout
     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)
     {\tt residual\_convolution}\,(O\_1,\,O\_2)
     forward_triples (x: torch.Tensor) \rightarrow torch.Tensor
              Parameters
                  x
     forward_k_vs_all (x: torch.Tensor)
          Given a head entity and a relation (h,r), we compute scores for all entities. [score(h,r,x)|x in Entities] =>
          [0.0,0.1,...,0.8], shape=> (1, |Entities|) Given a batch of head entities and relations => shape (size of batch,|
          Entities()
class dicee.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:

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.

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

 $\textbf{k_vs_all_score} \ (bpe_head_ent_emb, bpe_rel_ent_emb, E)$

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
```

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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.

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|)

```
\verb"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() \rightarrow Tuple[numpy.ndarray, None]
forward_k_vs_all(x) \rightarrow torch.FloatTensor
forward_triples(x) \rightarrow torch.FloatTensor

Parameters
    x

Returns
```

```
class dicee.LFMult(args)
     Bases: dicee.models.base_model.BaseKGE
     Embedding with polynomial functions. We represent all entities and relations in the polynomial space as: f(x) =
     sum_{i=0}^{d-1} a_k x^{i}d and use the three differents scoring function as in the paper to evaluate the score.
     We also consider combining with Neural Networks.
     name = 'LFMult'
     entity_embeddings
     relation_embeddings
     degree
     m
     x_values
     forward_triples (idx_triple)
               Parameters
     construct_multi_coeff(x)
     poly_NN(x, coefh, coefr, coeft)
           Constructing a 2 layers NN to represent the embeddings. h = sigma(wh^T x + bh), r = sigma(wr^T x + br),
           t = sigma(wt^T x + bt)
     linear(x, w, b)
     scalar_batch_NN(a, b, c)
           element wise multiplication between a,b and c: Inputs: a, b, c ====> torch.tensor of size batch_size x m x
           d Output: a tensor of size batch_size x d
     tri_score (coeff_h, coeff_r, coeff_t)
           this part implement the trilinear scoring techniques:
           score(h,r,t) = int_{0}{1} h(x)r(x)t(x) dx = sum_{i,j,k} = 0}^{d-1} dfrac{a_i*b_j*c_k}{1+(i+j+k)%d}
            1. generate the range for i, j and k from [0 d-1]
           2. perform dfrac\{a_i*b_j*c_k\}\{1+(i+j+k)\%d\} in parallel for every batch
            3. take the sum over each batch
     vtp\_score(h, r, t)
           this part implement the vector triple product scoring techniques:
           score(h,r,t) = int_{0}{1} h(x)r(x)t(x) dx = sum_{i,j,k} = 0}^{d-1} dfrac_{a_i}c_j*b_k
           b\_i*c\_j*a\_k\}\{(1+(i+j)\%d)(1+k)\}
            1. generate the range for i,j and k from [0 d-1]
            2. Compute the first and second terms of the sum
```

 $comp_func(h, r, t)$

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

3. Multiply with then denominator and take the sum

4. take the sum over each batch

```
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:

 $h = h.reshape(len(x), self.embedding_dim, self.last_dim) r = r.reshape(len(x), self.embedding_dim, self.last_dim) t = t.reshape(len(x), self.embedding_dim, self.last_dim)$

(3) Compute the triple score return self.interaction.score(h=h, r=r, t=t, slice_size=None, slice_dim=0)

abstract forward_k_vs_sample (x: torch.LongTensor, target_entity_idx)

```
class dicee.BytE(*args, **kwargs)
```

Bases: dicee.models.base model.BaseKGE

Base class for all neural network modules.

Your models should also subclass this class.

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

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

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

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

args

```
embedding_dim = None
num_entities = None
num_relations = None
num_tokens = None
```

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

```
forward (x: torch.LongTensor | Tuple[torch.LongTensor, torch.LongTensor],
                 y idx: torch.LongTensor = None
              Parameters
                  • x
                  y_idx
                  • ordered_bpe_entities
     forward_triples (x: torch.LongTensor) → torch.Tensor
              Parameters
     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)
     get_embeddings() → Tuple[numpy.ndarray, numpy.ndarray]
dicee.create_recipriocal_triples(x)
     Add inverse triples into dask dataframe :param x: :return:
dicee.get_er_vocab(data, file_path: str = None)
dicee.get_re_vocab(data, file_path: str = None)
dicee.get_ee_vocab(data, file_path: str = None)
dicee.timeit(func)
dicee.save_pickle(*, data: object = None, file_path=str)
dicee.load_pickle(file_path=str)
dicee.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) \rightarrow None
     Store Pytorch model into disk
dicee.store(trainer, trained_model, model_name: str = 'model', full_storage_path: str = None,
            save\_embeddings\_as\_csv=False) \rightarrow None
     Store trained_model model and save embeddings into csv file. :param trainer: an instance of trainer class :param
     full storage path: path to save parameters. :param model name: string representation of the name of the model.
     :param trained_model: an instance of BaseKGE see core.models.base_model . :param save_embeddings_as_csv:
     for easy access of embeddings. :return:
dicee.add_noisy_triples(train_set: pandas.DataFrame, add_noise_rate: float) → 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
                                                 "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.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

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

```
Bases: dicee.abstracts.BaseInteractiveKGE
```

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

```
__str__()
```

to (*device*: str) \rightarrow None

 $\verb|get_transductive_entity_embeddings| (indices: torch.LongTensor \mid List[str],$

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)

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

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

Parameter

relation: Union[List[str], str]

String representation of selected relations.

tail_entity: Union[List[str], str]

String representation of selected entities.

k: int

Highest ranked k entities.

Returns: Tuple

Highest K scores and entities

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

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

Parameter

head_entity: List[str]

String representation of selected entities.

tail_entity: List[str]

String representation of selected entities.

k: int

Highest ranked k entities.

Returns: Tuple

Highest K scores and entities

```
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() ${\tt read_preprocess_index_serialize_data}~()~\to None$

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

```
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

```
\verb|dicee.mapping_from_first_two_cols_to_third| (\textit{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 DataLoader. Subclasses could also optionally implement __getitems__(), for speedup batched samples loading. This method accepts list of indices of samples of batch and returns list of samples.



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



```
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

 $\textbf{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.

you be reloaded The dataloader 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.

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:

→ See also

- move_data_to_device()
- apply_to_collection()

prepare_data(*args, **kwargs)

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

Warning

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

Example:

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

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

In a distributed environment, prepare_data can be called in two ways (using prepare_data_per_node)

- 1. Once per node. This is the default and is only called on LOCAL_RANK=0.
- 2. Once in total. Only called on GLOBAL_RANK=0.

Example:

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

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

This is called before requesting the dataloaders:

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

class dicee. **QueryGenerator** (*train_path*, *val_path*: *str*, *test_path*: *str*, *ent2id*: *Dict* = *None*, *rel2id*: *Dict* = *None*, *seed*: *int* = 1, *gen_valid*: *bool* = *False*, *gen_test*: *bool* = *True*)

```
train_path
val_path
test_path
gen_valid
gen_test
seed
max_ans_num = 1000000.0
mode
ent2id
rel2id: Dict
ent_in: Dict
ent_out: Dict
query_name_to_struct
list2tuple (list_data)
tuple2list (x: List \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'
```

Python Module Index

d

```
dicee. 12
dicee. main ,115
dicee.abstracts, 115
dicee.analyse_experiments, 121
dicee.callbacks, 123
dicee.config, 130
dicee.dataset_classes, 133
dicee.eval static funcs, 144
dicee.evaluator, 145
dicee.executer, 146
dicee.knowledge_graph, 149
dicee.knowledge_graph_embeddings, 150
dicee.models, 12
dicee.models.base model, 12
dicee.models.clifford, 21
dicee.models.complex, 29
dicee.models.dualE, 31
dicee.models.function_space, 33
dicee.models.octonion, 36
dicee.models.pykeen_models, 39
dicee.models.quaternion, 41
dicee.models.real,44
dicee.models.static funcs, 45
dicee.models.transformers, 46
dicee.query_generator, 155
dicee.read_preprocess_save_load_kg, 100
dicee.read_preprocess_save_load_kg.preprocess,
dicee.read_preprocess_save_load_kg.read_from_disk,
dicee.read_preprocess_save_load_kg.save_load_disk,
dicee.read_preprocess_save_load_kg.util,
dicee.sanity_checkers, 156
dicee.scripts, 106
dicee.scripts.index, 106
dicee.scripts.run, 107
dicee.scripts.serve, 107
dicee.static_funcs, 157
dicee.static_funcs_training, 160
dicee.static_preprocess_funcs, 160
dicee.trainer, 108
dicee.trainer.dice_trainer, 108
dicee.trainer.torch_trainer,110
dicee.trainer.torch_trainer_ddp, 111
```

Index

Non-alphabetical

```
__call__() (dicee.models.base_model.IdentityClass method), 21
__call__() (dicee.models.IdentityClass method), 62, 73, 79
__getitem__() (dicee.AllvsAll method), 201
__getitem__() (dicee.BPE_NegativeSamplingDataset method), 198
__getitem__() (dicee.dataset_classes.AllvsAll method), 137
__getitem__() (dicee.dataset_classes.BPE_NegativeSamplingDataset method), 134
  _getitem__() (dicee.dataset_classes.KvsAll method), 137
__getitem__() (dicee.dataset_classes.KvsSampleDataset method), 138
__getitem__() (dicee.dataset_classes.MultiClassClassificationDataset method), 135
__getitem__() (dicee.dataset_classes.MultiLabelDataset method), 135
__getitem__() (dicee.dataset_classes.NegSampleDataset method), 139
  _getitem__() (dicee.dataset_classes.OnevsAllDataset method), 136
__getitem__() (dicee.dataset_classes.TriplePredictionDataset method), 140
__getitem__() (dicee.KvsAll method), 200
__getitem__() (dicee.KvsSampleDataset method), 202
__getitem__() (dicee.MultiClassClassificationDataset method), 199
  _getitem__() (dicee.MultiLabelDataset method), 198
__getitem__() (dicee.NegSampleDataset method), 203
__getitem__() (dicee.OnevsAllDataset method), 199
__getitem__() (dicee.TriplePredictionDataset method), 203
  _iter___() (dicee.config.Namespace method), 133
  _len__() (dicee.AllvsAll method), 201
__len__() (dicee.BPE_NegativeSamplingDataset method), 198
__len__() (dicee.dataset_classes.AllvsAll method), 137
__len__() (dicee.dataset_classes.BPE_NegativeSamplingDataset method), 134
__len__() (dicee.dataset_classes.KvsAll method), 137
__len__() (dicee.dataset_classes.KvsSampleDataset method), 138
__len__() (dicee.dataset_classes.MultiClassClassificationDataset method), 135
__len__() (dicee.dataset_classes.MultiLabelDataset method), 135
__len__() (dicee.dataset_classes.NegSampleDataset method), 139
  _len__() (dicee.dataset_classes.OnevsAllDataset method), 136
__len__() (dicee.dataset_classes.TriplePredictionDataset method), 140
__len__() (dicee.KvsAll method), 200
__len__() (dicee.KvsSampleDataset method), 202
__len__() (dicee.MultiClassClassificationDataset method), 199
  _len__() (dicee.MultiLabelDataset method), 198
__len__() (dicee.NegSampleDataset method), 202
__len__() (dicee.OnevsAllDataset method), 199
__len__() (dicee.TriplePredictionDataset method), 203
__str__() (dicee.KGE method), 191
  _str__() (dicee.knowledge_graph_embeddings.KGE method), 150
__version__(in module dicee), 208
Α
AbstractCallback (class in dicee.abstracts), 119
AbstractPPECallback (class in dicee.abstracts), 120
AbstractTrainer (class in dicee.abstracts), 115
AccumulateEpochLossCallback (class in dicee.callbacks), 124
achieve_answer() (dicee.query_generator.QueryGenerator method), 155
achieve_answer() (dicee.QueryGenerator method), 208
AConEx (class in dicee), 175
AConEx (class in dicee.models), 69
AConEx (class in dicee.models.complex), 30
AConvO (class in dicee), 175
AConvO (class in dicee.models), 81
AConvO (class in dicee.models.octonion), 39
AConvQ (class in dicee), 176
AConvQ (class in dicee.models), 76
AConvQ (class in dicee.models.quaternion), 43
adaptive_swa (dicee.config.Namespace attribute), 133
add_new_entity_embeddings() (dicee.abstracts.BaseInteractiveKGE method), 118
add_noise_rate (dicee.config.Namespace attribute), 131
add_noise_rate (dicee.knowledge_graph.KG attribute), 149
```

```
add noisy triples() (in module dicee), 189
add_noisy_triples() (in module dicee.static_funcs), 159
add_noisy_triples_into_training() (dicee.read_preprocess_save_load_kg.read_from_disk.ReadFromDisk method), 102
add_noisy_triples_into_training() (dicee.read_preprocess_save_load_kg.ReadFromDisk method), 106
add_reciprical (dicee.knowledge_graph.KG attribute), 149
AllvsAll (class in dicee), 200
AllvsAll (class in dicee.dataset_classes), 137
alphas (dicee.abstracts.AbstractPPECallback attribute), 121
alphas (dicee.callbacks.ASWA attribute), 127
analyse() (in module dicee.analyse_experiments), 123
answer_multi_hop_query() (dicee.KGE method), 194
answer_multi_hop_query() (dicee.knowledge_graph_embeddings.KGE method), 153
app (in module dicee.scripts.serve), 108
apply_coefficients() (dicee.DeCaL method), 171
apply_coefficients() (dicee. Keci method), 168
apply_coefficients() (dicee.models.clifford.DeCaL method), 27
apply_coefficients() (dicee.models.clifford.Keci method), 24
apply_coefficients() (dicee.models.DeCaL method), 88
apply_coefficients() (dicee.models.Keci method), 83
apply_reciprical_or_noise() (in module dicee.read_preprocess_save_load_kg.util), 103
apply_semantic_constraint (dicee.abstracts.BaseInteractiveKGE attribute), 117
apply_unit_norm(dicee.BaseKGE attribute), 187
apply_unit_norm(dicee.models.base_model.BaseKGE attribute), 18
apply_unit_norm(dicee.models.BaseKGE attribute), 60, 63, 67, 71, 77, 91, 94
args (dicee.BaseKGE attribute), 186
args (dicee.DICE_Trainer attribute), 190
args (dicee.evaluator.Evaluator attribute), 145
args (dicee.Execute attribute), 196
args (dicee.executer.ContinuousExecute attribute), 148
args (dicee.executer.Execute attribute), 146
args (dicee.models.base_model.BaseKGE attribute), 18
args (dicee.models.base model.IdentityClass attribute), 21
args (dicee.models.BaseKGE attribute), 60, 63, 66, 71, 77, 91, 94
args (dicee.models.IdentityClass attribute), 62, 73, 79
args (dicee.models.pykeen_models.PykeenKGE attribute), 40
args (dicee.models.PykeenKGE attribute), 93
args (dicee.PykeenKGE attribute), 183
args (dicee.trainer.DICE_Trainer attribute), 113
args (dicee.trainer.dice_trainer.DICE_Trainer attribute), 109
ASWA (class in dicee.callbacks), 127
\verb"aswa" (dicee. analyse\_experiments. Experiment attribute), 122
attn (dicee.models.transformers.Block attribute), 51
attn_dropout (dicee.models.transformers.CausalSelf Attention attribute), 49
attributes (dicee.abstracts.AbstractTrainer attribute), 115
В
backend (dicee.config.Namespace attribute), 131
backend (dicee.knowledge graph.KG attribute), 149
BaseInteractiveKGE (class in dicee.abstracts), 117
BaseKGE (class in dicee), 186
BaseKGE (class in dicee.models), 59, 62, 66, 70, 76, 90, 93
{\tt BaseKGE}~(\textit{class in dicee.models.base\_model}),~18
BaseKGELightning (class in dicee.models), 54
BaseKGELightning (class in dicee.models.base_model), 12
batch_kronecker_product() (dicee.callbacks.KronE static method), 129
batch_size (dicee.analyse_experiments.Experiment attribute), 122
batch_size (dicee.callbacks.PseudoLabellingCallback attribute), 127
batch_size (dicee.config.Namespace attribute), 131
batch_size (dicee.CVDataModule attribute), 204
batch_size (dicee.dataset_classes.CVDataModule attribute), 140
bias (dicee.models.transformers.GPTConfig attribute), 51
bias (dicee.models.transformers.LayerNorm attribute), 48
Block (class in dicee.models.transformers), 50
block_size (dicee.BaseKGE attribute), 187
block_size (dicee.config.Namespace attribute), 133
block_size (dicee.dataset_classes.MultiClassClassificationDataset attribute), 135
block_size (dicee.models.base_model.BaseKGE attribute), 19
```

```
block size (dicee.models.BaseKGE attribute), 61, 64, 67, 72, 78, 91, 95
block_size (dicee.models.transformers.GPTConfig attribute), 51
block_size (dicee.MultiClassClassificationDataset attribute), 199
bn_conv1 (dicee.AConvQ attribute), 176
bn_conv1 (dicee.ConvQ attribute), 177
bn_conv1 (dicee.models.AConvQ attribute), 76
bn_conv1 (dicee.models.ConvQ attribute), 75
bn conv1 (dicee.models.quaternion.AConvO attribute), 43
bn_conv1 (dicee.models.quaternion.ConvQ attribute), 43
bn_conv2 (dicee.AConvQ attribute), 176
bn_conv2 (dicee.ConvQ attribute), 177
bn_conv2 (dicee.models.AConvQ attribute), 76
bn_conv2 (dicee.models.ConvQ attribute), 75
bn_conv2 (dicee.models.quaternion.AConvQ attribute), 43
bn_conv2 (dicee.models.quaternion.ConvQ attribute), 43
bn_conv2d (dicee.AConEx attribute), 175
bn_conv2d (dicee.AConvO attribute), 176
bn_conv2d (dicee.ConEx attribute), 178
bn_conv2d (dicee.ConvO attribute), 178
bn_conv2d (dicee.models.AConEx attribute), 69
bn_conv2d (dicee.models.AConvO attribute), 82
bn_conv2d (dicee.models.complex.AConEx attribute), 30
bn_conv2d (dicee.models.complex.ConEx attribute), 29
bn_conv2d (dicee.models.ConEx attribute), 69
bn_conv2d (dicee.models.ConvO attribute), 81
bn_conv2d (dicee.models.octonion.AConvO attribute), 39
bn_conv2d (dicee.models.octonion.ConvO attribute), 38
BPE_NegativeSamplingDataset (class in dicee), 197
BPE_NegativeSamplingDataset (class in dicee.dataset_classes), 134
build_chain_funcs() (dicee.models.FMult2 method), 97
build_chain_funcs() (dicee.models.function_space.FMult2 method), 34
build func() (dicee.models.FMult2 method), 97
build_func() (dicee.models.function_space.FMult2 method), 34
BytE (class in dicee), 184
BytE (class in dicee.models.transformers), 46
byte_pair_encoding (dicee.analyse_experiments.Experiment attribute), 122
byte pair encoding (dicee.BaseKGE attribute), 187
byte_pair_encoding (dicee.config.Namespace attribute), 132
byte_pair_encoding (dicee.knowledge_graph.KG attribute), 149
byte_pair_encoding (dicee.models.base_model.BaseKGE attribute), 19
byte_pair_encoding (dicee.models.BaseKGE attribute), 61, 64, 67, 72, 78, 91, 95
c_attn (dicee.models.transformers.CausalSelfAttention attribute), 49
\verb|c_fc| (\textit{dicee.models.transformers.MLP attribute}), 50
c_proj (dicee.models.transformers.CausalSelfAttention attribute), 49
c_proj (dicee.models.transformers.MLP attribute), 50
callbacks (dicee.abstracts.AbstractTrainer attribute), 115
callbacks (dicee.analyse_experiments.Experiment attribute), 122
callbacks (dicee.config.Namespace attribute), 131
callbacks (dicee.trainer.torch_trainer_ddp.DDPTrainer attribute), 113
callbacks (dicee.trainer.torch_trainer_ddp.NodeTrainer attribute), 112
CausalSelfAttention (class in dicee.models.transformers), 48
chain_func() (dicee.models.FMult method), 96
chain_func() (dicee.models.function_space.FMult method), 33
chain_func() (dicee.models.function_space.GFMult method), 34
chain_func() (dicee.models.GFMult method), 96
cl_pgr() (dicee.DeCaL method), 170
cl_pqr() (dicee.models.clifford.DeCaL method), 26
cl_pqr() (dicee.models.DeCaL method), 87
clifford_mul() (dicee.CMult method), 165
clifford_mul() (dicee.models.clifford.CMult method), 22
clifford_mul() (dicee.models.CMult method), 86
clifford_multiplication() (dicee.Keci method), 168
clifford_multiplication() (dicee.models.clifford.Keci method), 24
clifford_multiplication() (dicee.models.Keci method), 84
CMult (class in dicee), 164
```

```
CMult (class in dicee.models), 85
CMult (class in dicee.models.clifford), 21
collate fn (dicee. Allvs All attribute), 201
collate_fn (dicee.dataset_classes.AllvsAll attribute), 137
collate_fn (dicee.dataset_classes.KvsAll attribute), 136
collate_fn (dicee.dataset_classes.KvsSampleDataset attribute), 138
collate_fn (dicee.dataset_classes.MultiClassClassificationDataset attribute), 135
collate fn (dicee.dataset classes.MultiLabelDataset attribute), 135
collate_fn (dicee.dataset_classes.OnevsAllDataset attribute), 136
collate_fn (dicee.KvsAll attribute), 200
collate_fn (dicee.KvsSampleDataset attribute), 202
collate_fn (dicee.MultiClassClassificationDataset attribute), 199
collate_fn (dicee.MultiLabelDataset attribute), 198
collate_fn (dicee.OnevsAllDataset attribute), 199
collate_fn() (dicee.BPE_NegativeSamplingDataset method), 198
collate_fn() (dicee.dataset_classes.BPE_NegativeSamplingDataset method), 134
collate_fn() (dicee.dataset_classes.TriplePredictionDataset method), 140
collate_fn() (dicee.TriplePredictionDataset method), 203
collection_name (dicee.scripts.serve.NeuralSearcher attribute), 108
comp_func() (dicee.LFMult method), 182
comp_func() (dicee.models.function_space.LFMult method), 36
comp func () (dicee.models.LFMult method), 99
Complex (class in dicee), 174
Complex (class in dicee.models), 69
Complex (class in dicee.models.complex), 30
compute_convergence() (in module dicee.callbacks), 127
compute_func() (dicee.models.FMult method), 96
compute_func() (dicee.models.FMult2 method), 97
compute_func() (dicee.models.function_space.FMult method), 33
compute_func() (dicee.models.function_space.FMult2 method), 34
compute_func() (dicee.models.function_space.GFMult method), 34
compute func () (dicee.models.GFMult method), 96
compute_mrr() (dicee.callbacks.ASWA static method), 127
compute_sigma_pp() (dicee.DeCaL method), 171
compute_sigma_pp() (dicee.Keci method), 167
compute_sigma_pp() (dicee.models.clifford.DeCaL method), 27
compute_sigma_pp() (dicee.models.clifford.Keci method), 23
compute_sigma_pp() (dicee.models.DeCaL method), 88
compute_sigma_pp() (dicee.models.Keci method), 83
compute_sigma_pq() (dicee.DeCaL method), 172
compute_sigma_pq() (dicee.Keci method), 167
compute_sigma_pq() (dicee.models.clifford.DeCaL method), 28
compute_sigma_pq() (dicee.models.clifford.Keci method), 24
compute_sigma_pq() (dicee.models.DeCaL method), 89
compute_sigma_pq() (dicee.models.Keci method), 83
compute_sigma_pr() (dicee.DeCaL method), 172
compute_sigma_pr() (dicee.models.clifford.DeCaL method), 29
compute_sigma_pr() (dicee.models.DeCaL method), 90
compute_sigma_qq() (dicee.DeCaL method), 172
compute_sigma_qq() (dicee.Keci method), 167
\verb|compute_sigma_qq()| \textit{(dicee.models.clifford.DeCaL method)}, 28
compute_sigma_qq() (dicee.models.clifford.Keci method), 23
compute_sigma_qq() (dicee.models.DeCaL method), 89
compute_sigma_gg() (dicee.models.Keci method), 83
compute_sigma_qr() (dicee.DeCaL method), 173
compute_sigma_qr() (dicee.models.clifford.DeCaL method), 29
compute_sigma_qr() (dicee.models.DeCaL method), 90
compute_sigma_rr() (dicee.DeCaL method), 172
compute_sigma_rr() (dicee.models.clifford.DeCaL method), 28
compute_sigma_rr() (dicee.models.DeCaL method), 89
compute sigmas multivect() (dicee.DeCaL method), 171
compute_sigmas_multivect() (dicee.models.clifford.DeCaL method), 27
compute_sigmas_multivect() (dicee.models.DeCaL method), 88
compute_sigmas_single() (dicee.DeCaL method), 170
\verb|compute_sigmas_single()| \textit{(dicee.models.clifford.DeCaL method)}, 26
compute_sigmas_single() (dicee.models.DeCaL method), 87
ConEx (class in dicee), 178
ConEx (class in dicee.models), 68
```

```
ConEx (class in dicee.models.complex), 29
config (dicee.BytE attribute), 184
config (dicee.models.transformers.BytE attribute), 47
config (dicee.models.transformers.GPT attribute), 52
configs (dicee.abstracts.BaseInteractiveKGE attribute), 117
configure_optimizers() (dicee.models.base_model.BaseKGELightning method), 16
configure_optimizers() (dicee.models.BaseKGELightning method), 58
configure optimizers () (dicee.models.transformers.GPT method), 52
construct_cl_multivector() (dicee.DeCaL method), 171
construct_cl_multivector() (dicee.Keci method), 168
construct_cl_multivector() (dicee.models.clifford.DeCaL method), 27
construct_cl_multivector() (dicee.models.clifford.Keci method), 24
construct_cl_multivector() (dicee.models.DeCaL method), 88
construct_cl_multivector() (dicee.models.Keci method), 84
construct_dataset() (in module dicee), 197
construct_dataset() (in module dicee.dataset_classes), 134
construct_ensemble (dicee.abstracts.BaseInteractiveKGE attribute), 117
construct_graph() (dicee.query_generator.QueryGenerator method), 155
construct_graph() (dicee.QueryGenerator method), 208
construct_input_and_output() (dicee.abstracts.BaseInteractiveKGE method), 119
construct_multi_coeff() (dicee.LFMult method), 182
construct_multi_coeff() (dicee.models.function_space.LFMult method), 35
construct_multi_coeff() (dicee.models.LFMult method), 98
continual_learning (dicee.config.Namespace attribute), 133
continual_start() (dicee.DICE_Trainer method), 190
continual_start() (dicee.executer.ContinuousExecute method), 148
continual_start() (dicee.trainer.DICE_Trainer method), 114
continual_start() (dicee.trainer.dice_trainer.DICE_Trainer method), 109
continual_training_setup_executor() (in module dicee), 189
continual_training_setup_executor() (in module dicee.static_funcs), 159
Continuous Execute (class in dicee.executer), 148
conv2d (dicee.AConEx attribute), 175
conv2d (dicee. AConvO attribute), 175
conv2d (dicee. AConvQ attribute), 176
conv2d (dicee.ConEx attribute), 178
conv2d (dicee.ConvO attribute), 178
conv2d (dicee.ConvO attribute), 177
conv2d (dicee.models.AConEx attribute), 69
conv2d (dicee.models.AConvO attribute), 81
conv2d (dicee.models.AConvQ attribute), 76
conv2d (dicee.models.complex.AConEx attribute), 30
conv2d (dicee.models.complex.ConEx attribute), 29
conv2d (dicee.models.ConEx attribute), 68
conv2d (dicee.models.ConvO attribute), 81
conv2d (dicee.models.ConvQ attribute), 75
conv2d (dicee.models.octonion.AConvO attribute), 39
conv2d (dicee.models.octonion.ConvO attribute), 38
conv2d (dicee.models.quaternion.AConvQ attribute), 43
conv2d (dicee.models.quaternion.ConvQ attribute), 43
ConvO (class in dicee), 177
ConvO (class in dicee.models), 80
ConvO (class in dicee.models.octonion), 38
ConvQ (class in dicee), 176
ConvQ (class in dicee.models), 75
ConvQ (class in dicee.models.quaternion), 42
create_constraints() (in module dicee.read_preprocess_save_load_kg.util), 104
create_constraints() (in module dicee.static_preprocess_funcs), 161
create_experiment_folder() (in module dicee), 189
create_experiment_folder() (in module dicee.static_funcs), 159
create_random_data() (dicee.callbacks.PseudoLabellingCallback method), 127
create_recipriocal_triples() (in module dicee), 188
create_recipriocal_triples() (in module dicee.read_preprocess_save_load_kg.util), 104
create_recipriocal_triples() (in module dicee.static_funcs), 158
create_vector_database() (dicee.KGE method), 191
create_vector_database() (dicee.knowledge_graph_embeddings.KGE method), 150
crop_block_size() (dicee.models.transformers.GPT method), 52
CVDataModule (class in dicee), 203
CVDataModule (class in dicee.dataset_classes), 140
```

```
D
data_module (dicee.callbacks.PseudoLabellingCallback attribute), 127
dataset_dir (dicee.config.Namespace attribute), 130
dataset_dir (dicee.knowledge_graph.KG attribute), 149
dataset_sanity_checking() (in module dicee.read_preprocess_save_load_kg.util), 104
DDPTrainer (class in dicee.trainer.torch_trainer_ddp), 113
DeCaL (class in dicee), 169
DeCal (class in dicee.models), 86
DeCaL (class in dicee.models.clifford), 25
decide() (dicee.callbacks.ASWA method), 127
degree (dicee.LFMult attribute), 182
degree (dicee.models.function_space.LFMult attribute), 35
degree (dicee.models.LFMult attribute), 98
deploy() (dicee.KGE method), 195
{\tt deploy} \ () \ ({\it dicee.knowledge\_graph\_embeddings.KGE\ method}), \ 154
deploy_head_entity_prediction() (in module dicee), 189
deploy_head_entity_prediction() (in module dicee.static_funcs), 159
deploy_relation_prediction() (in module dicee), 189
deploy_relation_prediction() (in module dicee.static_funcs), 159
deploy_tail_entity_prediction() (in module dicee), 189
deploy_tail_entity_prediction() (in module dicee.static_funcs), 159
deploy_triple_prediction() (in module dicee), 189
deploy_triple_prediction() (in module dicee.static_funcs), 159
DICE_Trainer (class in dicee), 190
DICE_Trainer (class in dicee.trainer), 113
DICE_Trainer (class in dicee.trainer.dice_trainer), 109
dicee
    module, 12
dicee.___main_
    module, 115
dicee.abstracts
     module, 115
dicee.analyse_experiments
     module, 121
dicee.callbacks
    module, 123
dicee.config
    module, 130
dicee.dataset_classes
    module, 133
dicee.eval_static_funcs
    module, 144
dicee.evaluator
     module, 145
dicee.executer
    module, 146
dicee.knowledge_graph
    module, 149
\verb|dicee.knowledge_graph_embeddings|
    module, 150
dicee.models
    module, 12
dicee.models.base_model
    module, 12
dicee.models.clifford
    module, 21
dicee.models.complex
    module, 29
dicee.models.dualE
    module, 31
dicee.models.function_space
     module, 33
dicee.models.octonion
    module, 36
dicee.models.pykeen_models
    module, 39
dicee.models.quaternion
     module, 41
```

```
dicee.models.real
     module, 44
dicee.models.static_funcs
     module, 45
dicee.models.transformers
    module, 46
dicee.query_generator
    module, 155
dicee.read_preprocess_save_load_kg
    module, 100
dicee.read_preprocess_save_load_kg.preprocess
    module, 100
dicee.read_preprocess_save_load_kg.read_from_disk
    module, 101
dicee.read_preprocess_save_load_kg.save_load_disk
    module, 102
dicee.read_preprocess_save_load_kg.util
    module, 103
dicee.sanity_checkers
    module, 156
dicee.scripts
    module, 106
dicee.scripts.index
    module, 106
dicee.scripts.run
    module, 107
dicee.scripts.serve
    module, 107
dicee.static_funcs
    module, 157
dicee.static_funcs_training
    module, 160
dicee.static_preprocess_funcs
    module, 160
dicee.trainer
    module, 108
dicee.trainer.dice_trainer
    module, 108
dicee.trainer.torch_trainer
    module, 110
dicee.trainer.torch_trainer_ddp
    module, 111
discrete_points (dicee.models.FMult2 attribute), 97
discrete_points (dicee.models.function_space.FMult2 attribute), 34
dist_func (dicee.models.Pyke attribute), 66
dist_func (dicee.models.real.Pyke attribute), 45
dist_func (dicee.Pyke attribute), 165
DistMult (class in dicee), 165
DistMult (class in dicee.models), 65
DistMult (class in dicee.models.real), 44
download_file() (in module dicee), 190
download_file() (in module dicee.static_funcs), 159
download_files_from_url() (in module dicee), 190
download_files_from_url() (in module dicee.static_funcs), 159
download_pretrained_model() (in module dicee), 190
download_pretrained_model() (in module dicee.static_funcs), 160
dropout (dicee.models.transformers.CausalSelfAttention attribute), 49
dropout (dicee.models.transformers.GPTConfig attribute), 51
dropout (dicee.models.transformers.MLP attribute), 50
DualE (class in dicee), 173
DualE (class in dicee.models), 99
DualE (class in dicee.models.dualE), 32
dummy_eval() (dicee.evaluator.Evaluator method), 146
dummy_id (dicee.knowledge_graph.KG attribute), 150
during_training (dicee.evaluator.Evaluator attribute), 145
```

F

ee_vocab (dicee.evaluator.Evaluator attribute), 145

```
efficient zero grad() (in module dicee.static funcs training), 160
embedding_dim (dicee.analyse_experiments.Experiment attribute), 122
embedding_dim (dicee.BaseKGE attribute), 186
embedding_dim (dicee.config.Namespace attribute), 131
embedding_dim (dicee.models.base_model.BaseKGE attribute), 18
embedding_dim (dicee.models.BaseKGE attribute), 60, 63, 66, 71, 77, 91, 94
enable_log (in module dicee.static_preprocess_funcs), 161
enc (dicee.knowledge_graph.KG attribute), 150
end() (dicee.Execute method), 197
end() (dicee.executer.Execute method), 148
ent2id (dicee.query_generator.QueryGenerator attribute), 155
ent2id (dicee.QueryGenerator attribute), 207
ent_in (dicee.query_generator.QueryGenerator attribute), 155
ent_in (dicee.QueryGenerator attribute), 207
ent_out (dicee.query_generator.QueryGenerator attribute), 155
ent_out (dicee.QueryGenerator attribute), 207
entities_str (dicee.knowledge_graph.KG property), 150
entity_embeddings (dicee.AConvQ attribute), 176
entity_embeddings (dicee.CMult attribute), 164
entity_embeddings (dicee.ConvQ attribute), 177
entity_embeddings (dicee.DeCaL attribute), 170
entity_embeddings (dicee.DualE attribute), 173
entity_embeddings (dicee.LFMult attribute), 182
entity_embeddings (dicee.models.AConvQ attribute), 76
entity_embeddings (dicee.models.clifford.CMult attribute), 21
entity_embeddings (dicee.models.clifford.DeCaL attribute), 26
entity_embeddings (dicee.models.CMult attribute), 86
entity_embeddings (dicee.models.ConvQ attribute), 75
entity_embeddings (dicee.models.DeCaL attribute), 87
entity_embeddings (dicee.models.DualE attribute), 99
entity_embeddings (dicee.models.dualE.DualE attribute), 32
entity_embeddings (dicee.models.FMult attribute), 96
entity_embeddings (dicee.models.FMult2 attribute), 97
entity_embeddings (dicee.models.function_space.FMult attribute), 33
entity_embeddings (dicee.models.function_space.FMult2 attribute), 34
entity_embeddings (dicee.models.function_space.GFMult attribute), 34
entity embeddings (dicee.models.function space.LFMult attribute), 35
entity_embeddings (dicee.models.function_space.LFMult1 attribute), 35
entity_embeddings (dicee.models.GFMult attribute), 96
entity_embeddings (dicee.models.LFMult attribute), 98
entity_embeddings (dicee.models.LFMult1 attribute), 97
entity_embeddings (dicee.models.pykeen_models.PykeenKGE attribute), 40
entity_embeddings (dicee.models.PykeenKGE attribute), 93
entity_embeddings (dicee.models.quaternion.AConvQ attribute), 43
entity_embeddings (dicee.models.quaternion.ConvQ attribute), 43
entity_embeddings (dicee.PykeenKGE attribute), 183
entity_to_idx (dicee.knowledge_graph.KG attribute), 149
epoch_count (dicee.abstracts.AbstractPPECallback attribute), 121
epoch_count (dicee.callbacks.ASWA attribute), 127
epoch_counter (dicee.callbacks.Eval attribute), 128
epoch_counter(dicee.callbacks.KGESaveCallback attribute), 125
epoch_ratio (dicee.callbacks.Eval attribute), 128
er_vocab (dicee.evaluator.Evaluator attribute), 145
estimate_mfu() (dicee.models.transformers.GPT method), 52
estimate_q() (in module dicee.callbacks), 127
Eval (class in dicee.callbacks), 128
eval () (dicee.evaluator.Evaluator method), 145
eval_lp_performance() (dicee.KGE method), 191
eval_lp_performance() (dicee.knowledge_graph_embeddings.KGE method), 151
eval_model (dicee.config.Namespace attribute), 132
eval_model (dicee.knowledge_graph.KG attribute), 149
eval_rank_of_head_and_tail_byte_pair_encoded_entity() (dicee.evaluator.Evaluator method), 145
\verb|eval_rank_of_head_and_tail_entity()| \textit{(dicee.evaluator.Evaluator method)}, 145
eval_with_bpe_vs_all() (dicee.evaluator.Evaluator method), 146
eval_with_byte() (dicee.evaluator.Evaluator method), 145
eval_with_data() (dicee.evaluator.Evaluator method), 146
eval_with_vs_all() (dicee.evaluator.Evaluator method), 146
evaluate() (in module dicee), 190
```

```
evaluate() (in module dicee.static funcs), 159
evaluate_bpe_lp() (in module dicee.static_funcs_training), 160
evaluate_link_prediction_performance() (in module dicee.eval_static_funcs), 144
evaluate_link_prediction_performance_with_bpe() (in module dicee.eval_static_funcs), 144
evaluate_link_prediction_performance_with_bpe_reciprocals() (in module dicee.eval_static_funcs), 144
evaluate_link_prediction_performance_with_reciprocals() (in module dicee.eval_static_funcs), 144
evaluate_lp() (dicee.evaluator.Evaluator method), 146
evaluate lp() (in module dicee.static funcs training), 160
evaluate_lp_bpe_k_vs_all() (dicee.evaluator.Evaluator method), 146
\verb|evaluate_lp_bpe_k_vs_all()| \textit{(in module dicee.eval\_static\_funcs)}, 144
evaluate_lp_k_vs_all() (dicee.evaluator.Evaluator method), 146
evaluate_lp_with_byte() (dicee.evaluator.Evaluator method), 146
Evaluator (class in dicee.evaluator), 145
evaluator (dicee.DICE_Trainer attribute), 190
evaluator (dicee. Execute attribute), 196
evaluator (dicee.executer.Execute attribute), 147
evaluator (dicee.trainer.DICE_Trainer attribute), 114
evaluator (dicee.trainer.dice_trainer.DICE_Trainer attribute), 109
every_x_epoch (dicee.callbacks.KGESaveCallback attribute), 125
Execute (class in dicee), 195
Execute (class in dicee.executer), 146
Experiment (class in dicee.analyse_experiments), 122
explicit (dicee.models.QMult attribute), 74
explicit (dicee.models.quaternion.QMult attribute), 42
explicit (dicee.QMult attribute), 179
exponential_function() (in module dicee), 189
exponential_function() (in module dicee.static_funcs), 159
extract_input_outputs() (dicee.trainer.torch_trainer_ddp.DDPTrainer method), 113
extract_input_outputs() (dicee.trainer.torch_trainer_ddp.NodeTrainer method), 112
extract_input_outputs_set_device() (dicee.trainer.torch_trainer.TorchTrainer method), 111
f (dicee.callbacks.KronE attribute), 129
fc1 (dicee.AConEx attribute), 175
fc1 (dicee.AConvO attribute), 176
fc1 (dicee.AConvQ attribute), 176
fc1 (dicee.ConEx attribute), 178
fc1 (dicee.ConvO attribute), 178
fc1 (dicee.ConvQ attribute), 177
fc1 (dicee.models.AConEx attribute), 69
fc1 (dicee.models.AConvO attribute), 82
fc1 (dicee.models.AConvQ attribute), 76
fc1 (dicee.models.complex.AConEx attribute), 30
fc1 (dicee.models.complex.ConEx attribute), 29
fc1 (dicee.models.ConEx attribute), 68
fc1 (dicee.models.ConvO attribute), 81
fc1 (dicee.models.ConvQ attribute), 75
fc1 (dicee.models.octonion.AConvO attribute), 39
fc1 (dicee.models.octonion.ConvO attribute), 38
fc1 (dicee.models.quaternion.AConvQ attribute), 43
fc1 (dicee.models.quaternion.ConvQ attribute), 43
fc_num_input (dicee.AConEx attribute), 175
fc_num_input (dicee.AConvO attribute), 176
fc_num_input (dicee.AConvQ attribute), 176
fc_num_input (dicee.ConEx attribute), 178
fc_num_input (dicee.ConvO attribute), 178
fc_num_input (dicee.ConvQ attribute), 177
fc_num_input (dicee.models.AConEx attribute), 69
fc_num_input (dicee.models.AConvO attribute), 82
fc_num_input (dicee.models.AConvQ attribute), 76
fc_num_input (dicee.models.complex.AConEx attribute), 30
fc_num_input (dicee.models.complex.ConEx attribute), 29
fc_num_input (dicee.models.ConEx attribute), 68
fc_num_input (dicee.models.ConvO attribute), 81
fc_num_input (dicee.models.ConvQ attribute), 75
fc_num_input (dicee.models.octonion.AConvO attribute), 39
fc_num_input (dicee.models.octonion.ConvO attribute), 38
```

```
fc num input (dicee.models.quaternion.AConvO attribute), 43
fc_num_input (dicee.models.quaternion.ConvQ attribute), 43
feature_map_dropout (dicee.AConEx attribute), 175
feature_map_dropout (dicee.AConvO attribute), 176
feature_map_dropout (dicee.AConvQ attribute), 176
feature_map_dropout (dicee.ConEx attribute), 178
feature_map_dropout (dicee.ConvO attribute), 178
feature map dropout (dicee. ConvO attribute), 177
feature_map_dropout (dicee.models.AConEx attribute), 69
feature_map_dropout (dicee.models.AConvO attribute), 82
feature_map_dropout (dicee.models.AConvQ attribute), 76
feature_map_dropout (dicee.models.complex.AConEx attribute), 30
feature_map_dropout (dicee.models.complex.ConEx attribute), 30
feature_map_dropout (dicee.models.ConEx attribute), 69
feature_map_dropout (dicee.models.ConvO attribute), 81
feature_map_dropout (dicee.models.ConvQ attribute), 75
feature_map_dropout (dicee.models.octonion.AConvO attribute), 39
feature_map_dropout (dicee.models.octonion.ConvO attribute), 38
feature_map_dropout (dicee.models.quaternion.AConvQ attribute), 43
feature_map_dropout (dicee.models.quaternion.ConvQ attribute), 43
feature_map_dropout_rate (dicee.BaseKGE attribute), 187
feature_map_dropout_rate (dicee.config.Namespace attribute), 132
feature_map_dropout_rate (dicee.models.base_model.BaseKGE attribute), 19
feature_map_dropout_rate (dicee.models.BaseKGE attribute), 60, 63, 67, 71, 77, 91, 94
fill_query() (dicee.query_generator.QueryGenerator method), 155
fill_query() (dicee.QueryGenerator method), 208
find_missing_triples() (dicee.KGE method), 195
find_missing_triples() (dicee.knowledge_graph_embeddings.KGE method), 154
\verb|fit()| (dicee.trainer.torch\_trainer\_ddp.TorchDDPTrainer method), 112|
fit () (dicee.trainer.torch_trainer.TorchTrainer method), 110
flash (dicee.models.transformers.CausalSelfAttention attribute), 49
FMult (class in dicee.models), 96
FMult (class in dicee.models.function_space), 33
FMult2 (class in dicee.models), 97
FMult2 (class in dicee.models.function_space), 34
form_of_labelling (dicee.DICE_Trainer attribute), 190
form of labelling (dicee.trainer.DICE Trainer attribute), 114
form_of_labelling (dicee.trainer.dice_trainer.DICE_Trainer attribute), 109
forward() (dicee.BaseKGE method), 187
forward() (dicee.BytE method), 185
{\tt forward()} \ ({\it dicee.models.base\_model.BaseKGE\ method}), \, 19
forward() (dicee.models.base_model.IdentityClass static method), 21
forward() (dicee.models.BaseKGE method), 61, 64, 68, 72, 78, 92, 95
forward() (dicee.models.IdentityClass static method), 62, 73, 79
forward() (dicee.models.transformers.Block method), 51
forward() (dicee.models.transformers.BytE method), 47
forward() (dicee.models.transformers.CausalSelfAttention method), 49
forward() (dicee.models.transformers.GPT method), 52
forward() (dicee.models.transformers.LayerNorm method), 48
forward() (dicee.models.transformers.MLP method), 50
forward backward update() (dicee.trainer.torch trainer.TorchTrainer method), 111
forward_byte_pair_encoded_k_vs_all() (dicee.BaseKGE method), 187
forward_byte_pair_encoded_k_vs_all() (dicee.models.base_model.BaseKGE method), 19
forward_byte_pair_encoded_k_vs_all() (dicee.models.BaseKGE method), 61, 64, 67, 72, 78, 91, 95
forward_byte_pair_encoded_triple() (dicee.BaseKGE method), 187
forward_byte_pair_encoded_triple() (dicee.models.base_model.BaseKGE method), 19
forward_byte_pair_encoded_triple() (dicee.models.BaseKGE method), 61, 64, 67, 72, 78, 92, 95
forward_k_vs_all() (dicee.AConEx method), 175
forward_k_vs_all() (dicee.AConvO method), 176
forward_k_vs_all() (dicee.AConvQ method), 176
forward_k_vs_all() (dicee.BaseKGE method), 188
forward_k_vs_all() (dicee.CMult method), 165
forward_k_vs_all() (dicee.ComplEx method), 175
forward_k_vs_all() (dicee.ConEx method), 179
forward_k_vs_all() (dicee.ConvO method), 178
forward_k_vs_all() (dicee.ConvQ method), 177
forward_k_vs_all() (dicee.DeCaL method), 171
forward_k_vs_all() (dicee.DistMult method), 166
```

```
forward k vs all() (dicee.DualE method), 174
forward_k_vs_all() (dicee.Keci method), 168
forward_k_vs_all() (dicee.models.AConEx method), 69
forward_k_vs_all() (dicee.models.AConvO method), 82
forward_k_vs_all() (dicee.models.AConvQ method), 76
forward_k_vs_all() (dicee.models.base_model.BaseKGE method), 20
forward_k_vs_all() (dicee.models.BaseKGE method), 61, 64, 68, 72, 78, 92, 95
forward k vs all() (dicee.models.clifford.CMult method), 22
forward_k_vs_all() (dicee.models.clifford.DeCaL method), 27
forward_k_vs_all() (dicee.models.clifford.Keci method), 24
forward_k_vs_all() (dicee.models.CMult method), 86
forward_k_vs_all() (dicee.models.ComplEx method), 70
forward_k_vs_all() (dicee.models.complex.AConEx method), 30
forward_k_vs_all() (dicee.models.complex.ComplEx method), 31
forward_k_vs_all() (dicee.models.complex.ConEx method), 30
forward_k_vs_all() (dicee.models.ConEx method), 69
forward_k_vs_all() (dicee.models.ConvO method), 81
forward_k_vs_all() (dicee.models.ConvQ method), 76
forward_k_vs_all() (dicee.models.DeCaL method), 88
forward_k_vs_all() (dicee.models.DistMult method), 65
forward_k_vs_all() (dicee.models.DualE method), 100
forward_k_vs_all() (dicee.models.dualE.DualE method), 32
forward_k_vs_all() (dicee.models.Keci method), 84
forward_k_vs_all() (dicee.models.octonion.AConvO method), 39
forward_k_vs_all() (dicee.models.octonion.ConvO method), 39
forward_k_vs_all() (dicee.models.octonion.OMult method), 38
forward_k_vs_all() (dicee.models.OMult method), 80
forward_k_vs_all() (dicee.models.pykeen_models.PykeenKGE method), 40
forward_k_vs_all() (dicee.models.PykeenKGE method), 93
forward_k_vs_all() (dicee.models.QMult method), 75
forward_k_vs_all() (dicee.models.quaternion.AConvQ method), 44
forward_k_vs_all() (dicee.models.quaternion.ConvQ method), 43
forward_k_vs_all() (dicee.models.quaternion.QMult method), 42
forward_k_vs_all() (dicee.models.real.DistMult method), 44
forward_k_vs_all() (dicee.models.real.Shallom method), 45
forward_k_vs_all() (dicee.models.real.TransE method), 45
forward k vs all() (dicee.models.Shallom method), 65
forward_k_vs_all() (dicee.models.TransE method), 65
forward_k_vs_all() (dicee.OMult method), 181
forward_k_vs_all() (dicee.PykeenKGE method), 183
forward_k_vs_all() (dicee.QMult method), 180
forward_k_vs_all() (dicee.Shallom method), 181
forward_k_vs_all() (dicee.TransE method), 169
forward_k_vs_sample() (dicee.AConEx method), 175
forward_k_vs_sample() (dicee.BaseKGE method), 188
forward_k_vs_sample() (dicee.ConEx method), 179
forward_k_vs_sample() (dicee.DistMult method), 166
forward_k_vs_sample() (dicee.Keci method), 168
forward_k_vs_sample() (dicee.models.AConEx method), 69
forward_k_vs_sample() (dicee.models.base_model.BaseKGE method), 20
forward_k_vs_sample() (dicee.models.BaseKGE method), 61, 64, 68, 72, 78, 92, 95
forward_k_vs_sample() (dicee.models.clifford.Keci method), 25
forward_k_vs_sample() (dicee.models.complex.AConEx method), 30
forward_k_vs_sample() (dicee.models.complex.ConEx method), 30
forward_k_vs_sample() (dicee.models.ConEx method), 69
forward_k_vs_sample() (dicee.models.DistMult method), 65
forward_k_vs_sample() (dicee.models.Keci method), 84
\verb|forward_k_vs_sample()| \textit{(dicee.models.pykeen\_models.PykeenKGE method)}, 40
forward_k_vs_sample() (dicee.models.PykeenKGE method), 93
forward_k_vs_sample() (dicee.models.QMult method), 75
forward_k_vs_sample() (dicee.models.quaternion.QMult method), 42
forward_k_vs_sample() (dicee.models.real.DistMult method), 44
forward_k_vs_sample() (dicee.PykeenKGE method), 184
forward_k_vs_sample() (dicee.QMult method), 180
forward_k_vs_with_explicit() (dicee.Keci method), 168
forward_k_vs_with_explicit() (dicee.models.clifford.Keci method), 24
forward_k_vs_with_explicit() (dicee.models.Keci method), 84
forward_triples() (dicee.AConEx method), 175
```

```
forward triples () (dicee. AConvO method), 176
forward_triples() (dicee.AConvQ method), 176
forward_triples() (dicee.BaseKGE method), 188
forward_triples() (dicee.CMult method), 165
forward_triples() (dicee.ConEx method), 179
forward_triples() (dicee.ConvO method), 178
forward_triples() (dicee.ConvQ method), 177
forward triples() (dicee.DeCaL method), 170
forward_triples() (dicee.DualE method), 173
forward_triples() (dicee.Keci method), 169
forward_triples() (dicee.LFMult method), 182
forward_triples() (dicee.models.AConEx method), 69
forward_triples() (dicee.models.AConvO method), 82
forward_triples() (dicee.models.AConvQ method), 76
forward_triples() (dicee.models.base_model.BaseKGE method), 20
forward_triples() (dicee.models.BaseKGE method), 61, 64, 68, 72, 78, 92, 95
forward_triples() (dicee.models.clifford.CMult method), 22
forward_triples() (dicee.models.clifford.DeCaL method), 26
forward_triples() (dicee.models.clifford.Keci method), 25
forward_triples() (dicee.models.CMult method), 86
forward_triples() (dicee.models.complex.AConEx method), 30
forward_triples() (dicee.models.complex.ConEx method), 30
forward_triples() (dicee.models.ConEx method), 69
forward_triples() (dicee.models.ConvO method), 81
forward_triples() (dicee.models.ConvQ method), 75
forward_triples() (dicee.models.DeCaL method), 87
forward_triples() (dicee.models.DualE method), 99
forward_triples() (dicee.models.dualE.DualE method), 32
forward_triples() (dicee.models.FMult method), 96
forward_triples() (dicee.models.FMult2 method), 97
forward_triples() (dicee.models.function_space.FMult method), 33
forward triples() (dicee.models.function space.FMult2 method), 35
forward_triples() (dicee.models.function_space.GFMult method), 34
forward_triples() (dicee.models.function_space.LFMult method), 35
forward_triples() (dicee.models.function_space.LFMult1 method), 35
forward_triples() (dicee.models.GFMult method), 96
forward triples () (dicee.models.Keci method), 85
forward_triples() (dicee.models.LFMult method), 98
forward_triples() (dicee.models.LFMult1 method), 97
forward_triples() (dicee.models.octonion.AConvO method), 39
forward_triples() (dicee.models.octonion.ConvO method), 39
forward_triples() (dicee.models.Pyke method), 66
forward_triples() (dicee.models.pykeen_models.PykeenKGE method), 40
forward_triples() (dicee.models.PykeenKGE method), 93
forward_triples() (dicee.models.quaternion.AConvQ method), 43
forward_triples() (dicee.models.quaternion.ConvQ method), 43
forward_triples() (dicee.models.real.Pyke method), 45
forward_triples() (dicee.models.real.Shallom method), 45
forward_triples() (dicee.models.Shallom method), 65
forward_triples() (dicee.Pyke method), 165
forward_triples() (dicee.PykeenKGE method). 183
forward_triples() (dicee.Shallom method), 181
frequency (dicee.callbacks.Perturb attribute), 130
from_pretrained() (dicee.models.transformers.GPT class method), 52
full_storage_path (dicee.analyse_experiments.Experiment attribute), 122
func_triple_to_bpe_representation (dicee.evaluator.Evaluator attribute), 145
func_triple_to_bpe_representation() (dicee.knowledge_graph.KG method), 150
function() (dicee.models.FMult2 method), 97
function() (dicee.models.function_space.FMult2 method), 34
G
gamma (dicee.models.FMult attribute), 96
gamma (dicee.models.function_space.FMult attribute), 33
gelu (dicee.models.transformers.MLP attribute), 50
gen_test (dicee.query_generator.QueryGenerator attribute), 155
gen_test (dicee.QueryGenerator attribute), 207
gen_valid (dicee.query_generator.QueryGenerator attribute), 155
```

```
gen valid (dicee. Ouery Generator attribute), 207
generate() (dicee.BytE method), 185
generate() (dicee.KGE method), 191
generate() (dicee.knowledge_graph_embeddings.KGE method), 151
generate() (dicee.models.transformers.BytE method), 47
generate_queries() (dicee.query_generator.QueryGenerator method), 156
generate_queries() (dicee.QueryGenerator method), 208
get () (dicee.scripts.serve.NeuralSearcher method), 108
get_aswa_state_dict() (dicee.callbacks.ASWA method), 127
get_bpe_head_and_relation_representation() (dicee.BaseKGE method), 188
get_bpe_head_and_relation_representation() (dicee.models.base_model.BaseKGE method), 20
get_bpe_token_representation() (dicee.abstracts.BaseInteractiveKGE method), 117
get_callbacks() (in module dicee.trainer.dice_trainer), 109
get_default_arguments() (in module dicee.analyse_experiments), 122
get_default_arguments() (in module dicee.scripts.index), 106
get_default_arguments() (in module dicee.scripts.run), 107
get_default_arguments() (in module dicee.scripts.serve), 108
get_ee_vocab() (in module dicee), 188
get_ee_vocab() (in module dicee.read_preprocess_save_load_kg.util), 104
get_ee_vocab() (in module dicee.static_funcs), 158
get_ee_vocab() (in module dicee.static_preprocess_funcs), 161
get_embeddings() (dicee.BaseKGE method), 188
get_embeddings() (dicee.models.base_model.BaseKGE method), 20
get_embeddings() (dicee.models.BaseKGE method), 61, 65, 68, 73, 79, 92, 96
get_embeddings() (dicee.models.real.Shallom method), 45
get_embeddings() (dicee.models.Shallom method), 65
get_embeddings() (dicee.Shallom method), 181
get_entity_embeddings() (dicee.abstracts.BaseInteractiveKGE method), 118
get_entity_index() (dicee.abstracts.BaseInteractiveKGE method), 118
get_er_vocab() (in module dicee), 188
get_er_vocab() (in module dicee.read_preprocess_save_load_kg.util), 104
get_er_vocab() (in module dicee.static_funcs), 158
get_er_vocab() (in module dicee.static_preprocess_funcs), 161
get_eval_report() (dicee.abstracts.BaseInteractiveKGE method), 117
get_head_relation_representation() (dicee.BaseKGE method), 188
get_head_relation_representation() (dicee.models.base_model.BaseKGE method), 20
get_head_relation_representation() (dicee.models.BaseKGE method), 61, 64, 68, 72, 78, 92, 95
get_kronecker_triple_representation() (dicee.callbacks.KronE method), 129
get_num_params() (dicee.models.transformers.GPT method), 52
get_padded_bpe_triple_representation() (dicee.abstracts.BaseInteractiveKGE method), 117
get_queries() (dicee.query_generator.QueryGenerator method), 156
get_queries() (dicee.QueryGenerator method), 208
get_re_vocab() (in module dicee), 188
get_re_vocab() (in module dicee.read_preprocess_save_load_kg.util), 104
get_re_vocab() (in module dicee.static_funcs), 158
get_re_vocab() (in module dicee.static_preprocess_funcs), 161
get_relation_embeddings() (dicee.abstracts.BaseInteractiveKGE method), 119
get_relation_index() (dicee.abstracts.BaseInteractiveKGE method), 118
get_sentence_representation() (dicee.BaseKGE method), 188
get_sentence_representation() (dicee.models.base_model.BaseKGE method), 20
get_sentence_representation() (dicee.models.BaseKGE method), 61, 64, 68, 72, 78, 92, 95
get_transductive_entity_embeddings() (dicee.KGE method), 191
get_transductive_entity_embeddings() (dicee.knowledge_graph_embeddings.KGE method), 150
get_triple_representation() (dicee.BaseKGE method), 188
get_triple_representation() (dicee.models.base_model.BaseKGE method), 20
get_triple_representation() (dicee.models.BaseKGE method), 61, 64, 68, 72, 78, 92, 95
GFMult (class in dicee.models), 96
GFMult (class in dicee.models.function_space), 34
global_rank (dicee.trainer.torch_trainer_ddp.NodeTrainer attribute), 112
GPT (class in dicee.models.transformers), 51
GPTConfig (class in dicee.models.transformers), 51
gpu_id (dicee.trainer.torch_trainer_ddp.DDPTrainer attribute), 113
gpus (dicee.config.Namespace attribute), 131
gradient_accumulation_steps (dicee.config.Namespace attribute), 132
ground_queries() (dicee.query_generator.QueryGenerator method), 156
ground_queries() (dicee.QueryGenerator method), 208
```

```
Н
hidden_dropout (dicee.BaseKGE attribute), 187
hidden_dropout (dicee.models.base_model.BaseKGE attribute), 19
hidden_dropout (dicee.models.BaseKGE attribute), 60, 64, 67, 72, 78, 91, 95
hidden_dropout_rate (dicee.BaseKGE attribute), 187
hidden_dropout_rate (dicee.config.Namespace attribute), 132
hidden_dropout_rate (dicee.models.base_model.BaseKGE attribute), 18
hidden_dropout_rate (dicee.models.BaseKGE attribute), 60, 63, 67, 71, 77, 91, 94
hidden_normalizer (dicee.BaseKGE attribute), 187
hidden_normalizer (dicee.models.base_model.BaseKGE attribute), 19
hidden_normalizer (dicee.models.BaseKGE attribute), 60, 64, 67, 72, 78, 91, 95
IdentityClass (class in dicee.models), 62, 73, 79
IdentityClass (class in dicee.models.base model), 20
idx_entity_to_bpe_shaped (dicee.knowledge_graph.KG attribute), 150
index_triple() (dicee.abstracts.BaseInteractiveKGE method), 118
index_triples_with_pandas() (in module dicee.read_preprocess_save_load_kg.util), 104
init_param (dicee.config.Namespace attribute), 132
init_params_with_sanity_checking() (dicee.BaseKGE method), 187
init_params_with_sanity_checking() (dicee.models.base_model.BaseKGE method), 19
init params with sanity checking () (dicee.models.BaseKGE method), 61, 64, 68, 72, 78, 92, 95
initial_eval_setting (dicee.callbacks.ASWA attribute), 127
initialize_dataloader() (dicee.DICE_Trainer method), 191
initialize_dataloader() (dicee.trainer.DICE_Trainer method), 114
initialize_dataloader() (dicee.trainer.dice_trainer.DICE_Trainer method), 109
initialize_dataset() (dicee.DICE_Trainer method), 191
initialize_dataset() (dicee.trainer.DICE_Trainer method), 114
initialize_dataset() (dicee.trainer.dice_trainer.DICE_Trainer method), 109
initialize_or_load_model()(dicee.DICE_Trainer method), 191
initialize_or_load_model() (dicee.trainer.DICE_Trainer method), 114
initialize_or_load_model() (dicee.trainer.dice_trainer.DICE_Trainer method), 109
initialize_trainer() (dicee.DICE_Trainer method), 191
initialize_trainer() (dicee.trainer.DICE_Trainer method), 114
initialize_trainer() (dicee.trainer.dice_trainer.DICE_Trainer method), 109
initialize_trainer() (in module dicee.trainer.dice_trainer), 109
input_dp_ent_real (dicee.BaseKGE attribute), 187
input_dp_ent_real (dicee.models.base_model.BaseKGE attribute), 19
input_dp_ent_real (dicee.models.BaseKGE attribute), 60, 64, 67, 72, 78, 91, 95
input_dp_rel_real (dicee.BaseKGE attribute), 187
input_dp_rel_real (dicee.models.base_model.BaseKGE attribute), 19
input_dp_rel_real (dicee.models.BaseKGE attribute), 60, 64, 67, 72, 78, 91, 95
input_dropout_rate (dicee.BaseKGE attribute), 187
input_dropout_rate (dicee.config.Namespace attribute), 132
input_dropout_rate (dicee.models.base_model.BaseKGE attribute), 18
input_dropout_rate (dicee.models.BaseKGE attribute), 60, 63, 67, 71, 77, 91, 94
intialize_model() (in module dicee), 189
intialize_model() (in module dicee.static_funcs), 159
is_continual_training (dicee.DICE_Trainer attribute), 190
is_continual_training (dicee.evaluator.Evaluator attribute), 145
is_continual_training (dicee.Execute attribute), 196
is_continual_training (dicee.executer.Execute attribute), 146
is_continual_training (dicee.trainer.DICE_Trainer attribute), 114
is_continual_training (dicee.trainer.dice_trainer.DICE_Trainer attribute), 109
is_global_zero (dicee.abstracts.AbstractTrainer attribute), 115
is_seen() (dicee.abstracts.BaseInteractiveKGE method), 118
is_sparql_endpoint_alive() (in module dicee.sanity_checkers), 156
K
k (dicee.models.FMult attribute), 96
k (dicee.models.FMult2 attribute), 97
k (dicee.models.function_space.FMult attribute), 33
k (dicee.models.function_space.FMult2 attribute), 34
k (dicee.models.function_space.GFMult attribute), 34
```

k (dicee.models.GFMult attribute), 96

k_fold_cross_validation() (dicee.DICE_Trainer method), 191

```
k fold cross validation() (dicee.trainer.DICE Trainer method), 114
k_fold_cross_validation() (dicee.trainer.dice_trainer.DICE_Trainer method), 110
k_vs_all_score() (dicee.ComplEx static method), 175
k_vs_all_score() (dicee.DistMult method), 166
k_vs_all_score() (dicee.Keci method), 168
k_vs_all_score() (dicee.models.clifford.Keci method), 24
k_vs_all_score() (dicee.models.ComplEx static method), 70
k vs all score() (dicee.models.complex.ComplEx static method), 31
k_vs_all_score() (dicee.models.DistMult method), 65
k_vs_all_score() (dicee.models.Keci method), 84
k_vs_all_score() (dicee.models.octonion.OMult method), 38
k_vs_all_score() (dicee.models.OMult method), 80
k_vs_all_score() (dicee.models.QMult method), 75
k_vs_all_score() (dicee.models.quaternion.QMult method), 42
k_vs_all_score() (dicee.models.real.DistMult method), 44
k_vs_all_score() (dicee.OMult method), 181
k_vs_all_score() (dicee.QMult method), 180
Keci (class in dicee), 166
Keci (class in dicee.models), 82
Keci (class in dicee.models.clifford), 22
KeciBase (class in dicee), 166
KeciBase (class in dicee.models), 85
KeciBase (class in dicee.models.clifford), 25
kernel_size (dicee.BaseKGE attribute), 187
kernel_size (dicee.config.Namespace attribute), 132
kernel_size (dicee.models.base_model.BaseKGE attribute), 19
kernel_size(dicee.models.BaseKGE attribute), 60, 63, 67, 71, 77, 91, 94
KG (class in dicee.knowledge_graph), 149
kg (dicee.callbacks.PseudoLabellingCallback attribute), 127
kg (dicee.read_preprocess_save_load_kg.LoadSaveToDisk attribute), 106
kg (dicee.read_preprocess_save_load_kg.PreprocessKG attribute), 105
kg (dicee.read_preprocess_save_load_kg.preprocess.PreprocessKG attribute), 100
kg (dicee.read_preprocess_save_load_kg.read_from_disk.ReadFromDisk attribute), 101
kg (dicee.read_preprocess_save_load_kg.ReadFromDisk attribute), 106
kg (dicee.read_preprocess_save_load_kg.save_load_disk.LoadSaveToDisk attribute), 102
KGE (class in dicee), 191
KGE (class in dicee.knowledge_graph_embeddings), 150
KGESaveCallback (class in dicee.callbacks), 125
knowledge_graph (dicee.Execute attribute), 196
knowledge_graph (dicee.executer.Execute attribute), 147
KronE (class in dicee.callbacks), 129
KvsAll (class in dicee), 199
KvsAll (class in dicee.dataset_classes), 136
kvsall_score() (dicee.DualE method), 173
kvsall_score() (dicee.models.DualE method), 99
{\tt kvsall\_score} \ () \ \textit{(dicee.models.dualE.DualE method)}, 32
KvsSampleDataset (class in dicee), 201
KvsSampleDataset (class in dicee.dataset_classes), 137
label_smoothing_rate (dicee.AllvsAll attribute), 201
label_smoothing_rate (dicee.config.Namespace attribute), 132
label_smoothing_rate (dicee.dataset_classes.AllvsAll attribute), 137
label_smoothing_rate (dicee.dataset_classes.KvsAll attribute), 136
label_smoothing_rate (dicee.dataset_classes.KvsSampleDataset attribute), 138
label_smoothing_rate (dicee.dataset_classes.TriplePredictionDataset attribute), 139
label_smoothing_rate (dicee.KvsAll attribute), 200
label_smoothing_rate (dicee.KvsSampleDataset attribute), 202
label_smoothing_rate (dicee. TriplePredictionDataset attribute), 203
LayerNorm (class in dicee.models.transformers), 48
learning_rate (dicee.BaseKGE attribute), 186
learning_rate (dicee.models.base_model.BaseKGE attribute), 18
learning_rate (dicee.models.BaseKGE attribute), 60, 63, 67, 71, 77, 91, 94
length (dicee.dataset_classes.NegSampleDataset attribute), 139
length (dicee.dataset_classes.TriplePredictionDataset attribute), 140
length (dicee.NegSampleDataset attribute), 202
length (dicee. Triple Prediction Dataset attribute), 203
```

```
level (dicee.callbacks.Perturb attribute), 130
LFMult (class in dicee), 181
LFMult (class in dicee.models), 98
LFMult (class in dicee.models.function_space), 35
LFMult1 (class in dicee.models), 97
LFMult1 (class in dicee.models.function_space), 35
linear() (dicee.LFMult method), 182
linear() (dicee.models.function space.LFMult method), 35
linear() (dicee.models.LFMult method), 98
list2tuple() (dicee.query_generator.QueryGenerator method), 155
list2tuple() (dicee.QueryGenerator method), 207
lm_head (dicee.BytE attribute), 184
lm_head (dicee.models.transformers.BytE attribute), 47
lm_head (dicee.models.transformers.GPT attribute), 52
ln_1 (dicee.models.transformers.Block attribute), 51
ln_2 (dicee.models.transformers.Block attribute), 51
load() (dicee.read_preprocess_save_load_kg.LoadSaveToDisk method), 106
load() (dicee.read_preprocess_save_load_kg.save_load_disk.LoadSaveToDisk method), 102
load_indexed_data() (dicee.Execute method), 196
load_indexed_data() (dicee.executer.Execute method), 147
load_json() (in module dicee), 189
load_json() (in module dicee.static_funcs), 159
load_model() (in module dicee), 188
load_model() (in module dicee.static_funcs), 158
load_model_ensemble() (in module dicee), 188
load_model_ensemble() (in module dicee.static_funcs), 158
load_numpy() (in module dicee), 189
load_numpy() (in module dicee.static_funcs), 159
load_numpy_ndarray() (in module dicee.read_preprocess_save_load_kg.util), 104
load_pickle() (in module dicee), 188, 197
load_pickle() (in module dicee.read_preprocess_save_load_kg.util), 104
load_pickle() (in module dicee.static_funcs), 158
load_queries() (dicee.query_generator.QueryGenerator method), 156
load_queries() (dicee.QueryGenerator method), 208
load_queries_and_answers() (dicee.query_generator.QueryGenerator static method), 156
load_queries_and_answers() (dicee.QueryGenerator static method), 208
load with pandas () (in module dicee.read preprocess save load kg.util), 104
LoadSaveToDisk (class in dicee.read_preprocess_save_load_kg), 105
LoadSaveToDisk (class in dicee.read_preprocess_save_load_kg.save_load_disk), 102
local_rank (dicee.trainer.torch_trainer_ddp.NodeTrainer attribute), 112
loss (dicee.BaseKGE attribute), 187
loss (dicee.models.base_model.BaseKGE attribute), 19
loss (dicee.models.BaseKGE attribute), 60, 63, 67, 71, 77, 91, 94
loss_func (dicee.trainer.torch_trainer_ddp.DDPTrainer attribute), 113
loss_func (dicee.trainer.torch_trainer_ddp.NodeTrainer attribute), 112
loss_function (dicee.trainer.torch_trainer.TorchTrainer attribute), 110
loss_function() (dicee.BytE method), 184
loss_function() (dicee.models.base_model.BaseKGELightning method), 14
loss_function() (dicee.models.BaseKGELightning method), 55
loss_function() (dicee.models.transformers.BytE method), 47
loss_history (dicee.BaseKGE attribute), 187
loss_history (dicee.models.base_model.BaseKGE attribute), 19
loss_history (dicee.models.BaseKGE attribute), 61, 64, 67, 72, 78, 91, 95
loss_history (dicee.models.pykeen_models.PykeenKGE attribute), 40
loss_history (dicee.models.PykeenKGE attribute), 93
loss_history (dicee.PykeenKGE attribute), 183
loss_history (dicee.trainer.torch_trainer_ddp.DDPTrainer attribute), 113
loss_history (dicee.trainer.torch_trainer_ddp.NodeTrainer attribute), 112
1r (dicee.analyse_experiments.Experiment attribute), 122
1r (dicee.config.Namespace attribute), 131
Μ
m (dicee.LFMult attribute), 182
m (dicee.models.function_space.LFMult attribute), 35
m (dicee.models.LFMult attribute), 98
main() (in module dicee.scripts.index), 106
main() (in module dicee.scripts.run), 107
```

```
main() (in module dicee.scripts.serve), 108
make_iterable_verbose() (in module dicee.trainer.torch_trainer_ddp), 112
mapping_from_first_two_cols_to_third() (in module dicee), 197
mapping_from_first_two_cols_to_third() (in module dicee.static_preprocess_funcs), 161
margin (dicee.models.Pyke attribute), 66
margin (dicee.models.real.Pyke attribute), 45
margin (dicee.models.real.TransE attribute), 44
margin (dicee.models.TransE attribute), 65
margin (dicee. Pyke attribute), 165
margin (dicee. TransE attribute), 169
max_ans_num (dicee.query_generator.QueryGenerator attribute), 155
max_ans_num (dicee.QueryGenerator attribute), 207
max_epochs (dicee.callbacks.KGESaveCallback attribute), 125
max_length_subword_tokens (dicee.BaseKGE attribute), 187
max_length_subword_tokens (dicee.knowledge_graph.KG attribute), 150
max_length_subword_tokens (dicee.models.base_model.BaseKGE attribute), 19
max_length_subword_tokens (dicee.models.BaseKGE attribute), 61, 64, 67, 72, 78, 91, 95
mem_of_model() (dicee.models.base_model.BaseKGELightning method), 13
mem_of_model() (dicee.models.BaseKGELightning method), 54
method (dicee.callbacks.Perturb attribute), 130
MLP (class in dicee.models.transformers), 49
mlp (dicee.models.transformers.Block attribute), 51
mode (dicee.query_generator.QueryGenerator attribute), 155
mode (dicee. Query Generator attribute), 207
model (dicee.config.Namespace attribute), 131
model (dicee.models.pykeen_models.PykeenKGE attribute), 40
model (dicee.models.PykeenKGE attribute), 93
model (dicee.PykeenKGE attribute), 183
model (dicee.scripts.serve.NeuralSearcher attribute), 108
model (dicee.trainer.torch_trainer_ddp.DDPTrainer attribute), 113
model (dicee.trainer.torch_trainer_ddp.NodeTrainer attribute), 112
model (dicee.trainer.torch trainer.TorchTrainer attribute), 110
model_kwargs (dicee.models.pykeen_models.PykeenKGE attribute), 40
model_kwargs (dicee.models.PykeenKGE attribute), 92
model_kwargs (dicee.PykeenKGE attribute), 183
model_name (dicee.analyse_experiments.Experiment attribute), 122
module
     dicee, 12
     dicee.___main___, 115
     dicee.abstracts, 115
     dicee.analyse_experiments, 121
     dicee.callbacks, 123
     dicee.config, 130
     dicee.dataset_classes, 133
     dicee.eval_static_funcs, 144
     dicee.evaluator.145
     dicee.executer, 146
     dicee.knowledge_graph, 149
     dicee.knowledge_graph_embeddings, 150
     dicee.models, 12
     dicee.models.base_model, 12
     dicee.models.clifford, 21
     dicee.models.complex, 29
     dicee.models.dualE,31
     dicee.models.function_space, 33
     dicee.models.octonion, 36
     dicee.models.pykeen_models, 39
     dicee.models.quaternion,41
     dicee.models.real,44
     dicee.models.static_funcs,45
     dicee.models.transformers.46
     dicee.query_generator, 155
     dicee.read_preprocess_save_load_kg, 100
     dicee.read_preprocess_save_load_kg.preprocess, 100
     dicee.read_preprocess_save_load_kg.read_from_disk, 101
     dicee.read_preprocess_save_load_kg.save_load_disk, 102
     dicee.read_preprocess_save_load_kg.util, 103
     dicee.sanity_checkers, 156
```

```
dicee.scripts, 106
      dicee.scripts.index, 106
      dicee.scripts.run, 107
      dicee.scripts.serve, 107
      dicee.static_funcs, 157
      dicee.static_funcs_training, 160
      dicee.static_preprocess_funcs, 160
      dicee.trainer, 108
      dicee.trainer.dice_trainer, 108
      dicee.trainer.torch_trainer,110
      dicee.trainer.torch_trainer_ddp, 111
MultiClassClassificationDataset (class in dicee), 198
MultiClassClassificationDataset (class in dicee.dataset_classes), 135
MultiLabelDataset (class in dicee), 198
MultiLabelDataset (class in dicee.dataset_classes), 134
Ν
n (dicee.models.FMult2 attribute), 97
n (dicee.models.function_space.FMult2 attribute), 34
n_embd (dicee.models.transformers.CausalSelfAttention attribute), 49
n_embd (dicee.models.transformers.GPTConfig attribute), 51
n_head (dicee.models.transformers.CausalSelfAttention attribute), 49
n_head (dicee.models.transformers.GPTConfig attribute), 51
n_layer (dicee.models.transformers.GPTConfig attribute), 51
n_layers (dicee.models.FMult2 attribute), 97
n_layers (dicee.models.function_space.FMult2 attribute), 34
name (dicee.abstracts.BaseInteractiveKGE property), 118
name (dicee.AConEx attribute), 175
name (dicee.AConvO attribute), 175
name (dicee. AConvQ attribute), 176
name (dicee.BytE attribute), 184
name (dicee.CMult attribute), 164
name (dicee.ComplEx attribute), 175
name (dicee.ConEx attribute), 178
name (dicee.ConvO attribute), 178
name (dicee.ConvQ attribute), 177
name (dicee.DeCaL attribute), 170
name (dicee.DistMult attribute), 166
name (dicee.DualE attribute), 173
name (dicee.Keci attribute), 167
name (dicee. KeciBase attribute), 166
name (dicee.LFMult attribute), 182
name (dicee.models.AConEx attribute), 69
name (dicee.models.AConvO attribute), 81
name (dicee.models.AConvQ attribute), 76
name (dicee.models.clifford.CMult attribute), 21
name (dicee.models.clifford.DeCaL attribute), 26
name (dicee.models.clifford.Keci attribute), 23
name (dicee.models.clifford.KeciBase attribute), 25
name (dicee.models.CMult attribute), 85
name (dicee.models.ComplEx attribute), 70
name (dicee.models.complex.AConEx attribute), 30
name (dicee.models.complex.ComplEx attribute), 31
name (dicee.models.complex.ConEx attribute), 29
name (dicee.models.ConEx attribute), 68
name (dicee.models.ConvO attribute), 81
name (dicee.models.ConvQ attribute), 75
name (dicee.models.DeCaL attribute), 87
name (dicee.models.DistMult attribute), 65
name (dicee.models.DualE attribute), 99
name (dicee.models.dualE.DualE attribute), 32
name (dicee.models.FMult attribute), 96
name (dicee.models.FMult2 attribute), 97
\verb"name" (\textit{dicee.models.function\_space.FMult attribute}), 33
name (dicee.models.function_space.FMult2 attribute), 34
name (dicee.models.function_space.GFMult attribute), 34
```

name (dicee.models.function_space.LFMult attribute), 35

```
name (dicee.models.function space.LFMult1 attribute), 35
name (dicee.models.GFMult attribute), 96
name (dicee.models.Keci attribute), 83
name (dicee.models.KeciBase attribute), 85
name (dicee.models.LFMult attribute), 98
name (dicee.models.LFMult1 attribute), 97
name (dicee.models.octonion.AConvO attribute), 39
name (dicee.models.octonion.ConvO attribute), 38
name (dicee.models.octonion.OMult attribute), 37
name (dicee.models.OMult attribute), 80
name (dicee.models.Pyke attribute), 66
name (dicee.models.pykeen_models.PykeenKGE attribute), 40
name (dicee.models.PykeenKGE attribute), 93
name (dicee.models.QMult attribute), 74
name (dicee.models.quaternion.AConvQ attribute), 43
name (dicee.models.quaternion.ConvQ attribute), 43
name (dicee.models.quaternion.QMult attribute), 42
name (dicee.models.real.DistMult attribute), 44
name (dicee.models.real.Pyke attribute), 45
name (dicee.models.real.Shallom attribute), 45
name (dicee.models.real.TransE attribute), 44
name (dicee.models.Shallom attribute), 65
name (dicee.models.TransE attribute), 65
name (dicee.models.transformers.BytE attribute), 47
name (dicee.OMult attribute), 181
name (dicee.Pyke attribute), 165
name (dicee.PykeenKGE attribute), 183
name (dicee.QMult attribute), 179
name (dicee.Shallom attribute), 181
name (dicee. TransE attribute), 169
Name space (class in dicee.config), 130
neg_ratio (dicee.BPE_NegativeSamplingDataset attribute), 198
neg_ratio (dicee.config.Namespace attribute), 131
neg_ratio (dicee.dataset_classes.BPE_NegativeSamplingDataset attribute), 134
neg_sample_ratio (dicee.CVDataModule attribute), 204
neg_sample_ratio (dicee.dataset_classes.CVDataModule attribute), 140
neg sample ratio (dicee.dataset classes.KvsSampleDataset attribute), 138
neg_sample_ratio (dicee.dataset_classes.NegSampleDataset attribute), 139
neg_sample_ratio (dicee.dataset_classes.TriplePredictionDataset attribute), 140
neg_sample_ratio (dicee.KvsSampleDataset attribute), 202
neg_sample_ratio (dicee.NegSampleDataset attribute), 202
neg_sample_ratio (dicee. TriplePredictionDataset attribute), 203
negnorm() (dicee.KGE method), 194
negnorm() (dicee.knowledge_graph_embeddings.KGE method), 153
NegSampleDataset (class in dicee), 202
NegSampleDataset (class in dicee.dataset_classes), 138
neural_searcher (in module dicee.scripts.serve), 108
Neural Searcher (class in dicee.scripts.serve), 108
NodeTrainer (class in dicee.trainer.torch_trainer_ddp), 112
norm_fc1 (dicee.AConEx attribute), 175
norm_fc1 (dicee.AConvO attribute), 176
norm_fc1 (dicee.ConEx attribute), 178
norm_fc1 (dicee.ConvO attribute), 178
norm_fc1 (dicee.models.AConEx attribute), 69
norm_fc1 (dicee.models.AConvO attribute), 82
norm_fc1 (dicee.models.complex.AConEx attribute), 30
norm_fc1 (dicee.models.complex.ConEx attribute), 29
norm_fc1 (dicee.models.ConEx attribute), 68
norm_fc1 (dicee.models.ConvO attribute), 81
{\tt norm\_fc1} (dicee.models.octonion.AConvO attribute), 39
norm fc1 (dicee.models.octonion.ConvO attribute), 38
normalization (dicee.analyse_experiments.Experiment attribute), 123
normalization (dicee.config.Namespace attribute), 131
normalize_head_entity_embeddings (dicee.BaseKGE attribute), 187
normalize_head_entity_embeddings (dicee.models.base_model.BaseKGE attribute), 19
normalize_head_entity_embeddings (dicee.models.BaseKGE attribute), 60, 63, 67, 71, 77, 91, 94
normalize_relation_embeddings (dicee.BaseKGE attribute), 187
normalize_relation_embeddings (dicee.models.base_model.BaseKGE attribute), 19
```

```
normalize relation embeddings (dicee.models.BaseKGE attribute), 60, 63, 67, 72, 77, 91, 94
normalize_tail_entity_embeddings (dicee.BaseKGE attribute), 187
normalize_tail_entity_embeddings (dicee.models.base_model.BaseKGE attribute), 19
normalize_tail_entity_embeddings (dicee.models.BaseKGE attribute), 60, 63, 67, 72, 77, 91, 94
normalizer_class (dicee.BaseKGE attribute), 187
normalizer_class (dicee.models.base_model.BaseKGE attribute), 19
normalizer_class (dicee.models.BaseKGE attribute), 60, 63, 67, 71, 77, 91, 94
num bpe entities (dicee.BPE NegativeSamplingDataset attribute), 198
num_bpe_entities (dicee.dataset_classes.BPE_NegativeSamplingDataset attribute), 134
num_bpe_entities (dicee.knowledge_graph.KG attribute), 150
num_core (dicee.config.Namespace attribute), 132
num_datapoints (dicee.BPE_NegativeSamplingDataset attribute), 198
num_datapoints (dicee.dataset_classes.BPE_NegativeSamplingDataset attribute), 134
num_datapoints (dicee.dataset_classes.MultiLabelDataset attribute), 135
num_datapoints (dicee.MultiLabelDataset attribute), 198
num_ent (dicee.DualE attribute), 173
num_ent (dicee.models.DualE attribute), 99
num_ent (dicee.models.dualE.DualE attribute), 32
num_entities (dicee.BaseKGE attribute), 186
num_entities (dicee.CVDataModule attribute), 204
num_entities (dicee.dataset_classes.CVDataModule attribute), 140
num_entities (dicee.dataset_classes.KvsSampleDataset attribute), 138
num_entities (dicee.dataset_classes.NegSampleDataset attribute), 139
num_entities (dicee.dataset_classes.TriplePredictionDataset attribute), 140
num_entities (dicee.evaluator.Evaluator attribute), 145
num_entities (dicee.knowledge_graph.KG attribute), 149
num_entities (dicee.KvsSampleDataset attribute), 202
num_entities (dicee.models.base_model.BaseKGE attribute), 18
num_entities (dicee.models.BaseKGE attribute), 60, 63, 67, 71, 77, 91, 94
num_entities (dicee.NegSampleDataset attribute), 202
num_entities (dicee. TriplePredictionDataset attribute), 203
num epochs (dicee.abstracts.AbstractPPECallback attribute), 121
num_epochs (dicee.analyse_experiments.Experiment attribute), 122
num_epochs (dicee.callbacks.ASWA attribute), 127
num_epochs (dicee.config.Namespace attribute), 131
num_epochs (dicee.trainer.torch_trainer_ddp.DDPTrainer attribute), 113
num epochs (dicee.trainer.torch trainer ddp.NodeTrainer attribute), 112
num_folds_for_cv (dicee.config.Namespace attribute), 132
num_of_data_points (dicee.dataset_classes.MultiClassClassificationDataset attribute), 135
num_of_data_points (dicee.MultiClassClassificationDataset attribute), 199
num_of_epochs (dicee.callbacks.PseudoLabellingCallback attribute), 127
num_of_output_channels (dicee.BaseKGE attribute), 187
num_of_output_channels (dicee.config.Namespace attribute), 132
\verb|num_of_output_channels| \textit{(dicee.models.base\_model.BaseKGE attribute)}, 19
num_of_output_channels (dicee.models.BaseKGE attribute), 60, 63, 67, 71, 77, 91, 94
num_params (dicee.analyse_experiments.Experiment attribute), 122
num_relations (dicee.BaseKGE attribute), 186
num_relations (dicee.CVDataModule attribute), 204
num_relations (dicee.dataset_classes.CVDataModule attribute), 140
num_relations (dicee.dataset_classes.KvsSampleDataset attribute), 138
num_relations (dicee.dataset_classes.NegSampleDataset attribute), 139
num_relations (dicee.dataset_classes.TriplePredictionDataset attribute), 140
num_relations (dicee.evaluator.Evaluator attribute), 145
num_relations (dicee.knowledge_graph.KG attribute), 149
num_relations (dicee.KvsSampleDataset attribute), 202
num_relations (dicee.models.base_model.BaseKGE attribute), 18
num_relations (dicee.models.BaseKGE attribute), 60, 63, 67, 71, 77, 91, 94
num_relations (dicee.NegSampleDataset attribute), 202
num_relations (dicee. TriplePredictionDataset attribute), 203
num_sample (dicee.models.FMult attribute), 96
num_sample (dicee.models.function_space.FMult attribute), 33
num_sample (dicee.models.function_space.GFMult attribute), 34
num_sample (dicee.models.GFMult attribute), 96
num_tokens (dicee.BaseKGE attribute), 186
\verb|num_tokens| (\textit{dicee.knowledge\_graph.KG attribute}), 150
num_tokens (dicee.models.base_model.BaseKGE attribute), 18
num_tokens (dicee.models.BaseKGE attribute), 60, 63, 67, 71, 77, 91, 94
num_workers (dicee.CVDataModule attribute), 204
```

```
num workers (dicee.dataset classes.CVDataModule attribute), 140
numpy_data_type_changer() (in module dicee), 189
numpy_data_type_changer() (in module dicee.static_funcs), 158
octonion_mul() (in module dicee.models), 79
octonion_mul() (in module dicee.models.octonion), 37
octonion_mul_norm() (in module dicee.models), 79
octonion_mul_norm() (in module dicee.models.octonion), 37
octonion_normalizer() (dicee.AConvO static method), 176
octonion_normalizer() (dicee.ConvO static method), 178
octonion_normalizer() (dicee.models.AConvO static method), 82
octonion_normalizer() (dicee.models.ConvO static method), 81
octonion_normalizer() (dicee.models.octonion.AConvO static method), 39
octonion_normalizer() (dicee.models.octonion.ConvO static method), 38
octonion_normalizer() (dicee.models.octonion.OMult static method), 37
octonion_normalizer() (dicee.models.OMult static method), 80
octonion_normalizer() (dicee.OMult static method), 181
OMult (class in dicee), 180
OMult (class in dicee.models), 79
OMult (class in dicee.models.octonion), 37
on_epoch_end() (dicee.callbacks.KGESaveCallback method), 126
on_epoch_end() (dicee.callbacks.PseudoLabellingCallback method), 127
on_fit_end() (dicee.abstracts.AbstractCallback method), 120
on_fit_end() (dicee.abstracts.AbstractPPECallback method), 121
on_fit_end() (dicee.abstracts.AbstractTrainer method), 116
on_fit_end() (dicee.callbacks.AccumulateEpochLossCallback method), 124
on_fit_end() (dicee.callbacks.ASWA method), 127
on_fit_end() (dicee.callbacks.Eval method), 128
on_fit_end() (dicee.callbacks.KGESaveCallback method), 126
on_fit_end() (dicee.callbacks.PrintCallback method), 124
on_fit_start() (dicee.abstracts.AbstractCallback method), 119
on_fit_start() (dicee.abstracts.AbstractPPECallback method), 121
on_fit_start() (dicee.abstracts.AbstractTrainer method), 115
on_fit_start() (dicee.callbacks.Eval method), 128
on_fit_start() (dicee.callbacks.KGESaveCallback method), 126
on_fit_start() (dicee.callbacks.KronE method), 129
on_fit_start() (dicee.callbacks.PrintCallback method), 124
on_init_end() (dicee.abstracts.AbstractCallback method), 119
on_init_start() (dicee.abstracts.AbstractCallback method), 119
on_train_batch_end() (dicee.abstracts.AbstractCallback method), 120
on_train_batch_end() (dicee.abstracts.AbstractTrainer method), 116
on_train_batch_end() (dicee.callbacks.Eval method), 129
on_train_batch_end() (dicee.callbacks.KGESaveCallback method), 125
\verb"on_train_batch_end()" (\textit{dicee.callbacks.PrintCallback method}), 125
on_train_batch_start() (dicee.callbacks.Perturb method), 130
on_train_epoch_end() (dicee.abstracts.AbstractCallback method), 120
on_train_epoch_end() (dicee.abstracts.AbstractTrainer method), 116
on_train_epoch_end() (dicee.callbacks.ASWA method), 128
on_train_epoch_end() (dicee.callbacks.Eval method), 129
on_train_epoch_end() (dicee.callbacks.KGESaveCallback method), 126
on_train_epoch_end() (dicee.callbacks.PrintCallback method), 125
on_train_epoch_end() (dicee.models.base_model.BaseKGELightning method), 14
on_train_epoch_end() (dicee.models.BaseKGELightning method), 55
OnevsAllDataset (class in dicee), 199
OnevsAllDataset (class in dicee.dataset_classes), 135
optim (dicee.config.Namespace attribute), 131
optimizer (dicee.trainer.torch_trainer_ddp.DDPTrainer attribute), 113
optimizer (dicee.trainer.torch_trainer_ddp.NodeTrainer attribute), 112
optimizer (dicee.trainer.torch_trainer.TorchTrainer attribute), 110
optimizer_name (dicee.BaseKGE attribute), 187
\verb"optimizer_name" (\textit{dicee.models.base\_model.BaseKGE attribute}), 19
optimizer_name (dicee.models.BaseKGE attribute), 60, 63, 67, 71, 77, 91, 94
ordered_bpe_entities (dicee.BPE_NegativeSamplingDataset attribute), 198
ordered_bpe_entities (dicee.dataset_classes.BPE_NegativeSamplingDataset attribute), 134
ordered_bpe_entities (dicee.knowledge_graph.KG attribute), 150
ordered_shaped_bpe_tokens (dicee.knowledge_graph.KG attribute), 149
```

P

```
p (dicee.CMult attribute), 165
p (dicee.config.Namespace attribute), 132
p (dicee.DeCaL attribute), 170
p (dicee.Keci attribute), 167
p (dicee.models.clifford.CMult attribute), 21
p (dicee.models.clifford.DeCaL attribute), 26
p (dicee.models.clifford.Keci attribute), 23
p (dicee.models.CMult attribute), 86
p (dicee.models.DeCaL attribute), 87
p (dicee.models.Keci attribute), 83
padding (dicee.knowledge_graph.KG attribute), 150
param_init (dicee.BaseKGE attribute), 187
param_init (dicee.models.base_model.BaseKGE attribute), 19
param_init (dicee.models.BaseKGE attribute), 60, 64, 67, 72, 78, 91, 95
parameters () (dicee.abstracts.BaseInteractiveKGE method), 119
path (dicee.abstracts.AbstractPPECallback attribute), 121
path (dicee.callbacks.AccumulateEpochLossCallback attribute), 124
path (dicee.callbacks.ASWA attribute), 127
path (dicee.callbacks.Eval attribute), 128
path (dicee.callbacks.KGESaveCallback attribute), 125
path_dataset_folder (dicee.analyse_experiments.Experiment attribute), 122
path_for_deserialization (dicee.knowledge_graph.KG attribute), 149
path_for_serialization (dicee.knowledge_graph.KG attribute), 149
path_single_kg (dicee.config.Namespace attribute), 131
path_single_kg (dicee.knowledge_graph.KG attribute), 149
path_to_store_single_run (dicee.config.Namespace attribute), 131
Perturb (class in dicee.callbacks), 130
poly_NN() (dicee.LFMult method), 182
poly_NN() (dicee.models.function_space.LFMult method), 35
poly_NN() (dicee.models.LFMult method), 98
polynomial () (dicee.LFMult method), 182
polynomial() (dicee.models.function_space.LFMult method), 36
polynomial () (dicee.models.LFMult method), 99
pop() (dicee.LFMult method), 183
pop() (dicee.models.function_space.LFMult method), 36
pop () (dicee.models.LFMult method), 99
pq (dicee.analyse_experiments.Experiment attribute), 122
predict () (dicee.KGE method), 193
predict() (dicee.knowledge_graph_embeddings.KGE method), 152
predict_dataloader() (dicee.models.base_model.BaseKGELightning method), 15
predict_dataloader() (dicee.models.BaseKGELightning method), 57
predict_missing_head_entity() (dicee.KGE method), 191
predict_missing_head_entity() (dicee.knowledge_graph_embeddings.KGE method), 151
predict_missing_relations() (dicee.KGE method), 192
predict_missing_relations() (dicee.knowledge_graph_embeddings.KGE method), 151
predict_missing_tail_entity() (dicee.KGE method), 192
predict_missing_tail_entity() (dicee.knowledge_graph_embeddings.KGE method), 152
predict_topk() (dicee.KGE method), 193
predict_topk() (dicee.knowledge_graph_embeddings.KGE method), 152
prepare_data() (dicee.CVDataModule method), 206
prepare_data() (dicee.dataset_classes.CVDataModule method), 142
preprocess_with_byte_pair_encoding() (dicee.read_preprocess_save_load_kg.PreprocessKG method), 105
preprocess_with_byte_pair_encoding() (dicee.read_preprocess_save_load_kg.preprocess.PreprocessKG method), 101
preprocess_with_byte_pair_encoding_with_padding() (dicee.read_preprocess_save_load_kg.PreprocessKG method), 105
preprocess_with_byte_pair_encoding_with_padding() (dicee.read_preprocess_save_load_kg.preprocess.PreprocessKG method),
preprocess_with_pandas() (dicee.read_preprocess_save_load_kg.PreprocessKG method), 105
preprocess_with_pandas() (dicee.read_preprocess_save_load_kg.preprocess.PreprocessKG method), 101
preprocess_with_polars() (dicee.read_preprocess_save_load_kg.PreprocessKG method), 105
preprocess_with_polars() (dicee.read_preprocess_save_load_kg.preprocess.PreprocessKG method), 101
preprocesses_input_args() (in module dicee.static_preprocess_funcs), 161
PreprocessKG (class in dicee.read_preprocess_save_load_kg), 105
PreprocessKG (class in dicee.read_preprocess_save_load_kg.preprocess), 100
previous_args (dicee.executer.ContinuousExecute attribute), 148
print_peak_memory() (in module dicee.trainer.torch_trainer_ddp), 112
PrintCallback (class in dicee.callbacks), 124
process (dicee.trainer.torch_trainer.TorchTrainer attribute), 110
```

```
PseudoLabellingCallback (class in dicee.callbacks), 126
Pyke (class in dicee), 165
Pyke (class in dicee.models), 66
Pyke (class in dicee.models.real), 45
pykeen_model_kwargs (dicee.config.Namespace attribute), 132
PykeenKGE (class in dicee), 183
PykeenKGE (class in dicee.models), 92
PykeenKGE (class in dicee.models.pykeen_models), 40
q (dicee.CMult attribute), 165
q (dicee.config.Namespace attribute), 132
q (dicee.DeCaL attribute), 170
q (dicee.Keci attribute), 167
q (dicee.models.clifford.CMult attribute), 22
q (dicee.models.clifford.DeCaL attribute), 26
q (dicee.models.clifford.Keci attribute), 23
q (dicee.models.CMult attribute), 86
q (dicee.models.DeCaL attribute), 87
q (dicee.models.Keci attribute), 83
qdrant_client (dicee.scripts.serve.NeuralSearcher attribute), 108
QMult (class in dicee), 179
QMult (class in dicee.models), 73
QMult (class in dicee.models.quaternion), 41
quaternion_mul() (in module dicee.models), 70
quaternion_mul() (in module dicee.models.static_funcs), 46
quaternion_mul_with_unit_norm() (in module dicee.models), 73
quaternion_mul_with_unit_norm() (in module dicee.models.quaternion), 41
quaternion_multiplication_followed_by_inner_product() (dicee.models.QMult method), 74
quaternion_multiplication_followed_by_inner_product() (dicee.models.quaternion.QMult method), 42
quaternion_multiplication_followed_by_inner_product() (dicee.QMult method), 179
quaternion_normalizer() (dicee.models.QMult static method), 74
quaternion_normalizer() (dicee.models.quaternion.QMult static method), 42
quaternion_normalizer() (dicee.QMult static method), 180
query_name_to_struct (dicee.query_generator.QueryGenerator attribute), 155
query_name_to_struct (dicee.QueryGenerator attribute), 207
QueryGenerator (class in dicee), 207
QueryGenerator (class in dicee.query_generator), 155
r (dicee.DeCaL attribute), 170
r (dicee.Keci attribute), 167
r (dicee.models.clifford.DeCaL attribute), 26
r (dicee.models.clifford.Keci attribute), 23
r (dicee.models.DeCaL attribute), 87
r (dicee.models.Keci attribute), 83
random_prediction() (in module dicee), 189
random_prediction() (in module dicee.static_funcs), 159
random_seed (dicee.config.Namespace attribute), 132
ratio (dicee.callbacks.Perturb attribute), 130
re (dicee.DeCaL attribute), 170
re (dicee.models.clifford.DeCaL attribute), 26
re (dicee.models.DeCaL attribute), 87
re_vocab (dicee.evaluator.Evaluator attribute), 145
read_from_disk() (in module dicee.read_preprocess_save_load_kg.util), 103
read_from_triple_store() (in module dicee.read_preprocess_save_load_kg.util), 104
read_only_few (dicee.config.Namespace attribute), 132
read_only_few (dicee.knowledge_graph.KG attribute), 149
read_or_load_kg() (dicee.Execute method), 196
read_or_load_kg() (dicee.executer.Execute method), 147
read_or_load_kg() (in module dicee), 189
read_or_load_kg() (in module dicee.static_funcs), 159
read_preprocess_index_serialize_data() (dicee.Execute method), 196
read_preprocess_index_serialize_data() (dicee.executer.Execute method), 147
read_with_pandas() (in module dicee.read_preprocess_save_load_kg.util), 103
read_with_polars() (in module dicee.read_preprocess_save_load_kg.util), 103
ReadFromDisk (class in dicee.read_preprocess_save_load_kg), 106
```

```
ReadFromDisk (class in dicee.read preprocess save load kg.read from disk), 101
rel2id (dicee.query_generator.QueryGenerator attribute), 155
rel2id (dicee. Ouery Generator attribute), 207
relation_embeddings (dicee.AConvQ attribute), 176
relation_embeddings (dicee.CMult attribute), 165
relation_embeddings (dicee.ConvQ attribute), 177
relation_embeddings (dicee.DeCaL attribute), 170
relation embeddings (dicee. DualE attribute), 173
relation_embeddings (dicee.LFMult attribute), 182
relation_embeddings (dicee.models.AConvQ attribute), 76
relation_embeddings (dicee.models.clifford.CMult attribute), 21
{\tt relation\_embeddings}~(\textit{dicee.models.clifford.DeCaL attribute}), 26
relation_embeddings (dicee.models.CMult attribute), 86
relation_embeddings (dicee.models.ConvQ attribute), 75
relation_embeddings (dicee.models.DeCaL attribute), 87
relation_embeddings (dicee.models.DualE attribute), 99
relation_embeddings (dicee.models.dualE.DualE attribute), 32
relation_embeddings (dicee.models.FMult attribute), 96
relation_embeddings (dicee.models.FMult2 attribute), 97
relation_embeddings (dicee.models.function_space.FMult attribute), 33
relation_embeddings (dicee.models.function_space.FMult2 attribute), 34
relation_embeddings (dicee.models.function_space.GFMult attribute), 34
relation_embeddings (dicee.models.function_space.LFMult attribute), 35
relation_embeddings (dicee.models.function_space.LFMult1 attribute), 35
relation_embeddings (dicee.models.GFMult attribute), 96
relation_embeddings (dicee.models.LFMult attribute), 98
relation_embeddings (dicee.models.LFMult1 attribute), 97
relation_embeddings (dicee.models.pykeen_models.PykeenKGE attribute), 40
relation_embeddings (dicee.models.PykeenKGE attribute), 93
relation_embeddings (dicee.models.quaternion.AConvQ attribute), 43
relation_embeddings (dicee.models.quaternion.ConvQ attribute), 43
relation embeddings (dicee. Pykeen KGE attribute), 183
relation_to_idx (dicee.knowledge_graph.KG attribute), 149
relations_str (dicee.knowledge_graph.KG property), 150
reload_dataset() (in module dicee), 197
reload_dataset() (in module dicee.dataset_classes), 134
remove_triples_from_train_with_condition() (dicee.read_preprocess_save_load_kg.PreprocessKG method), 105
remove_triples_from_train_with_condition() (dicee.read_preprocess_save_load_kg.preprocess_Preprocess_Greendod), 101
report (dicee.DICE_Trainer attribute), 190
report (dicee.evaluator.Evaluator attribute), 145
report (dicee. Execute attribute), 196
report (dicee.executer.Execute attribute), 147
report (dicee.trainer.DICE_Trainer attribute), 113
report (dicee.trainer.dice_trainer.DICE_Trainer attribute), 109
reports (dicee.callbacks.Eval attribute), 128
requires_grad_for_interactions (dicee.Keci attribute), 167
requires_grad_for_interactions (dicee. KeciBase attribute), 166
requires_grad_for_interactions (dicee.models.clifford.Keci attribute), 23
requires_grad_for_interactions (dicee.models.clifford.KeciBase attribute), 25
requires_grad_for_interactions (dicee.models.Keci attribute), 83
requires_grad_for_interactions (dicee.models.KeciBase attribute), 85
resid_dropout (dicee.models.transformers.CausalSelfAttention attribute), 49
residual_convolution() (dicee.AConEx method), 175
residual_convolution() (dicee.AConvO method), 176
residual_convolution() (dicee.AConvQ method), 176
residual_convolution() (dicee.ConEx method), 178
residual_convolution() (dicee.ConvO method), 178
residual_convolution() (dicee.ConvQ method), 177
residual_convolution() (dicee.models.AConEx method), 69
residual_convolution() (dicee.models.AConvO method), 82
residual convolution() (dicee.models.AConvO method), 76
residual_convolution() (dicee.models.complex.AConEx method), 30
residual_convolution() (dicee.models.complex.ConEx method), 30
residual_convolution() (dicee.models.ConEx method), 69
residual_convolution() (dicee.models.ConvO method), 81
residual_convolution() (dicee.models.ConvQ method), 75
residual_convolution() (dicee.models.octonion.AConvO method), 39
residual_convolution() (dicee.models.octonion.ConvO method), 39
```

```
residual convolution() (dicee.models.guaternion.AConvO method), 43
residual_convolution() (dicee.models.quaternion.ConvQ method), 43
retrieve_embeddings() (in module dicee.scripts.serve), 108
return_multi_hop_query_results() (dicee.KGE method), 194
return_multi_hop_query_results() (dicee.knowledge_graph_embeddings.KGE method), 153
root () (in module dicee.scripts.serve), 108
roots (dicee.models.FMult attribute), 96
roots (dicee.models.function space.FMult attribute), 33
roots (dicee.models.function_space.GFMult attribute), 34
roots (dicee.models.GFMult attribute), 96
runtime (dicee.analyse_experiments.Experiment attribute), 123
S
{\tt sample\_counter}~(\textit{dicee.abstracts.AbstractPPECallback~attribute}),~121
sample_entity() (dicee.abstracts.BaseInteractiveKGE method), 118
sample_relation() (dicee.abstracts.BaseInteractiveKGE method), 118
sample_triples_ratio (dicee.config.Namespace attribute), 132
sample_triples_ratio (dicee.knowledge_graph.KG attribute), 149
sanity_checking_with_arguments() (in module dicee.sanity_checkers), 156
save () (dicee.abstracts.BaseInteractiveKGE method), 118
save() (dicee.read_preprocess_save_load_kg.LoadSaveToDisk method), 106
save() (dicee.read_preprocess_save_load_kg.save_load_disk.LoadSaveToDisk method), 102
save_checkpoint() (dicee.abstracts.AbstractTrainer static method), 116
save_checkpoint_model() (in module dicee), 189
save_checkpoint_model() (in module dicee.static_funcs), 158
save_embeddings() (in module dicee), 189
save_embeddings() (in module dicee.static_funcs), 159
save_embeddings_as_csv (dicee.config.Namespace attribute), 130
save_experiment() (dicee.analyse_experiments.Experiment method), 123
save_model_at_every_epoch (dicee.config.Namespace attribute), 132
save_numpy_ndarray() (in module dicee), 189
save_numpy_ndarray() (in module dicee.read_preprocess_save_load_kg.util), 104
save_numpy_ndarray() (in module dicee.static_funcs), 158
save_pickle() (in module dicee), 188
save_pickle() (in module dicee.read_preprocess_save_load_kg.util), 104
save_pickle() (in module dicee.static_funcs), 158
save_queries() (dicee.query_generator.QueryGenerator method), 156
save_queries() (dicee.QueryGenerator method), 208
save_queries_and_answers() (dicee.query_generator.QueryGenerator static method), 156
save_queries_and_answers() (dicee.QueryGenerator static method), 208
save_trained_model() (dicee.Execute method), 196
save_trained_model() (dicee.executer.Execute method), 147
scalar_batch_NN() (dicee.LFMult method), 182
scalar_batch_NN() (dicee.models.function_space.LFMult method), 36
scalar_batch_NN() (dicee.models.LFMult method), 98
scaler (dicee.callbacks.Perturb attribute), 130
score() (dicee.CMult method), 165
score () (dicee.ComplEx static method), 175
score() (dicee.DistMult method), 166
score () (dicee. Keci method), 169
score() (dicee.models.clifford.CMult method), 22
score () (dicee.models.clifford.Keci method), 25
score () (dicee.models.CMult method), 86
score() (dicee.models.ComplEx static method), 70
score () (dicee.models.complex.ComplEx static method), 31
score () (dicee.models.DistMult method), 65
score () (dicee.models.Keci method), 85
score() (dicee.models.octonion.OMult method), 37
score () (dicee.models.OMult method), 80
score () (dicee.models.QMult method), 75
score () (dicee.models.quaternion.QMult method), 42
score() (dicee.models.real.DistMult method), 44
score () (dicee.models.real.TransE method), 45
score () (dicee.models.TransE method), 65
score() (dicee.OMult method), 181
score() (dicee.QMult method), 180
score () (dicee. TransE method), 169
```

```
score func (dicee.models.FMult2 attribute), 97
score_func (dicee.models.function_space.FMult2 attribute), 34
scoring_technique (dicee.analyse_experiments.Experiment attribute), 123
scoring_technique (dicee.config.Namespace attribute), 131
search() (dicee.scripts.serve.NeuralSearcher method), 108
search_embeddings() (in module dicee.scripts.serve), 108
seed (dicee.query_generator.QueryGenerator attribute), 155
seed (dicee. Query Generator attribute), 207
select_model() (in module dicee), 188
select_model() (in module dicee.static_funcs), 158
selected_optimizer (dicee.BaseKGE attribute), 187
selected_optimizer (dicee.models.base_model.BaseKGE attribute), 19
selected_optimizer (dicee.models.BaseKGE attribute), 60, 63, 67, 71, 77, 91, 94
sequential_vocabulary_construction() (dicee.read_preprocess_save_load_kg.PreprocessKG method), 105
sequential\_vocabulary\_construction () \ (\textit{dicee.read\_preprocess\_save\_load\_kg.preprocess.Preprocess.Preprocess.Preprocess.Preprocess.Preprocess.Preprocess.Preprocess.Preprocess.Preprocess.Preprocess.Preprocess.Preprocess.Preprocess.Preprocess.Preprocess.Preprocess.Preprocess.Preprocess.Preprocess.Preprocess.Preprocess.Preprocess.Preprocess.Preprocess.Preprocess.Preprocess.Preprocess.Preprocess.Preprocess.Preprocess.Preprocess.Preprocess.Preprocess.Preprocess.Preprocess.Preprocess.Preprocess.Preprocess.Preprocess.Preprocess.Preprocess.Preprocess.Preprocess.Preprocess.Preprocess.Preprocess.Preprocess.Preprocess.Preprocess.Preprocess.Preprocess.Preprocess.Preprocess.Preprocess.Preprocess.Preprocess.Preprocess.Preprocess.Preprocess.Preprocess.Preprocess.Preprocess.Preprocess.Preprocess.Preprocess.Preprocess.Preprocess.Preprocess.Preprocess.Preprocess.Preprocess.Preprocess.Preprocess.Preprocess.Preprocess.Preprocess.Preprocess.Preprocess.Preprocess.Preprocess.Preprocess.Preprocess.Preprocess.Preprocess.Preprocess.Preprocess.Preprocess.Preprocess.Preprocess.Preprocess.Preprocess.Preprocess.Preprocess.Preprocess.Preprocess.Preprocess.Preprocess.Preprocess.Preprocess.Preprocess.Preprocess.Preprocess.Preprocess.Preprocess.Preprocess.Preprocess.Preprocess.Preprocess.Preprocess.Preprocess.Preprocess.Preprocess.Preprocess.Preprocess.Preprocess.Preprocess.Preprocess.Preprocess.Preprocess.Preprocess.Preprocess.Preprocess.Preprocess.Preprocess.Preprocess.Preprocess.Preprocess.Preprocess.Preprocess.Preprocess.Preprocess.Preprocess.Preprocess.Preprocess.Preprocess.Preprocess.Preprocess.Preprocess.Preprocess.Preprocess.Preprocess.Preprocess.Preprocess.Preprocess.Preprocess.Preprocess.Preprocess.Preprocess.Preprocess.Preprocess.Preprocess.Preprocess.Preprocess.Preprocess.Preprocess.Preprocess.Preprocess.Preprocess.Preprocess.Preprocess.Preprocess.Preprocess.Preprocess.Preprocess.Preprocess.Preprocess.Preprocess.Preprocess.Preprocess.Preprocess.Preprocess.Preprocess.Preprocess.Preprocess.Preprocess.Preprocess.Preprocess.Preproce
set_global_seed() (dicee.query_generator.QueryGenerator method), 155
set_global_seed() (dicee.QueryGenerator method), 207
set_model_eval_mode() (dicee.abstracts.BaseInteractiveKGE method), 118
set_model_train_mode() (dicee.abstracts.BaseInteractiveKGE method), 117
setup() (dicee.CVDataModule method), 205
setup() (dicee.dataset_classes.CVDataModule method), 141
Shallom (class in dicee), 181
Shallom (class in dicee.models), 65
Shallom (class in dicee.models.real), 45
shallom (dicee.models.real.Shallom attribute), 45
shallom (dicee.models.Shallom attribute), 65
shallom (dicee.Shallom attribute), 181
shallom_width (dicee.models.real.Shallom attribute), 45
shallom_width (dicee.models.Shallom attribute), 65
shallom_width (dicee.Shallom attribute), 181
single_hop_query_answering() (dicee.KGE method), 194
single_hop_query_answering() (dicee.knowledge_graph_embeddings.KGE method), 153
sparql_endpoint (dicee.config.Namespace attribute), 131
sparql_endpoint (dicee.knowledge_graph.KG attribute), 149
start() (dicee.DICE_Trainer method), 191
start() (dicee.Execute method), 197
start() (dicee.executer.Execute method), 148
start() (dicee.read_preprocess_save_load_kg.PreprocessKG method), 105
\verb|start()| (dicee.read\_preprocess\_save\_load\_kg.preprocess.PreprocessKG method), 100
start() (dicee.read_preprocess_save_load_kg.read_from_disk.ReadFromDisk method), 101
start() (dicee.read_preprocess_save_load_kg.ReadFromDisk method), 106
start () (dicee.trainer.DICE_Trainer method), 114
start() (dicee.trainer.dice_trainer.DICE_Trainer method), 110
start_time (dicee.callbacks.PrintCallback attribute), 124
start_time (dicee.Execute attribute), 196
start time (dicee.executer.Execute attribute), 147
storage_path (dicee.config.Namespace attribute), 130
storage_path (dicee.DICE_Trainer attribute), 190
storage_path (dicee.trainer.DICE_Trainer attribute), 114
storage_path (dicee.trainer.dice_trainer.DICE_Trainer attribute), 109
store (dicee, Allys All attribute), 201
store (dicee.dataset_classes.AllvsAll attribute), 137
store (dicee.dataset_classes.KvsSampleDataset attribute), 138
store (dicee.KvsSampleDataset attribute), 202
store() (in module dicee), 189
store() (in module dicee.static_funcs), 159
store_ensemble() (dicee.abstracts.AbstractPPECallback method), 121
strategy (dicee.abstracts.AbstractTrainer attribute), 115
swa (dicee.config.Namespace attribute), 133
T() (dicee.DualE method), 174
T() (dicee.models.DualE method), 100
T() (dicee.models.dualE.DualE method), 33
t_conorm() (dicee.KGE method), 194
t_conorm() (dicee.knowledge_graph_embeddings.KGE method), 153
t_norm() (dicee.KGE method), 194
```

```
t norm() (dicee.knowledge graph embeddings.KGE method), 153
target_dim (dicee. Allvs All attribute), 201
target dim (dicee.dataset classes.AllvsAll attribute), 137
target_dim (dicee.dataset_classes.MultiLabelDataset attribute), 135
target_dim (dicee.dataset_classes.OnevsAllDataset attribute), 136
target_dim (dicee.knowledge_graph.KG attribute), 150
target_dim (dicee.MultiLabelDataset attribute), 198
target dim (dicee. Onevs All Dataset attribute), 199
temperature (dicee. BytE attribute), 184
temperature (dicee.models.transformers.BytE attribute), 47
tensor_t_norm() (dicee.KGE method), 194
tensor_t_norm() (dicee.knowledge_graph_embeddings.KGE method), 153
test_dataloader() (dicee.models.base_model.BaseKGELightning method), 14
test_dataloader() (dicee.models.BaseKGELightning method), 56
test_epoch_end() (dicee.models.base_model.BaseKGELightning method), 14
test_epoch_end() (dicee.models.BaseKGELightning method), 56
test_h1 (dicee.analyse_experiments.Experiment attribute), 122
test_h3 (dicee.analyse_experiments.Experiment attribute), 122
test_h10 (dicee.analyse_experiments.Experiment attribute), 123
test_mrr (dicee.analyse_experiments.Experiment attribute), 122
test_path (dicee.query_generator.QueryGenerator attribute), 155
test_path (dicee.QueryGenerator attribute), 207
timeit() (in module dicee), 188, 197
timeit() (in module dicee.read_preprocess_save_load_kg.util), 103
timeit() (in module dicee.static_funcs), 158
timeit() (in module dicee.static_preprocess_funcs), 161
to() (dicee.KGE method), 191
to () (dicee.knowledge_graph_embeddings.KGE method), 150
to_df() (dicee.analyse_experiments.Experiment method), 123
topk (dicee.BytE attribute), 184
topk (dicee.models.transformers.BytE attribute), 47
torch_ordered_shaped_bpe_entities (dicee.dataset_classes.MultiLabelDataset attribute), 135
torch_ordered_shaped_bpe_entities (dicee.MultiLabelDataset attribute), 198
TorchDDPTrainer (class in dicee.trainer.torch_trainer_ddp), 112
TorchTrainer (class in dicee.trainer.torch_trainer), 110
train() (dicee.KGE method), 195
train() (dicee.knowledge_graph_embeddings.KGE method), 154
train() (dicee.trainer.torch_trainer_ddp.DDPTrainer method), 113
train() (dicee.trainer.torch_trainer_ddp.NodeTrainer method), 113
train_data (dicee. Allvs All attribute), 201
train_data (dicee.dataset_classes.AllvsAll attribute), 137
train_data (dicee.dataset_classes.KvsAll attribute), 136
train_data (dicee.dataset_classes.KvsSampleDataset attribute), 138
train_data (dicee.dataset_classes.MultiClassClassificationDataset attribute), 135
train_data (dicee.dataset_classes.OnevsAllDataset attribute), 136
train data (dicee. KvsAll attribute), 200
train_data (dicee.KvsSampleDataset attribute), 202
train_data (dicee.MultiClassClassificationDataset attribute), 199
train_data (dicee. Onevs All Dataset attribute), 199
train_dataloader() (dicee.CVDataModule method), 204
train dataloader() (dicee.dataset classes.CVDataModule method), 140
train_dataloader() (dicee.models.base_model.BaseKGELightning method), 16
train_dataloader() (dicee.models.BaseKGELightning method), 57
train_dataloaders (dicee.trainer.torch_trainer.TorchTrainer attribute), 110
train_dataset_loader (dicee.trainer.torch_trainer_ddp.DDPTrainer attribute), 113
train_dataset_loader (dicee.trainer.torch_trainer_ddp.NodeTrainer attribute), 112
train_h1 (dicee.analyse_experiments.Experiment attribute), 122
train_h3 (dicee.analyse_experiments.Experiment attribute), 122
train_h10 (dicee.analyse_experiments.Experiment attribute), 122
train_indices_target (dicee.dataset_classes.MultiLabelDataset attribute), 135
train_indices_target (dicee.MultiLabelDataset attribute), 198
train_k_vs_all() (dicee.KGE method), 195
\verb|train_k_vs_all()| \textit{(dicee.knowledge\_graph\_embeddings.KGE method)}, 154|
train_mrr (dicee.analyse_experiments.Experiment attribute), 122
train_path (dicee.query_generator.QueryGenerator attribute), 155
train_path (dicee.QueryGenerator attribute), 207
train_set (dicee.BPE_NegativeSamplingDataset attribute), 198
train_set (dicee.dataset_classes.BPE_NegativeSamplingDataset attribute), 134
```

```
train set (dicee.dataset classes.MultiLabelDataset attribute), 135
train_set (dicee.dataset_classes.NegSampleDataset attribute), 139
train set (dicee.dataset classes.TriplePredictionDataset attribute), 140
train_set (dicee.MultiLabelDataset attribute), 198
train_set (dicee.NegSampleDataset attribute), 202
train_set (dicee.TriplePredictionDataset attribute), 203
train_set_idx (dicee.CVDataModule attribute), 204
train set idx (dicee.dataset classes.CVDataModule attribute), 140
train_set_target (dicee.knowledge_graph.KG attribute), 150
train_target (dicee. Allvs All attribute), 201
train_target (dicee.dataset_classes.AllvsAll attribute), 137
train_target (dicee.dataset_classes.KvsAll attribute), 136
train_target (dicee.dataset_classes.KvsSampleDataset attribute), 138
train_target (dicee.KvsAll attribute), 200
train_target (dicee.KvsSampleDataset attribute), 202
train_target_indices (dicee.knowledge_graph.KG attribute), 150
train_triples() (dicee.KGE method), 195
train_triples() (dicee.knowledge_graph_embeddings.KGE method), 154
trained_model (dicee.Execute attribute), 196
trained_model (dicee.executer.Execute attribute), 147
trainer (dicee.config.Namespace attribute), 131
trainer (dicee.DICE Trainer attribute), 190
trainer (dicee. Execute attribute), 196
trainer (dicee.executer.Execute attribute), 147
trainer (dicee.trainer.DICE_Trainer attribute), 113
trainer (dicee.trainer.dice_trainer.DICE_Trainer attribute), 109
trainer (dicee.trainer.torch_trainer_ddp.NodeTrainer attribute), 112
training_step (dicee.trainer.torch_trainer.TorchTrainer attribute), 110
training_step() (dicee.BytE method), 185
training_step() (dicee.models.base_model.BaseKGELightning method), 13
training_step() (dicee.models.BaseKGELightning method), 54
training_step() (dicee.models.transformers.BytE method), 47
training_step_outputs (dicee.models.base_model.BaseKGELightning attribute), 13
training_step_outputs (dicee.models.BaseKGELightning attribute), 54
training_technique (dicee.knowledge_graph.KG attribute), 150
TransE (class in dicee), 169
TransE (class in dicee.models), 65
TransE (class in dicee.models.real), 44
transfer_batch_to_device() (dicee.CVDataModule method), 205
transfer_batch_to_device() (dicee.dataset_classes.CVDataModule method), 141
transformer (dicee. BytE attribute), 184
transformer (dicee.models.transformers.BytE attribute), 47
transformer (dicee.models.transformers.GPT attribute), 52
trapezoid() (dicee.models.FMult2 method), 97
trapezoid() (dicee.models.function_space.FMult2 method), 35
tri_score() (dicee.LFMult method), 182
tri_score() (dicee.models.function_space.LFMult method), 36
tri_score() (dicee.models.function_space.LFMult1 method), 35
tri_score() (dicee.models.LFMult method), 98
tri_score() (dicee.models.LFMult1 method), 97
triple_score() (dicee.KGE method), 194
triple_score() (dicee.knowledge_graph_embeddings.KGE method), 153
TriplePredictionDataset (class in dicee), 203
TriplePredictionDataset (class in dicee.dataset_classes), 139
tuned_embedding_dim (dicee.models.FMult2 attribute), 97
tuned_embedding_dim (dicee.models.function_space.FMult2 attribute), 34
tuple2list() (dicee.query_generator.QueryGenerator method), 155
tuple2list() (dicee.QueryGenerator method), 207
U
unlabelled_size (dicee.callbacks.PseudoLabellingCallback attribute), 127
unmap () (dicee.query_generator.QueryGenerator method), 156
unmap () (dicee.QueryGenerator method), 208
unmap_query() (dicee.query_generator.QueryGenerator method), 156
unmap_query() (dicee.QueryGenerator method), 208
```

```
٧
```

```
val_aswa (dicee.callbacks.ASWA attribute), 127
val_dataloader() (dicee.models.base_model.BaseKGELightning method), 15
val_dataloader() (dicee.models.BaseKGELightning method), 56
val_h1 (dicee.analyse_experiments.Experiment attribute), 122
val_h3 (dicee.analyse_experiments.Experiment attribute), 122
val_h10 (dicee.analyse_experiments.Experiment attribute), 122
val_mrr (dicee.analyse_experiments.Experiment attribute), 122
val_path (dicee.query_generator.QueryGenerator attribute), 155
val_path (dicee.QueryGenerator attribute), 207
validate_knowledge_graph() (in module dicee.sanity_checkers), 156
vocab_preparation() (dicee.evaluator.Evaluator method), 145
vocab_size (dicee.models.transformers.GPTConfig attribute), 51
vocab_to_parquet() (in module dicee), 189
vocab_to_parquet() (in module dicee.static_funcs), 159
vtp_score() (dicee.LFMult method), 182
\verb|vtp_score|()| \textit{(dicee.models.function\_space.LFMult method)}, 36
vtp_score() (dicee.models.function_space.LFMult1 method), 35
vtp_score() (dicee.models.LFMult method), 98
vtp_score() (dicee.models.LFMult1 method), 98
W
weight (dicee.BytE attribute), 184
weight (dicee.models.transformers.BytE attribute), 47
weight (dicee.models.transformers.GPT attribute), 52
weight (dicee.models.transformers.LayerNorm attribute), 48
weight_decay (dicee.BaseKGE attribute), 187
weight_decay (dicee.config.Namespace attribute), 131
weight_decay (dicee.models.base_model.BaseKGE attribute), 19
weight_decay (dicee.models.BaseKGE attribute), 60, 63, 67, 71, 77, 91, 94
weights (dicee.models.FMult attribute), 96
weights (dicee.models.function_space.FMult attribute), 33
weights (dicee.models.function_space.GFMult attribute), 34
weights (dicee.models.GFMult attribute), 96
write_links() (dicee.query_generator.QueryGenerator method), 155
write_links() (dicee.QueryGenerator method), 208
write_report() (dicee.Execute method), 197
write_report() (dicee.executer.Execute method), 148
Χ
x_values (dicee.LFMult attribute), 182
x_values (dicee.models.function_space.LFMult attribute), 35
x_values (dicee.models.LFMult attribute), 98
```