DICE Embeddings

Release 0.1.3.2

Caglar Demir

Apr 10, 2025

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	8
13	How to cite	10
14	dicee 14.1 Submodules 14.2 Attributes 14.3 Classes 14.4 Functions 14.5 Package Contents	12 12 161 161 162 164
Py	thon Module Index	209

Index 210

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

Contact: caglar.demir@upb.de

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

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

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

- 1. 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 &&_ 
cd dice-embeddings && 
pip3 install -e .
```

or

```
pip install dicee
```

3 Download Knowledge Graphs

```
wget https://files.dice-research.org/datasets/dice-embeddings/KGs.zip --no-check-

→certificate && unzip KGs.zip
```

To test the Installation

```
python -m pytest -p no:warnings -x # Runs >114 tests leading to > 15 mins

python -m pytest -p no:warnings --lf # run only the last failed test

python -m pytest -p no:warnings --ff # to run the failures first and then the rest of the tests.
```

4 Knowledge Graph Embedding Models

- 1. TransE, DistMult, ComplEx, ConEx, QMult, OMult, ConvO, ConvQ, Keci
- 2. All 44 models available in https://github.com/pykeen/pykeen#models For more, please refer to examples.

5 How to Train

To Train a KGE model (KECI) and evaluate it on the train, validation, and test sets of the UMLS benchmark dataset.

```
from dicee.executer import Execute
from dicee.config import Namespace
args = Namespace()
args.model = 'Keci'
args.scoring_technique = "KvsAll" # 1vsAll, or AllvsAll, or NegSample
args.dataset_dir = "KGs/UMLS"
args.path_to_store_single_run = "Keci_UMLS"
args.num_epochs = 100
args.embedding_dim = 32
args.batch_size = 1024
reports = Execute(args).start()
print(reports["Train"]["MRR"]) # => 0.9912
print(reports["Trest"]["MRR"]) # => 0.8155
# See the Keci_UMLS folder embeddings and all other files
```

where the data is in the following form

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

A KGE model can also be trained from the command line

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

dicee automaticaly detects available GPUs and trains a model with distributed data parallels technique. Under the hood, dicee uses lighning as a default trainer.

```
# Train a model by only using the GPU-0

CUDA_VISIBLE_DEVICES=0 dicee --dataset_dir "KGs/UMLS" --model Keci --eval_model

--"train_val_test"

# Train a model by only using GPU-1

CUDA_VISIBLE_DEVICES=1 dicee --dataset_dir "KGs/UMLS" --model Keci --eval_model

--"train_val_test"

NCCL_P2P_DISABLE=1 CUDA_VISIBLE_DEVICES=0,1 python dicee/scripts/run.py --trainer PL -

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

Under the hood, dicee executes run.py script and uses lighning as a default trainer

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

Similarly, models can be easily trained with torchrun

```
torchrun --standalone --nnodes=1 --nproc_per_node=gpu dicee/scripts/run.py --trainer_
→torchDDP --dataset_dir "KGs/UMLS" --model Keci --eval_model "train_val_test"

# Evaluate Keci on Train set: Evaluate Keci on Train set: Evaluate Keci on Train set

# {'H@1': 0.9518788343558282, 'H@3': 0.9988496932515337, 'H@10': 1.0, 'MRR': 0.

→9753123402351737}

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

# {'H@1': 0.6932515337423313, 'H@3': 0.9041411042944786, 'H@10': 0.9754601226993865,

→'MRR': 0.8072499937521418}

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

{'H@1': 0.6951588502269289, 'H@3': 0.9039334341906202, 'H@10': 0.9750378214826021,

→'MRR': 0.8064032293278861}
```

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

```
torchrun --nnodes 2 --nproc_per_node=gpu --node_rank 0 --rdzv_id 455 --rdzv_backend_

--c10d --rdzv_endpoint=nebula dicee/scripts/run.py --trainer torchDDP --dataset_dir_

--KGS/UMLS

torchrun --nnodes 2 --nproc_per_node=gpu --node_rank 1 --rdzv_id 455 --rdzv_backend_

--c10d --rdzv_endpoint=nebula dicee/scripts/run.py --trainer torchDDP --dataset_dir_

--KGS/UMLS
```

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

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

where the data is in the following form

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

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

For more, please refer to examples.

6 Creating an Embedding Vector Database

6.1 Learning Embeddings

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

6.2 Loading Embeddings into Qdrant Vector Database

6.3 Launching Webservice

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

→location "localhost"
```

Retrieve and Search

Get embedding of germany

```
curl -X 'GET' 'http://0.0.0.8000/api/get?q=germany' -H 'accept: application/json'
```

Get most similar things to europe

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

7 Answering Complex Queries

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

```
pre_trained_kge = KGE(path=result['path_experiment_folder'])
# (3) Single-hop query answering
# Query: ?E : \exist E.hasSibling(E, F9M167)
# Question: Who are the siblings of F9M167?
# Answer: [F9M157, F9F141], as (F9M167, hasSibling, F9M157) and (F9M167, hasSibling,
\hookrightarrow F9F141)
predictions = pre_trained_kge.answer_multi_hop_query(query_type="1p",
                                                      query=('http://www.benchmark.org/
→family#F9M167',
                                                             ('http://www.benchmark.
→org/family#hasSibling',)),
                                                      tnorm="min", k=3)
top_entities = [topk_entity for topk_entity, query_score in predictions]
assert "http://www.benchmark.org/family#F9F141" in top_entities
assert "http://www.benchmark.org/family#F9M157" in top_entities
# (2) Two-hop query answering
# Query: ?D : \exist E.Married(D, E) \land hasSibling(E, F9M167)
# Question: To whom a sibling of F9M167 is married to?
# Answer: [F9F158, F9M142] as (F9M157 #married F9F158) and (F9F141 #married F9M142)
predictions = pre_trained_kge.answer_multi_hop_query(query_type="2p",
                                                      query=("http://www.benchmark.org/
→family#F9M167",
                                                             ("http://www.benchmark.
→org/family#hasSibling",
                                                              "http://www.benchmark.
→org/family#married")),
                                                     tnorm="min", k=3)
top_entities = [topk_entity for topk_entity, query_score in predictions]
assert "http://www.benchmark.org/family#F9M142" in top_entities
assert "http://www.benchmark.org/family#F9F158" in top_entities
# (3) Three-hop query answering
# Query: ?T : \exist D.type(D,T) \land Married(D,E) \land hasSibling(E, F9M167)
# Question: What are the type of people who are married to a sibling of F9M167?
# (3) Answer: [Person, Male, Father] since F9M157 is [Brother Father Grandfather_
→Male] and F9M142 is [Male Grandfather Father]
predictions = pre_trained_kge.answer_multi_hop_query(query_type="3p", query=("http://
→www.benchmark.org/family#F9M167",
                                                                               ("http://
→www.benchmark.org/family#hasSibling",
                                                                              "http://
→www.benchmark.org/family#married",
                                                                              "http://
\rightarrowwww.w3.org/1999/02/22-rdf-syntax-ns#type")),
                                                     tnorm="min", k=5)
top_entities = [topk_entity for topk_entity, query_score in predictions]
print (top_entities)
assert "http://www.benchmark.org/family#Person" in top_entities
assert "http://www.benchmark.org/family#Father" in top_entities
assert "http://www.benchmark.org/family#Male" in top_entities
```

For more, please refer to examples/multi_hop_query_answering.

8 Predicting Missing Links

```
from dicee import KGE
# (1) Train a knowledge graph embedding model..
# (2) Load a pretrained model
pre_trained_kge = KGE(path='..')
# (3) Predict missing links through head entity rankings
pre_trained_kge.predict_topk(h=[".."],r=[".."],topk=10)
# (4) Predict missing links through relation rankings
pre_trained_kge.predict_topk(h=[".."],t=[".."],topk=10)
# (5) Predict missing links through tail entity rankings
pre_trained_kge.predict_topk(r=[".."],t=[".."],topk=10)
```

9 Downloading Pretrained Models

```
from dicee import KGE
# (1) Load a pretrained ConEx on DBpedia
model = KGE(url="https://files.dice-research.org/projects/DiceEmbeddings/KINSHIP-Keci-
-dim128-epoch256-KvsAll")
```

For more please look at dice-research.org/projects/DiceEmbeddings/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
```

12 Coverage Report

The coverage report is generated using coverage.py¹²:

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

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

¹² https://coverage.readthedocs.io/en/7.6.0/

```
→123, 146-147, 152, 165, 197, 240-254, 257-260, 263-266, 301, 314-317, 320-324, 364-
\Rightarrow375, 390-398, 413, 424-428, 555-575, 581-585, 589-591
dicee/callbacks.py
                                                           245
                                                                  102
\hookrightarrow67-73, 76, 88-93, 98-103, 106-109, 116-133, 138-142, 146-147, 276-280, 286-287, 305-
→311, 314, 319-320, 332-338, 344-353, 358-360, 405, 416-429, 433-468, 480-486
dicee/config.py
                                                            93
                                                                    2
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dicee/dataset_classes.py
                                                           299
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→87, 93, 99-106, 109, 112, 115-139, 195-201, 204, 207-209, 314, 325-328, 344, 410-

→411, 429, 528-536, 539, 543-557, 700-707, 710-714

dicee/eval_static_funcs.py
                                                           227
                                                                   95
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→ 111, 258-353, 360-411
dicee/evaluator.py
                                                           262
                                                                   51
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                                                                                46, 51,_
→56, 84, 89-90, 93, 109, 126, 137, 141, 146, 177-188, 195-206, 314, 344-367, 455, □
→465, 482-487
dicee/executer.py
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                                                           113
⇒259, 291
dicee/knowledge_graph.py
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⇔114
dicee/knowledge_graph_embeddings.py
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→31, 39-52, 57-90, 93-127, 131-139, 170-184, 215-228, 254-274, 324-327, 330-333, 346,
→ 381-426, 484-486, 502-503, 509-517, 522-525, 528-533, 538, 547, 592-598, 630, 688-
→1053, 1084-1145, 1149-1177, 1200, 1227-1265
dicee/models/__init__.py
                                                             9
                                                                        100%
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dicee/models/base_model.py
                                                                                54, 56, ...
→82, 88-103, 157, 190, 230, 236, 245, 248, 252, 259, 263, 265, 280, 288-289, 296-297,

→ 351, 354, 427, 439

dicee/models/clifford.py
                                                                  357
→68-117, 122-133, 156-168, 190-220, 235, 237, 241, 248-249, 276-280, 303-311, 325-
→327, 332-333, 364-384, 406, 413, 417-478, 495-499, 511, 514, 519, 524, 571-607, 625-
→631, 644, 647, 652, 657, 686-692, 705, 708, 713, 718, 728-737, 753-754, 774-845, □
→856-859, 884-909, 933-966, 1002-1006, 1019, 1029, 1032, 1037, 1042, 1047, 1051, □
→1055, 1064-1065, 1095, 1102, 1107, 1135-1139, 1167-1176, 1186-1194, 1212-1214, 1232-
→1234, 1250-1252
dicee/models/complex.py
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dicee/models/dualE.py
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→142-156
                                                           262
                                                                  221
dicee/models/function_space.py
                                                                         16%
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\Rightarrow28-37, 40-49, 53-70, 77-86, 89-98, 101-110, 114-126, 134-156, 159-165, 168-185, 188-
→194, 197-205, 208, 213-234, 243-246, 250-254, 258-267, 271-292, 301-307, 311-328, □
→332-335, 344-352, 355, 366-372, 392-406, 424-438, 443-453, 461-465, 474-478
                                                           227
                                                                   83
                                                                         63%
dicee/models/octonion.py
                                                                                21-44,_
\Rightarrow320-329, 334-345, 348-370, 374-416, 426-474
dicee/models/pykeen_models.py
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dicee/models/quaternion.py
                                                                                7-21, 30-
                                                           192
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→55, 68-72, 107, 185, 328-342, 345-364, 368-389, 399-426
dicee/models/real.py
                                                            61
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\leftrightarrow 66-69, 87, 103-106
dicee/models/static_funcs.py
                                                            10
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dicee/models/transformers.py
                                                           236
                                                                  189
→46, 60-75, 84-102, 105-116, 123-125, 128, 134-151, 155-180, 186-190, 193-197, 203-
→207, 210-212, 229-256, 265-268, 271-276, 279-304, 310-315, 319-372, 376-398, 404-414
```

```
dicee/query_generator.py
                                                              374
                                                                      346
                                                                               7%
                                                                                    18-52,_
\hookrightarrow56, 62-65, 69-70, 78-92, 100-147, 155-188, 192-206, 212-269, 274-303, 307-443, 453-
\hookrightarrow472, 480-501, 508-512, 517, 522-528
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dicee/read_preprocess_save_load_kg/__init__.py
dicee/read_preprocess_save_load_kg/preprocess.py
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\hookrightarrow78, 102-127, 133, 138-151, 184, 214, 388-389, 444
dicee/read_preprocess_save_load_kg/read_from_disk.py
                                                               36
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\hookrightarrow40, 47, 55, 58-72
dicee/read_preprocess_save_load_kg/save_load_disk.py
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dicee/read_preprocess_save_load_kg/util.py
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→72-73, 91-97, 100-102, 107-109, 121, 134, 140-143, 148-156, 161-167, 172-177, 182-
→187, 199-220, 226-282, 286-290, 294-295, 299, 303-304, 334, 351, 356, 363-364
                                                                       23
                                                                             57%
dicee/sanity_checkers.py
                                                               54
                                                                                    8-12, 21-
\rightarrow31, 46, 51, 58, 64-79, 85, 89, 96
dicee/static_funcs.py
                                                                      163
                                                                             61%
                                                                                    40, 50, _
                                                              418
→56-61, 83, 105-106, 115, 138, 152, 157-159, 163-165, 167, 194-198, 246, 254, 263-
→268, 290-304, 316-336, 340-357, 362, 386-387, 392-393, 410-411, 413-414, 416-417, □
→419-420, 428, 446-450, 467-470, 474-479, 483-487, 491-492, 498-500, 526-527, 539-
\hookrightarrow 542, 547-550, 559-610, 615-627, 644-658, 661-669
dicee/static_funcs_training.py
                                                              123
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⇔223-224
dicee/static_preprocess_funcs.py
                                                              100
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\hookrightarrow 52, 56, 64, 67, 78, 91-115, 120-123, 128-131, 136-139
dicee/trainer/__init__.py
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dicee/trainer/dice_trainer.py
                                                              126
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\hookrightarrow 91, 98, 103-108, 147
dicee/trainer/torch_trainer.py
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→207-208
dicee/trainer/torch_trainer_ddp.py
                                                              152
                                                                      128
                                                                             16%
                                                                                    13-14,_
→43, 47-72, 83-112, 131-137, 140-149, 164-194, 204-217, 226-246, 251-260, 263-272, □
⇒275-299, 302-309
TOTAL
                                                             6181
                                                                     2828
                                                                             54%
```

13 How to cite

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

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

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

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

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

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

14 dicee

14.1 Submodules

dicee.__main__

dicee.abstracts

Classes

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

Module Contents

class dicee.abstracts.AbstractTrainer(args, callbacks)

Abstract class for Trainer class for knowledge graph embedding models

Parameter

```
args
    [str]?

callbacks: list
    ?

attributes

callbacks

is_global_zero = True
global_rank = 0

local_rank = 0

strategy = None
```

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

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

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

```
Parameter
     trainer:
     model:
         rtype
             None
on_init_end(*args, **kwargs)
     Call at the beginning of the training.
     Parameter
     trainer:
     model:
         rtype
             None
\verb"on_fit_start" (\textit{trainer}, model)
     Call at the beginning of the training.
     Parameter
     trainer:
     model:
         rtype
             None
on_train_epoch_end(trainer, model)
     Call at the end of each epoch during training.
     Parameter
     trainer:
     model:
         rtype
             None
on_train_batch_end(*args, **kwargs)
     Call at the end of each mini-batch during the training.
     Parameter
     trainer:
     model:
         rtype
             None
on_fit_end(*args, **kwargs)
```

Call at the end of the training.

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

dicee.analyse_experiments

 $store_ensemble (param_ensemble) \rightarrow None$

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

Classes

```
Experiment
```

Functions

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

Module Contents

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

```
val_h10 = []

test_mrr = []

test_h1 = []

test_h3 = []

test_h10 = []

runtime = []

normalization = []

scoring_technique = []

save_experiment(x)

to_df()

dicee.analyse_experiments.analyse(args)
```

dicee.callbacks

Classes

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

Functions

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

Module Contents

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

Abstract class for Callback class for knowledge graph embedding models

```
Parameter
```

```
path
      on\_fit\_end(\mathit{trainer}, \mathit{model}) \rightarrow None
           Store epoch loss
           Parameter
           trainer:
           model:
                rtype
                    None
class dicee.callbacks.PrintCallback
      Bases: dicee.abstracts.AbstractCallback
      Abstract class for Callback class for knowledge graph embedding models
      Parameter
      start_time
      \verb"on_fit_start" (\textit{trainer}, \textit{pl}\_\textit{module})
           Call at the beginning of the training.
           Parameter
           trainer:
           model:
                rtype
                    None
      on_fit_end(trainer, pl_module)
           Call at the end of the training.
           Parameter
           trainer:
           model:
                rtype
                    None
      on_train_batch_end(*args, **kwargs)
           Call at the end of each mini-batch during the training.
           Parameter
           trainer:
           model:
```

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

```
Parameter
          trainer:
          model:
              rtype
                 None
     on fit end(*args, **kwargs)
          Call at the end of the training.
          Parameter
          trainer:
          model:
              rtype
                 None
     on_epoch_end (model, trainer, **kwargs)
class dicee.callbacks.PseudoLabellingCallback(data_module, kg, batch_size)
     Bases: dicee.abstracts.AbstractCallback
     Abstract class for Callback class for knowledge graph embedding models
     Parameter
     data_module
     kg
     num_of_epochs = 0
     unlabelled_size
     batch_size
     create_random_data()
     on_epoch_end(trainer, model)
dicee.callbacks.estimate_q(eps)
     estimate rate of convergence q from sequence esp
dicee.callbacks.compute_convergence(seq, i)
class dicee.callbacks.ASWA (num_epochs, path)
     Bases: dicee.abstracts.AbstractCallback
     Adaptive stochastic weight averaging ASWE keeps track of the validation performance and update s the ensemble
     model accordingly.
     path
     num_epochs
     initial_eval_setting = None
```

```
epoch_count = 0
     alphas = []
     val_aswa = -1
     on_fit_end(trainer, model)
          Call at the end of the training.
          Parameter
          trainer:
          model:
              rtype
                  None
     static compute\_mrr(trainer, model) \rightarrow float
     get_aswa_state_dict(model)
     {\tt decide} \ (running\_model\_state\_dict,\ ensemble\_state\_dict,\ val\_running\_model,
                 mrr_updated_ensemble_model)
          Perform Hard Update, software or rejection
              Parameters
                   • running_model_state_dict
                   • ensemble_state_dict
                   • val_running_model
                   • mrr_updated_ensemble_model
     on_train_epoch_end(trainer, model)
          Call at the end of each epoch during training.
          Parameter
          trainer:
          model:
              rtype
                  None
class dicee.callbacks.Eval (path, epoch_ratio: int = None)
     Bases: dicee.abstracts.AbstractCallback
     Abstract class for Callback class for knowledge graph embedding models
     Parameter
     path
     reports = []
     epoch_ratio = None
```

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

Abstract class for Callback class for knowledge graph embedding models

Parameter

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

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

Parameter Perturbation:

```
Output Perturbation:

level = 'input'

ratio = 0.0

method = None

scaler = None

frequency = None

on_train_batch_start (trainer, model, batch, batch_idx)

Called when the train batch begins.
```

dicee.config

Classes

Namespace

Simple object for storing attributes.

Module Contents

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

```
backend: str = 'pandas'
    Backend to read, process, and index input knowledge graph. pandas, polars and rdflib available
separator: str = '\\s+'
    separator for extracting head, relation and tail from a triple
trainer: str = 'torchCPUTrainer'
    Trainer for knowledge graph embedding model
scoring_technique: str = 'KvsAll'
    Scoring technique for knowledge graph embedding models
neg_ratio: int = 0
    Negative ratio for a true triple in NegSample training_technique
weight_decay: float = 0.0
    Weight decay for all trainable params
normalization: str = 'None'
    LayerNorm, BatchNorm1d, or None
init_param: str = None
    xavier_normal or None
gradient_accumulation_steps: int = 0
    Not tested e
num_folds_for_cv: int = 0
    Number of folds for CV
eval_model: str = 'train_val_test'
    ["None", "train", "train_val", "train_val_test", "test"]
            Evaluate trained model choices
save_model_at_every_epoch: int = None
    Not tested
label_smoothing_rate: float = 0.0
num core: int = 0
    Number of CPUs to be used in the mini-batch loading process
random seed: int = 0
    Random Seed
sample_triples_ratio: float = None
    Read some triples that are uniformly at random sampled. Ratio being between 0 and 1
read_only_few: int = None
    Read only first few triples
pykeen_model_kwargs
    Additional keyword arguments for pykeen models
kernel size: int = 3
    Size of a square kernel in a convolution operation
```

```
num_of_output_channels: int = 32
    Number of slices in the generated feature map by convolution.
p: int = 0
    P parameter of Clifford Embeddings
q: int = 1
    Q parameter of Clifford Embeddings
input_dropout_rate: float = 0.0
    Dropout rate on embeddings of input triples
hidden_dropout_rate: float = 0.0
    Dropout rate on hidden representations of input triples
feature_map_dropout_rate: float = 0.0
     Dropout rate on a feature map generated by a convolution operation
byte_pair_encoding: bool = False
    Byte pair encoding
        Type
             WIP
adaptive_swa: bool = False
     Adaptive stochastic weight averaging
swa: bool = False
    Stochastic weight averaging
block_size: int = None
    block size of LLM
continual_learning = None
    Path of a pretrained model size of LLM
auto_batch_finding = False
     A flag for using auto batch finding
__iter__()
```

dicee.dataset_classes

Classes

BPE_NegativeSamplingDataset	An abstract class representing a Dataset.
MultiLabelDataset	An abstract class representing a Dataset.
MultiClassClassificationDataset	Dataset for the 1vsALL training strategy
OnevsAllDataset	Dataset for the 1vsALL training strategy
KvsAll	Creates a dataset for KvsAll training by inheriting from
	torch.utils.data.Dataset.
AllvsAll	Creates a dataset for AllvsAll training by inheriting from
	torch.utils.data.Dataset.
OnevsSample	A custom PyTorch Dataset class for knowledge graph em-
	beddings, which includes
KvsSampleDataset	KvsSample a Dataset:
NegSampleDataset	An abstract class representing a Dataset.
TriplePredictionDataset	Triple Dataset
CVDataModule	Create a Dataset for cross validation

Functions

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

Module Contents

Reload the files from disk to construct the Pytorch dataset

dicee.dataset_classes.construct_dataset (*, train_set: numpy.ndarray | list, valid_set=None, test_set=None, ordered_bpe_entities=None, train_target_indices=None, target_dim: int = None, entity_to_idx: dict, relation_to_idx: dict, form_of_labelling: str, scoring_technique: str, neg_ratio: int, label_smoothing_rate: float, byte_pair_encoding=None, block_size: int = None)

→ torch.utils.data.Dataset

Bases: torch.utils.data.Dataset

An abstract class representing a Dataset.

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



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

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

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

samples loading. This method accepts list of indices of samples of batch and returns list of samples.

1 Note

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

```
• entity_idxs - mapping.
```

- relation_idxs mapping.
- form ?
- num_workers int for https://pytorch.org/docs/stable/data.html#torch.utils.data.

 DataLoader

Return type

torch.utils.data.Dataset

```
train_data
block_size = 8
num_of_data_points
collate_fn = None
__len__()
__getitem__(idx)
```

class dicee.dataset_classes.OnevsAllDataset(train_set_idx: numpy.ndarray, entity_idxs)

Bases: torch.utils.data.Dataset

Dataset for the 1vsALL training strategy

Parameters

- train_set_idx Indexed triples for the training.
- entity_idxs mapping.
- relation_idxs mapping.
- form ?
- num_workers int for https://pytorch.org/docs/stable/data.html#torch.utils.data.
 DataLoader

Return type

torch.utils.data.Dataset

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

Bases: torch.utils.data.Dataset

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

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



TODO

train_set_idx

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

entity_idxs

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

relation idxs

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

self: torch.utils.data.Dataset

```
>>> a = KvsAll()
```

```
train data = None
train target = None
label_smoothing_rate
collate_fn = None
__len__()
\__getitem_(idx)
```

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

Bases: torch.utils.data.Dataset

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

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

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



1 Note

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

only with 0s.

train_set_idx

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

entity idxs

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

relation idxs

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

self: torch.utils.data.Dataset

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

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

class dicee.dataset_classes.OnevsSample ($train_set$: numpy.ndarray, $num_entities$, $num_relations$, neg sample ratio: int = None, label smoothing rate: <math>float = 0.0)

Bases: torch.utils.data.Dataset

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

Parameters

- train_set (np.ndarray) A numpy array containing triples of knowledge graph data. Each triple consists of (head_entity, relation, tail_entity).
- num_entities (int) The number of unique entities in the knowledge graph.
- num_relations (int) The number of unique relations in the knowledge graph.
- neg_sample_ratio (int, optional) The number of negative samples to be generated per positive sample. Must be a positive integer and less than num_entities.
- label_smoothing_rate (float, optional) A label smoothing rate to apply to the positive and negative labels. Defaults to 0.0.

train_data

The input data converted into a PyTorch tensor.

```
Type torch. Tensor
```

num entities

Number of entities in the dataset.

```
Type int
```

num_relations

Number of relations in the dataset.

```
Type int
```

```
neg_sample_ratio
```

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

```
Type int
```

label_smoothing_rate

The smoothing factor applied to the labels.

Type

torch.Tensor

collate_fn

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

Type

function, optional

```
train_data
num_entities
num_relations
neg_sample_ratio = None
label_smoothing_rate
collate_fn = None
__len__()
    Returns the number of sam
```

Returns the number of samples in the dataset.

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

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

Parameters

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

Returns

A tuple consisting of:

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

Return type

tuple

 $\begin{tabular}{ll} {\tt classe} & \tt dicee.dataset_classes. {\tt KvsSampleDataset} ({\it train_set_idx: numpy.ndarray, entity_idxs, relation_idxs, form, store=None, neg_ratio=None, label_smoothing_rate: float = 0.0) \end{tabular}$

Bases: torch.utils.data.Dataset

KvsSample a Dataset:

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

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

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

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



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

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

- num_relations relation to index mapping.
- batch_size int
- form ?
- num_workers int for https://pytorch.org/docs/stable/data.html#torch.utils.data.
 DataLoader

Return type

?

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

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

An iterable or collection of iterables specifying training samples.

For more information about multiple dataloaders, see this section.

The dataloader you return will not be reloaded unless you set **:param-ref:~pytorch_lightning.trainer.trainer.Trainer.reload_dataloaders_every_n_epochs**` to a positive integer.

For data processing use the following pattern:

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

However, the above are only necessary for distributed processing.

A Warning

do not assign state in prepare_data

• fit()

- prepare_data()
- setup()

1 Note

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

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

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

Parameters

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

Example:

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

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

# don't do this
        self.something = else

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

transfer_batch_to_device(*args, **kwargs)

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

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

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

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

1 Note

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

Parameters

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

Returns

A reference to the data on the new device.

Example:

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

See also

- move_data_to_device()
- apply_to_collection()

prepare_data(*args, **kwargs)

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

▲ Warning

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

Example:

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

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

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

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

Example:

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

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

This is called before requesting the dataloaders:

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

dicee.eval_static_funcs

Functions

```
evaluate_link_prediction_performance(→
Dict)
evaluate_link_prediction_performance_with_.

evaluate_link_prediction_performance_with_i

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

Module Contents

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

Parameters

• model

- triples
- er_vocab
- re_vocab

Parameters

- model
- triples
- within_entities
- er_vocab
- re_vocab

dicee.evaluator

Classes

Evaluator Evaluator Class to evaluate KGE models in various downstream tasks

Module Contents

class dicee.evaluator.Evaluator(args, is_continual_training=None)

Evaluator class to evaluate KGE models in various downstream tasks

Arguments

```
re_vocab = None
er_vocab = None
ee_vocab = None
func_triple_to_bpe_representation = None
is_continual_training = None
num_entities = None
```

```
num relations = None
args
report
during_training = False
vocab\_preparation(dataset) \rightarrow None
     A function to wait future objects for the attributes of executor
         Return type
             None
eval (dataset: dicee.knowledge_graph.KG, trained_model, form_of_labelling, during_training=False)
             \rightarrow None
eval_rank_of_head_and_tail_entity(*, train_set, valid_set=None, test_set=None, trained_model)
eval_rank_of_head_and_tail_byte_pair_encoded_entity(*, train_set=None, valid_set=None,
             test_set=None, ordered_bpe_entities, trained_model)
eval_with_byte (*, raw_train_set, raw_valid_set=None, raw_test_set=None, trained_model,
            form of labelling) \rightarrow None
     Evaluate model after reciprocal triples are added
eval with bpe vs all (*, raw train set, raw valid set=None, raw test set=None, trained model,
            form\_of\_labelling) \rightarrow None
     Evaluate model after reciprocal triples are added
eval_with_vs_all (*, train_set, valid_set=None, test_set=None, trained_model, form_of_labelling)
     Evaluate model after reciprocal triples are added
evaluate_lp_k_vs_all (model, triple_idx, info=None, form_of_labelling=None)
     Filtered link prediction evaluation. :param model: :param triple_idx: test triples :param info: :param
     form_of_labelling: :return:
evaluate_lp_with_byte (model, triples: List[List[str]], info=None)
evaluate_lp_bpe_k_vs_all (model, triples: List[List[str]], info=None, form_of_labelling=None)
         Parameters
              • model
              • triples (List of lists)
              • info
              • form_of_labelling
evaluate_lp (model, triple_idx, info: str)
dummy_eval (trained_model, form_of_labelling: str)
eval_with_data(dataset, trained_model, triple_idx: numpy.ndarray, form_of_labelling: str)
```

dicee.executer

Classes

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

Module Contents

class dicee.executer.Execute(args, continuous_training=False)

A class for Training, Retraining and Evaluation a model.

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

```
args
```

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

 ${\tt save_trained_model}\,()\,\to None$

Save a knowledge graph embedding model

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

Parameter

rtype

None

end $(form_of_labelling: str) \rightarrow dict$

End training

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

Parameter

rtype

A dict containing information about the training and/or evaluation

$write_report() \rightarrow None$

Report training related information in a report.json file

 $start() \rightarrow dict$

Start training

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

Parameter

rtype

A dict containing information about the training and/or evaluation

class dicee.executer.ContinuousExecute(args)

Bases: Execute

A subclass of Execute Class for retraining

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

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

 ${\tt continual_start}\,()\,\to dict$

Start Continual Training

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

Parameter

rtype

A dict containing information about the training and/or evaluation

dicee.knowledge_graph

Classes

KG Knowledge Graph

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

```
target_dim = None

train_target_indices = None

ordered_bpe_entities = None

separator = None

description_of_input = None

describe() \rightarrow None

property entities_str: List

property relations_str: List

exists(h: str, r: str, t: str)

__iter___()

__len___()

func_triple_to_bpe_representation(triple: List[str])
```

dicee.knowledge_graph_embeddings

Classes

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

```
class dicee.knowledge_graph_embeddings.KGE (path=None, url=None, construct_ensemble=False,
             model name=None)
      Bases: dicee.abstracts.BaseInteractiveKGE
      Knowledge Graph Embedding Class for interactive usage of pre-trained models
      __str__()
      to (device: str) \rightarrow None
      get_transductive_entity_embeddings (indices: torch.LongTensor | List[str], as_pytorch=False,
                   as\_numpy = False, as\_list = True) \rightarrow torch.FloatTensor | numpy.ndarray | List[float]
      create_vector_database (collection_name: str, distance: str, location: str = 'localhost',
                   port: int = 6333)
      generate (h=", r=")
      eval_lp_performance (dataset=List[Tuple[str, str, str]], filtered=True)
      predict_missing_head_entity(relation: List[str] | str, tail_entity: List[str] | str, within=None)
                    \rightarrow Tuple
           Given a relation and a tail entity, return top k ranked head entity.
           argmax_{e} in E \} f(e,r,t), where r in R, t in E.
```

Parameter

relation: Union[List[str], str]

String representation of selected relations.

tail_entity: Union[List[str], str]

String representation of selected entities.

k: int

Highest ranked k entities.

Returns: Tuple

Highest K scores and entities

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

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

Parameter

head_entity: List[str]

String representation of selected entities.

tail_entity: List[str]

String representation of selected entities.

k: int

Highest ranked k entities.

Returns: Tuple

Highest K scores and entities

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

Given a head entity and a relation, return top k ranked entities

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

Parameter

head_entity: List[str]

String representation of selected entities.

tail_entity: List[str]

String representation of selected entities.

Returns: Tuple

```
scores
```

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

Parameters

- logits
- h
- r
- t
- within

Predict missing item in a given triple.

Parameter

head_entity: Union[str, List[str]]

String representation of selected entities.

relation: Union[str, List[str]]

String representation of selected relations.

tail_entity: Union[str, List[str]]

String representation of selected entities.

k: int

Highest ranked k item.

Returns: Tuple

Highest K scores and items

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

Predict triple score

Parameter

head_entity: List[str]

String representation of selected entities.

relation: List[str]

String representation of selected relations.

tail_entity: List[str]

String representation of selected entities.

logits: bool

If logits is True, unnormalized score returned

Returns: Tuple

```
pytorch tensor of triple score
```

```
t norm (tens 1: torch. Tensor, tens 2: torch. Tensor, tnorm: str = 'min') \rightarrow torch. Tensor
```

 $tensor_t_norm(subquery_scores: torch.FloatTensor, tnorm: str = 'min') \rightarrow torch.FloatTensor$

Compute T-norm over [0,1] ^{n imes d} where n denotes the number of hops and d denotes number of entities

```
t\_conorm (tens_1: torch. Tensor, tens_2: torch. Tensor, tconorm: str = 'min') \rightarrow torch. Tensor
```

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

```
return_multi_hop_query_results (aggregated_query_for_all_entities, k: int, only_scores)
```

```
single_hop_query_answering (query: tuple, only_scores: bool = True, k: int = None)
```

```
answer_multi_hop_query (query_type: str = None, query: Tuple[str | Tuple[str, str], Ellipsis] = None, queries: List[Tuple[str | Tuple[str, str], Ellipsis]] = None, tnorm: str = 'prod', neg_norm: str = 'standard', lambda_: float = 0.0, k: int = 10, only_scores=False)

→ List[Tuple[str, torch.Tensor]]
```

@TODO: Refactoring is needed # @TODO: Score computation for each query type should be done in a static function

Find an answer set for EPFO queries including negation and disjunction

Parameter

```
query_type: str The type of the query, e.g., "2p".
```

query: Union[str, Tuple[str, Tuple[str, str]]] The query itself, either a string or a nested tuple.

queries: List of Tuple[Union[str, Tuple[str, str]], ...]

tnorm: str The t-norm operator.

neg_norm: str The negation norm.

lambda_: float lambda parameter for sugeno and yager negation norms

k: int The top-k substitutions for intermediate variables.

returns

- List[Tuple[str, torch.Tensor]]
- · Entities and corresponding scores sorted in the descening order of scores

```
find_missing_triples (confidence: float, entities: List[str] = None, relations: List[str] = None, topk: int = 10, at_most: int = sys.maxsize) \rightarrow Set
```

Find missing triples

Iterative over a set of entities E and a set of relation R:

orall e in E and orall r in R f(e,r,x)

Return (e,r,x)

otin G and f(e,r,x) >confidence

```
confidence: float
          A threshold for an output of a sigmoid function given a triple.
          topk: int
          Highest ranked k item to select triples with f(e,r,x) > confidence.
          at most: int
          Stop after finding at_most missing triples
          \{(e,r,x) \mid f(e,r,x) > \text{confidence land } (e,r,x)\}
     otin G
deploy(share: bool = False, top_k: int = 10)
train_triples (h: List[str], r: List[str], t: List[str], labels: List[float], iteration=2, optimizer=None)
train_k_vs_all(h, r, iteration=1, lr=0.001)
     Train k vs all :param head_entity: :param relation: :param iteration: :param lr: :return:
train(kg, lr=0.1, epoch=10, batch\_size=32, neg\_sample\_ratio=10, num\_workers=1) \rightarrow None
     Retrained a pretrain model on an input KG via negative sampling.
```

dicee.models

Submodules

dicee.models.adopt

Classes

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

Functions

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

Module Contents

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

Base class for all optimizers.



Warning

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

Parameters

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

clip_lambda

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

Perform a single optimization step.

Parameters

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

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

Functional API that performs ADOPT algorithm computation.

dicee.models.base model

Classes

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

Module Contents

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

Bases: lightning.LightningModule

Base class for all neural network modules.

Your models should also subclass this class.

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

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

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

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

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

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

1 Note

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

Variables

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

```
\label{eq:training_step_outputs} \textbf{ = []} \label{eq:mem_of_model()} \rightarrow \text{Dict}
```

Size of model in MB and number of params

training_step(batch, batch_idx=None)

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

Parameters

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

Returns

- Tensor The loss tensor
- dict A dictionary which can include any keys, but must include the key 'loss' in the case of automatic optimization.
- None In automatic optimization, this will skip to the next batch (but is not supported for multi-GPU, TPU, or DeepSpeed). For manual optimization, this has no special meaning, as returning the loss is not required.

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

Example:

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

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

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

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

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

1 Note

When accumulate_grad_batches > 1, the loss returned here will be automatically normalized by accumulate_grad_batches internally.

loss_function(yhat_batch: torch.FloatTensor, y_batch: torch.FloatTensor)

Parameters

- yhat_batch
- y_batch

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

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

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

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

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

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

test_epoch_end(outputs: List[Any])

$test_dataloader() \rightarrow None$

An iterable or collection of iterables specifying test samples.

For more information about multiple dataloaders, see this section.

For data processing use the following pattern:

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

However, the above are only necessary for distributed processing.

Warning

do not assign state in prepare_data

- test()
- prepare_data()
- setup()

1 Note

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

1 Note

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

${\tt val_dataloader}\,()\,\to None$

An iterable or collection of iterables specifying validation samples.

For more information about multiple dataloaders, see this section.

The reloaded :paramdataloader you return will not be unless you ref: `~lightning.pytorch.trainer.trainer.Trainer.reload_dataloaders_every_n_epochs` a positive integer.

It's recommended that all data downloads and preparation happen in prepare_data().

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

1 Note

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

1 Note

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

$\texttt{predict_dataloader}() \rightarrow None$

An iterable or collection of iterables specifying prediction samples.

For more information about multiple dataloaders, see this section.

It's recommended that all data downloads and preparation happen in prepare_data().

- predict()
- prepare_data()
- setup()

1 Note

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

Returns

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

$train_dataloader() \rightarrow None$

An iterable or collection of iterables specifying training samples.

For more information about multiple dataloaders, see this section.

The dataloader you return will not be reloaded unless you set **:param-ref: ~lightning.pytorch.trainer.trainer.Trainer.reload_dataloaders_every_n_epochs** to a positive integer.

For data processing use the following pattern:

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

However, the above are only necessary for distributed processing.

A Warning

do not assign state in prepare_data

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

1 Note

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

configure_optimizers (parameters=None)

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

Returns

Any of these 6 options.

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

The lr_scheduler_config is a dictionary which contains the scheduler and its associated configuration. The default configuration is shown below.

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

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

Metrics can be made available to monitor by simply logging it using self.log('metric_to_track', metric_val) in your LightningModule.

1 Note

Some things to know:

- Lightning calls .backward() and .step() automatically in case of automatic optimization.
- If a learning rate scheduler is specified in <code>configure_optimizers()</code> with key "interval" (default "epoch") in the scheduler configuration, Lightning will call the scheduler's <code>.step()</code> method automatically in case of automatic optimization.
- If you use 16-bit precision (precision=16), Lightning will automatically handle the optimizer.
- If you use torch.optim.LBFGS, Lightning handles the closure function automatically for you.
- If you use multiple optimizers, you will have to switch to 'manual optimization' mode and step them yourself.
- If you need to control how often the optimizer steps, override the optimizer_step() hook.

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

Bases: BaseKGELightning

Base class for all neural network modules.

Your models should also subclass this class.

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

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

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

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

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

1 Note

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

Variables

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

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

```
forward_byte_pair_encoded_triple(x: Tuple[torch.LongTensor, torch.LongTensor])
          byte pair encoded neural link predictors
              Parameters
     init_params_with_sanity_checking()
     forward(x: torch.LongTensor | Tuple[torch.LongTensor, torch.LongTensor],
                 y idx: torch.LongTensor = None
              Parameters
                  • x
                  • y_idx
                  • ordered_bpe_entities
     forward_triples (x: torch.LongTensor) \rightarrow torch.Tensor
              Parameters
     forward_k_vs_all(*args, **kwargs)
     forward_k_vs_sample(*args, **kwargs)
     get_triple_representation(idx_hrt)
     get_head_relation_representation(indexed_triple)
     get_sentence_representation(x: torch.LongTensor)
              Parameters
                  • (b (x shape)
                  • 3
                  • t)
     get_bpe_head_and_relation_representation(x: torch.LongTensor)
                  \rightarrow Tuple[torch.FloatTensor, torch.FloatTensor]
              Parameters
                  x (B x 2 x T)
     \mathtt{get\_embeddings}() \rightarrow Tuple[numpy.ndarray, numpy.ndarray]
class dicee.models.base_model.IdentityClass(args=None)
     Bases: torch.nn.Module
```

Base class for all neural network modules.

Your models should also subclass this class.

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

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

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

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

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

1 Note

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

Variables

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

```
args = None
_call__(x)
static forward(x)
```

dicee.models.clifford

Classes

Keci	Base class for all neural network modules.
CKeci	Without learning dimension scaling
DeCaL	Base class for all neural network modules.

Module Contents

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

Base class for all neural network modules.

Your models should also subclass this class.

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

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

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

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

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

1 Note

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

Variables

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

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

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

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

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

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

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

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

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

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

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

```
results = [] for j in range(q - 1):
                             for k in range(j + 1, q):
                                  results.append(hq[:, :, j] * rq[:, :, k] - hq[:, :, k] * rq[:, :, j])
                    sigma_q = torch.stack(results, dim=2) assert sigma_qq.shape == (b, r, int((q * (q - 1)) / 2))
           Yet, this computation would be quite inefficient. Instead, we compute interactions along all p, e.g., e1e1,
           e1e2, e1e3,
                    e2e1, e2e2, e2e3, e3e1, e3e2, e3e3
           Then select the triangular matrix without diagonals: e1e2, e1e3, e2e3.
compute_sigma_pq(*, hp, hq, rp, rq)
           sum_{i=1}^{p} sum_{j=p+1}^{p+q} (h_i r_j - h_j r_i) e_i e_j
           results = [] sigma_pq = torch.zeros(b, r, p, q) for i in range(p):
                    for i in range(q):
                             sigma_pq[:, :, i, j] = hp[:, :, i] * rq[:, :, j] - hq[:, :, j] * rp[:, :, i]
           print(sigma_pq.shape)
apply_coefficients(hp, hq, rp, rq)
           Multiplying a base vector with its scalar coefficient
clifford_multiplication (h0, hp, hq, r0, rp, rq)
           Compute our CL multiplication
                    h = h_0 + sum_{i=1}^p h_i e_i + sum_{j=p+1}^p h_j e_j r = r_0 + sum_{i=1}^p r_i e_i + sum_{j=p+1}^n h_j e_j r = r_0 + sum_{i=1}^n h_j e_j r = r_0 + sum_{i
                    sum_{j=p+1}^{p+q} r_j e_j
                    ei ^2 = +1 for i = < i = < p ej ^2 = -1 for p < j = < p+q ei ej = -eje1 for i
           eq j
                    h r = sigma_0 + sigma_p + sigma_q + sigma_{pp} + sigma_{q} + sigma_{pq}  where
                    (1) sigma_0 = h_0 r_0 + sum_{i=1}^p (h_0 r_i) e_i - sum_{j=p+1}^{p+q} (h_j r_j) e_j
                    (2) sigma p = sum \{i=1\}^p (h \ 0 \ r \ i + h \ i \ r \ 0) e \ i
                    (3) sigma_q = sum_{j=p+1}^{p+q} (h_0 r_j + h_j r_0) e_j
                    (4) sigma_{pp} = sum_{i=1}^{p-1} sum_{k=i+1}^p (h_i r_k - h_k r_i) e_i e_k
                    (5) sigma_{qq} = sum_{j=1}^{p+q-1} sum_{k=j+1}^{p+q} (h_j r_k - h_k r_j) e_j e_k
                    (6) sigma \{pq\} = sum \{i=1\}^{p} sum \{j=p+1\}^{p+q} (h ir j-h jr i) e ie j
construct_cl_multivector(x: torch.FloatTensor, r: int, p: int, q: int)
                             → tuple[torch.FloatTensor, torch.FloatTensor, torch.FloatTensor]
           Construct a batch of multivectors Cl_{p,q}(mathbb\{R\}^d)
           Parameter
           x: torch.FloatTensor with (n,d) shape
```

returns

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

```
forward_k_vs_with_explicit(x: torch.Tensor)
      k_vs_all_score (bpe_head_ent_emb, bpe_rel_ent_emb, E)
      forward_k_vs_all(x: torch.Tensor) \rightarrow torch.FloatTensor
           Kvsall training
           (1) Retrieve real-valued embedding vectors for heads and relations mathbb{R}^d.
           (2) Construct head entity and relation embeddings according to Cl_{p,q}(mathbb\{R\}^d).
           (3) Perform Cl multiplication
           (4) Inner product of (3) and all entity embeddings
           forward_k_vs_with_explicit and this funcitons are identical Parameter ----- x: torch.LongTensor with
           (n,2) shape :rtype: torch.FloatTensor with (n, |E|) shape
      construct_batch_selected_cl_multivector(x: torch.FloatTensor, r: int, p: int, q: int)
                    → tuple[torch.FloatTensor, torch.FloatTensor, torch.FloatTensor]
           Construct a batch of batchs multivectors Cl_{p,q}(mathbb\{R\}^d)
           Parameter
           x: torch.FloatTensor with (n,k, d) shape
                returns
                    • a0 (torch.FloatTensor with (n,k, m) shape)
                    • ap (torch.FloatTensor with (n,k, m, p) shape)
                    • aq (torch.FloatTensor with (n,k, m, q) shape)
      forward_k\_vs\_sample (x: torch.LongTensor, target_entity_idx: torch.LongTensor) \rightarrow torch.FloatTensor
           Parameter
           x: torch.LongTensor with (n,2) shape
           target_entity_idx: torch.LongTensor with (n, k) shape k denotes the selected number of examples.
                    torch.FloatTensor with (n, k) shape
      score (h, r, t)
      forward\_triples (x: torch.Tensor) \rightarrow torch.FloatTensor
           Parameter
           x: torch.LongTensor with (n,3) shape
                rtype
                    torch.FloatTensor with (n) shape
class dicee.models.clifford.CKeci(args)
      Bases: Keci
      Without learning dimension scaling
      name = 'CKeci'
```

requires_grad_for_interactions = False

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

Base class for all neural network modules.

Your models should also subclass this class.

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

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

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

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

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

1 Note

As per the example above, an $__{init}_{_}()$ call to the parent class must be made before assignment on the child.

Variables

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

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

Parameter

x: torch.LongTensor with (n,) shape

rtype

torch.FloatTensor with (n) shape

 $cl_pqr(a: torch.tensor) \rightarrow torch.tensor$

Input: tensor(batch_size, emb_dim) \longrightarrow output: tensor with 1+p+q+r components with size (batch_size, emb_dim/(1+p+q+r)) each.

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

compute_sigmas_single (list_h_emb, list_r_emb, list_t_emb)

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

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

and return:

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

compute_sigmas_multivect(list_h_emb, list_r_emb)

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

For same bases vectors interaction we have

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

For different base vector interactions, we have

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

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

Kvsall training

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

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

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

Multiplying a base vector with its scalar coefficient

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

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

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

Parameter

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

returns

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

 $compute_sigma_pp(hp, rp)$

Compute .. math:

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

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

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

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

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

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

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

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

 $compute_sigma_qq(hq, rq)$

Compute

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

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

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

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

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

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

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

 $compute_sigma_rr(hk, rk)$

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

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

Compute

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

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

for j in range(q):

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

print(sigma_pq.shape)

 $\texttt{compute_sigma_pr} \ (*, hp, hk, rp, rk)$

Compute

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

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

for j in range(q):

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

print(sigma_pq.shape)

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

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

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

for j in range(q):

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

print(sigma_pq.shape)

dicee.models.complex

Classes

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

Module Contents

class dicee.models.complex.ConEx(args)

Bases: dicee.models.base_model.BaseKGE

Convolutional ComplEx Knowledge Graph Embeddings

name = 'ConEx'

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

conv2d

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

Base class for all neural network modules.

Your models should also subclass this class.

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

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

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

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

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

1 Note

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

Variables

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

Parameters

- emb_h
- emb_r
- emb E

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

forward_k_vs_sample (x: torch.LongTensor, target_entity_idx: torch.LongTensor)

dicee.models.dualE

Classes

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

```
class dicee.models.dualE.DualE(args)
                         Bases: \ \textit{dicee.models.base\_model.BaseKGE}
                         Dual Quaternion Knowledge Graph Embeddings (https://ojs.aaai.org/index.php/AAAI/article/download/16850/
                         16657)
                         name = 'DualE'
                         entity_embeddings
                         relation_embeddings
                        num_ent = None
                        {\tt kvsall\_score}\,(e\_1\_h,e\_2\_h,e\_3\_h,e\_4\_h,e\_5\_h,e\_6\_h,e\_7\_h,e\_8\_h,e\_1\_t,e\_2\_t,e\_3\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e\_4\_t,e_4\_t,e_4\_t,e_4\_t,e_4\_t,e_4\_t,e_4\_t,e_4\_t,e_4\_t,e_4\_t,e_4\_t,e_4\_t,e_4\_t,e_4\_t,e_4\_t,e_4\_t,e_4\_t,e_4\_t,e_4\_t,e_4\_t,e_4\_t,e_4\_t,e_4\_t,e_4\_t,e_4\_t,e_4\_t,e_4\_t,e_4\_
                                                                               e\_5\_t, e\_6\_t, e\_7\_t, e\_8\_t, r\_1, r\_2, r\_3, r\_4, r\_5, r\_6, r\_7, r\_8) \rightarrow \text{torch.tensor}
                                               KvsAll scoring function
                                               Input
                                               x: torch.LongTensor with (n, ) shape
                                               Output
                                               torch.FloatTensor with (n) shape
                         \textbf{forward\_triples} \ (\textit{idx\_triple: torch.tensor}) \ \rightarrow \textbf{torch.tensor}) \ \rightarrow \textbf{torch.tensor}
                                               Negative Sampling forward pass:
                                               Input
                                               x: torch.LongTensor with (n, ) shape
                                               Output
                                               torch.FloatTensor with (n) shape
                         {\tt forward\_k\_vs\_all}\;(\mathcal{X})
                                               KvsAll forward pass
                                               Input
                                               x: torch.LongTensor with (n, ) shape
```

Output

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

dicee.models.ensemble

Classes

EnsembleKGE

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

dicee.models.function space

Classes

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

```
class dicee.models.function_space.FMult(args)
      Bases: dicee.models.base_model.BaseKGE
      Learning Knowledge Neural Graphs
      name = 'FMult'
      entity_embeddings
      relation_embeddings
      num_sample = 50
      gamma
      roots
      weights
      \verb|compute_func| (\textit{weights: torch.FloatTensor}, \textit{x}) \rightarrow \textit{torch.FloatTensor}
      chain_func(weights, x: torch.FloatTensor)
      \textbf{forward\_triples} \ (\textit{idx\_triple: torch.Tensor}) \ \rightarrow \textbf{torch.Tensor}) \ \rightarrow \textbf{torch.Tensor}
                Parameters
                    x
class dicee.models.function_space.GFMult(args)
      Bases: dicee.models.base_model.BaseKGE
      Learning Knowledge Neural Graphs
      name = 'GFMult'
      entity_embeddings
      relation_embeddings
      num_sample = 250
```

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

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

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

```
comp func(h, r, t)
```

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

```
polynomial (coeff, x, degree)
```

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

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

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

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

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

dicee.models.octonion

Classes

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

Functions

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

Module Contents

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

Base class for all neural network modules.

Your models should also subclass this class.

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

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

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

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

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

1 Note

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

Variables

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

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

```
class dicee.models.octonion.ConvO(args: dict)
Bases: dicee.models.base model.BaseKGE
```

Base class for all neural network modules.

Your models should also subclass this class.

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

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

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

(continued from previous page)

```
self.conv1 = nn.Conv2d(1, 20, 5)
    self.conv2 = nn.Conv2d(20, 20, 5)
def forward(self, x):
    x = F.relu(self.conv1(x))
    return F.relu(self.conv2(x))
```

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



conv2d

1 Note

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

Variables

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

```
name = 'ConvO'
     conv2d
     fc_num_input
     fc1
     bn conv2d
     norm_fc1
     feature_map_dropout
     static octonion_normalizer(emb_rel_e0, emb_rel_e1, emb_rel_e2, emb_rel_e3, emb_rel_e4,
                  emb_rel_e5, emb_rel_e6, emb_rel_e7)
     residual\_convolution(O\_1, O\_2)
     forward\_triples(x: torch.Tensor) \rightarrow torch.Tensor
               Parameters
                   x
     forward_k_vs_all (x: torch.Tensor)
          Given a head entity and a relation (h,r), we compute scores for all entities. [score(h,r,x)|x in Entities] =>
          [0.0,0.1,...,0.8], shape=> (1, |Entities|) Given a batch of head entities and relations => shape (size of batch,)
          Entities()
class dicee.models.octonion.AConvO(args: dict)
     Bases: dicee.models.base_model.BaseKGE
     Additive Convolutional Octonion Knowledge Graph Embeddings
     name = 'AConvO'
```

```
fc_num_input

fc1

bn_conv2d

norm_fc1

feature_map_dropout

static octonion_normalizer(emb_rel_e0, emb_rel_e1, emb_rel_e2, emb_rel_e3, emb_rel_e4, emb_rel_e5, emb_rel_e6, emb_rel_e7)

residual_convolution(O_1, O_2)

forward_triples(x: torch.Tensor) \rightarrow torch.Tensor

Parameters

x

forward_k_vs_all(x: torch.Tensor)
```

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

dicee.models.pykeen_models

Classes

PykeenKGE A class for using knowledge graph embedding models implemented in Pykeen

Module Contents

```
class dicee.models.pykeen_models.PykeenKGE (args: dict)
    Bases: dicee.models.base_model.BaseKGE
    A class for using knowledge graph embedding models implemented in Pykeen
```

Notes: Pykeen_DistMult: C Pykeen_ComplEx: Pykeen_QuatE: Pykeen_MuRE: Pykeen_CP: Pykeen_HolE: Pykeen_HolE: Pykeen_TransD: Pykeen_TransE: Pykeen_TransF: Pykeen_TransH: Pykeen_TransR:

```
model_kwargs
name
model
loss_history = []
args
entity_embeddings = None
relation_embeddings = None
```

forward_k_vs_all (x: torch.LongTensor)

- # => Explicit version by this we can apply bn and dropout
- # (1) Retrieve embeddings of heads and relations + apply Dropout & Normalization if given. h, $r = self.get_head_relation_representation(x) # (2) Reshape (1). if <math>self.last_dim > 0$:
 - $h = h.reshape(len(x), self.embedding_dim, self.last_dim) r = r.reshape(len(x), self.embedding_dim, self.last_dim)$
- # (3) Reshape all entities. if self.last dim > 0:
 - t = self.entity_embeddings.weight.reshape(self.num_entities, self.embedding_dim, self.last_dim)

else:

- t = self.entity_embeddings.weight
- # (4) Call the score_t from interactions to generate triple scores. return self.interaction.score_t(h=h, r=r, all_entities=t, slice_size=1)
- $forward_triples$ (x: torch.LongTensor) \rightarrow torch.FloatTensor
 - # => Explicit version by this we can apply bn and dropout
 - # (1) Retrieve embeddings of heads, relations and tails and apply Dropout & Normalization if given. h, r, t = self.get_triple_representation(x) # (2) Reshape (1). if self.last_dim > 0:
 - $h = h.reshape(len(x), self.embedding_dim, self.last_dim) r = r.reshape(len(x), self.embedding_dim, self.last_dim) t = t.reshape(len(x), self.embedding_dim, self.last_dim)$
 - # (3) Compute the triple score return self.interaction.score(h=h, r=r, t=t, slice size=None, slice dim=0)
- abstract forward_k_vs_sample (x: torch.LongTensor, target_entity_idx)

dicee.models.quaternion

Classes

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

Functions

 $quaternion_mul_with_unit_norm(*, Q_1, Q_2)$

Module Contents

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

class dicee.models.quaternion.QMult(args)

Bases: dicee.models.base_model.BaseKGE

Base class for all neural network modules.

Your models should also subclass this class.

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

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

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

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

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



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

Variables

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

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

Parameters

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

Returns

Triple scores.

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

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

Absolute value of a quaternion

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

L2 norm of quaternion vector:

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

```
Parameters
                   \mathbf{x} – The vector.
               Returns
                   The normalized vector.
     score (head_ent_emb: torch.FloatTensor, rel_ent_emb: torch.FloatTensor,
                  tail ent emb: torch.FloatTensor)
     k_vs_all_score (bpe_head_ent_emb, bpe_rel_ent_emb, E)
               Parameters
                    • bpe_head_ent_emb
                    • bpe_rel_ent_emb
                   • E
     {\tt forward\_k\_vs\_all}\;(\mathcal{X})
               Parameters
     forward_k_vs_sample (x, target_entity_idx)
           Completed. Given a head entity and a relation (h,r), we compute scores for all possible triples, i.e.,
           [score(h,r,x)|x \text{ in Entities}] => [0.0,0.1,...,0.8], shape=> (1, |Entities|) Given a batch of head entities and
           relations => shape (size of batch, | Entities|)
class dicee.models.quaternion.ConvQ(args)
     Bases: dicee.models.base_model.BaseKGE
     Convolutional Quaternion Knowledge Graph Embeddings
     name = 'ConvQ'
     entity_embeddings
     relation_embeddings
     conv2d
     fc_num_input
     fc1
     bn_conv1
     bn_conv2
     feature_map_dropout
     residual\_convolution(Q_1, Q_2)
     forward\_triples (indexed\_triple: torch.Tensor) \rightarrow torch.Tensor
               Parameters
                   x
     forward_k_vs_all (x: torch.Tensor)
           Given a head entity and a relation (h,r), we compute scores for all entities. [score(h,r,x)|x in Entities] =>
```

Entities₍₎

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

```
class dicee.models.quaternion.AConvQ(args)
     Bases: dicee.models.base_model.BaseKGE
     Additive Convolutional Quaternion Knowledge Graph Embeddings
     name = 'AConvQ'
     entity_embeddings
     relation_embeddings
     conv2d
     fc_num_input
     fc1
     bn_conv1
     bn_conv2
     feature_map_dropout
     \verb"residual_convolution" (Q\_1, Q\_2)
     forward\_triples (indexed_triple: torch.Tensor) \rightarrow torch.Tensor
               Parameters
     forward_k_vs_all (x: torch.Tensor)
           Given a head entity and a relation (h,r), we compute scores for all entities. [score(h,r,x)|x in Entities] =>
           [0.0,0.1,...,0.8], shape=> (1, |Entities|) Given a batch of head entities and relations => shape (size of batch,|
```

dicee.models.real

Entities()

Classes

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

Module Contents

```
class dicee.models.real.DistMult(args)
    Bases: dicee.models.base_model.BaseKGE
    Embedding Entities and Relations for Learning and Inference in Knowledge Bases https://arxiv.org/abs/1412.6575
    name = 'DistMult'
```

```
k_vs_all_score (emb_h: torch.FloatTensor, emb_r: torch.FloatTensor, emb_E: torch.FloatTensor)
               Parameters
                   • emb h
                   • emb_r
                   • emb E
     forward_k_vs_all (x: torch.LongTensor)
     forward_k_vs_sample (x: torch.LongTensor, target_entity_idx: torch.LongTensor)
     score (h, r, t)
class dicee.models.real.TransE(args)
     Bases: dicee.models.base_model.BaseKGE
     Translating Embeddings for Modeling Multi-relational Data https://proceedings.neurips.cc/paper/2013/file/
     1cecc7a77928ca8133fa24680a88d2f9-Paper.pdf
     name = 'TransE'
     margin = 4
     score (head_ent_emb, rel_ent_emb, tail_ent_emb)
     \textbf{forward\_k\_vs\_all} \ (\textit{x: torch.Tensor}) \ \rightarrow \text{torch.FloatTensor}
class dicee.models.real.Shallom(args)
     Bases: dicee.models.base_model.BaseKGE
     A shallow neural model for relation prediction (https://arxiv.org/abs/2101.09090)
     name = 'Shallom'
     shallom
     \texttt{get\_embeddings}\,() \, \to Tuple[numpy.ndarray,\,None]
     forward_k_vs_all (x) \rightarrow \text{torch.FloatTensor}
     forward\_triples(x) \rightarrow torch.FloatTensor
               Parameters
               Returns
class dicee.models.real.Pyke(args)
     Bases: dicee.models.base_model.BaseKGE
     A Physical Embedding Model for Knowledge Graphs
     name = 'Pyke'
     dist_func
     margin = 1.0
     forward_triples (x: torch.LongTensor)
               Parameters
                   x
```

dicee.models.static_funcs

Functions

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

Module Contents

```
\label{eq:dicee.models.static_funcs.quaternion_mul} (*, Q_1, Q_2) \\ \rightarrow Tuple[torch.Tensor, torch.Tensor, torch.Tensor, torch.Tensor] \\ Perform quaternion multiplication :param Q_1: :param Q_2: :return:
```

dicee.models.transformers

Full definition of a GPT Language Model, all of it in this single file. References: 1) the official GPT-2 TensorFlow implementation released by OpenAI: https://github.com/openai/gpt-2/blob/master/src/model.py 2) hugging-face/transformers PyTorch implementation: https://github.com/huggingface/transformers/blob/main/src/transformers/models/gpt2/modeling_gpt2.py

Classes

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

Module Contents

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

Base class for all neural network modules.

Your models should also subclass this class.

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

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

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

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

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



1 Note

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

Variables

name = 'BytE'

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

```
config
temperature = 0.5
topk = 2
transformer
lm_head
loss_function(yhat_batch, y_batch)
```

Parameters

- yhat_batch
- y_batch

forward (x: torch.LongTensor)

Parameters

```
x (B by T tensor)
```

generate (idx, max_new_tokens, temperature=1.0, top_k=None)

Take a conditioning sequence of indices idx (LongTensor of shape (b,t)) and complete the sequence max_new_tokens times, feeding the predictions back into the model each time. Most likely you'll want to make sure to be in model.eval() mode of operation for this.

```
training_step(batch, batch_idx=None)
```

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

Parameters

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

Returns

- Tensor The loss tensor
- dict A dictionary which can include any keys, but must include the key 'loss' in the case of automatic optimization.
- None In automatic optimization, this will skip to the next batch (but is not supported for multi-GPU, TPU, or DeepSpeed). For manual optimization, this has no special meaning, as returning the loss is not required.

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

Example:

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

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

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

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

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

1 Note

When accumulate_grad_batches > 1, the loss returned here will be automatically normalized by accumulate_grad_batches internally.

```
class dicee.models.transformers.LayerNorm(ndim, bias)
```

Bases: torch.nn.Module

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

weight

bias

forward(input)

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

Bases: torch.nn.Module

Base class for all neural network modules.

Your models should also subclass this class.

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

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

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

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

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

1 Note

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

Variables

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

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

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

Base class for all neural network modules.

Your models should also subclass this class.

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

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

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

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

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

1 Note

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

Variables

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

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

Base class for all neural network modules.

Your models should also subclass this class.

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

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

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

(continued from previous page)

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

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

1 Note

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

Variables

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

```
ln_1
  attn
  ln_2
  mlp
  forward(x)

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

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

Base class for all neural network modules.

Your models should also subclass this class.

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

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

class Model (nn.Module):
```

(continued from previous page)

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

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

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

1 Note

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

Variables

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

config

transformer

lm_head

```
get_num_params (non_embedding=True)
```

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

Classes

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

Table 1 - continued from previous page

	r - continued from previous page
TransE	Translating Embeddings for Modeling
Shallom	A shallow neural model for relation prediction (https:
	//arxiv.org/abs/2101.09090)
Pyke	A Physical Embedding Model for Knowledge Graphs
BaseKGE	Base class for all neural network modules.
ConEx	Convolutional ComplEx Knowledge Graph Embeddings
AConEx	Additive Convolutional ComplEx Knowledge Graph Embeddings
ComplEx	Base class for all neural network modules.
BaseKGE	Base class for all neural network modules.
IdentityClass	Base class for all neural network modules.
QMult	Base class for all neural network modules.
ConvQ	Convolutional Quaternion Knowledge Graph Embeddings
AConvQ	Additive Convolutional Quaternion Knowledge Graph Embeddings
BaseKGE	Base class for all neural network modules.
IdentityClass	Base class for all neural network modules.
OMult	Base class for all neural network modules.
ConvO	Base class for all neural network modules.
AConv0	Additive Convolutional Octonion Knowledge Graph Embeddings
Keci	Base class for all neural network modules.
CKeci	Without learning dimension scaling
DeCaL	Base class for all neural network modules.
BaseKGE	Base class for all neural network modules.
PykeenKGE	A class for using knowledge graph embedding models implemented in Pykeen
BaseKGE	Base class for all neural network modules.
FMult	Learning Knowledge Neural Graphs
GFMult	Learning Knowledge Neural Graphs
FMult2	Learning Knowledge Neural Graphs
LFMult1	Embedding with trigonometric functions. We represent all entities and relations in the complex number space as:
LFMult	Embedding with polynomial functions. We represent all entities and relations in the polynomial space as:
DualE	Dual Quaternion Knowledge Graph Embeddings (https://ojs.aaai.org/index.php/AAAI/article/download/16850/16657)

Functions

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

Package Contents

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

Base class for all optimizers.

Warning

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

Parameters

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

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

Parameters

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

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

Bases: lightning.LightningModule

Base class for all neural network modules.

Your models should also subclass this class.

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

```
import torch.nn as nn
import torch.nn.functional as F
class Model(nn.Module):
   def __init__(self) -> None:
       super().__init__()
       self.conv1 = nn.Conv2d(1, 20, 5)
       self.conv2 = nn.Conv2d(20, 20, 5)
    def forward(self, x):
       x = F.relu(self.conv1(x))
       return F.relu(self.conv2(x))
```

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



1 Note

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

Variables

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

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

Size of model in MB and number of params

```
training_step(batch, batch_idx=None)
```

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

Parameters

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

Returns

- Tensor The loss tensor
- · dict A dictionary which can include any keys, but must include the key 'loss' in the case of automatic optimization.
- None In automatic optimization, this will skip to the next batch (but is not supported for multi-GPU, TPU, or DeepSpeed). For manual optimization, this has no special meaning, as returning the loss is not required.

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

Example:

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

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

```
def __init__(self):
   super().__init__()
    self.automatic_optimization = False
# Multiple optimizers (e.g.: GANs)
```

(continued from previous page)

```
def training_step(self, batch, batch_idx):
    opt1, opt2 = self.optimizers()

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

1 Note

When accumulate_grad_batches > 1, the loss returned here will be automatically normalized by accumulate_grad_batches internally.

loss_function(yhat_batch: torch.FloatTensor, y_batch: torch.FloatTensor)

Parameters

- yhat_batch
- y_batch

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

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

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

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

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

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

test_epoch_end (outputs: List[Any])

```
\texttt{test\_dataloader}() \rightarrow None
```

An iterable or collection of iterables specifying test samples.

For more information about multiple dataloaders, see this section.

For data processing use the following pattern:

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

However, the above are only necessary for distributed processing.

A Warning

do not assign state in prepare_data

- test()
- prepare_data()
- setup()

1 Note

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

1 Note

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

$val_dataloader() \rightarrow None$

An iterable or collection of iterables specifying validation samples.

For more information about multiple dataloaders, see this section.

The dataloader you return will not be reloaded unless you set :param-ref:`~lightning.pytorch.trainer.trainer.Trainer.reload_dataloaders_every_n_epochs` to a positive integer.

It's recommended that all data downloads and preparation happen in prepare_data().

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

1 Note

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

1 Note

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

$predict_dataloader() \rightarrow None$

An iterable or collection of iterables specifying prediction samples.

For more information about multiple dataloaders, see this section.

It's recommended that all data downloads and preparation happen in prepare_data().

- predict()
- prepare_data()
- setup()

1 Note

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

Returns

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

$train_dataloader() \rightarrow None$

An iterable or collection of iterables specifying training samples.

For more information about multiple dataloaders, see this section.

dataloader will not be reloaded unless you set :paramref: "~lightning.pytorch.trainer.trainer.Trainer.reload_dataloaders_every_n_epochs" to a positive integer.

For data processing use the following pattern:

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

However, the above are only necessary for distributed processing.

Warning

do not assign state in prepare_data

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

1 Note

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

configure_optimizers (parameters=None)

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

Returns

Any of these 6 options.

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

The lr_scheduler_config is a dictionary which contains the scheduler and its associated configuration. The default configuration is shown below.

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

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

Metrics can be made available to monitor by simply logging it using self.log('metric_to_track', metric_val) in your LightningModule.



1 Note

Some things to know:

- Lightning calls .backward() and .step() automatically in case of automatic optimization.
- If a learning rate scheduler is specified in <code>configure_optimizers()</code> with key "interval" (default "epoch") in the scheduler configuration, Lightning will call the scheduler's <code>.step()</code> method automatically in case of automatic optimization.
- If you use 16-bit precision (precision=16), Lightning will automatically handle the optimizer.
- If you use torch.optim.LBFGS, Lightning handles the closure function automatically for you.
- If you use multiple optimizers, you will have to switch to 'manual optimization' mode and step them yourself.
- If you need to control how often the optimizer steps, override the optimizer_step() hook.

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

Bases: BaseKGELightning

Base class for all neural network modules.

Your models should also subclass this class.

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

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

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

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

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

1 Note

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

Variables

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

args

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

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

```
forward (x: torch.LongTensor | Tuple[torch.LongTensor, torch.LongTensor],
                 y idx: torch.LongTensor = None)
              Parameters
                  • x
                  y_idx
                  • ordered_bpe_entities
     \texttt{forward\_triples} \ (x: torch.LongTensor) \ \to torch.Tensor
              Parameters
     forward_k_vs_all(*args, **kwargs)
     forward_k_vs_sample(*args, **kwargs)
     get_triple_representation(idx_hrt)
     get_head_relation_representation (indexed_triple)
     get_sentence_representation(x: torch.LongTensor)
              Parameters
                  • (b (x shape)
                  • 3
                  • t)
     get_bpe_head_and_relation_representation(x: torch.LongTensor)
                  → Tuple[torch.FloatTensor, torch.FloatTensor]
              Parameters
                  x (B x 2 x T)
     get_embeddings() → Tuple[numpy.ndarray, numpy.ndarray]
class dicee.models.IdentityClass(args=None)
     Bases: torch.nn.Module
     Base class for all neural network modules.
     Your models should also subclass this class.
     modules as regular attributes:
```

init_params_with_sanity_checking()

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

```
import torch.nn as nn
import torch.nn.functional as F
class Model(nn.Module):
    def __init__(self) -> None:
        super().__init__()
        self.conv1 = nn.Conv2d(1, 20, 5)
        self.conv2 = nn.Conv2d(20, 20, 5)
```

(continued from previous page)

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

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

1 Note

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

Variables

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

```
args = None
__call__(x)
static forward(x)

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

Base class for all neural network modules.

Your models should also subclass this class.

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

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

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

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

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

1 Note

As per the example above, an $__{init}_{_}()$ call to the parent class must be made before assignment on the child.

Variables

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

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

```
forward_byte_pair_encoded_k_vs_all(x: torch.LongTensor)
              Parameters
                 x (B x 2 x T)
     forward_byte_pair_encoded_triple (x: Tuple[torch.LongTensor, torch.LongTensor])
          byte pair encoded neural link predictors
              Parameters
     init_params_with_sanity_checking()
     forward(x: torch.LongTensor | Tuple[torch.LongTensor, torch.LongTensor],
                 y_idx: torch.LongTensor = None
              Parameters
                  • x
                  • y_idx
                  • ordered_bpe_entities
     forward\_triples(x: torch.LongTensor) \rightarrow torch.Tensor
              Parameters
     forward_k_vs_all(*args, **kwargs)
     forward_k_vs_sample(*args, **kwargs)
     get_triple_representation(idx_hrt)
     get_head_relation_representation(indexed_triple)
     get_sentence_representation(x: torch.LongTensor)
              Parameters
                  • (b(x shape)
                  • 3
                  • t)
     get_bpe_head_and_relation_representation(x: torch.LongTensor)
                 → Tuple[torch.FloatTensor, torch.FloatTensor]
              Parameters
                  x (B x 2 x T)
     get_embeddings() → Tuple[numpy.ndarray, numpy.ndarray]
class dicee.models.DistMult (args)
     Bases: dicee.models.base_model.BaseKGE
     Embedding Entities and Relations for Learning and Inference in Knowledge Bases https://arxiv.org/abs/1412.6575
     name = 'DistMult'
```

```
k_vs_all_score (emb_h: torch.FloatTensor, emb_r: torch.FloatTensor, emb_E: torch.FloatTensor)
               Parameters
                   • emb h
                   • emb_r
                   • emb_E
     forward_k_vs_all (x: torch.LongTensor)
     forward_k_vs_sample(x: torch.LongTensor, target_entity_idx: torch.LongTensor)
     score(h, r, t)
class dicee.models.TransE(args)
     Bases: dicee.models.base_model.BaseKGE
     Translating Embeddings for Modeling Multi-relational Data https://proceedings.neurips.cc/paper/2013/file/
     1cecc7a77928ca8133fa24680a88d2f9-Paper.pdf
     name = 'TransE'
     margin = 4
     score (head_ent_emb, rel_ent_emb, tail_ent_emb)
     forward_k_vs_all(x: torch.Tensor) \rightarrow torch.FloatTensor
class dicee.models.Shallom(args)
     Bases: dicee.models.base_model.BaseKGE
     A shallow neural model for relation prediction (https://arxiv.org/abs/2101.09090)
     name = 'Shallom'
     shallom
     \texttt{get\_embeddings}\,() \, \to Tuple[numpy.ndarray,\,None]
     \mathbf{forward\_k\_vs\_all}\;(x)\;\to \mathrm{torch.FloatTensor}
     forward_triples (x) \rightarrow \text{torch.FloatTensor}
               Parameters
               Returns
class dicee.models.Pyke(args)
     Bases: dicee.models.base_model.BaseKGE
     A Physical Embedding Model for Knowledge Graphs
     name = 'Pyke'
     dist_func
     margin = 1.0
```

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

Parameters

x

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

Bases: BaseKGELightning

Base class for all neural network modules.

Your models should also subclass this class.

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

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

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

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

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

1 Note

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

Variables

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

args

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

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

```
forward_triples (x: torch.LongTensor) \rightarrow torch.Tensor
               Parameters
                   x
     forward_k_vs_all(*args, **kwargs)
     forward_k_vs_sample(*args, **kwargs)
     get_triple_representation(idx_hrt)
     get_head_relation_representation (indexed_triple)
     get_sentence_representation(x: torch.LongTensor)
               Parameters
                   • (b (x shape)
                   • 3
                   • t)
     get_bpe_head_and_relation_representation (x: torch.LongTensor)
                  → Tuple[torch.FloatTensor, torch.FloatTensor]
               Parameters
                  x (B x 2 x T)
     \mathtt{get\_embeddings}() \rightarrow Tuple[numpy.ndarray, numpy.ndarray]
class dicee.models.ConEx(args)
     Bases: dicee.models.base_model.BaseKGE
     Convolutional ComplEx Knowledge Graph Embeddings
     name = 'ConEx'
     conv2d
     fc_num_input
     fc1
     norm_fc1
     bn_conv2d
     feature_map_dropout
     residual_convolution(C_1: Tuple[torch.Tensor, torch.Tensor],
                  C_2: Tuple[torch.Tensor, torch.Tensor]) \rightarrow torch.FloatTensor
          Compute residual score of two complex-valued embeddings. :param C_1: a tuple of two pytorch tensors
          that corresponds complex-valued embeddings :param C_2: a tuple of two pytorch tensors that corresponds
          complex-valued embeddings :return:
     forward_k_vs_all(x: torch.Tensor) \rightarrow torch.FloatTensor
     forward\_triples(x: torch.Tensor) \rightarrow torch.FloatTensor
               Parameters
                  x
```

```
forward_k_vs_sample (x: torch.Tensor, target_entity_idx: torch.Tensor)
class dicee.models.AConEx(args)
     Bases: dicee.models.base_model.BaseKGE
     Additive Convolutional ComplEx Knowledge Graph Embeddings
     name = 'AConEx'
     conv2d
     fc_num_input
     fc1
     norm_fc1
     bn_conv2d
     feature_map_dropout
     residual_convolution (C_1: Tuple[torch.Tensor, torch.Tensor],
                  C_2: Tuple[torch.Tensor, torch.Tensor]) \rightarrow torch.FloatTensor
           Compute residual score of two complex-valued embeddings. :param C_1: a tuple of two pytorch tensors
           that corresponds complex-valued embeddings :param C_2: a tuple of two pytorch tensors that corresponds
           complex-valued embeddings :return:
     forward_k_vs_all(x: torch.Tensor) \rightarrow torch.FloatTensor
     forward\_triples(x: torch.Tensor) \rightarrow torch.FloatTensor
               Parameters
     forward_k_vs_sample (x: torch.Tensor, target_entity_idx: torch.Tensor)
class dicee.models.ComplEx (args)
     Bases: dicee.models.base_model.BaseKGE
     Base class for all neural network modules.
     Your models should also subclass this class.
     Modules can also contain other Modules, allowing them to be nested in a tree structure. You can assign the sub-
     modules as regular attributes:
      import torch.nn as nn
      import torch.nn.functional as F
```

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

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

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

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



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

Variables

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

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

forward_k_vs_sample (x: torch.LongTensor, target_entity_idx: torch.LongTensor)

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

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

Perform quaternion multiplication :param Q_1: :param Q_2: :return:

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

Bases: BaseKGELightning

Base class for all neural network modules.

Your models should also subclass this class.

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

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

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

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

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



1 Note

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

Variables

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

```
args
embedding_dim = None
num_entities = None
num_relations = None
num_tokens = None
learning_rate = None
apply_unit_norm = None
input_dropout_rate = None
hidden_dropout_rate = None
optimizer_name = None
feature_map_dropout_rate = None
kernel_size = None
num_of_output_channels = None
weight_decay = None
loss
selected_optimizer = None
normalizer_class = None
normalize_head_entity_embeddings
normalize_relation_embeddings
normalize_tail_entity_embeddings
hidden_normalizer
param_init
input_dp_ent_real
input_dp_rel_real
```

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

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

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

Bases: torch.nn.Module

Base class for all neural network modules.

Your models should also subclass this class.

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

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

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

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

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

1 Note

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

Variables

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

```
args = None
__call__(x)
static forward(x)

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

class dicee.models.QMult(args)

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

Base class for all neural network modules.

Your models should also subclass this class.

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

```
import torch.nn as nn
import torch.nn.functional as F
(continues on next page)
```

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

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

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



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

Variables

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

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

Parameters

- h shape: (*batch_dims, dim) The head representations.
- \mathbf{r} shape: (*batch_dims, dim) The head representations.
- t shape: (*batch_dims, dim) The tail representations.

Returns

Triple scores.

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

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

Absolute value of a quaternion

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

L2 norm of quaternion vector:

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

Parameters

 \mathbf{x} – The vector.

Returns

The normalized vector.

```
score (head_ent_emb: torch.FloatTensor, rel_ent_emb: torch.FloatTensor,
                   tail ent emb: torch.FloatTensor)
      k\_vs\_all\_score (bpe_head_ent_emb, bpe_rel_ent_emb, E)
                Parameters
                    • bpe_head_ent_emb
                    • bpe_rel_ent_emb
      forward_k_vs_all(x)
                Parameters
                    x
      forward_k_vs_sample (x, target_entity_idx)
           Completed. Given a head entity and a relation (h,r), we compute scores for all possible triples, i.e.,
           [score(h,r,x)|x \text{ in Entities}] => [0.0,0.1,...,0.8], shape=> (1, |Entities|) Given a batch of head entities and
           relations => shape (size of batch,| Entities|)
class dicee.models.ConvQ(args)
      Bases: dicee.models.base_model.BaseKGE
      Convolutional Quaternion Knowledge Graph Embeddings
      name = 'ConvQ'
      entity_embeddings
      relation_embeddings
      conv2d
      fc_num_input
      fc1
      bn conv1
      bn_conv2
      feature_map_dropout
      residual_convolution (Q_1, Q_2)
      \textbf{forward\_triples} \ (\textit{indexed\_triple: torch.Tensor}) \ \rightarrow \textbf{torch.Tensor}) \ \rightarrow \textbf{torch.Tensor}
                Parameters
      forward_k_vs_all (x: torch.Tensor)
           Given a head entity and a relation (h,r), we compute scores for all entities. [score(h,r,x)|x in Entities] =>
           [0.0,0.1,...,0.8], shape=> (1, |Entities|) Given a batch of head entities and relations => shape (size of batch,)
           Entities()
class dicee.models.AConvQ(args)
      Bases: dicee.models.base_model.BaseKGE
      Additive Convolutional Quaternion Knowledge Graph Embeddings
```

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

Bases: BaseKGELightning

Base class for all neural network modules.

Your models should also subclass this class.

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

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

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

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

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

1 Note

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

Variables

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

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

```
loss_history = []
byte_pair_encoding
max_length_subword_tokens
block_size
forward_byte_pair_encoded_k_vs_all (x: torch.LongTensor)
         Parameters
             x (B x 2 x T)
forward_byte_pair_encoded_triple (x: Tuple[torch.LongTensor, torch.LongTensor])
     byte pair encoded neural link predictors
         Parameters
init_params_with_sanity_checking()
forward (x: torch.LongTensor | Tuple[torch.LongTensor, torch.LongTensor],
            y_idx: torch.LongTensor = None)
         Parameters
             • x
             • y_idx
             • ordered_bpe_entities
forward\_triples(x: torch.LongTensor) \rightarrow torch.Tensor
         Parameters
forward_k_vs_all(*args, **kwargs)
forward_k_vs_sample(*args, **kwargs)
get_triple_representation(idx_hrt)
get_head_relation_representation(indexed_triple)
get_sentence_representation(x: torch.LongTensor)
         Parameters
             • (b (x shape)
             • 3
             • t)
get_bpe_head_and_relation_representation(x: torch.LongTensor)
             → Tuple[torch.FloatTensor, torch.FloatTensor]
         Parameters
             x (B x 2 x T)
\mathtt{get\_embeddings}() \rightarrow \mathsf{Tuple}[\mathsf{numpy}.\mathsf{ndarray}, \mathsf{numpy}.\mathsf{ndarray}]
```

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

Bases: torch.nn.Module

Base class for all neural network modules.

Your models should also subclass this class.

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

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

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

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

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

1 Note

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

Variables

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

```
args = None
__call__(x)
static forward(x)
dicee.models.octonion_mul(*, O_1, O_2)
dicee.models.octonion_mul_norm(*, O_1, O_2)
class dicee.models.OMult(args)
Bases: dicee.models.base_model.BaseKGE
```

Base class for all neural network modules.

Your models should also subclass this class.

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

(continued from previous page)

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

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

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



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

Variables

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

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

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

Bases: dicee.models.base_model.BaseKGE

Base class for all neural network modules.

Your models should also subclass this class.

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

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

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

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

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

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

1 Note

conv2d

fc_num_input

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

Variables

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

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

```
fc1
```

bn_conv2d

norm_fc1

feature_map_dropout

static octonion_normalizer(emb_rel_e0, emb_rel_e1, emb_rel_e2, emb_rel_e3, emb_rel_e4,
emb_rel_e5, emb_rel_e6, emb_rel_e7)

 ${\tt residual_convolution}\,(O_1,\,O_2)$

 $forward_triples(x: torch.Tensor) \rightarrow torch.Tensor$

Parameters

x

forward k vs all (x: torch. Tensor)

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

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

Bases: dicee.models.base model.BaseKGE

Base class for all neural network modules.

Your models should also subclass this class.

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

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

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

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

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

1 Note

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

Variables

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

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

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

Compute our CL multiplication

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

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

eq j

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

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

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

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

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

Parameter

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

returns

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

forward_k_vs_with_explicit(x: torch.Tensor)

 $k_vs_all_score$ (bpe_head_ent_emb, bpe_rel_ent_emb, E)

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

Kvsall training

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

forward_k_vs_with_explicit and this funcitons are identical Parameter — x: torch.LongTensor with (n,2) shape :rtype: torch.FloatTensor with (n, |E|) shape

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

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

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

Parameter

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

returns

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

 $forward_k_vs_sample$ (x: torch.LongTensor, target_entity_idx: torch.LongTensor) \rightarrow torch.FloatTensor

Parameter

```
x: torch.LongTensor with (n,2) shape target_entity_idx: torch.LongTensor with (n, k) shape k denotes the selected number of examples. 

rtype torch.FloatTensor with (n, k) shape score (h, r, t)

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

Parameter

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

rtvpe

torch.FloatTensor with (n) shape

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

Without learning dimension scaling

```
name = 'CKeci'
```

requires_grad_for_interactions = False

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

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

Base class for all neural network modules.

Your models should also subclass this class.

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

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

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

(continues on next page)

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

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

1 Note

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

Variables

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

name = 'DeCaL'

entity_embeddings

relation_embeddings

q

r

re

forward_triples (x: torch.Tensor) \rightarrow torch.FloatTensor

Parameter

x: torch.LongTensor with (n,) shape

rtype

torch.FloatTensor with (n) shape

 $cl_pqr(a: torch.tensor) \rightarrow torch.tensor$

Input: tensor(batch_size, emb_dim) —> output: tensor with 1+p+q+r components with size (batch_size, $emb_dim/(1+p+q+r)$) each.

1) takes a tensor of size (batch_size, emb_dim), split it into 1 + p + q + r components, hence 1+p+q+r must be a divisor of the emb_dim. 2) Return a list of the 1+p+q+r components vectors, each are tensors of size $(batch_size, emb_dim/(1+p+q+r))$

compute_sigmas_single (list_h_emb, list_r_emb, list_t_emb)

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

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

and return:

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

compute_sigmas_multivect(list_h_emb, list_r_emb)

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

For same bases vectors interaction we have

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

For different base vector interactions, we have

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

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

Kvsall training

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

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

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

Multiplying a base vector with its scalar coefficient

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

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

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

Parameter

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

returns

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

 $compute_sigma_pp(hp, rp)$

Compute .. math:

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

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

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

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

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

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

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

$compute_sigma_qq(hq, rq)$

Compute

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

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

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

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

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

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

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

 $compute_sigma_rr(hk, rk)$

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

compute_sigma_pq(*, hp, hq, rp, rq)

Compute

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

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

for j in range(q):

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

print(sigma_pq.shape)

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

Compute

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

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

```
\begin{aligned} & \textbf{for j in range(q):} \\ & \text{sigma\_pq[:,:,i,j] = hp[:,:,i] * rq[:,:,j] - hq[:,:,j] * rp[:,:,i]} \\ & print(sigma\_pq.shape) \\ & \textbf{compute\_sigma\_qr}(*,hq,hk,rq,rk) \\ & \sum_{i=1}^{p} \sum_{j=p+1}^{p+q} (h_i r_j - h_j r_i) e_i e_j \\ & \text{results = [] sigma\_pq = torch.zeros(b, r, p, q) for i in range(p):} \\ & \textbf{for j in range(q):} \\ & \text{sigma\_pq[:,:,i,j] = hp[:,:,i] * rq[:,:,j] - hq[:,:,j] * rp[:,:,i]} \\ & \text{print(sigma\_pq.shape)} \\ & \textbf{class dicee.models.BaseKGE}(\textit{args: dict}) \\ & \text{Bases: } \textit{BaseKGELightning} \end{aligned}
```

Base class for all neural network modules.

Your models should also subclass this class.

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

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

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

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

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

1 Note

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

Variables

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

```
args
embedding_dim = None
num_entities = None
```

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

```
init_params_with_sanity_checking()
     forward (x: torch.LongTensor | Tuple[torch.LongTensor, torch.LongTensor],
                 y idx: torch.LongTensor = None)
              Parameters
                  • x
                  y_idx
                  • ordered_bpe_entities
     \texttt{forward\_triples} \ (x: torch.LongTensor) \ \to torch.Tensor
              Parameters
     forward_k_vs_all(*args, **kwargs)
     forward_k_vs_sample(*args, **kwargs)
     get_triple_representation(idx_hrt)
     get_head_relation_representation(indexed_triple)
     get_sentence_representation(x: torch.LongTensor)
              Parameters
                  • (b (x shape)
                  • 3
                  • t)
     get_bpe_head_and_relation_representation(x: torch.LongTensor)
                 → Tuple[torch.FloatTensor, torch.FloatTensor]
              Parameters
                 x (B x 2 x T)
     get_embeddings() → Tuple[numpy.ndarray, numpy.ndarray]
class dicee.models.PykeenKGE(args: dict)
     Bases: dicee.models.base_model.BaseKGE
     A class for using knowledge graph embedding models implemented in Pykeen
     Notes: Pykeen_DistMult: C Pykeen_ComplEx: Pykeen_QuatE: Pykeen_MuRE: Pykeen_CP: Pykeen_HolE: Py-
     keen_HolE: Pykeen_HolE: Pykeen_TransD: Pykeen_TransE: Pykeen_TransF: Pykeen_TransH: Pykeen_TransR:
     model_kwargs
     name
     model
     loss_history = []
     args
```

```
entity_embeddings = None
relation_embeddings = None
forward_k_vs_all (x: torch.LongTensor)
              # => Explicit version by this we can apply bn and dropout
              # (1) Retrieve embeddings of heads and relations + apply Dropout & Normalization if given. h, r =
              self.get_head_relation_representation(x) \# (2) Reshape (1). if self.last_dim > 0:
                          h = h.reshape(len(x), self.embedding dim, self.last dim) r = r.reshape(len(x), self.embedding dim,
                          self.last dim)
              # (3) Reshape all entities. if self.last_dim > 0:
                          t = self.entity_embeddings.weight.reshape(self.num_entities, self.embedding_dim, self.last_dim)
              else:
                          t = self.entity\_embeddings.weight
              # (4) Call the score_t from interactions to generate triple scores. return self.interaction.score_t(h=h, r=r,
              all_entities=t, slice_size=1)
forward\_triples(x: torch.LongTensor) \rightarrow torch.FloatTensor
              # => Explicit version by this we can apply bn and dropout
              # (1) Retrieve embeddings of heads, relations and tails and apply Dropout & Normalization if given. h, r, t =
              self.get\_triple\_representation(x) \# (2) Reshape (1). if <math>self.last\_dim > 0:
                          h = h.reshape(len(x), self.embedding_dim, self.last_dim) r = r.reshape(len(x), self.embedding_dim, self.embedding_di
                          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 them to be nested in a tree structure. You can assign the sub-modules as regular attributes:

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

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

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

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



1 Note

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

Variables

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

```
args
embedding_dim = None
num_entities = None
num_relations = None
num_tokens = None
learning_rate = None
apply_unit_norm = None
input_dropout_rate = None
hidden_dropout_rate = None
optimizer_name = None
feature_map_dropout_rate = None
kernel_size = None
num_of_output_channels = None
weight_decay = None
loss
selected_optimizer = None
normalizer_class = None
normalize_head_entity_embeddings
normalize_relation_embeddings
normalize_tail_entity_embeddings
hidden_normalizer
param_init
input_dp_ent_real
input_dp_rel_real
```

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

```
\mathtt{get\_embeddings}() \rightarrow Tuple[numpy.ndarray, numpy.ndarray]
class dicee.models.FMult(args)
     Bases: dicee.models.base_model.BaseKGE
     Learning Knowledge Neural Graphs
     name = 'FMult'
     entity_embeddings
     relation_embeddings
     num_sample = 50
     gamma
     roots
     weights
     compute\_func(weights: torch.FloatTensor, x) \rightarrow torch.FloatTensor
     chain_func(weights, x: torch.FloatTensor)
     forward\_triples(idx\_triple: torch.Tensor) \rightarrow torch.Tensor
               Parameters
                   x
class dicee.models.GFMult (args)
     Bases: dicee.models.base_model.BaseKGE
     Learning Knowledge Neural Graphs
     name = 'GFMult'
     entity_embeddings
     relation_embeddings
     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
                   x
```

```
class dicee.models.FMult2(args)
     Bases: dicee.models.base_model.BaseKGE
     Learning Knowledge Neural Graphs
     name = 'FMult2'
     n_{ayers} = 3
     n = 50
     score_func = 'compositional'
     discrete_points
     entity_embeddings
     relation_embeddings
     {\tt build\_func}\,(\mathit{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.LFMult1 (args)
     Bases: dicee.models.base_model.BaseKGE
     Embedding with trigonometric functions. We represent all entities and relations in the complex number space as:
     f(x) = sum_{k=0}^{k=0}^{k=d-1}wk e^{kix}, and use the three differents scoring function as in the paper to evaluate
     the score
     name = 'LFMult1'
     entity_embeddings
     relation_embeddings
     forward_triples (idx_triple)
               Parameters
     tri_score(h, r, t)
     \mathtt{vtp\_score}(h, r, t)
```

```
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
\mathtt{vtp\_score}(h, r, t)
     this part implement the vector triple product scoring techniques:
     score(h,r,t) = int_{0}{1} h(x)r(x)t(x) dx = sum_{i,j,k} = 0}^{d-1} dfrac_{a_i}c_j*b_k
     b\_i*c\_j*a\_k\}\{(1+(i+j)\%d)(1+k)\}
      1. generate the range for i,j and k from [0 d-1]
      2. Compute the first and second terms of the sum
      3. Multiply with then denominator and take the sum
      4. take the sum over each batch
comp func (h, r, t)
```

class dicee.models.LFMult(args)

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

```
polynomial(coeff, x, degree)
           This function takes a matrix tensor of coefficients (coeff), a tensor vector of points x and range of integer
           [0,1,...d] and return a vector tensor (coeff[0][0] + coeff[0][1]x +...+ coeff[0][d]x^d,
                coeff[1][0] + coeff[1][1]x + ... + coeff[1][d]x^d
      pop (coeff, x, degree)
           This function allow us to evaluate the composition of two polynomes without for loops:) it takes a matrix
           tensor of coefficients (coeff), a matrix tensor of points x and range of integer [0,1,...d]
                and return a tensor (coeff[0][0] + coeff[0][1]x + ... + coeff[0][d]x^d,
                    coeff[1][0] + coeff[1][1]x + ... + coeff[1][d]x^d
class dicee.models.DualE(args)
      Bases: dicee.models.base_model.BaseKGE
      Dual Quaternion Knowledge Graph Embeddings (https://ojs.aaai.org/index.php/AAAI/article/download/16850/
      16657)
      name = 'DualE'
      entity_embeddings
      relation embeddings
      num ent = None
      kvsall_score (e_1_h, e_2_h, e_3_h, e_4_h, e_5_h, e_6_h, e_7_h, e_8_h, e_1_t, e_2_t, e_3_t, e_4_t,
                   e_5_t, e_6_t, e_7_t, e_8_t, r_1, r_2, r_3, r_4, r_5, r_6, r_7, r_8) \rightarrow \text{torch.tensor}
           KvsAll scoring function
           Input
           x: torch.LongTensor with (n, ) shape
           Output
           torch.FloatTensor with (n) shape
      forward\_triples(idx\_triple: torch.tensor) \rightarrow torch.tensor
           Negative Sampling forward pass:
           Input
           x: torch.LongTensor with (n, ) shape
           Output
           torch.FloatTensor with (n) shape
      forward_k_vs_all(x)
```

KvsAll forward pass

Input

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

Output

```
torch.FloatTensor with (n) shape

T (x: torch.tensor) → torch.tensor

Transpose function

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

dicee.query_generator

Classes

QueryGenerator

Module Contents

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

```
set_global_seed(seed: int)
           Set seed
      construct\_graph(paths: List[str]) \rightarrow Tuple[Dict, Dict]
           Construct graph from triples Returns dicts with incoming and outgoing edges
      fill_query(query\_structure: List[str | List], ent_in: Dict, ent_out: Dict, answer: int) \rightarrow bool
           Private method for fill_query logic.
      achieve\_answer(query: List[str \mid List], ent\_in: Dict, ent\_out: Dict) \rightarrow set
           Private method for achieve_answer logic. @TODO: Document the code
      write_links(ent_out, small_ent_out)
      ground_queries (query_structure: List[str | List], ent_in: Dict, ent_out: Dict, small_ent_in: Dict,
                   small_ent_out: Dict, gen_num: int, query_name: str)
           Generating queries and achieving answers
      unmap (query_type, queries, tp_answers, fp_answers, fn_answers)
      unmap_query (query_structure, query, id2ent, id2rel)
      generate_queries (query_struct: List, gen_num: int, query_type: str)
           Passing incoming and outgoing edges to ground queries depending on mode [train valid or text] and getting
           queries and answers in return @ TODO: create a class for each single query struct
      save_queries (query_type: str, gen_num: int, save_path: str)
      abstract load_queries(path)
      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.read_preprocess_save_load_kg
Submodules
dicee.read_preprocess_save_load_kg.preprocess
Classes
```

PreprocessKG

Preprocess the data in memory

Module Contents

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

Parameter

rtype

None

```
\label{eq:preprocess_with_byte_pair} $$preprocess_with_byte_pair_encoding_with_padding() \to None $$preprocess_with_pandas() \to None $$preprocess_with_pandas() \to None $$$preprocess_with_pandas() \to None $$$$preprocess_with_pandas() \to None $$$$$$$$$$
```

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

 $\label{eq:preprocess_with_polars()} \textbf{\rightarrow None}$ $\mbox{sequential_vocabulary_construction()} \rightarrow None$

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

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

dicee.read_preprocess_save_load_kg.read_from_disk

Classes

ReadFromDisk

Read the data from disk into memory

Module Contents

class dicee.read_preprocess_save_load_kg.read_from_disk.ReadFromDisk (kg) Read the data from disk into memory kg start () \rightarrow None

Read a knowledge graph from disk into memory

Data will be available at the train_set, test_set, valid_set attributes.

Parameter

```
None

rtype

None

add_noisy_triples_into_training()
```

dicee.read_preprocess_save_load_kg.save_load_disk

Classes

LoadSaveToDisk

Module Contents

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

dicee.read_preprocess_save_load_kg.util

Functions

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

Module Contents

```
dicee.read_preprocess_save_load_kg.util.polars_dataframe_indexer( df_polars: polars.DataFrame, idx_entity: polars.DataFrame, idx_relation: polars.DataFrame) <math>\rightarrow polars.DataFrame
```

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

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

Parameters:

df polars

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

idx_entity

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

idx relation

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

Returns:

polars.DataFrame

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

Example Usage:

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

Steps:

- 1. Join the input DataFrame *df_polars* on the 'relation' column with *idx_relation* to replace the relations with their indices.
- 2. Join on 'subject' to replace it with the corresponding entity index using a left join on idx_entity.
- 3. Join on 'object' to replace it with the corresponding entity index using a left join on idx_entity.
- 4. Select only the 'subject', 'relation', and 'object' columns to return the final result.

```
dicee.read_preprocess_save_load_kg.util.pandas_dataframe_indexer(  df\_pandas: pandas.DataFrame, idx\_entity: pandas.DataFrame, idx\_relation: pandas.DataFrame) \\ \rightarrow pandas.DataFrame
```

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

Parameters:

df_pandas

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

idx_entity

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

idx relation

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

Returns:

pd.DataFrame

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

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

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

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

read_only_few: int = None, sample_triples_ratio: float = None, separator: str = None) $\rightarrow polars.DataFrame$

Load and Preprocess via Polars

```
dicee.read_preprocess_save_load_kg.util.read_with_pandas(data_path, read_only_few: int = None, sample_triples_ratio: float = None, separator: str = None)
```

```
dicee.read_preprocess_save_load_kg.util.read_from_disk(data_path: str, read_only_few: int = None, sample_triples_ratio: float = None, backend: str = None, separator: str = None) → Tuple[polars.DataFrame, pandas.DataFrame]
```

```
dicee.read_preprocess_save_load_kg.util.read_from_triple_store(endpoint: str = None)
```

Read triples from triple store into pandas dataframe

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

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

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

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

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

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

Deserialize data

Classes

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

Package Contents

(3) Index datasets

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

Preprocess the data in memory

kg

start () → None

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

Parameter

rtype

None

preprocess_with_byte_pair_encoding()

preprocess_with_byte_pair_encoding_with_padding() → None

preprocess_with_pandas() → None

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

(1) Add recipriocal or noisy triples

(2) Construct vocabulary
```

Parameter

```
rtvpe
                   None
     {\tt preprocess\_with\_polars}\, () \, \to None
     \verb|sequential_vocabulary_construction|()| \to None
           (1) Read input data into memory
           (2) Remove triples with a condition
           (3) Serialize vocabularies in a pandas dataframe where
                   => the index is integer and => a single column is string (e.g. URI)
class dicee.read_preprocess_save_load_kg.LoadSaveToDisk(kg)
     kg
     save()
     load()
class dicee.read_preprocess_save_load_kg.ReadFromDisk(kg)
     Read the data from disk into memory
     kg
     \mathtt{start}() \rightarrow \mathrm{None}
           Read a knowledge graph from disk into memory
           Data will be available at the train_set, test_set, valid_set attributes.
           Parameter
           None
               rtype
                   None
     add_noisy_triples_into_training()
```

dicee.sanity checkers

Functions

Module Contents

dicee.sanity_checkers.is_sparql_endpoint_alive(sparql_endpoint: str = None)

```
dicee.sanity_checkers.validate_knowledge_graph (args)

Validating the source of knowledge graph
```

dicee.sanity_checkers.sanity_checking_with_arguments(args)

dicee.scripts

Submodules

dicee.scripts.index_serve

\$ docker pull qdrant/qdrant && docker run -p 6333:6333 -p 6334:6334 -v \$(pwd)/qdrant_storage:/qdrant/storage:z qdrant/qdrant \$ dicee_vector_db -index -serve -path CountryEmbeddings -collection "countries_vdb"

Attributes

```
app
neural_searcher
```

Classes

NeuralSearcher	
StringListRequest	!!! abstract "Usage Documentation"

Functions

```
get_default_arguments()
index(args)

root()
search_embeddings(q)

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

main()
```

Module Contents

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

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

dicee.scripts.run

Functions

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

Module Contents

dicee.static_funcs

Functions

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

continues on next page

Table 2 - continued from previous page

```
deploy_head_entity_prediction(pre_trained_kge,
deploy_relation_prediction(pre_trained_kge,
...)
 vocab_to_parquet(vocab_to_idx, name, ...)
create_experiment_folder([folder_name])
continual_training_setup_executor(→ None)
exponential\_function(\rightarrow torch.FloatTensor)
load_numpy(→ numpy.ndarray)
                                                    # @TODO: CD: Renamed this function
evaluate(entity_to_idx,
                           scores,
                                      easy answers,
hard answers)
 download_file(url[, destination_folder])
download\_files\_from\_url(\rightarrow None)
download_pretrained_model(\rightarrow str)
write_csv_from_model_parallel(path)
                                                     Create
 from_pretrained_model_write_embeddings_into
None)
```

Module Contents

```
dicee.static_funcs.create_recipriocal_triples(x)
     Add inverse triples into dask dataframe :param x: :return:
dicee.static_funcs.get_er_vocab(data, file_path: str = None)
dicee.static_funcs.get_re_vocab(data, file_path: str = None)
dicee.static_funcs.get_ee_vocab(data, file_path: str = None)
dicee.static_funcs.timeit(func)
dicee.static_funcs.save_pickle(*, data: object = None, file_path=str)
dicee.static_funcs.load_pickle(file_path=str)
dicee.static_funcs.load_term_mapping(file_path=str)
dicee.static_funcs.select_model(args: dict, is_continual_training: bool = None,
           storage\_path: str = None)
dicee.static_funcs.load_model(path_of_experiment_folder: str, model_name='model.pt', verbose=0)
            → Tuple[object, Tuple[dict, dict]]
     Load weights and initialize pytorch module from namespace arguments
dicee.static_funcs.load_model_ensemble(path_of_experiment_folder: str)
            → Tuple[dicee.models.base_model.BaseKGE, Tuple[pandas.DataFrame, pandas.DataFrame]]
     Construct Ensemble Of weights and initialize pytorch module from namespace arguments
```

- (1) Detect models under given path
- (2) Accumulate parameters of detected models
- (3) Normalize parameters
- (4) Insert (3) into model.

```
dicee.static_funcs.save_numpy_ndarray(*, data: numpy.ndarray, file_path: str)
```

Detect most efficient data type for a given triples :param train_set: :param num: :return:

```
dicee.static_funcs.save_checkpoint_model (model, path: str) \rightarrow None
```

Store Pytorch model into disk

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

Add randomly constructed triples :param train_set: :param add_noise_rate: :return:

```
dicee.static_funcs.read_or_load_kg(args, cls)
```

```
dicee.static_funcs.intialize_model(args: dict, verbose=0) \rightarrow Tuple[object, str]
```

```
dicee.static_funcs.load_json(p: str) \rightarrow dict
```

dicee.static_funcs.save_embeddings (embeddings: numpy.ndarray, indexes, path: $str) \rightarrow None$ Save it as CSV if memory allows. :param embeddings: :param indexes: :param path: :return:

```
dicee.static_funcs.random_prediction(pre_trained_kge)
```

dicee.static_funcs.deploy_tail_entity_prediction($pre_trained_kge$, $str_subject$, $str_predicate$, top_k)

 $\label{local_discrete_discrete} \verb|discrete_static_funcs.deploy_head_entity_prediction|| (pre_trained_kge, str_object, str_predicate, top_k)|$

dicee.static_funcs.deploy_relation_prediction(pre_trained_kge, str_subject, str_object, top_k)

dicee.static_funcs.vocab_to_parquet(vocab_to_idx, name, path_for_serialization, print_into)

dicee.static_funcs.create_experiment_folder(folder_name='Experiments')

dicee.static_funcs.continual_training_setup_executor(executor) \rightarrow None

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

dicee.static_funcs.load_numpy(path) \rightarrow numpy.ndarray

dicee.static_funcs.evaluate(entity_to_idx, scores, easy_answers, hard_answers)

#@TODO: CD: Renamed this function Evaluate multi hop query answering on different query types dicee.static_funcs.download_file (url, destination_folder='.')

```
dicee.static_funcs.download_files_from_url(base\_url: str, destination\_folder='.') 	o None
```

Parameters

- base_url (e.g. "https://files.dice-research.org/projects/DiceEmbeddings/ KINSHIP-Keci-dim128-epoch256-KvsAll")
- destination_folder(e.g. "KINSHIP-Keci-dim128-epoch256-KvsA11")

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

dicee.static_funcs.write_csv_from_model_parallel(path: str)

Create

 $\texttt{dicee.static_funcs.from_pretrained_model_write_embeddings_into_csv} \ (\textit{path: str}) \rightarrow None$

dicee.static_funcs_training

Functions

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

Module Contents

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

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

dicee.static_funcs_training.efficient_zero_grad(model)

dicee.static_preprocess_funcs

Attributes

enable_log

Functions

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

Module Contents

- (1) Extract domains and ranges of relations
- (2) Store a mapping from relations to entities that are outside of the domain and range. Create constraints entities based on the range of relations :param triples: :return:

```
dicee.static_preprocess_funcs.get_er_vocab(data)
dicee.static_preprocess_funcs.get_re_vocab(data)
dicee.static_preprocess_funcs.get_ee_vocab(data)
dicee.static_preprocess_funcs.mapping_from_first_two_cols_to_third(train_set_idx)
```

dicee.trainer

Submodules

dicee.trainer.dice_trainer

Classes

DICE_Trainer implement

Functions

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

Module Contents

```
dicee.trainer.dice_trainer.load_term_mapping(file_path=str)
dicee.trainer.dice_trainer.initialize_trainer(args, callbacks)
            \rightarrow dicee.trainer.torch_trainer.Torch_trainer.Torch_trainer.ddp.arallelism.TensorParallel \(\) dicee.trainer.torch_trainer_ddp.
dicee.trainer.dice_trainer.get_callbacks(args)
class dicee.trainer.dice_trainer.DICE_Trainer(args, is_continual_training: bool, storage_path,
            evaluator=None)
     DICE Trainer implement
          1- Pytorch Lightning trainer (https://pytorch-lightning.readthedocs.io/en/stable/common/trainer.html)
          2- Multi-GPU Trainer(https://pytorch.org/docs/stable/generated/torch.nn.parallel.DistributedDataParallel.
          html) 3- CPU Trainer
          args
          is_continual_training:bool
          storage_path:str
          evaluator:
          report:dict
     report
     args
     trainer = None
     is_continual_training
     storage_path
     evaluator = None
     form_of_labelling = None
     continual_start (knowledge_graph)
           (1) Initialize training.
           (2) Load model
          (3) Load trainer (3) Fit model
```

Parameter

returns

- model
- form_of_labelling (str)

initialize_trainer(callbacks: List)

→ lightning.Trainer | dicee.trainer.model_parallelism.TensorParallel | dicee.trainer.torch_trainer.TorchTrainer | dicee.trainer.TorchTrainer | dicee.trainer.torch_trainer.TorchTrainer | dicee.trainer.torch_trainer.TorchTrainer | dicee.trainer.torch_trai

```
initialize_or_load_model()
```

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

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

start (knowledge_graph: dicee.knowledge_graph.KG | numpy.memmap)

→ Tuple[dicee.models.base model.BaseKGE, str]

Start the training

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

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

 $k_fold_cross_validation(dataset) \rightarrow Tuple[dicee.models.base_model.BaseKGE, str]$

Perform K-fold Cross-Validation

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

Parameters

- self
- dataset

Returns

model

dicee.trainer.model_parallelism

Classes

TensorParallel Abstract class for Knowledge graph embedding models

Functions

```
extract_input_outputs(z[, device])

find_good_batch_size(train_loader,

tp_ensemble_model)

forward_backward_update_loss(→ float)
```

Module Contents

dicee.trainer.torch_trainer

Classes

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

Module Contents

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

Bases: dicee.abstracts.AbstractTrainer

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

Arguments

callbacks: list of Abstract callback instances

loss_function = None
```

```
optimizer = None
model = None
train_dataloaders = None
training_step = None
process
fit (*args, train\_dataloaders, **kwargs) \rightarrow None
           Training starts
           Arguments
      kwargs:Tuple
           empty dictionary
           Return type
                batch loss (float)
\textbf{forward\_backward\_update} \ (x\_\textit{batch: torch.Tensor}, \ y\_\textit{batch: torch.Tensor}) \ \to \ \text{torch.Tensor}) \ \to \ \text{torch.Tensor})
           Compute forward, loss, backward, and parameter update
           Arguments
           Return type
                batch loss (float)
\textbf{extract\_input\_outputs\_set\_device} \ (\textit{batch: list}) \ \rightarrow \textbf{Tuple}
           Construct inputs and outputs from a batch of inputs with outputs From a batch of inputs and put
           Arguments
           Return type
                (tuple) mini-batch on select device
```

dicee.trainer.torch_trainer_ddp

Classes

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

Functions

 $make_iterable_verbose(\rightarrow Iterable)$

Module Contents

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

```
extract_input_outputs (z: list)
train()
Training loop for DDP
```

Classes

DICE_Trainer

DICE_Trainer implement

Package Contents

class dicee.trainer.DICE_Trainer(args, is_continual_training: bool, storage_path, evaluator=None)

DICE_Trainer implement

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

args

is_continual_training:bool

storage_path:str

evaluator:

report:dict

report

args

trainer = None

is_continual_training

storage_path

evaluator = None

form_of_labelling = None

continual_start (knowledge_graph)

- (1) Initialize training.
- (2) Load model
- (3) Load trainer (3) Fit model

Parameter

returns

- model
- form_of_labelling (str)

initialize_trainer(callbacks: List)

→ lightning.Trainer | dicee.trainer.model_parallelism.TensorParallel | dicee.trainer.torch_trainer.TorchTrainer | dicee.trainer.TorchTrainer | dicee.trainer.torch_trainer.TorchTrainer | dicee.trainer.torch_trainer.TorchTrainer | dicee.trainer.torch_trai

initialize_or_load_model()

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

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

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

→ Tuple[dicee.models.base_model.BaseKGE, str]

Start the training

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

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

 $k_fold_cross_validation(dataset) \rightarrow Tuple[dicee.models.base_model.BaseKGE, str]$

Perform K-fold Cross-Validation

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

Parameters

- self
- dataset

Returns

model

14.2 Attributes

__version__

14.3 Classes

Pyke	A Physical Embedding Model for Knowledge Graphs
DistMult	Embedding Entities and Relations for Learning and Infer-
	ence in Knowledge Bases
CKeci	Without learning dimension scaling
Keci	Base class for all neural network modules.
TransE	Translating Embeddings for Modeling
DeCaL	Base class for all neural network modules.

continues on next page

Table 3 - continued from previous page

	continued from previous page
DualE	Dual Quaternion Knowledge Graph Embeddings (https://ojs.aaai.org/index.php/AAAI/article/download/16850/16657)
ComplEx	Base class for all neural network modules.
AConEx	Additive Convolutional ComplEx Knowledge Graph Em-
	beddings
AConv0	Additive Convolutional Octonion Knowledge Graph Embeddings
AConvQ	Additive Convolutional Quaternion Knowledge Graph Embeddings
ConvQ	Convolutional Quaternion Knowledge Graph Embeddings
ConvO	Base class for all neural network modules.
ConEx	Convolutional ComplEx Knowledge Graph Embeddings
QMult	Base class for all neural network modules.
OMult	Base class for all neural network modules.
Shallom	A shallow neural model for relation prediction (https:
SHATTOM	//arxiv.org/abs/2101.09090)
LFMult	Embedding with polynomial functions. We represent all
	entities and relations in the polynomial space as:
PykeenKGE	A class for using knowledge graph embedding models im-
	plemented in Pykeen
BytE	Base class for all neural network modules.
BaseKGE	Base class for all neural network modules.
EnsembleKGE	
DICE_Trainer	DICE_Trainer implement
KGE	Knowledge Graph Embedding Class for interactive usage
	of pre-trained models
Execute	A class for Training, Retraining and Evaluation a model.
BPE_NegativeSamplingDataset	An abstract class representing a Dataset.
MultiLabelDataset	An abstract class representing a Dataset.
MultiClassClassificationDataset	Dataset for the 1vsALL training strategy
OnevsAllDataset	Dataset for the 1vsALL training strategy
KvsAll	Creates a dataset for KvsAll training by inheriting from torch.utils.data.Dataset.
AllvsAll	Creates a dataset for AllvsAll training by inheriting from torch.utils.data.Dataset.
OnevsSample	A custom PyTorch Dataset class for knowledge graph embeddings, which includes
KvsSampleDataset	KvsSample a Dataset:
NegSampleDataset	An abstract class representing a Dataset.
TriplePredictionDataset	Triple Dataset
CVDataModule	Create a Dataset for cross validation
QueryGenerator	2

14.4 Functions

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

Table 4 - continued from previous page

```
get_er_vocab(data[, file_path])
get_re_vocab(data[, file_path])
get_ee_vocab(data[, file_path])
timeit(func)
save_pickle(*[, data, file_path])
load_pickle([file_path])
load_term_mapping([file_path])
                         is_continual_training,
select_model(args[,
                                                 stor-
age_path])
load_model(→ Tuple[object, Tuple[dict, dict]])
                                                        Load weights and initialize pytorch module from names-
                                                        pace arguments
                                                        Construct Ensemble Of weights and initialize pytorch
load_model_ensemble(...)
                                                        module from namespace arguments
save_numpy_ndarray(*, data, file_path)
numpy_data_type_changer(→ numpy.ndarray)
                                                        Detect most efficient data type for a given triples
save\_checkpoint\_model(\rightarrow None)
                                                        Store Pytorch model into disk
store(\rightarrow None)
add\_noisy\_triples(\rightarrow pandas.DataFrame)
                                                        Add randomly constructed triples
read_or_load_kg(args, cls)
intialize\_model(\rightarrow Tuple[object, str])
load_json(\rightarrow dict)
                                                        Save it as CSV if memory allows.
save\_embeddings(\rightarrow None)
random_prediction(pre_trained_kge)
deploy_triple_prediction(pre_trained_kge,
str subject, ...)
deploy_tail_entity_prediction(pre_trained_kge,
deploy_head_entity_prediction(pre_trained_kge,
deploy_relation_prediction(pre_trained_kge,
vocab_to_parquet(vocab_to_idx, name, ...)
create_experiment_folder([folder_name])
continual\_training\_setup\_executor(\rightarrow None)
exponential_function(\rightarrow torch.FloatTensor)
```

continues on next page

Table 4 - continued from previous page

```
load_numpy(\rightarrow numpy.ndarray)
                                                      # @TODO: CD: Renamed this function
 evaluate(entity_to_idx,
                            scores,
                                       easy_answers,
 hard answers)
 download_file(url[, destination_folder])
 download\_files\_from\_url(\rightarrow None)
 download\_pretrained\_model(\rightarrow str)
                                                      Create
write_csv_from_model_parallel(path)
 from_pretrained_model_write_embeddings_int
 None)
 mapping_from_first_two_cols_to_third(train_se
 timeit(func)
 load_term_mapping([file_path])
                                                      Reload the files from disk to construct the Pytorch dataset
 reload_dataset(path, form_of_labelling, ...)
 construct_dataset(→ torch.utils.data.Dataset)
14.5 Package Contents
class dicee.Pyke(args)
     Bases: dicee.models.base_model.BaseKGE
     A Physical Embedding Model for Knowledge Graphs
     name = 'Pyke'
     dist_func
     margin = 1.0
     forward_triples (x: torch.LongTensor)
              Parameters
class dicee.DistMult(args)
     Bases: dicee.models.base_model.BaseKGE
     Embedding Entities and Relations for Learning and Inference in Knowledge Bases https://arxiv.org/abs/1412.6575
     name = 'DistMult'
     \verb+k_vs_all_score+ (emb_h: torch.FloatTensor, emb_r: torch.FloatTensor, emb_E: torch.FloatTensor)
              Parameters
                   • emb h
                   • emb_r
                   • emb_E
```

```
forward_k_vs_all(x: torch.LongTensor)
forward_k_vs_sample(x: torch.LongTensor, target_entity_idx: torch.LongTensor)
score(h, r, t)

class dicee.CKeci(args)
Bases: Keci
Without learning dimension scaling
name = 'CKeci'
requires_grad_for_interactions = False

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

Base class for all neural network modules.

Your models should also subclass this class.

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

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

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

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

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

1 Note

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

Variables

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

```
name = 'Keci'
p
q
```

```
requires_grad_for_interactions = True
compute\_sigma\_pp(hp, rp)
          Compute sigma_{pp} = sum_{i=1}^{p-1} sum_{k=i+1}^p (h_i r_k - h_k r_i) e_i e_k
          sigma_{pp} captures the interactions between along p bases For instance, let p e_1, e_2, e_3, we compute
          interactions between e 1 e 2, e 1 e 3, and e 2 e 3 This can be implemented with a nested two for loops
                  results = [] for i in range(p - 1):
                          for k in range(i + 1, p):
                               results.append(hp[:, :, i] * rp[:, :, k] - hp[:, :, k] * rp[:, :, i])
                  sigma_pp = torch.stack(results, dim=2) assert sigma_pp.shape == (b, r, int((p * (p - 1)) / 2))
          Yet, this computation would be quite inefficient. Instead, we compute interactions along all p, e.g., e1e1,
          e1e2, e1e3,
                  e2e1, e2e2, e2e3, e3e1, e3e2, e3e3
          Then select the triangular matrix without diagonals: e1e2, e1e3, e2e3.
compute\_sigma\_qq(hq, rq)
          Compute sigma_{qq} = sum_{j=1}^{p+q-1} sum_{k=j+1}^{p+q} (h_j r_k - h_k r_j) e_j e_k sigma_{q}
          captures the interactions between along q bases For instance, let q e 1, e 2, e 3, we compute interactions
          between e 1 e 2, e 1 e 3, and e 2 e 3 This can be implemented with a nested two for loops
                  results = [] for j in range(q - 1):
                          for k in range(j + 1, q):
                               results.append(hq[:,:,j]*rq[:,:,k]-hq[:,:,k]*rq[:,:,j])\\
                  sigma_qq = torch.stack(results, dim=2) assert sigma_qq.shape == (b, r, int((q * (q - 1)) / 2))
          Yet, this computation would be quite inefficient. Instead, we compute interactions along all p, e.g., e1e1,
          e1e2, e1e3,
                  e2e1, e2e2, e2e3, e3e1, e3e2, e3e3
          Then select the triangular matrix without diagonals: e1e2, e1e3, e2e3.
compute_sigma_pq(*, hp, hq, rp, rq)
          sum_{i=1}^{p} sum_{j=p+1}^{p+q} (h_i r_j - h_j r_i) e_i e_j
          results = [] sigma_pq = torch.zeros(b, r, p, q) for i in range(p):
                  for j in range(q):
                          sigma_pq[:, :, i, j] = hp[:, :, i] * rq[:, :, j] - hq[:, :, j] * rp[:, :, i]
          print(sigma_pq.shape)
apply_coefficients(hp, hq, rp, rq)
          Multiplying a base vector with its scalar coefficient
clifford_multiplication (h0, hp, hq, r0, rp, rq)
          Compute our CL multiplication
                  h = h_0 + sum_{i=1}^p h_i e_i + sum_{j=p+1}^p h_j e_j r = r_0 + sum_{i=1}^p r_i e_i + sum_{i=1}^p r_i e_i + sum_{i=1}^n p_i e_j r = r_0 + sum_{i=1}^n p_i e_i + sum_{i=1}^n p_i e_j r = r_0 + sum_{i=1}^n p_i r = r_0 + sum_{i=1}^n p_i e_j r = r_0 
                  sum_{j=p+1}^{p+q} r_j e_j
                  ei ^2 = +1 for i =< i =< p ej ^2 = -1 for p < j =< p+q ei ej = -eje1 for i
          eq j
                  h r = sigma \ 0 + sigma \ p + sigma \ q + sigma \ \{pp\} + sigma \ \{q\} + sigma \ \{pq\}  where
```

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

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

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

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

Parameter

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

returns

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

forward_k_vs_with_explicit(x: torch.Tensor)

k_vs_all_score (bpe_head_ent_emb, bpe_rel_ent_emb, E)

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

Kvsall training

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

forward_k_vs_with_explicit and this functions are identical Parameter — x: torch.LongTensor with (n,2) shape :rtype: torch.FloatTensor with (n, |E|) shape

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

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

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

Parameter

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

returns

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

 $forward_k_vs_sample$ (x: torch.LongTensor, target_entity_idx: torch.LongTensor) \rightarrow torch.FloatTensor

Parameter

```
x: torch.LongTensor with (n,2) shape  \begin{aligned} &\text{target\_entity\_idx: torch.LongTensor with (n, k) shape k denotes the selected number of examples.} \\ & &\textbf{rtype} \\ & & & & & & & & & & & & & & & \\ & & & & & & & & & & & & & \\ & & & & & & & & & & & & \\ & & & & & & & & & & & & \\ & & & & & & & & & & & \\ & & & & & & & & & & & \\ & & & & & & & & & & & \\ & & & & & & & & & & \\ & & & & & & & & & & \\ & & & & & & & & & & \\ & & & & & & & & & & \\ & & & & & & & & & \\ & & & & & & & & & \\ & & & & & & & & & \\ & & & & & & & & & \\ & & & & & & & & & \\ & & & & & & & & & \\ & & & & & & & & \\ & & & & & & & & \\ & & & & & & & & \\ & & & & & & & & \\ & & & & & & & \\ & & & & & & & \\ & & & & & & & \\ & & & & & & & \\ & & & & & & & \\ & & & & & & & \\ & & & & & & & \\ & & & & & & & \\ & & & & & & & \\ & & & & & & & \\ & & & & & & & \\ & & & & & & & \\ & & & & & & & \\ & & & & & & & \\ & & & & & & & \\ & & & & & & \\ & & & & & & \\ & & & & & & \\ & & & & & & \\ & & & & & & \\ & & & & & & \\ & & & & & \\ & & & & & & \\ & & & & & & \\ & & & & & & \\ & & & & & & \\ & & & & & & \\ & & & & & \\ & & & & & \\ & & & & & \\ & & & & & \\ & & & & & \\ & & & & & \\ & & & & & \\ & & & & \\ & & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & \\ & & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & &
```

Parameter

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

rtype

torch.FloatTensor with (n) shape

```
class dicee.TransE(args)
```

Bases: dicee.models.base model.BaseKGE

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

```
name = 'TransE'

margin = 4

score (head_ent_emb, rel_ent_emb, tail_ent_emb)

forward_k_vs_all(x: torch.Tensor) → torch.FloatTensor

class dicee.DeCaL(args)

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

Base class for all neural network modules.

Your models should also subclass this class.

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

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

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

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

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

1 Note

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

Variables

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

name = 'DeCaL'

entity_embeddings

relation_embeddings

р

q

r

re

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

Parameter

x: torch.LongTensor with (n,) shape

rtype

torch.FloatTensor with (n) shape

 $cl_pqr(a: torch.tensor) \rightarrow torch.tensor$

Input: tensor(batch_size, emb_dim) \longrightarrow output: tensor with 1+p+q+r components with size (batch_size, emb_dim/(1+p+q+r)) each.

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

compute_sigmas_single (list_h_emb, list_r_emb, list_t_emb)

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

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

and return:

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

compute_sigmas_multivect(list_h_emb, list_r_emb)

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

For same bases vectors interaction we have

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

For different base vector interactions, we have

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

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

Kvsall training

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

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

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

Multiplying a base vector with its scalar coefficient

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

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

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

Parameter

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

returns

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

 $compute_sigma_pp(hp, rp)$

Compute .. math:

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

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

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

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

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

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

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

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

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

 $compute_sigma_qq(hq, rq)$

Compute

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

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

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

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

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

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

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

 $compute_sigma_rr(hk, rk)$

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

compute_sigma_pq(*, hp, hq, rp, rq)

Compute

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

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

for j in range(q):

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

print(sigma_pq.shape)

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

Compute

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

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

for j in range(q):

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

print(sigma_pq.shape)

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

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

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

```
for j in range(q):
                                                                       sigma_pq[:, :, i, j] = hp[:, :, i] * rq[:, :, j] - hq[:, :, j] * rp[:, :, i]
                                        print(sigma_pq.shape)
class dicee.DualE(args)
                     Bases: dicee.models.base_model.BaseKGE
                     Dual Quaternion Knowledge Graph Embeddings (https://ojs.aaai.org/index.php/AAAI/article/download/16850/
                     16657)
                     name = 'DualE'
                     entity_embeddings
                     relation_embeddings
                     num_ent = None
                     {\tt kvsall\_score}\ (e\_1\_h,\, e\_2\_h,\, e\_3\_h,\, e\_4\_h,\, e\_5\_h,\, e\_6\_h,\, e\_7\_h,\, e\_8\_h,\, e\_1\_t,\, e\_2\_t,\, e\_3\_t,\, e\_4\_t,\, e
                                                                    e\_5\_t, e\_6\_t, e\_7\_t, e\_8\_t, r\_1, r\_2, r\_3, r\_4, r\_5, r\_6, r\_7, r\_8) \rightarrow \text{torch.tensor}
                                         KvsAll scoring function
                                        Input
                                        x: torch.LongTensor with (n, ) shape
                                         Output
                                         torch.FloatTensor with (n) shape
                     \textbf{forward\_triples} \ (\textit{idx\_triple: torch.tensor}) \ \rightarrow \textbf{torch.tensor}) \ \rightarrow \textbf{torch.tensor}
                                         Negative Sampling forward pass:
                                        Input
                                        x: torch.LongTensor with (n, ) shape
                                         Output
                                         torch.FloatTensor with (n) shape
                     forward_k_vs_all(x)
                                        KvsAll forward pass
                                         Input
                                         x: torch.LongTensor with (n, ) shape
                                         Output
                                         torch.FloatTensor with (n) shape
                     T (x: torch.tensor) \rightarrow torch.tensor
                                         Transpose function
                                         Input: Tensor with shape (nxm) Output: Tensor with shape (mxn)
```

```
class dicee.ComplEx(args)
```

Bases: dicee.models.base_model.BaseKGE

Base class for all neural network modules.

Your models should also subclass this class.

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

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

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

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

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

1 Note

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

Variables

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

Parameters

- emb_h
- emb_r
- emb_E

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

forward_k_vs_sample(x: torch.LongTensor, target_entity_idx: torch.LongTensor)

```
class dicee.AConEx(args)
```

 $Bases: \ \textit{dicee.models.base_model.BaseKGE}$

Additive Convolutional ComplEx Knowledge Graph Embeddings

```
name = 'AConEx'
     conv2d
     fc_num_input
     fc1
     norm_fc1
     bn_conv2d
     feature_map_dropout
     {\tt residual\_convolution}~(C\_1: Tuple[torch.Tensor, torch.Tensor],
                  C_2: Tuple[torch.Tensor, torch.Tensor]) \rightarrow torch.FloatTensor
           Compute residual score of two complex-valued embeddings. :param C_1: a tuple of two pytorch tensors
           that corresponds complex-valued embeddings :param C_2: a tuple of two pytorch tensors that corresponds
           complex-valued embeddings :return:
     forward_k_vs_all(x: torch.Tensor) \rightarrow torch.FloatTensor
     forward\_triples(x: torch.Tensor) \rightarrow torch.FloatTensor
               Parameters
     forward_k_vs_sample (x: torch.Tensor, target_entity_idx: torch.Tensor)
class dicee.AConvO(args: dict)
     Bases: dicee.models.base_model.BaseKGE
     Additive Convolutional Octonion Knowledge Graph Embeddings
     name = 'AConvO'
     conv2d
     fc_num_input
     fc1
     bn_conv2d
     norm_fc1
     feature_map_dropout
     static octonion_normalizer(emb_rel_e0, emb_rel_e1, emb_rel_e2, emb_rel_e3, emb_rel_e4,
                  emb_rel_e5, emb_rel_e6, emb_rel_e7)
     {\tt residual\_convolution}\,(O\_1,\,O\_2)
     forward\_triples(x: torch.Tensor) \rightarrow torch.Tensor
               Parameters
                   x
```

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

forward_k_vs_all (x: torch.Tensor)

```
feature_map_dropout
```

```
residual_convolution (Q_1, Q_2)
```

 $forward_triples (indexed_triple: torch.Tensor) \rightarrow torch.Tensor$

Parameters

x

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

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

class dicee.ConvO(args: dict)

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

Base class for all neural network modules.

Your models should also subclass this class.

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

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

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

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

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

1 Note

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

Variables

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

```
name = 'ConvO'
conv2d
fc_num_input
fc1
```

```
bn_conv2d
     norm_fc1
     feature_map_dropout
     static octonion_normalizer(emb_rel_e0, emb_rel_e1, emb_rel_e2, emb_rel_e3, emb_rel_e4,
                  emb_rel_e5, emb_rel_e6, emb_rel_e7)
     residual\_convolution(O\_1, O\_2)
     forward\_triples(x: torch.Tensor) \rightarrow torch.Tensor
               Parameters
     forward k vs all(x: torch.Tensor)
           Given a head entity and a relation (h,r), we compute scores for all entities. [score(h,r,x)|x in Entities] =>
           [0.0,0.1,...,0.8], shape=> (1, |Entities|) Given a batch of head entities and relations => shape (size of batch,|
           Entities()
class dicee.ConEx(args)
     Bases: dicee.models.base model.BaseKGE
     Convolutional ComplEx Knowledge Graph Embeddings
     name = 'ConEx'
     conv2d
     fc_num_input
     fc1
     norm_fc1
     bn_conv2d
     feature_map_dropout
     residual_convolution(C_1: Tuple[torch.Tensor, torch.Tensor],
                  C_2: Tuple[torch.Tensor, torch.Tensor]) \rightarrow torch.FloatTensor
           Compute residual score of two complex-valued embeddings. :param C_1: a tuple of two pytorch tensors
           that corresponds complex-valued embeddings :param C_2: a tuple of two pytorch tensors that corresponds
           complex-valued embeddings :return:
     forward_k_vs_all(x: torch.Tensor) \rightarrow torch.FloatTensor
     forward\_triples(x: torch.Tensor) \rightarrow torch.FloatTensor
               Parameters
     forward_k_vs_sample (x: torch.Tensor, target_entity_idx: torch.Tensor)
class dicee.QMult(args)
     Bases: dicee.models.base_model.BaseKGE
     Base class for all neural network modules.
     Your models should also subclass this class.
```

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

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

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

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

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



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

Variables

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

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

Parameters

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

Returns

Triple scores.

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

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

Absolute value of a quaternion

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

L2 norm of quaternion vector:

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

Parameters

 \mathbf{x} – The vector.

Returns

The normalized vector.

 $k_vs_all_score$ (bpe_head_ent_emb, bpe_rel_ent_emb, E)

Parameters

- bpe_head_ent_emb
- bpe_rel_ent_emb
- E

forward_k_vs_all (X)

Parameters

x

 $forward_k_vs_sample(x, target_entity_idx)$

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

```
class dicee.OMult(args)
```

Bases: dicee.models.base_model.BaseKGE

Base class for all neural network modules.

Your models should also subclass this class.

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

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

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

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

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

1 Note

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

Variables

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

```
name = 'OMult'
     static octonion_normalizer(emb_rel_e0, emb_rel_e1, emb_rel_e2, emb_rel_e3, emb_rel_e4,
                  emb rel e5, emb rel e6, emb rel e7)
     \verb+score+ (head\_ent\_emb: torch.FloatTensor, rel\_ent\_emb: torch.FloatTensor,
                  tail_ent_emb: torch.FloatTensor)
     k_vs_all_score (bpe_head_ent_emb, bpe_rel_ent_emb, E)
     forward_k_vs_all(X)
           Completed. Given a head entity and a relation (h,r), we compute scores for all possible triples, i.e.,
           [score(h,r,x)|x \text{ in Entities}] => [0.0,0.1,...,0.8], shape=> (1, |Entities|) Given a batch of head entities and
           relations => shape (size of batch, | Entities|)
class dicee.Shallom(args)
     Bases: dicee.models.base_model.BaseKGE
     A shallow neural model for relation prediction (https://arxiv.org/abs/2101.09090)
     name = 'Shallom'
     shallom
     get_embeddings() → Tuple[numpy.ndarray, None]
     forward_k_vs_all (x) \rightarrow \text{torch.FloatTensor}
     forward_triples (x) \rightarrow \text{torch.FloatTensor}
               Parameters
                   x
               Returns
class dicee.LFMult(args)
     Bases: dicee.models.base_model.BaseKGE
     Embedding with polynomial functions. We represent all entities and relations in the polynomial space as: f(x) =
     sum_{i=0}^{d-1} a_k x^{i\%d} and use the three differents scoring function as in the paper to evaluate the score.
     We also consider combining with Neural Networks.
     name = 'LFMult'
     entity_embeddings
     relation_embeddings
     degree
     x values
     forward_triples (idx_triple)
               Parameters
                   x
     construct_multi_coeff(x)
```

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

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

linear(x, w, b)

$scalar_batch_NN(a, b, c)$

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

tri_score (coeff_h, coeff_r, coeff_t)

this part implement the trilinear scoring techniques:

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

$\mathtt{vtp_score}(h, r, t)$

this part implement the vector triple product scoring techniques:

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

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

$\mathtt{comp_func}\,(h,\,r,\,t)$

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

polynomial(coeff, x, degree)

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

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

pop (coeff, x, degree)

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

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

class dicee.PykeenKGE(args: dict)

Bases: dicee.models.base_model.BaseKGE

A class for using knowledge graph embedding models implemented in Pykeen

Notes: Pykeen_DistMult: C Pykeen_ComplEx: Pykeen_QuatE: Pykeen_MuRE: Pykeen_CP: Pykeen_HolE: Pykeen_HolE: Pykeen_TransD: Pykeen_TransE: Pykeen_TransF: Pykeen_TransH: Pykeen_TransR:

model_kwargs

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

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

Base class for all neural network modules.

Your models should also subclass this class.

Modules can also contain other Modules, allowing them to be nested in a tree structure. You can assign the submodules as regular attributes:

```
import torch.nn as nn
import torch.nn.functional as F
class Model(nn.Module):
    def __init__(self) -> None:
        super().__init__()
```

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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 also have their parameters converted when you call to(), etc.



1 Note

As per the example above, an __init__() call to the parent class must be made before assignment on the child.

Variables

training $(b \circ o 1)$ – Boolean represents whether this module is in training or evaluation mode.

```
name = 'BytE'
config
temperature = 0.5
topk = 2
transformer
lm_head
loss_function(yhat_batch, y_batch)
```

Parameters

- yhat_batch
- y_batch

forward(x: torch.LongTensor)

Parameters

```
\mathbf{x} (B by T tensor)
```

generate (idx, max_new_tokens, temperature=1.0, top_k=None)

Take a conditioning sequence of indices idx (LongTensor of shape (b,t)) and complete the sequence max_new_tokens times, feeding the predictions back into the model each time. Most likely you'll want to make sure to be in model.eval() mode of operation for this.

```
training_step(batch, batch_idx=None)
```

Here you compute and return the training loss and some additional metrics for e.g. the progress bar or logger.

Parameters

- batch The output of your data iterable, normally a DataLoader.
- batch_idx The index of this batch.

dataloader_idx – The index of the dataloader that produced this batch. (only if multiple dataloaders used)

Returns

- Tensor The loss tensor
- dict A dictionary which can include any keys, but must include the key 'loss' in the case of automatic optimization.
- None In automatic optimization, this will skip to the next batch (but is not supported for multi-GPU, TPU, or DeepSpeed). For manual optimization, this has no special meaning, as returning the loss is not required.

In this step you'd normally do the forward pass and calculate the loss for a batch. You can also do fancier things like multiple forward passes or something model specific.

Example:

```
def training_step(self, batch, batch_idx):
    x, y, z = batch
    out = self.encoder(x)
    loss = self.loss(out, x)
    return loss
```

To use multiple optimizers, you can switch to 'manual optimization' and control their stepping:

```
def __init__ (self):
    super().__init__()
    self.automatic_optimization = False

# Multiple optimizers (e.g.: GANs)
def training_step(self, batch, batch_idx):
    opt1, opt2 = self.optimizers()

# do training_step with encoder
    ...
    opt1.step()
    # do training_step with decoder
    ...
    opt2.step()
```

1 Note

When accumulate_grad_batches > 1, the loss returned here will be automatically normalized by accumulate_grad_batches internally.

class dicee.BaseKGE(args: dict)

Bases: BaseKGELightning

Base class for all neural network modules.

Your models should also subclass this class.

Modules can also contain other Modules, allowing them to be nested in a tree structure. You can assign the sub-modules as regular attributes:

```
import torch.nn as nn
import torch.nn.functional as F

class Model(nn.Module):
    def __init__(self) -> None:
        super().__init__()
        self.conv1 = nn.Conv2d(1, 20, 5)
        self.conv2 = nn.Conv2d(20, 20, 5)

    def forward(self, x):
        x = F.relu(self.conv1(x))
        return F.relu(self.conv2(x))
```

Submodules assigned in this way will be registered, and will also have their parameters converted when you call to(), etc.

1 Note

As per the example above, an $__{init}$ __() call to the parent class must be made before assignment on the child.

Variables

training (bool) – Boolean represents whether this module is in training or evaluation mode.

args

```
embedding_dim = None
num_entities = None
num_relations = None
num_tokens = None
learning_rate = None
learning_rate = None
apply_unit_norm = None
input_dropout_rate = None
hidden_dropout_rate = None
optimizer_name = None
feature_map_dropout_rate = None
kernel_size = None
num_of_output_channels = None
weight_decay = None
loss
selected_optimizer = None
```

```
normalizer_class = None
normalize_head_entity_embeddings
normalize_relation_embeddings
normalize_tail_entity_embeddings
hidden_normalizer
param_init
input_dp_ent_real
input_dp_rel_real
hidden_dropout
loss_history = []
byte_pair_encoding
max_length_subword_tokens
block_size
forward_byte_pair_encoded_k_vs_all (x: torch.LongTensor)
        Parameters
            x (B x 2 x T)
forward_byte_pair_encoded_triple (x: Tuple[torch.LongTensor, torch.LongTensor])
    byte pair encoded neural link predictors
        Parameters
init_params_with_sanity_checking()
forward(x: torch.LongTensor | Tuple[torch.LongTensor, torch.LongTensor],
           y_idx: torch.LongTensor = None)
        Parameters
            • x
            • y_idx
            • ordered_bpe_entities
forward\_triples(x: torch.LongTensor) \rightarrow torch.Tensor
        Parameters
forward_k_vs_all(*args, **kwargs)
forward_k_vs_sample(*args, **kwargs)
get_triple_representation(idx_hrt)
{\tt get\_head\_relation\_representation}\ (indexed\_triple)
```

```
get_sentence_representation(x: torch.LongTensor)
               Parameters
                   • (b (x shape)
                   • 3
                   • t)
     get_bpe_head_and_relation_representation(x: torch.LongTensor)
                  → Tuple[torch.FloatTensor, torch.FloatTensor]
               Parameters
                   x (B x 2 x T)
     \mathtt{get\_embeddings}() \rightarrow \mathsf{Tuple}[\mathsf{numpy}.\mathsf{ndarray}, \mathsf{numpy}.\mathsf{ndarray}]
class dicee.EnsembleKGE (seed_model=None, pretrained_models: List = None)
     name
     train_mode = True
     named_children()
     property example_input_array
     parameters()
     modules()
     __iter__()
     __len__()
     eval()
     to (device)
     mem_of_model()
     __call__(x_batch)
     step()
     get_embeddings()
     __str__()
dicee.create_recipriocal_triples(x)
     Add inverse triples into dask dataframe :param x: :return:
dicee.get_er_vocab(data, file_path: str = None)
dicee.get_re_vocab(data, file_path: str = None)
dicee.get_ee_vocab (data, file_path: str = None)
dicee.timeit(func)
dicee.save_pickle(*, data: object = None, file_path=str)
```

```
dicee.load_pickle(file_path=str)
dicee.load_term_mapping(file_path=str)
dicee.select_model(args: dict, is_continual_training: bool = None, storage_path: str = None)
dicee.load_model(path_of_experiment_folder: str, model_name='model.pt', verbose=0)
             → Tuple[object, Tuple[dict, dict]]
     Load weights and initialize pytorch module from namespace arguments
dicee.load_model_ensemble(path_of_experiment_folder: str)
             → Tuple[dicee.models.base_model.BaseKGE, Tuple[pandas.DataFrame, pandas.DataFrame]]
     Construct Ensemble Of weights and initialize pytorch module from namespace arguments
       (1) Detect models under given path
       (2) Accumulate parameters of detected models
       (3) Normalize parameters
       (4) Insert (3) into model.
dicee.save_numpy_ndarray(*, data: numpy.ndarray, file_path: str)
dicee.numpy_data_type_changer(train\_set: numpy.ndarray, num: int) \rightarrow numpy.ndarray
     Detect most efficient data type for a given triples :param train_set: :param num: :return:
dicee.save_checkpoint_model(model, path: str) \rightarrow None
     Store Pytorch model into disk
dicee.store(trained_model, model_name: str = 'model', full_storage_path: str = None,
            save\_embeddings\_as\_csv=False) \rightarrow None
dicee.add_noisy_triples(train\_set: pandas.DataFrame, add\_noise\_rate: float) \rightarrow pandas.DataFrame
     Add randomly constructed triples :param train_set: :param add_noise_rate: :return:
dicee.read_or_load_kg(args, cls)
dicee.intialize_model(args: dict, verbose=0) \rightarrow Tuple[object, str]
dicee.load_json(p: str) \rightarrow dict
dicee.save_embeddings(embeddings: numpy.ndarray, indexes, path: str) \rightarrow None
     Save it as CSV if memory allows. :param embeddings: :param indexes: :param path: :return:
dicee.random_prediction(pre_trained_kge)
dicee.deploy_triple_prediction(pre_trained_kge, str_subject, str_predicate, str_object)
dicee.deploy_tail_entity_prediction(pre_trained_kge, str_subject, str_predicate, top_k)
dicee.deploy_head_entity_prediction(pre_trained_kge, str_object, str_predicate, top_k)
dicee.deploy_relation_prediction(pre_trained_kge, str_subject, str_object, top_k)
dicee.vocab_to_parquet(vocab_to_idx, name, path_for_serialization, print_into)
dicee.create_experiment_folder(folder_name='Experiments')
dicee.continual_training_setup_executor(executor) \rightarrow None
```

```
dicee.exponential_function (x: numpy.ndarray, lam: float, ascending_order=True) \rightarrow torch.FloatTensor
dicee.load_numpy(path) \rightarrow numpy.ndarray
dicee.evaluate(entity_to_idx, scores, easy_answers, hard_answers)
     # @TODO: CD: Renamed this function Evaluate multi hop query answering on different query types
dicee.download_file (url, destination_folder='.')
dicee.download_files_from_url(base\_url: str, destination\_folder='.') \rightarrow None
           Parameters
                 base_url
                                                   "https://files.dice-research.org/projects/DiceEmbeddings/
                   KINSHIP-Keci-dim128-epoch256-KvsAll")
                 • destination_folder(e.g. "KINSHIP-Keci-dim128-epoch256-KvsAll")
dicee.download_pretrained_model(url: str) \rightarrow str
dicee.write_csv_from_model_parallel(path: str)
     Create
\texttt{dicee.from\_pretrained\_model\_write\_embeddings\_into\_csv}(\textit{path: str}) \rightarrow \texttt{None}
class dicee.DICE_Trainer(args, is_continual_training: bool, storage_path, evaluator=None)
     DICE Trainer implement
           1- Pytorch Lightning trainer (https://pytorch-lightning.readthedocs.io/en/stable/common/trainer.html)
           2- Multi-GPU Trainer(https://pytorch.org/docs/stable/generated/torch.nn.parallel.DistributedDataParallel.
           html) 3- CPU Trainer
           args
           is_continual_training:bool
           storage_path:str
           evaluator:
           report:dict
     report
     args
     trainer = None
     is_continual_training
     storage_path
     evaluator = None
     form_of_labelling = None
     continual_start (knowledge_graph)
           (1) Initialize training.
           (2) Load model
           (3) Load trainer (3) Fit model
```

Parameter

returns

- model
- form_of_labelling (str)

initialize_trainer(callbacks: List)

→ lightning.Trainer | dicee.trainer.model_parallelism.TensorParallel | dicee.trainer.torch_trainer.TorchTrainer | dicee.trainer.TorchTrainer | dicee.trainer.torch_trainer.TorchTrainer | dicee.trainer.torch_trainer.TorchTrainer | dicee.trainer.torch_trai

```
initialize_or_load_model()
```

 $init_dataloader(dataset: torch.utils.data.Dataset) \rightarrow torch.utils.data.DataLoader$

init_dataset() → torch.utils.data.Dataset

 $\begin{tabular}{ll} \textbf{start} & (knowledge_graph: dicee.knowledge_graph.KG \mid numpy.memmap) \\ & \rightarrow \textbf{Tuple}[dicee.models.base_model.BaseKGE, str] \\ \end{tabular}$

Start the training

- (1) Initialize Trainer
- (2) Initialize or load a pretrained KGE model

in DDP setup, we need to load the memory map of already read/index KG.

 $\textbf{k_fold_cross_validation} (\textit{dataset}) \rightarrow \text{Tuple}[\textit{dicee.models.base_model.BaseKGE}, \text{str}]$

Perform K-fold Cross-Validation

- 1. Obtain K train and test splits.
- 2. For each split,
 - 2.1 initialize trainer and model 2.2. Train model with configuration provided in args. 2.3. Compute the mean reciprocal rank (MRR) score of the model on the test respective split.
- 3. Report the mean and average MRR.

Parameters

- self
- dataset

Returns

model

class dicee. KGE (path=None, url=None, construct_ensemble=False, model_name=None)

Bases: dicee.abstracts.BaseInteractiveKGE

Knowledge Graph Embedding Class for interactive usage of pre-trained models

```
__str__()
```

to (device: str) \rightarrow None

 $\begin{tabular}{ll} \tt get_transductive_entity_embeddings (\it indices: torch.LongTensor \mid List[str], as_pytorch=False, \\ as_numpy=False, as_list=True) \rightarrow {\tt torch.FloatTensor \mid numpy.ndarray \mid List[float]} \\ \end{tabular}$

 $create_vector_database$ (collection_name: str, distance: str, location: str = 'localhost', port: int = 6333)

```
generate (h=", r=")
eval_lp_performance (dataset=List[Tuple[str, str, str]], filtered=True)
predict_missing_head_entity (relation: List[str] | str, tail_entity: List[str] | str, within=None)
               \rightarrow Tuple
     Given a relation and a tail entity, return top k ranked head entity.
     argmax_{e} in E  f(e,r,t), where r in R, t in E.
     Parameter
     relation: Union[List[str], str]
     String representation of selected relations.
     tail_entity: Union[List[str], str]
     String representation of selected entities.
     k: int
     Highest ranked k entities.
     Returns: Tuple
     Highest K scores and entities
predict_missing_relations (head_entity: List[str] | str, tail_entity: List[str] | str, within=None)
     Given a head entity and a tail entity, return top k ranked relations.
     argmax_{r in R} f(h,r,t), where h, t in E.
     Parameter
     head_entity: List[str]
     String representation of selected entities.
     tail_entity: List[str]
     String representation of selected entities.
     k: int
     Highest ranked k entities.
     Returns: Tuple
     Highest K scores and entities
predict_missing_tail_entity (head_entity: List[str] | str, relation: List[str] | str,
              within: List[str] = None \rightarrow torch.FloatTensor
     Given a head entity and a relation, return top k ranked entities
     argmax_{e} = in E  f(h,r,e), where h in E and r in R.
```

```
Parameter
```

```
head_entity: List[str]
```

String representation of selected entities.

```
tail_entity: List[str]
```

String representation of selected entities.

Returns: Tuple

scores

 $predict(*, h: List[str] | str = None, r: List[str] | str = None, t: List[str] | str = None, within=None, logits=True) <math>\rightarrow$ torch.FloatTensor

Parameters

- logits
- h
- r
- t
- within

Predict missing item in a given triple.

Parameter

head_entity: Union[str, List[str]]

String representation of selected entities.

relation: Union[str, List[str]]

String representation of selected relations.

tail_entity: Union[str, List[str]]

String representation of selected entities.

k: int

Highest ranked k item.

Returns: Tuple

Highest K scores and items

Predict triple score

```
Parameter
```

```
head entity: List[str]
     String representation of selected entities.
     relation: List[str]
     String representation of selected relations.
     tail_entity: List[str]
     String representation of selected entities.
     logits: bool
     If logits is True, unnormalized score returned
     Returns: Tuple
     pytorch tensor of triple score
t_norm(tens_1: torch.Tensor, tens_2: torch.Tensor, tnorm: str = 'min') \rightarrow torch.Tensor
tensor_t_norm (subquery_scores: torch.FloatTensor, tnorm: str = 'min') \rightarrow torch.FloatTensor
     Compute T-norm over [0,1] ^{n imes d} where n denotes the number of hops and d denotes number of
     entities
t\_conorm (tens_1: torch.Tensor, tens_2: torch.Tensor, tconorm: str = 'min') \rightarrow torch.Tensor
negnorm(tens\_1: torch.Tensor, lambda\_: float, neg\_norm: str = 'standard') \rightarrow torch.Tensor
return_multi_hop_query_results (aggregated_query_for_all_entities, k: int, only_scores)
single_hop_query_answering (query: tuple, only_scores: bool = True, k: int = None)
answer multi hop query (query type: str = None, query: Tuple[str | Tuple[str, str], Ellipsis] = None,
             queries: List[Tuple[str | Tuple[str, str], Ellipsis]] = None, tnorm: str = 'prod',
             neg_norm: str = 'standard', lambda_: float = 0.0, k: int = 10, only_scores=False)
              → List[Tuple[str, torch.Tensor]]
     # @TODO: Refactoring is needed # @TODO: Score computation for each query type should be done in a
     static function
     Find an answer set for EPFO queries including negation and disjunction
     Parameter
     query_type: str The type of the query, e.g., "2p".
     query: Union[str, Tuple[str, Tuple[str, str]]] The query itself, either a string or a nested tuple.
     queries: List of Tuple[Union[str, Tuple[str, str]], ...]
     tnorm: str The t-norm operator.
     neg_norm: str The negation norm.
     lambda_: float lambda parameter for sugeno and yager negation norms
     k: int The top-k substitutions for intermediate variables.
```

returns

• List[Tuple[str, torch.Tensor]]

```
• Entities and corresponding scores sorted in the descening order of scores
      find_missing_triples (confidence: float, entities: List[str] = None, relations: List[str] = None,
                   topk: int = 10, at_most: int = sys.maxsize) \rightarrow Set
                Find missing triples
                Iterative over a set of entities E and a set of relation R:
            orall e in E and orall r in R f(e,r,x)
                Return (e,r,x)
            otin G and f(e,r,x) > confidence
                confidence: float
                A threshold for an output of a sigmoid function given a triple.
                topk: int
                Highest ranked k item to select triples with f(e,r,x) > confidence.
                at_most: int
                Stop after finding at_most missing triples
                \{(e,r,x) \mid f(e,r,x) > \text{confidence land } (e,r,x)\}
           otin G
      deploy(share: bool = False, top\_k: int = 10)
      train_triples (h: List[str], r: List[str], t: List[str], labels: List[float], iteration=2, optimizer=None)
      train_k_vs_all(h, r, iteration=1, lr=0.001)
           Train k vs all :param head_entity: :param relation: :param iteration: :param lr: :return:
      train(kg, lr=0.1, epoch=10, batch\_size=32, neg\_sample\_ratio=10, num\_workers=1) \rightarrow None
            Retrained a pretrain model on an input KG via negative sampling.
class dicee.Execute(args, continuous_training=False)
      A class for Training, Retraining and Evaluation a model.
       (1) Loading & Preprocessing & Serializing input data.
       (2) Training & Validation & Testing
       (3) Storing all necessary info
      args
      is_continual_training = False
      trainer = None
      trained_model = None
      knowledge_graph = None
      report
      evaluator = None
```

start_time = None

```
setup\_executor() \rightarrow None
      {\tt save\_trained\_model}\,()\,\to None
            Save a knowledge graph embedding model
            (1) Send model to eval mode and cpu.
            (2) Store the memory footprint of the model.
            (3) Save the model into disk.
            (4) Update the stats of KG again?
            Parameter
                rtype
                    None
      end (form\_of\_labelling: str) \rightarrow dict
            End training
            (1) Store trained model.
            (2) Report runtimes.
            (3) Eval model if required.
            Parameter
                rtype
                    A dict containing information about the training and/or evaluation
      {\tt write\_report}\,()\,\to None
            Report training related information in a report.json file
      \mathtt{start}() \rightarrow \mathrm{dict}
            Start training
            # (1) Loading the Data # (2) Create an evaluator object. # (3) Create a trainer object. # (4) Start the training
            Parameter
                rtype
                     A dict containing information about the training and/or evaluation
dicee.mapping_from_first_two_cols_to_third(train_set_idx)
dicee.timeit(func)
dicee.load_term_mapping(file_path=str)
dicee.reload_dataset (path: str, form_of_labelling, scoring_technique, neg_ratio, label_smoothing_rate)
      Reload the files from disk to construct the Pytorch dataset
dicee.construct_dataset(*, train_set: numpy.ndarray| list, valid_set=None, test_set=None,
             ordered_bpe_entities=None, train_target_indices=None, target_dim: int = None, entity_to_idx: dict,
             relation to idx: dict, form of labelling: str, scoring technique: str, neg ratio: int,
             label_smoothing_rate: float, byte_pair_encoding=None, block_size: int = None)
```

→ torch.utils.data.Dataset

```
class dicee.BPE NegativeSamplingDataset (train set: torch.LongTensor,
            ordered_shaped_bpe_entities: torch.LongTensor, neg_ratio: int)
```

Bases: torch.utils.data.Dataset

An abstract class representing a Dataset.

All datasets that represent a map from keys to data samples should subclass it. All subclasses should overwrite __getitem__(), supporting fetching a data sample for a given key. Subclasses could also optionally overwrite __len__(), which is expected to return the size of the dataset by many Sampler implementations and the default options of DataLoader. Subclasses could also optionally implement __qetitems__(), for speedup batched samples loading. This method accepts list of indices of samples of batch and returns list of samples.

1 Note

DataLoader by default constructs an index sampler that yields integral indices. To make it work with a mapstyle dataset with non-integral indices/keys, a custom sampler must be provided.

```
train_set
ordered_bpe_entities
num_bpe_entities
neg_ratio
num_datapoints
__len__()
\__getitem\__(idx)
collate_fn (batch_shaped_bpe_triples: List[Tuple[torch.Tensor, torch.Tensor]])
```

class dicee.MultiLabelDataset (train_set: torch.LongTensor, train_indices_target: torch.LongTensor, target_dim: int, torch_ordered_shaped_bpe_entities: torch.LongTensor)

Bases: torch.utils.data.Dataset

An abstract class representing a Dataset.

All datasets that represent a map from keys to data samples should subclass it. All subclasses should overwrite __getitem__(), supporting fetching a data sample for a given key. Subclasses could also optionally overwrite _len__ (), which is expected to return the size of the dataset by many Sampler implementations and the default options of DataLoader. Subclasses could also optionally implement __getitems__(), for speedup batched samples loading. This method accepts list of indices of samples of batch and returns list of samples.

1 Note

DataLoader by default constructs an index sampler that yields integral indices. To make it work with a mapstyle dataset with non-integral indices/keys, a custom sampler must be provided.

```
train_set
train_indices_target
target_dim
```

```
num_datapoints
     torch_ordered_shaped_bpe_entities
     collate_fn = None
     __len__()
     \__getitem__(idx)
class dicee.MultiClassClassificationDataset (subword_units: numpy.ndarray, block_size: int = 8)
     Bases: torch.utils.data.Dataset
     Dataset for the 1vsALL training strategy
          Parameters
                • train_set_idx - Indexed triples for the training.
                • entity_idxs - mapping.
                • relation_idxs - mapping.
                • form - ?
                                                https://pytorch.org/docs/stable/data.html#torch.utils.data.
                • num_workers -
                                      int
                                          for
                  DataLoader
          Return type
              torch.utils.data.Dataset
     train_data
     block_size = 8
     num_of_data_points
     collate_fn = None
     __len__()
     \__{\texttt{getitem}} (idx)
class dicee.OnevsAllDataset (train_set_idx: numpy.ndarray, entity_idxs)
     Bases: torch.utils.data.Dataset
     Dataset for the 1vsALL training strategy
          Parameters
                • train_set_idx - Indexed triples for the training.
                • entity_idxs - mapping.
                • relation_idxs - mapping.
                • form - ?
                • num_workers - int for https://pytorch.org/docs/stable/data.html#torch.utils.data.
                  DataLoader
```

Return type

torch.utils.data.Dataset

Creates a dataset for KvsAll training by inheriting from torch.utils.data.Dataset.

Let D denote a dataset for KvsAll training and be defined as D:= $\{(x,y)_i\}_i ^N$, where x: (h,r) is an unique tuple of an entity h in E and a relation r in R that has been seed in the input graph. y: denotes a multi-label vector in $[0,1]^{\{E\}}$ is a binary label.

orall y_i =1 s.t. (h r E_i) in KG



train set idx

[numpy.ndarray] n by 3 array representing n triples

entity idxs

[dictonary] string representation of an entity to its integer id

relation_idxs

[dictonary] string representation of a relation to its integer id

self: torch.utils.data.Dataset

```
>>> a = KvsAll()
>>> a
? array([0, 1, 2, 3, 4, 5, 6, 7, 8, 9])
```

```
train_data = None
train_target = None
label_smoothing_rate
collate_fn = None
__len__()
__getitem__(idx)
```

class dicee. AllvsAll (train_set_idx: numpy.ndarray, entity_idxs, relation_idxs, label_smoothing_rate=0.0)

Bases: torch.utils.data.Dataset

Creates a dataset for AllvsAll training by inheriting from torch.utils.data.Dataset.

Let D denote a dataset for AllvsAll training and be defined as D:= $\{(x,y)_i\}_i^n N$, where x: (h,r) is a possible unique tuple of an entity h in E and a relation r in R. Hence $N = |E| \times |R| y$: denotes a multi-label vector in $[0,1]^{\{|E|\}}$ is a binary label.



1 Note

AllysAll extends KysAll via none existing (h,r). Hence, it adds data points that are labelled without 1s.

only with 0s.

train set idx

[numpy.ndarray] n by 3 array representing n triples

entity idxs

[dictonary] string representation of an entity to its integer id

relation_idxs

[dictonary] string representation of a relation to its integer id

self: torch.utils.data.Dataset

```
>>> a = AllvsAll()
>>> a
```

```
train_data = None
train_target = None
label_smoothing_rate
collate_fn = None
target_dim
__len__()
\__{\texttt{getitem}} (idx)
```

class dicee.OnevsSample(train_set: numpy.ndarray, num_entities, num_relations, neg_sample_ratio: int = None, label_smoothing_rate: float = 0.0)

Bases: torch.utils.data.Dataset

A custom PyTorch Dataset class for knowledge graph embeddings, which includes both positive and negative sampling for a given dataset for multi-class classification problem..

Parameters

- train_set (np.ndarray) A numpy array containing triples of knowledge graph data. Each triple consists of (head_entity, relation, tail_entity).
- num_entities (int) The number of unique entities in the knowledge graph.
- num_relations (int) The number of unique relations in the knowledge graph.
- neg sample ratio (int, optional) The number of negative samples to be generated per positive sample. Must be a positive integer and less than num_entities.
- label_smoothing_rate (float, optional) A label smoothing rate to apply to the positive and negative labels. Defaults to 0.0.

```
train_data
     The input data converted into a PyTorch tensor.
         Type
             torch.Tensor
num_entities
     Number of entities in the dataset.
         Type
             int
num_relations
     Number of relations in the dataset.
         Type
             int
neg_sample_ratio
     Ratio of negative samples to be drawn for each positive sample.
         Type
             int
label_smoothing_rate
     The smoothing factor applied to the labels.
         Type
             torch.Tensor
collate_fn
     A function that can be used to collate data samples into batches (set to None by default).
         Type
             function, optional
train_data
num_entities
num_relations
neg_sample_ratio = None
label_smoothing_rate
```

Returns the number of samples in the dataset.

 $__{getitem}_{_}(idx)$

__len__()

collate_fn = None

Retrieves a single data sample from the dataset at the given index.

Parameters

idx (int) - The index of the sample to retrieve.

Returns

A tuple consisting of:

• x (torch.Tensor): The head and relation part of the triple.

- y_idx (torch.Tensor): The concatenated indices of the true object (tail entity) and the indices of the negative samples.
- y_vec (torch.Tensor): A vector containing the labels for the positive and negative samples, with label smoothing applied.

```
Return type tuple
```

 $__getitem__(idx)$

```
class dicee.KvsSampleDataset(train_set_idx: numpy.ndarray, entity_idxs, relation_idxs, form,
            store=None, neg_ratio=None, label_smoothing_rate: float = 0.0)
     Bases: torch.utils.data.Dataset
           KvsSample a Dataset:
               D := \{(x,y)_i\}_i \ ^N, where
                   . x:(h,r) is a unique h in E and a relation r in R and . y in [0,1]^{\{E\}} is a binary label.
     orall y_i = 1 s.t. (h r E_i) in KG
               At each mini-batch construction, we subsample(y), hence n
                   lnew_yl << |E| new_y contains all 1's if sum(y)< neg_sample ratio new_y contains</pre>
           train_set_idx
               Indexed triples for the training.
           entity_idxs
               mapping.
           relation_idxs
               mapping.
           form
           store
           label_smoothing_rate
           torch.utils.data.Dataset
     train_data = None
     train_target = None
     neg_ratio = None
     num_entities
     label_smoothing_rate
     collate_fn = None
     max_num_of_classes
     __len__()
```

```
class dicee. NegSampleDataset (train_set: numpy.ndarray, num_entities: int, num_relations: int,
             neg\_sample\_ratio: int = 1)
```

Bases: torch.utils.data.Dataset

An abstract class representing a Dataset.

All datasets that represent a map from keys to data samples should subclass it. All subclasses should overwrite __getitem__(), supporting fetching a data sample for a given key. Subclasses could also optionally overwrite __len__(), which is expected to return the size of the dataset by many Sampler implementations and the default options of DataLoader. Subclasses could also optionally implement __getitems__(), for speedup batched samples loading. This method accepts list of indices of samples of batch and returns list of samples.

1 Note

DataLoader by default constructs an index sampler that yields integral indices. To make it work with a mapstyle dataset with non-integral indices/keys, a custom sampler must be provided.

```
neg_sample_ratio
      train_set
      length
      num_entities
      num_relations
      __len__()
      \__{\tt getitem}\_(idx)
class dicee. TriplePredictionDataset (train_set: numpy.ndarray, num_entities: int, num_relations: int,
             neg\_sample\_ratio: int = 1, label\_smoothing\_rate: float = 0.0)
      Bases: torch.utils.data.Dataset
            Triple Dataset
                D:=\{(x) \mid i \mid i \mid N, \text{ where }
                     . x:(h,r,t) in KG is a unique h in E and a relation r in R and . collact_fn => Generates
                     negative triples
                collect fn:
      orall (h,r,t) in G obtain, create negative triples \{(h,r,x),(r,t),(h,m,t)\}
                y:labels are represented in torch.float16
            train_set_idx
                Indexed triples for the training.
            entity idxs
                mapping.
            relation_idxs
                mapping.
            form
```

```
store
          label_smoothing_rate
          collate_fn: batch:List[torch.IntTensor] Returns ——- torch.utils.data.Dataset
     label_smoothing_rate
     neg_sample_ratio
     train_set
     length
     num_entities
     num_relations
     __len__()
     \__{\texttt{getitem}} (idx)
     collate_fn (batch: List[torch.Tensor])
class dicee. CVDataModule (train_set_idx: numpy.ndarray, num_entities, num_relations, neg_sample_ratio,
            batch_size, num_workers)
     Bases: pytorch_lightning.LightningDataModule
     Create a Dataset for cross validation
          Parameters
                • train_set_idx - Indexed triples for the training.
                • num_entities - entity to index mapping.
                • num_relations - relation to index mapping.
                • batch_size - int
                • form - ?
                                           for https://pytorch.org/docs/stable/data.html#torch.utils.data.
                • num_workers - int
                  DataLoader
          Return type
              ?
     train_set_idx
     num_entities
     num_relations
     neg_sample_ratio
     batch_size
     num_workers
```

train_dataloader() → torch.utils.data.DataLoader

An iterable or collection of iterables specifying training samples.

For more information about multiple dataloaders, see this section.

will dataloader return not be reloaded unless :paramyou ref: ~pytorch_lightning.trainer.trainer.Trainer.reload_dataloaders_every_n_epochs` to a positive integer.

For data processing use the following pattern:

- download in prepare_data()
- process and split in setup ()

However, the above are only necessary for distributed processing.

A Warning

do not assign state in prepare_data

- fit()
- prepare_data()
- setup()

1 Note

Lightning tries to add the correct sampler for distributed and arbitrary hardware. There is no need to set it yourself.

```
setup(*args, **kwargs)
```

Called at the beginning of fit (train + validate), validate, test, or predict. This is a good hook when you need to build models dynamically or adjust something about them. This hook is called on every process when using DDP.

```
stage - either 'fit', 'validate', 'test', or 'predict'
```

Example:

```
class LitModel(...):
   def __init__(self):
        self.11 = None
   def prepare_data(self):
        download_data()
        tokenize()
        # don't do this
        self.something = else
   def setup(self, stage):
        data = load_data(...)
        self.l1 = nn.Linear(28, data.num_classes)
```

transfer_batch_to_device(*args, **kwargs)

Override this hook if your DataLoader returns tensors wrapped in a custom data structure.

The data types listed below (and any arbitrary nesting of them) are supported out of the box:

- torch. Tensor or anything that implements .to(...)
- list
- dict
- tuple

For anything else, you need to define how the data is moved to the target device (CPU, GPU, TPU, ...).



This hook should only transfer the data and not modify it, nor should it move the data to any other device than the one passed in as argument (unless you know what you are doing). To check the current state of execution of this hook you can use self.trainer.training/testing/validating/predicting so that you can add different logic as per your requirement.

Parameters

- batch A batch of data that needs to be transferred to a new device.
- **device** The target device as defined in PyTorch.
- dataloader_idx The index of the dataloader to which the batch belongs.

Returns

A reference to the data on the new device.

Example:

```
def transfer_batch_to_device(self, batch, device, dataloader_idx):
    if isinstance(batch, CustomBatch):
        # move all tensors in your custom data structure to the device
        batch.samples = batch.samples.to(device)
        batch.targets = batch.targets.to(device)
    elif dataloader_idx == 0:
        # skip device transfer for the first dataloader or anything you wish
        pass
    else:
        batch = super().transfer_batch_to_device(batch, device, dataloader_
    →idx)
    return batch
```

→ See also

- move_data_to_device()
- apply_to_collection()

```
prepare_data(*args, **kwargs)
```

Use this to download and prepare data. Downloading and saving data with multiple processes (distributed settings) will result in corrupted data. Lightning ensures this method is called only within a single process, so you can safely add your downloading logic within.

Marning

DO NOT set state to the model (use setup instead) since this is NOT called on every device

Example:

```
def prepare_data(self):
    # good
    download_data()
    tokenize()
    etc()

# bad
self.split = data_split
self.some_state = some_other_state()
```

In a distributed environment, prepare_data can be called in two ways (using prepare_data_per_node)

- 1. Once per node. This is the default and is only called on LOCAL_RANK=0.
- 2. Once in total. Only called on GLOBAL_RANK=0.

Example:

```
# DEFAULT
# called once per node on LOCAL_RANK=0 of that node
class LitDataModule(LightningDataModule):
    def __init__(self):
        super().__init__()
        self.prepare_data_per_node = True

# call on GLOBAL_RANK=0 (great for shared file systems)
class LitDataModule(LightningDataModule):
    def __init__(self):
        super().__init__()
        self.prepare_data_per_node = False
```

This is called before requesting the dataloaders:

```
model.prepare_data()
initialize_distributed()
model.setup(stage)
model.train_dataloader()
model.val_dataloader()
model.test_dataloader()
model.predict_dataloader()
```

class dicee.QueryGenerator(train_path, val_path: str, test_path: str, ent2id: Dict = None, rel2id: Dict = None, seed: int = 1, gen_valid: bool = False, gen_test: bool = True)

```
train_path
val_path
test_path
gen_valid = False
gen_test = True
seed = 1
max_ans_num = 1000000.0
mode
ent2id = None
rel2id: Dict = None
ent_in: Dict
ent_out: Dict
query_name_to_struct
list2tuple(list data)
tuple2list(x: List | Tuple) \rightarrow List | Tuple
     Convert a nested tuple to a nested list.
set_global_seed (seed: int)
     Set seed
construct\_graph(paths: List[str]) \rightarrow Tuple[Dict, Dict]
     Construct graph from triples Returns dicts with incoming and outgoing edges
fill_query(query\_structure: List[str | List], ent_in: Dict, ent_out: Dict, answer: int) \rightarrow bool
     Private method for fill_query logic.
achieve\_answer(query: List[str \mid List], ent\_in: Dict, ent\_out: Dict) \rightarrow set
     Private method for achieve_answer logic. @TODO: Document the code
write_links (ent_out, small_ent_out)
ground_queries (query_structure: List[str | List], ent_in: Dict, ent_out: Dict, small_ent_in: Dict,
             small_ent_out: Dict, gen_num: int, query_name: str)
     Generating queries and achieving answers
unmap (query_type, queries, tp_answers, fp_answers, fn_answers)
unmap_query (query_structure, query, id2ent, id2rel)
generate_queries (query_struct: List, gen_num: int, query_type: str)
     Passing incoming and outgoing edges to ground queries depending on mode [train valid or text] and getting
     queries and answers in return @ TODO: create a class for each single query struct
save_queries (query_type: str, gen_num: int, save_path: str)
abstract load_queries(path)
```

Python Module Index

d

```
dicee, 12
dicee.__main__,12
dicee.abstracts, 12
dicee.analyse_experiments, 17
dicee.callbacks, 19
dicee.config, 25
dicee.dataset_classes, 28
dicee.eval_static_funcs, 40
dicee.evaluator, 41
dicee.executer, 43
dicee.knowledge_graph, 44
dicee.knowledge_graph_embeddings,46
dicee.models, 50
dicee.models.adopt, 50
dicee.models.base_model, 51
dicee.models.clifford, 60
dicee.models.complex, 67
dicee.models.dualE,70
dicee.models.ensemble, 71
dicee.models.function_space, 72
dicee.models.octonion, 75
dicee.models.pykeen_models, 78
dicee.models.quaternion, 79
dicee.models.real, 82
dicee.models.static_funcs, 84
dicee.models.transformers, 84
dicee.query_generator, 138
dicee.read_preprocess_save_load_kg, 139
dicee.read_preprocess_save_load_kg.preprocess,
        139
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,
       141
dicee.sanity_checkers, 146
dicee.scripts, 147
dicee.scripts.index_serve, 147
dicee.scripts.run, 149
dicee.static_funcs, 150
dicee.static_funcs_training, 153
dicee.static_preprocess_funcs, 153
dicee.trainer, 154
dicee.trainer.dice_trainer, 154
dicee.trainer.model_parallelism, 156
dicee.trainer.torch_trainer, 157
dicee.trainer.torch_trainer_ddp, 158
```

Index

Non-alphabetical

```
__call__() (dicee.EnsembleKGE method), 187
 _call__() (dicee.models.base_model.IdentityClass method), 60
__call__() (dicee.models.ensemble.EnsembleKGE method), 71
__call__() (dicee.models.IdentityClass method), 101, 112, 118
__class_vars__ (dicee.scripts.index_serve.StringListRequest attribute), 148
__getitem__() (dicee.AllvsAll method), 199
__getitem__() (dicee.BPE_NegativeSamplingDataset method), 196
__getitem__() (dicee.dataset_classes.AllvsAll method), 33
__getitem__() (dicee.dataset_classes.BPE_NegativeSamplingDataset method), 30
__getitem__() (dicee.dataset_classes.KvsAll method), 32
__getitem__() (dicee.dataset_classes.KvsSampleDataset method), 35
__getitem__() (dicee.dataset_classes.MultiClassClassificationDataset method), 31
__getitem__() (dicee.dataset_classes.MultiLabelDataset method), 30
__getitem__() (dicee.dataset_classes.NegSampleDataset method), 36
__getitem__() (dicee.dataset_classes.OnevsAllDataset method), 31
__getitem__() (dicee.dataset_classes.OnevsSample method), 34
__getitem__() (dicee.dataset_classes.TriplePredictionDataset method), 36
__getitem__() (dicee.KvsAll method), 198
__getitem__() (dicee.KvsSampleDataset method), 201
__getitem__() (dicee.MultiClassClassificationDataset method), 197
__getitem__() (dicee.MultiLabelDataset method), 197
__getitem__() (dicee.NegSampleDataset method), 202
__getitem__() (dicee.OnevsAllDataset method), 198
__getitem__() (dicee.OnevsSample method), 200
__getitem__() (dicee.TriplePredictionDataset method), 203
__iter__() (dicee.config.Namespace method), 28
__iter__() (dicee.EnsembleKGE method), 187
__iter__() (dicee.knowledge_graph.KG method), 46
__iter__() (dicee.models.ensemble.EnsembleKGE method), 71
__len__() (dicee.AllvsAll method), 199
  _len__() (dicee.BPE_NegativeSamplingDataset method), 196
__len__() (dicee.dataset_classes.AllvsAll method), 33
__len__() (dicee.dataset_classes.BPE_NegativeSamplingDataset method), 30
__len__() (dicee.dataset_classes.KvsAll method), 32
__len__() (dicee.dataset_classes.KvsSampleDataset method), 35
__len__() (dicee.dataset_classes.MultiClassClassificationDataset method), 31
__len__() (dicee.dataset_classes.MultiLabelDataset method), 30
__len__() (dicee.dataset_classes.NegSampleDataset method), 36
__len__() (dicee.dataset_classes.OnevsAllDataset method), 31
__len__() (dicee.dataset_classes.OnevsSample method), 34
__len__() (dicee.dataset_classes.TriplePredictionDataset method), 36
__len__() (dicee.EnsembleKGE method), 187
__len__() (dicee.knowledge_graph.KG method), 46
__len__() (dicee.KvsAll method), 198
  _len__() (dicee.KvsSampleDataset method), 201
__len__() (dicee.models.ensemble.EnsembleKGE method), 71
__len__() (dicee.MultiClassClassificationDataset method), 197
__len__() (dicee.MultiLabelDataset method), 197
__len__() (dicee.NegSampleDataset method), 202
__len__() (dicee.OnevsAllDataset method), 198
__len__() (dicee.OnevsSample method), 200
__len__() (dicee.TriplePredictionDataset method), 203
__private_attributes__ (dicee.scripts.index_serve.StringListRequest attribute), 148
__pydantic_complete__ (dicee.scripts.index_serve.StringListRequest attribute), 148
__pydantic_computed_fields__ (dicee.scripts.index_serve.StringListRequest attribute), 149
__pydantic_core_schema__ (dicee.scripts.index_serve.StringListRequest attribute), 148
__pydantic_custom_init__ (dicee.scripts.index_serve.StringListRequest attribute), 148
__pydantic_decorators__ (dicee.scripts.index_serve.StringListRequest attribute), 148
__pydantic_extra__ (dicee.scripts.index_serve.StringListRequest attribute), 149
__pydantic_fields__ (dicee.scripts.index_serve.StringListRequest attribute), 149
__pydantic_fields_set__ (dicee.scripts.index_serve.StringListRequest attribute), 149
__pydantic_generic_metadata__ (dicee.scripts.index_serve.StringListRequest attribute), 148
__pydantic_parent_namespace__ (dicee.scripts.index_serve.StringListRequest attribute), 149
__pydantic_post_init__ (dicee.scripts.index_serve.StringListRequest attribute), 149
```

```
__pydantic_private__ (dicee.scripts.index_serve.StringListRequest attribute), 149
__pydantic_root_model__ (dicee.scripts.index_serve.StringListRequest attribute), 149
__pydantic_serializer__ (dicee.scripts.index_serve.StringListRequest attribute), 149
__pydantic_validator__ (dicee.scripts.index_serve.StringListRequest attribute), 149
__setstate__() (dicee.models.ADOPT method), 92
__setstate__() (dicee.models.adopt.ADOPT method), 51
__signature__ (dicee.scripts.index_serve.StringListRequest attribute), 148
__str__() (dicee.EnsembleKGE method), 187
__str__() (dicee.KGE method), 190
__str__() (dicee.knowledge_graph_embeddings.KGE method), 46
__str__() (dicee.models.ensemble.EnsembleKGE method), 71
__version__ (in module dicee), 208
Α
AbstractCallback (class in dicee.abstracts), 15
AbstractPPECallback (class in dicee.abstracts), 17
AbstractTrainer (class in dicee.abstracts), 12
AccumulateEpochLossCallback (class in dicee.callbacks), 19
achieve answer () (dicee.query generator.QueryGenerator method), 139
achieve_answer() (dicee.QueryGenerator method), 207
AConEx (class in dicee), 173
AConEx (class in dicee.models), 108
AConEx (class in dicee.models.complex), 68
AConvo (class in dicee), 174
AConvO (class in dicee.models), 120
AConvo (class in dicee.models.octonion), 77
AConvo (class in dicee), 175
AConvQ (class in dicee.models), 114
AConvQ (class in dicee.models.quaternion), 81
adaptive_swa (dicee.config.Namespace attribute), 28
add_new_entity_embeddings() (dicee.abstracts.BaseInteractiveKGE method), 15
add_noise_rate (dicee.config.Namespace attribute), 26
\verb|add_noise_rate| (\textit{dicee.knowledge\_graph.KG attribute}), 45
add_noisy_triples() (in module dicee), 188
add_noisy_triples() (in module dicee.static_funcs), 152
add_noisy_triples_into_training() (dicee.read_preprocess_save_load_kg.read_from_disk.ReadFromDisk method), 141
add_noisy_triples_into_training() (dicee.read_preprocess_save_load_kg.ReadFromDisk method), 146
add_reciprocal (dicee.knowledge_graph.KG attribute), 45
ADOPT (class in dicee.models), 92
ADOPT (class in dicee.models.adopt), 50
adopt () (in module dicee.models.adopt), 51
AllvsAll (class in dicee), 198
AllvsAll (class in dicee.dataset_classes), 32
alphas (dicee.abstracts.AbstractPPECallback attribute), 17
alphas (dicee.callbacks.ASWA attribute), 23
analyse () (in module dicee.analyse_experiments), 19
answer_multi_hop_query() (\emph{dicee.KGE method}), 193
answer_multi_hop_query() (dicee.knowledge_graph_embeddings.KGE method), 49
app (in module dicee.scripts.index_serve), 148
{\tt apply\_coefficients()} \ (\textit{dicee.DeCaL method}), \, 170
apply_coefficients() (dicee.Keci method), 166
apply_coefficients() (dicee.models.clifford.DeCaL method), 65
apply_coefficients() (dicee.models.clifford.Keci method), 62
apply_coefficients() (dicee.models.DeCaL method), 126
apply_coefficients() (dicee.models.Keci method), 122
apply_reciprical_or_noise() (in module dicee.read_preprocess_save_load_kg.util), 144
apply_semantic_constraint (dicee.abstracts.BaseInteractiveKGE attribute), 14
apply_unit_norm (dicee.BaseKGE attribute), 185
apply_unit_norm (dicee.models.base_model.BaseKGE attribute), 58
apply_unit_norm (dicee.models.BaseKGE attribute), 99, 102, 105, 110, 116, 129, 132
args (dicee.BaseKGE attribute), 185
args (dicee.DICE_Trainer attribute), 189
args (dicee.evaluator.Evaluator attribute), 42
args (dicee. Execute attribute), 194
args (dicee.executer.Execute attribute), 43
args (dicee.models.base_model.BaseKGE attribute), 57
args (dicee.models.base_model.IdentityClass attribute), 60
```

```
args (dicee.models.BaseKGE attribute), 98, 102, 105, 110, 116, 128, 132
args (dicee.models.IdentityClass attribute), 101, 112, 118
args (dicee.models.pykeen models.PykeenKGE attribute), 78
args (dicee.models.PykeenKGE attribute), 130
args (dicee.PykeenKGE attribute), 182
args (dicee.trainer.DICE_Trainer attribute), 160
args (dicee.trainer.dice_trainer.DICE_Trainer attribute), 155
ASWA (class in dicee.callbacks), 22
aswa (dicee.analyse_experiments.Experiment attribute), 18
attn (dicee.models.transformers.Block attribute), 89
attn_dropout (dicee.models.transformers.CausalSelfAttention attribute), 87
attributes (dicee.abstracts.AbstractTrainer attribute), 12
auto_batch_finding (dicee.config.Namespace attribute), 28
В
backend (dicee.config.Namespace attribute), 26
backend (dicee.knowledge_graph.KG attribute), 45
BaseInteractiveKGE (class in dicee.abstracts), 13
BaseKGE (class in dicee), 184
BaseKGE (class in dicee.models), 98, 101, 105, 109, 115, 128, 131
BaseKGE (class in dicee.models.base_model), 57
BaseKGELightning (class in dicee.models), 92
BaseKGELightning (class in dicee.models.base_model), 51
batch_kronecker_product() (dicee.callbacks.KronE static method), 25
batch_size (dicee.analyse_experiments.Experiment attribute), 18
batch_size (dicee.callbacks.PseudoLabellingCallback attribute), 22
batch_size (dicee.config.Namespace attribute), 26
batch_size (dicee.CVDataModule attribute), 203
batch_size (dicee.dataset_classes.CVDataModule attribute), 37
bias (dicee.models.transformers.GPTConfig attribute), 89
bias (dicee.models.transformers.LayerNorm attribute), 86
Block (class in dicee.models.transformers), 88
block_size (dicee.BaseKGE attribute), 186
block_size (dicee.config.Namespace attribute), 28
\verb|block_size| (\textit{dicee.dataset\_classes.MultiClassClassificationDataset attribute}), 31
block_size (dicee.models.base_model.BaseKGE attribute), 58
block_size (dicee.models.BaseKGE attribute), 99, 102, 106, 111, 117, 129, 133
block_size (dicee.models.transformers.GPTConfig attribute), 89
block_size (dicee.MultiClassClassificationDataset attribute), 197
bn_conv1 (dicee.AConvQ attribute), 175
bn conv1 (dicee.ConvO attribute), 175
bn_conv1 (dicee.models.AConvQ attribute), 115
bn_conv1 (dicee.models.ConvQ attribute), 114
bn_conv1 (dicee.models.quaternion.AConvQ attribute), 82
bn_conv1 (dicee.models.quaternion.ConvQ attribute), 81
bn_conv2 (dicee.AConvQ attribute), 175
bn_conv2 (dicee.ConvQ attribute), 175
bn_conv2 (dicee.models.AConvQ attribute), 115
bn_conv2 (dicee.models.ConvQ attribute), 114
bn_conv2 (dicee.models.quaternion.AConvQ attribute), 82
bn_conv2 (dicee.models.quaternion.ConvQ attribute), 81
bn_conv2d (dicee.AConEx attribute), 174
bn_conv2d (dicee.AConvO attribute), 174
bn_conv2d (dicee.ConEx attribute), 177
bn_conv2d (dicee.ConvO attribute), 176
bn_conv2d (dicee.models.AConEx attribute), 108
bn_conv2d (dicee.models.AConvO attribute), 121
bn_conv2d (dicee.models.complex.AConEx attribute), 68
bn_conv2d (dicee.models.complex.ConEx attribute), 68
bn_conv2d (dicee.models.ConEx attribute), 107
bn_conv2d (dicee.models.ConvO attribute), 120
bn_conv2d (dicee.models.octonion.AConvO attribute), 78
bn_conv2d (dicee.models.octonion.ConvO attribute), 77
BPE_NegativeSamplingDataset (class in dicee), 195
BPE_NegativeSamplingDataset (class in dicee.dataset_classes), 29
build_chain_funcs() (dicee.models.FMult2 method), 135
build_chain_funcs() (dicee.models.function_space.FMult2 method), 73
```

```
build func() (dicee.models.FMult2 method), 135
build_func() (dicee.models.function_space.FMult2 method), 73
Byt E (class in dicee), 182
BytE (class in dicee.models.transformers), 84
byte_pair_encoding (dicee.analyse_experiments.Experiment attribute), 18
byte_pair_encoding (dicee.BaseKGE attribute), 186
byte_pair_encoding (dicee.config.Namespace attribute), 28
byte_pair_encoding (dicee.knowledge_graph.KG attribute), 45
byte_pair_encoding (dicee.models.base_model.BaseKGE attribute), 58
byte_pair_encoding (dicee.models.BaseKGE attribute), 99, 102, 106, 111, 117, 129, 133
c_attn (dicee.models.transformers.CausalSelfAttention attribute), 87
c_fc (dicee.models.transformers.MLP attribute), 88
c_proj (dicee.models.transformers.CausalSelfAttention attribute), 87
c_proj (dicee.models.transformers.MLP attribute), 88
callbacks (dicee.abstracts.AbstractTrainer attribute), 12
callbacks (dicee.analyse_experiments.Experiment attribute), 18
callbacks (dicee.config.Namespace attribute), 26
callbacks (dicee.trainer.torch_trainer_ddp.NodeTrainer attribute), 159
CausalSelfAttention (class in dicee.models.transformers), 86
chain_func() (dicee.models.FMult method), 134
\verb|chain_func()| (\textit{dicee.models.function\_space.FMult method}), 72
chain_func() (dicee.models.function_space.GFMult method), 73
chain_func() (dicee.models.GFMult method), 134
CKeci (class in dicee), 165
CKeci (class in dicee.models), 124
CKeci (class in dicee.models.clifford), 63
cl_pgr() (dicee.DeCaL method), 169
cl_pqr() (dicee.models.clifford.DeCaL method), 65
cl_pgr() (dicee.models.DeCaL method), 125
clifford_multiplication() (dicee.Keci method), 166
clifford_multiplication() (dicee.models.clifford.Keci method), 62
clifford_multiplication() (dicee.models.Keci method), 122
clip_lambda (dicee.models.ADOPT attribute), 92
clip_lambda (dicee.models.adopt.ADOPT attribute), 51
collate_fn (dicee.AllvsAll attribute), 199
collate_fn (dicee.dataset_classes.AllvsAll attribute), 33
collate_fn (dicee.dataset_classes.KvsAll attribute), 32
collate_fn (dicee.dataset_classes.KvsSampleDataset attribute), 35
collate fn (dicee.dataset classes.MultiClassClassificationDataset attribute), 31
collate_fn (dicee.dataset_classes.MultiLabelDataset attribute), 30
collate_fn (dicee.dataset_classes.OnevsAllDataset attribute), 31
collate_fn (dicee.dataset_classes.OnevsSample attribute), 34
collate_fn (dicee.KvsAll attribute), 198
collate_fn (dicee.KvsSampleDataset attribute), 201
collate_fn (dicee.MultiClassClassificationDataset attribute), 197
collate fn (dicee.MultiLabelDataset attribute), 197
collate_fn (dicee.OnevsAllDataset attribute), 198
collate_fn (dicee.OnevsSample attribute), 200
collate_fn() (dicee.BPE_NegativeSamplingDataset method), 196
collate_fn() (dicee.dataset_classes.BPE_NegativeSamplingDataset method), 30
collate_fn() (dicee.dataset_classes.TriplePredictionDataset method), 37
collate_fn() (dicee. TriplePredictionDataset method), 203
collection_name (dicee.scripts.index_serve.NeuralSearcher attribute), 148
comp_func() (dicee.LFMult method), 181
comp_func() (dicee.models.function_space.LFMult method), 75
comp_func() (dicee.models.LFMult method), 136
Complex (class in dicee), 172
Complex (class in dicee.models), 108
Complex (class in dicee.models.complex), 68
compute_convergence() (in module dicee.callbacks), 22
compute_func() (dicee.models.FMult method), 134
compute_func() (dicee.models.FMult2 method), 135
compute_func() (dicee.models.function_space.FMult method), 72
compute_func() (dicee.models.function_space.FMult2 method), 73
compute_func() (dicee.models.function_space.GFMult method), 73
```

```
compute func () (dicee.models.GFMult method), 134
compute_mrr() (dicee.callbacks.ASWA static method), 23
compute_sigma_pp() (dicee.DeCaL method), 170
compute_sigma_pp() (dicee.Keci method), 166
compute_sigma_pp() (dicee.models.clifford.DeCaL method), 66
compute_sigma_pp() (dicee.models.clifford.Keci method), 61
compute_sigma_pp() (dicee.models.DeCaL method), 126
compute_sigma_pp() (dicee.models.Keci method), 122
compute_sigma_pq() (dicee.DeCaL method), 171
compute_sigma_pq() (dicee.Keci method), 166
compute_sigma_pq() (dicee.models.clifford.DeCaL method), 67
compute_sigma_pq() (dicee.models.clifford.Keci method), 62
compute_sigma_pq() (dicee.models.DeCaL method), 127
compute_sigma_pq() (dicee.models.Keci method), 122
compute_sigma_pr() (dicee.DeCaL method), 171
compute_sigma_pr() (dicee.models.clifford.DeCaL method), 67
compute_sigma_pr() (dicee.models.DeCaL method), 127
compute_sigma_gq() (dicee.DeCaL method), 170
compute_sigma_qq() (dicee.Keci method), 166
compute_sigma_qq() (dicee.models.clifford.DeCaL method), 66
compute_sigma_qq() (dicee.models.clifford.Keci method), 61
compute_sigma_qq() (dicee.models.DeCaL method), 127
compute_sigma_gg() (dicee.models.Keci method), 122
compute_sigma_qr() (dicee.DeCaL method), 171
compute_sigma_gr() (dicee.models.clifford.DeCaL method), 67
compute_sigma_gr() (dicee.models.DeCaL method), 128
compute_sigma_rr() (dicee.DeCaL method), 171
compute_sigma_rr() (dicee.models.clifford.DeCaL method), 66
compute_sigma_rr() (dicee.models.DeCaL method), 127
compute_sigmas_multivect() (dicee.DeCaL method), 169
compute_sigmas_multivect() (dicee.models.clifford.DeCaL method), 65
compute sigmas multivect() (dicee.models.DeCaL method), 126
compute_sigmas_single() (dicee.DeCaL method), 169
compute_sigmas_single() (dicee.models.clifford.DeCaL method), 65
compute_sigmas_single() (dicee.models.DeCaL method), 125
ConEx (class in dicee), 177
ConEx (class in dicee.models), 107
ConEx (class in dicee.models.complex), 67
config (dicee.BytE attribute), 183
config (dicee.models.transformers.BytE attribute), 85
config (dicee.models.transformers.GPT attribute), 90
configs (dicee.abstracts.BaseInteractiveKGE attribute), 14
configure_optimizers() (dicee.models.base_model.BaseKGELightning method), 56
configure_optimizers() (dicee.models.BaseKGELightning method), 96
\verb|configure_optimizers()| \textit{(dicee.models.transformers.GPT method)}, 90
construct_batch_selected_cl_multivector() (dicee.Keci method), 167
construct_batch_selected_cl_multivector() (dicee.models.clifford.Keci method), 63
construct_batch_selected_cl_multivector() (dicee.models.Keci method), 123
construct_cl_multivector() (dicee.DeCaL method), 170
construct_cl_multivector() (dicee.Keci method), 167
construct_cl_multivector() (dicee.models.clifford.DeCaL method), 65
construct_cl_multivector() (dicee.models.clifford.Keci method), 62
construct_cl_multivector() (dicee.models.DeCaL method), 126
construct_cl_multivector() (dicee.models.Keci method), 123
construct_dataset() (in module dicee), 195
construct_dataset() (in module dicee.dataset_classes), 29
construct_ensemble (dicee.abstracts.BaseInteractiveKGE attribute), 14
construct_graph() (dicee.query_generator.QueryGenerator method), 139
construct_graph() (dicee.QueryGenerator method), 207
construct_input_and_output() (dicee.abstracts.BaseInteractiveKGE method), 15
construct_multi_coeff() (dicee.LFMult method), 180
construct_multi_coeff() (dicee.models.function_space.LFMult method), 74
\verb|construct_multi_coeff()| \textit{(dicee.models.LFMult method)}, 136
continual_learning (dicee.config.Namespace attribute), 28
continual_start() (dicee.DICE_Trainer method), 189
continual_start() (dicee.executer.ContinuousExecute method), 44
continual_start() (dicee.trainer.DICE_Trainer method), 160
continual_start() (dicee.trainer.dice_trainer.DICE_Trainer method), 155
```

```
\verb|continual_training_setup_executor()| \textit{(in module dicee)}, 188
continual_training_setup_executor() (in module dicee.static_funcs), 152
ContinuousExecute (class in dicee.executer), 44
conv2d (dicee.AConEx attribute), 174
conv2d (dicee.AConvO attribute), 174
conv2d (dicee.AConvQ attribute), 175
conv2d (dicee.ConEx attribute), 177
conv2d (dicee.ConvO attribute), 176
conv2d (dicee.ConvQ attribute), 175
conv2d (dicee.models.AConEx attribute), 108
conv2d (dicee.models.AConvO attribute), 120
conv2d (dicee.models.AConvQ attribute), 115
conv2d (dicee.models.complex.AConEx attribute), 68
conv2d (dicee.models.complex.ConEx attribute), 67
conv2d (dicee.models.ConEx attribute), 107
conv2d (dicee.models.ConvO attribute), 120
conv2d (dicee.models.ConvQ attribute), 114
conv2d (dicee.models.octonion.AConvO attribute), 77
conv2d (dicee.models.octonion.ConvO attribute), 77
conv2d (dicee.models.quaternion.AConvQ attribute), 82
conv2d (dicee.models.quaternion.ConvQ attribute), 81
ConvO (class in dicee), 176
ConvO (class in dicee.models), 119
ConvO (class in dicee.models.octonion), 76
ConvQ (class in dicee), 175
ConvQ (class in dicee.models), 114
ConvQ (class in dicee.models.quaternion), 81
create_constraints() (in module dicee.read_preprocess_save_load_kg.util), 144
create_constraints() (in module dicee.static_preprocess_funcs), 154
create_experiment_folder() (in module dicee), 188
create_experiment_folder() (in module dicee.static_funcs), 152
create_random_data() (dicee.callbacks.PseudoLabellingCallback method), 22
create_recipriocal_triples() (in module dicee), 187
\verb|create_recipriocal_triples(|)| \textit{ (in module dicee.read\_preprocess\_save\_load\_kg.util)}, 145
create_recipriocal_triples() (in module dicee.static_funcs), 151
create_vector_database() (dicee.KGE method), 190
create vector database() (dicee.knowledge graph embeddings.KGE method), 46
crop_block_size() (dicee.models.transformers.GPT method), 90
ctx (dicee.trainer.torch_trainer_ddp.NodeTrainer attribute), 159
CVDataModule (class in dicee), 203
CVDataModule (class in dicee.dataset_classes), 37
D
data_module (dicee.callbacks.PseudoLabellingCallback attribute), 22
dataset_dir (dicee.config.Namespace attribute), 26
dataset_dir (dicee.knowledge_graph.KG attribute), 45
dataset_sanity_checking() (in module dicee.read_preprocess_save_load_kg.util), 145
DeCaL (class in dicee), 168
DeCaL (class in dicee.models), 124
DeCal (class in dicee.models.clifford), 64
decide() (dicee.callbacks.ASWA method), 23
degree (dicee.LFMult attribute), 180
degree (dicee.models.function_space.LFMult attribute), 74
degree (dicee.models.LFMult attribute), 136
deploy() (dicee.KGE method), 194
deploy() (dicee.knowledge_graph_embeddings.KGE method), 50
deploy_head_entity_prediction() (in module dicee), 188
deploy_head_entity_prediction() (in module dicee.static_funcs), 152
deploy_relation_prediction() (in module dicee), 188
deploy_relation_prediction() (in module dicee.static_funcs), 152
deploy_tail_entity_prediction() (in module dicee), 188
deploy_tail_entity_prediction() (in module dicee.static_funcs), 152
deploy_triple_prediction() (in module dicee), 188
deploy_triple_prediction() (in module dicee.static_funcs), 152
describe() (dicee.knowledge_graph.KG method), 46
description_of_input (dicee.knowledge_graph.KG attribute), 46
DICE_Trainer (class in dicee), 189
```

```
DICE_Trainer (class in dicee.trainer), 160
DICE_Trainer (class in dicee.trainer.dice_trainer), 155
dicee
    module, 12
dicee.___main_
    module, 12
dicee.abstracts
    module, 12
dicee.analyse_experiments
    module, 17
dicee.callbacks
    module, 19
dicee.config
    module, 25
dicee.dataset_classes
    module, 28
dicee.eval_static_funcs
    module, 40
dicee.evaluator
    module.41
dicee.executer
    module, 43
dicee.knowledge_graph
    module, 44
dicee.knowledge_graph_embeddings
    module, 46
dicee.models
    module, 50
dicee.models.adopt
    module, 50
dicee.models.base_model
    module, 51
dicee.models.clifford
    module, 60
dicee.models.complex
    module, 67
dicee.models.dualE
    module, 70
dicee.models.ensemble
    module, 71
dicee.models.function_space
    module, 72
dicee.models.octonion
    module, 75
dicee.models.pykeen_models
    module, 78
dicee.models.quaternion
    module, 79
dicee.models.real
    module, 82
dicee.models.static_funcs
    module, 84
\verb|dicee.models.transformers|\\
    module, 84
dicee.query_generator
    module, 138
dicee.read_preprocess_save_load_kg
    module, 139
dicee.read_preprocess_save_load_kg.preprocess
     module, 139
dicee.read_preprocess_save_load_kg.read_from_disk
    module, 140
dicee.read_preprocess_save_load_kg.save_load_disk
    module, 141
dicee.read_preprocess_save_load_kg.util
    module, 141
dicee.sanity_checkers
    module, 146
```

```
dicee.scripts
     module, 147
dicee.scripts.index_serve
     module, 147
dicee.scripts.run
     module, 149
dicee.static_funcs
     module, 150
dicee.static_funcs_training
     module, 153
dicee.static_preprocess_funcs
     module, 153
dicee.trainer
     module, 154
dicee.trainer.dice trainer
     module, 154
dicee.trainer.model_parallelism
     module, 156
dicee.trainer.torch_trainer
     module, 157
dicee.trainer.torch_trainer_ddp
     module, 158
discrete_points (dicee.models.FMult2 attribute), 135
discrete_points (dicee.models.function_space.FMult2 attribute), 73
dist_func (dicee.models.Pyke attribute), 104
dist_func (dicee.models.real.Pyke attribute), 83
dist_func (dicee.Pyke attribute), 164
DistMult (class in dicee), 164
DistMult (class in dicee.models), 103
DistMult (class in dicee.models.real), 82
download_file() (in module dicee), 189
download_file() (in module dicee.static_funcs), 152
download_files_from_url() (in module dicee), 189
download_files_from_url() (in module dicee.static_funcs), 152
download_pretrained_model() (in module dicee), 189
download_pretrained_model() (in module dicee.static_funcs), 153
dropout (dicee.models.transformers.CausalSelfAttention attribute), 87
dropout (dicee.models.transformers.GPTConfig attribute), 89
dropout (dicee.models.transformers.MLP attribute), 88
DualE (class in dicee), 172
DualE (class in dicee.models), 137
DualE (class in dicee.models.dualE), 70
dummy_eval() (dicee.evaluator.Evaluator method), 42
dummy_id (dicee.knowledge_graph.KG attribute), 45
during_training (dicee.evaluator.Evaluator attribute), 42
E
ee vocab (dicee.evaluator.Evaluator attribute), 41
efficient_zero_grad() (in module dicee.static_funcs_training), 153
embedding_dim (dicee.analyse_experiments.Experiment attribute), 18
embedding_dim (dicee.BaseKGE attribute), 185
\verb|embedding_dim| (\textit{dicee.config.Namespace attribute}), 26
embedding_dim (dicee.models.base_model.BaseKGE attribute), 58
embedding_dim (dicee.models.BaseKGE attribute), 98, 102, 105, 110, 116, 128, 132
enable_log (in module dicee.static_preprocess_funcs), 154
enc (dicee.knowledge_graph.KG attribute), 45
end() (dicee.Execute method), 195
end() (dicee.executer.Execute method), 43
EnsembleKGE (class in dicee), 187
EnsembleKGE (class in dicee.models.ensemble), 71
ent2id (dicee.query_generator.QueryGenerator attribute), 138
ent2id (dicee.QueryGenerator attribute), 207
ent_in (dicee.query_generator.QueryGenerator attribute), 138
ent_in (dicee.QueryGenerator attribute), 207
ent_out (dicee.query_generator.QueryGenerator attribute), 138
ent_out (dicee.QueryGenerator attribute), 207
entities_str (dicee.knowledge_graph.KG property), 46
```

```
entity embeddings (dicee. AConvO attribute), 175
entity_embeddings (dicee.ConvQ attribute), 175
entity_embeddings (dicee.DeCaL attribute), 169
entity_embeddings (dicee.DualE attribute), 172
entity_embeddings (dicee.LFMult attribute), 180
entity_embeddings (dicee.models.AConvQ attribute), 115
entity_embeddings (dicee.models.clifford.DeCaL attribute), 64
entity embeddings (dicee.models.ConvO attribute), 114
entity_embeddings (dicee.models.DeCaL attribute), 125
entity_embeddings (dicee.models.DualE attribute), 137
entity_embeddings (dicee.models.dualE.DualE attribute), 70
entity_embeddings (dicee.models.FMult attribute), 134
entity_embeddings (dicee.models.FMult2 attribute), 135
entity_embeddings (dicee.models.function_space.FMult attribute), 72
entity_embeddings (dicee.models.function_space.FMult2 attribute), 73
entity_embeddings (dicee.models.function_space.GFMult attribute), 72
entity_embeddings (dicee.models.function_space.LFMult attribute), 74
entity_embeddings (dicee.models.function_space.LFMult1 attribute), 73
entity_embeddings (dicee.models.GFMult attribute), 134
entity_embeddings (dicee.models.LFMult attribute), 136
entity_embeddings (dicee.models.LFMult1 attribute), 135
entity_embeddings (dicee.models.pykeen_models.PykeenKGE attribute), 78
entity_embeddings (dicee.models.PykeenKGE attribute), 130
entity_embeddings (dicee.models.quaternion.AConvQ attribute), 82
entity_embeddings (dicee.models.quaternion.ConvQ attribute), 81
entity_embeddings (dicee.PykeenKGE attribute), 182
entity_to_idx (dicee.knowledge_graph.KG attribute), 45
entity_to_idx (dicee.scripts.index_serve.NeuralSearcher attribute), 148
epoch_count (dicee.abstracts.AbstractPPECallback attribute), 17
epoch_count (dicee.callbacks.ASWA attribute), 22
epoch_counter (dicee.callbacks.Eval attribute), 23
epoch counter (dicee.callbacks.KGESaveCallback attribute), 21
epoch_ratio (dicee.callbacks.Eval attribute), 23
er_vocab (dicee.evaluator.Evaluator attribute), 41
estimate_mfu() (dicee.models.transformers.GPT method), 90
estimate_q() (in module dicee.callbacks), 22
Eval (class in dicee.callbacks), 23
eval() (dicee. Ensemble KGE method), 187
eval () (dicee.evaluator.Evaluator method), 42
eval() (dicee.models.ensemble.EnsembleKGE method), 71
eval_lp_performance() (dicee.KGE method), 191
eval_lp_performance() (dicee.knowledge_graph_embeddings.KGE method), 46
eval_model (dicee.config.Namespace attribute), 27
eval_model (dicee.knowledge_graph.KG attribute), 45
eval_rank_of_head_and_tail_byte_pair_encoded_entity() (dicee.evaluator.Evaluator method), 42
eval_rank_of_head_and_tail_entity() (dicee.evaluator.Evaluator method), 42
eval_with_bpe_vs_all() (dicee.evaluator.Evaluator method), 42
eval_with_byte() (dicee.evaluator.Evaluator method), 42
eval_with_data() (dicee.evaluator.Evaluator method), 42
eval_with_vs_all() (dicee.evaluator.Evaluator method), 42
evaluate() (in module dicee), 189
evaluate() (in module dicee.static_funcs), 152
evaluate_bpe_lp() (in module dicee.static_funcs_training), 153
evaluate_link_prediction_performance() (in module dicee.eval_static_funcs), 40
evaluate_link_prediction_performance_with_bpe() (in module dicee.eval_static_funcs), 41
{\tt evaluate\_link\_prediction\_performance\_with\_bpe\_reciprocals} \ () \ \textit{(in module dicee.eval\_static\_funcs)}, 41 \\
evaluate_link_prediction_performance_with_reciprocals() (in module dicee.eval_static_funcs), 41
evaluate lp() (dicee.evaluator.Evaluator method), 42
evaluate_lp() (in module dicee.static_funcs_training), 153
evaluate_lp_bpe_k_vs_all() (dicee.evaluator.Evaluator method), 42
evaluate_lp_bpe_k_vs_all() (in module dicee.eval_static_funcs), 41
evaluate_lp_k_vs_all() (dicee.evaluator.Evaluator method), 42
evaluate_lp_with_byte() (dicee.evaluator.Evaluator method), 42
Evaluator (class in dicee.evaluator), 41
evaluator (dicee.DICE_Trainer attribute), 189
evaluator (dicee. Execute attribute), 194
evaluator (dicee.executer.Execute attribute), 43
evaluator (dicee.trainer.DICE_Trainer attribute), 160
```

```
evaluator (dicee.trainer.dice trainer.DICE Trainer attribute), 155
every_x_epoch (dicee.callbacks.KGESaveCallback attribute), 21
example_input_array (dicee.EnsembleKGE property), 187
example_input_array (dicee.models.ensemble.EnsembleKGE property), 71
Execute (class in dicee), 194
Execute (class in dicee.executer), 43
exists() (dicee.knowledge_graph.KG method), 46
Experiment (class in dicee.analyse experiments), 18
explicit (dicee.models.QMult attribute), 113
{\tt explicit}~(\textit{dicee.models.quaternion.QMult~attribute}),\,80
explicit (dicee.QMult attribute), 178
exponential_function() (in module dicee), 188
exponential_function() (in module dicee.static_funcs), 152
extract_input_outputs() (dicee.trainer.torch_trainer_ddp.NodeTrainer method), 159
extract_input_outputs() (in module dicee.trainer.model_parallelism), 157
extract_input_outputs_set_device() (dicee.trainer.torch_trainer.TorchTrainer method), 158
F
f (dicee.callbacks.KronE attribute), 25
fc1 (dicee.AConEx attribute), 174
fc1 (dicee.AConvO attribute), 174
fc1 (dicee.AConvQ attribute), 175
fc1 (dicee.ConEx attribute), 177
fc1 (dicee.ConvO attribute), 176
fc1 (dicee.ConvQ attribute), 175
fc1 (dicee.models.AConEx attribute), 108
fc1 (dicee.models.AConvO attribute), 120
fc1 (dicee.models.AConvQ attribute), 115
fc1 (dicee.models.complex.AConEx attribute), 68
fc1 (dicee.models.complex.ConEx attribute), 68
fc1 (dicee.models.ConEx attribute), 107
fc1 (dicee.models.ConvO attribute), 120
fc1 (dicee.models.ConvQ attribute), 114
fc1 (dicee.models.octonion.AConvO attribute), 78
fc1 (dicee.models.octonion.ConvO attribute), 77
fc1 (dicee.models.quaternion.AConvQ attribute), 82
fc1 (dicee.models.quaternion.ConvQ attribute), 81
fc_num_input (dicee.AConEx attribute), 174
fc_num_input (dicee.AConvO attribute), 174
fc_num_input (dicee.AConvQ attribute), 175
fc_num_input (dicee.ConEx attribute), 177
fc_num_input (dicee.ConvO attribute), 176
fc_num_input (dicee.ConvQ attribute), 175
fc_num_input (dicee.models.AConEx attribute), 108
fc_num_input (dicee.models.AConvO attribute), 120
fc_num_input (dicee.models.AConvQ attribute), 115
fc_num_input (dicee.models.complex.AConEx attribute), 68
fc num input (dicee.models.complex.ConEx attribute), 68
fc_num_input (dicee.models.ConEx attribute), 107
fc_num_input (dicee.models.ConvO attribute), 120
fc_num_input (dicee.models.ConvQ attribute), 114
fc_num_input (dicee.models.octonion.AConvO attribute), 77
fc_num_input (dicee.models.octonion.ConvO attribute), 77
fc_num_input (dicee.models.quaternion.AConvQ attribute), 82
fc_num_input (dicee.models.quaternion.ConvQ attribute), 81
feature_map_dropout (dicee.AConEx attribute), 174
feature_map_dropout (dicee.AConvO attribute), 174
feature_map_dropout (dicee.AConvQ attribute), 175
feature_map_dropout (dicee.ConEx attribute), 177
feature_map_dropout (dicee.ConvO attribute), 177
feature_map_dropout (dicee.ConvQ attribute), 175
feature_map_dropout (dicee.models.AConEx attribute), 108
feature_map_dropout (dicee.models.AConvO attribute), 121
feature_map_dropout (dicee.models.AConvQ attribute), 115
feature_map_dropout (dicee.models.complex.AConEx attribute), 68
feature_map_dropout (dicee.models.complex.ConEx attribute), 68
feature_map_dropout (dicee.models.ConEx attribute), 107
```

```
feature_map_dropout (dicee.models.ConvO attribute), 120
feature_map_dropout (dicee.models.ConvQ attribute), 114
feature_map_dropout (dicee.models.octonion.AConvO attribute), 78
feature_map_dropout (dicee.models.octonion.ConvO attribute), 77
feature_map_dropout (dicee.models.quaternion.AConvQ attribute), 82
feature_map_dropout (dicee.models.quaternion.ConvQ attribute), 81
feature_map_dropout_rate (dicee.BaseKGE attribute), 185
feature_map_dropout_rate (dicee.config.Namespace attribute), 28
feature_map_dropout_rate (dicee.models.base_model.BaseKGE attribute), 58
feature_map_dropout_rate (dicee.models.BaseKGE attribute), 99, 102, 106, 110, 116, 129, 132
fill_query() (dicee.query_generator.QueryGenerator method), 139
fill_query() (dicee.QueryGenerator method), 207
find_good_batch_size() (in module dicee.trainer.model_parallelism), 157
find_missing_triples() (dicee.KGE method), 194
find_missing_triples() (dicee.knowledge_graph_embeddings.KGE method), 49
fit () (dicee.trainer.model_parallelism.TensorParallel method), 157
fit () (dicee.trainer.torch_trainer_ddp.TorchDDPTrainer method), 159
fit () (dicee.trainer.torch_trainer.TorchTrainer method), 158
flash (dicee.models.transformers.CausalSelfAttention attribute), 87
FMult (class in dicee.models), 134
FMult (class in dicee.models.function_space), 72
FMult2 (class in dicee.models), 134
FMult2 (class in dicee.models.function_space), 73
form_of_labelling (dicee.DICE_Trainer attribute), 189
form_of_labelling (dicee.trainer.DICE_Trainer attribute), 160
form_of_labelling (dicee.trainer.dice_trainer.DICE_Trainer attribute), 155
forward() (dicee.BaseKGE method), 186
forward() (dicee.BytE method), 183
{\tt forward()} \ ({\it dicee.models.base\_model.BaseKGE\ method}), 59
forward() (dicee.models.base_model.IdentityClass static method), 60
forward() (dicee.models.BaseKGE method), 100, 103, 106, 111, 117, 130, 133
forward() (dicee.models.IdentityClass static method), 101, 112, 118
forward() (dicee.models.transformers.Block method), 89
forward() (dicee.models.transformers.BytE method), 85
forward() (dicee.models.transformers.CausalSelfAttention method), 87
forward() (dicee.models.transformers.GPT method), 90
forward() (dicee.models.transformers.LayerNorm method), 86
forward() (dicee.models.transformers.MLP method), 88
\verb|forward_backward_update()| \textit{(dicee.trainer.torch\_trainer.TorchTrainer method)}, 158
forward_backward_update_loss() (in module dicee.trainer.model_parallelism), 157
forward_byte_pair_encoded_k_vs_all() (dicee.BaseKGE method), 186
forward_byte_pair_encoded_k_vs_all() (dicee.models.base_model.BaseKGE method), 58
forward_byte_pair_encoded_k_vs_all() (dicee.models.BaseKGE method), 99, 102, 106, 111, 117, 129, 133
forward_byte_pair_encoded_triple() (dicee.BaseKGE method), 186
forward_byte_pair_encoded_triple() (dicee.models.base_model.BaseKGE method), 58
forward_byte_pair_encoded_triple() (dicee.models.BaseKGE method), 99, 103, 106, 111, 117, 129, 133
forward_k_vs_all() (dicee.AConEx method), 174
forward_k_vs_all() (dicee.AConvO method), 174
forward_k_vs_all() (dicee.AConvQ method), 175
forward_k_vs_all() (dicee.BaseKGE method), 186
forward_k_vs_all() (dicee.ComplEx method), 173
forward_k_vs_all() (dicee.ConEx method), 177
forward_k_vs_all() (dicee.ConvO method), 177
forward_k_vs_all() (dicee.ConvQ method), 176
forward_k_vs_all() (dicee.DeCaL method), 170
forward_k_vs_all() (dicee.DistMult method), 165
forward_k_vs_all() (dicee.DualE method), 172
forward_k_vs_all() (dicee.Keci method), 167
forward_k_vs_all() (dicee.models.AConEx method), 108
forward_k_vs_all() (dicee.models.AConvO method), 121
forward_k_vs_all() (dicee.models.AConvQ method), 115
forward_k_vs_all() (dicee.models.base_model.BaseKGE method), 59
forward_k_vs_all() (dicee.models.BaseKGE method), 100, 103, 107, 111, 117, 130, 133
forward_k_vs_all() (dicee.models.clifford.DeCaL method), 65
forward_k_vs_all() (dicee.models.clifford.Keci method), 63
forward_k_vs_all() (dicee.models.ComplEx method), 109
forward_k_vs_all() (dicee.models.complex.AConEx method), 68
forward_k_vs_all() (dicee.models.complex.ComplEx method), 69
```

```
forward k vs all() (dicee.models.complex.ConEx method), 68
forward_k_vs_all() (dicee.models.ConEx method), 107
forward_k_vs_all() (dicee.models.ConvO method), 120
forward_k_vs_all() (dicee.models.ConvQ method), 114
forward_k_vs_all() (dicee.models.DeCaL method), 126
forward_k_vs_all() (dicee.models.DistMult method), 104
forward_k_vs_all() (dicee.models.DualE method), 137
forward k vs all() (dicee.models.dualE.DualE method), 70
forward_k_vs_all() (dicee.models.Keci method), 123
forward_k_vs_all() (dicee.models.octonion.AConvO method), 78
forward_k_vs_all() (dicee.models.octonion.ConvO method), 77
{\tt forward\_k\_vs\_all()} \ (\textit{dicee.models.octonion.OMult method}), 76
forward_k_vs_all() (dicee.models.OMult method), 119
forward_k_vs_all() (dicee.models.pykeen_models.PykeenKGE method), 78
forward_k_vs_all() (dicee.models.PykeenKGE method), 131
forward_k_vs_all() (dicee.models.QMult method), 114
forward_k_vs_all() (dicee.models.quaternion.AConvQ method), 82
forward_k_vs_all() (dicee.models.quaternion.ConvQ method), 81
forward_k_vs_all() (dicee.models.quaternion.QMult method), 81
forward_k_vs_all() (dicee.models.real.DistMult method), 83
forward_k_vs_all() (dicee.models.real.Shallom method), 83
forward_k_vs_all() (dicee.models.real.TransE method). 83
forward_k_vs_all() (dicee.models.Shallom method), 104
{\tt forward\_k\_vs\_all()} \ (\textit{dicee.models.TransE method}), \, 104
forward_k_vs_all() (dicee.OMult method), 180
forward_k_vs_all() (dicee.PykeenKGE method), 182
forward_k_vs_all() (dicee.QMult method), 179
forward_k_vs_all() (dicee.Shallom method), 180
{\tt forward\_k\_vs\_all()} \ (\textit{dicee.TransE method}), \, 168
forward_k_vs_sample() (dicee.AConEx method), 174
forward_k_vs_sample() (dicee.BaseKGE method), 186
forward_k_vs_sample() (dicee.ComplEx method), 173
forward_k_vs_sample() (dicee.ConEx method), 177
forward_k_vs_sample() (dicee.DistMult method), 165
forward_k_vs_sample() (dicee.Keci method), 167
forward_k_vs_sample() (dicee.models.AConEx method), 108
forward k vs sample() (dicee.models.base model.BaseKGE method), 59
forward_k_vs_sample() (dicee.models.BaseKGE method), 100, 103, 107, 111, 117, 130, 133
forward_k_vs_sample() (dicee.models.clifford.Keci method), 63
forward_k_vs_sample() (dicee.models.ComplEx method), 109
forward_k_vs_sample() (dicee.models.complex.AConEx method), 68
forward_k_vs_sample() (dicee.models.complex.ComplEx method), 69
forward_k_vs_sample() (dicee.models.complex.ConEx method), 68
forward_k_vs_sample() (dicee.models.ConEx method), 107
forward_k_vs_sample() (dicee.models.DistMult method), 104
forward_k_vs_sample() (dicee.models.Keci method), 124
forward_k_vs_sample() (dicee.models.pykeen_models.PykeenKGE method), 79
forward_k_vs_sample() (dicee.models.PykeenKGE method), 131
forward_k_vs_sample() (dicee.models.QMult method), 114
forward_k_vs_sample() (dicee.models.quaternion.QMult method), 81
forward_k_vs_sample() (dicee.models.real.DistMult method), 83
forward_k_vs_sample() (dicee.PykeenKGE method), 182
forward_k_vs_sample() (dicee.QMult method), 179
forward_k_vs_with_explicit() (dicee. Keci method), 167
forward_k_vs_with_explicit() (dicee.models.clifford.Keci method), 62
forward_k_vs_with_explicit() (dicee.models.Keci method), 123
forward_triples() (dicee.AConEx method), 174
forward_triples() (dicee.AConvO method), 174
forward_triples() (dicee.AConvQ method), 175
forward_triples() (dicee.BaseKGE method), 186
forward triples() (dicee.ConEx method), 177
forward_triples() (dicee.ConvO method), 177
forward_triples() (dicee.ConvQ method), 176
forward_triples() (dicee.DeCaL method), 169
forward_triples() (dicee.DualE method), 172
forward_triples() (dicee.Keci method), 168
forward_triples() (dicee.LFMult method), 180
forward_triples() (dicee.models.AConEx method), 108
```

```
forward triples() (dicee.models.AConvO method), 121
forward_triples() (dicee.models.AConvQ method), 115
forward triples() (dicee.models.base model.BaseKGE method), 59
forward_triples() (dicee.models.BaseKGE method), 100, 103, 106, 111, 117, 130, 133
{\tt forward\_triples()} \ \textit{(dicee.models.clifford.DeCaL method)}, 64
forward_triples() (dicee.models.clifford.Keci method), 63
forward_triples() (dicee.models.complex.AConEx method), 68
forward triples() (dicee.models.complex.ConEx method), 68
forward_triples() (dicee.models.ConEx method), 107
forward_triples() (dicee.models.ConvO method), 120
forward_triples() (dicee.models.ConvQ method), 114
forward_triples() (dicee.models.DeCaL method), 125
forward_triples() (dicee.models.DualE method), 137
forward_triples() (dicee.models.dualE.DualE method), 70
forward_triples() (dicee.models.FMult method), 134
forward_triples() (dicee.models.FMult2 method), 135
forward_triples() (dicee.models.function_space.FMult method), 72
forward_triples() (dicee.models.function_space.FMult2 method), 73
forward_triples() (dicee.models.function_space.GFMult method), 73
forward_triples() (dicee.models.function_space.LFMult method), 74
forward_triples() (dicee.models.function_space.LFMult1 method), 73
forward_triples() (dicee.models.GFMult method), 134
forward_triples() (dicee.models.Keci method), 124
forward_triples() (dicee.models.LFMult method), 136
forward_triples() (dicee.models.LFMult1 method), 135
forward_triples() (dicee.models.octonion.AConvO method), 78
forward_triples() (dicee.models.octonion.ConvO method), 77
forward_triples() (dicee.models.Pyke method), 104
forward_triples() (dicee.models.pykeen_models.PykeenKGE method), 79
forward_triples() (dicee.models.PykeenKGE method), 131
forward_triples() (dicee.models.quaternion.AConvQ method), 82
forward triples() (dicee.models.quaternion.ConvO method), 81
forward_triples() (dicee.models.real.Pyke method), 83
forward_triples() (dicee.models.real.Shallom method), 83
forward_triples() (dicee.models.Shallom method), 104
forward_triples() (dicee.Pyke method), 164
forward triples() (dicee.PykeenKGE method), 182
forward_triples() (dicee.Shallom method), 180
frequency (dicee.callbacks.Perturb attribute), 25
from_pretrained() (dicee.models.transformers.GPT class method), 90
from_pretrained_model_write_embeddings_into_csv() (in module dicee), 189
from_pretrained_model_write_embeddings_into_csv() (in module dicee.static_funcs), 153
full_storage_path (dicee.analyse_experiments.Experiment attribute), 18
func_triple_to_bpe_representation (dicee.evaluator.Evaluator attribute), 41
func_triple_to_bpe_representation() (dicee.knowledge_graph.KG method), 46
function() (dicee.models.FMult2 method), 135
function() (dicee.models.function_space.FMult2 method), 73
G
gamma (dicee.models.FMult attribute), 134
gamma (dicee.models.function_space.FMult attribute), 72
gelu (dicee.models.transformers.MLP attribute), 88
gen_test (dicee.query_generator.QueryGenerator attribute), 138
gen_test (dicee.QueryGenerator attribute), 207
gen_valid (dicee.query_generator.QueryGenerator attribute), 138
gen_valid (dicee.QueryGenerator attribute), 207
generate() (dicee.BytE method), 183
generate() (dicee.KGE method), 190
generate() (dicee.knowledge_graph_embeddings.KGE method), 46
generate() (dicee.models.transformers.BytE method), 85
generate_queries() (dicee.query_generator.QueryGenerator method), 139
generate_queries() (dicee.QueryGenerator method), 207
get_aswa_state_dict() (dicee.callbacks.ASWA method), 23
get_bpe_head_and_relation_representation() (dicee.BaseKGE method), 187
\verb|get_bpe_head_and_relation_representation()| \textit{(dicee.models.base\_model.BaseKGE method)}, 59|
get_bpe_head_and_relation_representation() (dicee.models.BaseKGE method), 100, 103, 107, 111, 117, 130, 133
get_bpe_token_representation() (dicee.abstracts.BaseInteractiveKGE method), 14
```

```
get callbacks() (in module dicee.trainer.dice trainer), 155
get_default_arguments() (in module dicee.analyse_experiments), 18
get_default_arguments() (in module dicee.scripts.index_serve), 148
get_default_arguments() (in module dicee.scripts.run), 150
get_ee_vocab() (in module dicee), 187
get_ee_vocab() (in module dicee.read_preprocess_save_load_kg.util), 144
get_ee_vocab() (in module dicee.static_funcs), 151
get ee vocab () (in module dicee.static preprocess funcs), 154
get_embeddings() (dicee.BaseKGE method), 187
get_embeddings() (dicee.EnsembleKGE method), 187
get_embeddings() (dicee.models.base_model.BaseKGE method), 59
get_embeddings() (dicee.models.BaseKGE method), 100, 103, 107, 111, 117, 130, 133
get_embeddings() (dicee.models.ensemble.EnsembleKGE method), 71
get_embeddings() (dicee.models.real.Shallom method), 83
get_embeddings() (dicee.models.Shallom method), 104
get_embeddings() (dicee.Shallom method), 180
get_entity_embeddings() (dicee.abstracts.BaseInteractiveKGE method), 15
get_entity_index() (dicee.abstracts.BaseInteractiveKGE method), 14
get_er_vocab() (in module dicee), 187
get_er_vocab() (in module dicee.read_preprocess_save_load_kg.util), 144
get_er_vocab() (in module dicee.static_funcs), 151
get_er_vocab() (in module dicee.static_preprocess_funcs), 154
get_eval_report() (dicee.abstracts.BaseInteractiveKGE method), 14
get_head_relation_representation() (dicee.BaseKGE method), 186
qet_head_relation_representation() (dicee.models.base_model.BaseKGE method), 59
get_head_relation_representation() (dicee.models.BaseKGE method), 100, 103, 107, 111, 117, 130, 133
get_kronecker_triple_representation() (dicee.callbacks.KronE method), 25
get_num_params() (dicee.models.transformers.GPT method), 90
\verb|get_padded_bpe_triple_representation()| \textit{(dicee.abstracts.BaseInteractiveKGE method)}, 14
get_queries() (dicee.query_generator.QueryGenerator method), 139
get_queries() (dicee.QueryGenerator method), 207
get re vocab () (in module dicee), 187
get_re_vocab() (in module dicee.read_preprocess_save_load_kg.util), 144
get_re_vocab() (in module dicee.static_funcs), 151
get_re_vocab() (in module dicee.static_preprocess_funcs), 154
\verb|get_relation_embeddings()| \textit{(dicee.abstracts.BaseInteractiveKGE method)}, 15
get relation index() (dicee.abstracts.BaseInteractiveKGE method), 14
get_sentence_representation() (dicee.BaseKGE method), 186
get_sentence_representation() (dicee.models.base_model.BaseKGE method), 59
get_sentence_representation() (dicee.models.BaseKGE method), 100, 103, 107, 111, 117, 130, 133
\verb"get_transductive_entity_embeddings"() \textit{ (dicee.KGE method)}, 190
get_transductive_entity_embeddings() (dicee.knowledge_graph_embeddings.KGE method), 46
get_triple_representation() (dicee.BaseKGE method), 186
get_triple_representation() (dicee.models.base_model.BaseKGE method), 59
get_triple_representation() (dicee.models.BaseKGE method), 100, 103, 107, 111, 117, 130, 133
GFMult (class in dicee.models), 134
GFMult (class in dicee.models.function_space), 72
global_rank (dicee.abstracts.AbstractTrainer attribute), 12
global_rank (dicee.trainer.torch_trainer_ddp.NodeTrainer attribute), 159
GPT (class in dicee.models.transformers), 89
GPTConfig (class in dicee.models.transformers), 89
gpus (dicee.config.Namespace attribute), 26
gradient_accumulation_steps (dicee.config.Namespace attribute), 27
ground_queries() (dicee.query_generator.QueryGenerator method), 139
ground_queries() (dicee.QueryGenerator method), 207
Н
hidden_dropout (dicee.BaseKGE attribute), 186
hidden_dropout (dicee.models.base_model.BaseKGE attribute), 58
hidden_dropout (dicee.models.BaseKGE attribute), 99, 102, 106, 110, 116, 129, 132
hidden_dropout_rate (dicee.BaseKGE attribute), 185
hidden_dropout_rate (dicee.config.Namespace attribute), 28
hidden_dropout_rate (dicee.models.base_model.BaseKGE attribute), 58
hidden_dropout_rate (dicee.models.BaseKGE attribute), 99, 102, 105, 110, 116, 129, 132
hidden_normalizer (dicee.BaseKGE attribute), 186
hidden_normalizer (dicee.models.base_model.BaseKGE attribute), 58
hidden_normalizer (dicee.models.BaseKGE attribute), 99, 102, 106, 110, 116, 129, 132
```

```
I
IdentityClass (class in dicee.models), 100, 112, 117
IdentityClass (class in dicee.models.base_model), 59
idx_entity_to_bpe_shaped (dicee.knowledge_graph.KG attribute), 45
index() (in module dicee.scripts.index_serve), 148
index_triple() (dicee.abstracts.BaseInteractiveKGE method), 15
init_dataloader() (dicee.DICE_Trainer method), 190
init\_dataloader() (dicee.trainer.DICE_Trainer method), 161
init_dataloader() (dicee.trainer.dice_trainer.DICE_Trainer method), 156
init_dataset() (dicee.DICE_Trainer method), 190
init_dataset() (dicee.trainer.DICE_Trainer method), 161
init_dataset() (dicee.trainer.dice_trainer.DICE_Trainer method), 156
init_param (dicee.config.Namespace attribute), 27
init_params_with_sanity_checking() (dicee.BaseKGE method), 186
init_params_with_sanity_checking() (dicee.models.base_model.BaseKGE method), 59
init_params_with_sanity_checking() (dicee.models.BaseKGE method), 99, 103, 106, 111, 117, 129, 133
initial_eval_setting (dicee.callbacks.ASWA attribute), 22
\verb|initialize_or_load_model()| \textit{(dicee.DICE\_Trainer method)}, 190
initialize_or_load_model() (dicee.trainer.DICE_Trainer method), 161
initialize_or_load_model() (dicee.trainer.dice_trainer.DICE_Trainer method), 156
initialize_trainer() (dicee.DICE_Trainer method), 190
initialize_trainer() (dicee.trainer.DICE_Trainer method), 160
initialize_trainer() (dicee.trainer.dice_trainer.DICE_Trainer method), 156
initialize_trainer() (in module dicee.trainer.dice_trainer), 155
input_dp_ent_real (dicee.BaseKGE attribute), 186
input_dp_ent_real (dicee.models.base_model.BaseKGE attribute), 58
input_dp_ent_real (dicee.models.BaseKGE attribute), 99, 102, 106, 110, 116, 129, 132
input_dp_rel_real (dicee.BaseKGE attribute), 186
input_dp_rel_real (dicee.models.base_model.BaseKGE attribute), 58
input_dp_rel_real (dicee.models.BaseKGE attribute), 99, 102, 106, 110, 116, 129, 132
input_dropout_rate (dicee.BaseKGE attribute), 185
input_dropout_rate (dicee.config.Namespace attribute), 28
input_dropout_rate (dicee.models.base_model.BaseKGE attribute), 58
input_dropout_rate (dicee.models.BaseKGE attribute), 99, 102, 105, 110, 116, 129, 132
intialize_model() (in module dicee), 188
intialize_model() (in module dicee.static_funcs), 152
is_continual_training (dicee.DICE_Trainer attribute), 189
is_continual_training (dicee.evaluator.Evaluator attribute), 41
is_continual_training (dicee.Execute attribute), 194
is_continual_training (dicee.executer.Execute attribute), 43
is_continual_training (dicee.trainer.DICE_Trainer attribute), 160
is_continual_training (dicee.trainer.dice_trainer.DICE_Trainer attribute), 155
is_global_zero (dicee.abstracts.AbstractTrainer attribute), 12
is_seen() (dicee.abstracts.BaseInteractiveKGE method), 14
is_spargl_endpoint_alive() (in module dicee.sanity_checkers), 146
k (dicee.models.FMult attribute), 134
k (dicee.models.FMult2 attribute), 135
k (dicee.models.function_space.FMult attribute), 72
k (dicee.models.function_space.FMult2 attribute), 73
k (dicee.models.function_space.GFMult attribute), 72
k (dicee.models.GFMult attribute), 134
k_fold_cross_validation() (dicee.DICE_Trainer method), 190
k_fold_cross_validation() (dicee.trainer.DICE_Trainer method), 161
k_fold_cross_validation() (dicee.trainer.dice_trainer.DICE_Trainer method), 156
k_vs_all_score() (dicee.ComplEx static method), 173
k_vs_all_score() (dicee.DistMult method), 164
k_vs_all_score() (dicee.Keci method), 167
k_vs_all_score() (dicee.models.clifford.Keci method), 63
k_vs_all_score() (dicee.models.ComplEx static method), 109
k_vs_all_score() (dicee.models.complex.ComplEx static method), 69
k_vs_all_score() (dicee.models.DistMult method), 103
k_vs_all_score() (dicee.models.Keci method), 123
k_vs_all_score() (dicee.models.octonion.OMult method), 76
k_vs_all_score() (dicee.models.OMult method), 119
k_vs_all_score() (dicee.models.QMult method), 114
```

```
k vs all score() (dicee.models.quaternion.QMult method), 81
k_vs_all_score() (dicee.models.real.DistMult method), 82
k_vs_all_score() (dicee.OMult method), 180
k_vs_all_score() (dicee.QMult method), 179
Keci (class in dicee), 165
Keci (class in dicee.models), 121
Keci (class in dicee.models.clifford), 60
kernel size (dicee.BaseKGE attribute), 185
kernel_size (dicee.config.Namespace attribute), 27
kernel_size (dicee.models.base_model.BaseKGE attribute), 58
kernel_size (dicee.models.BaseKGE attribute), 99, 102, 106, 110, 116, 129, 132
KG (class in dicee.knowledge_graph), 44
kg (dicee.callbacks.PseudoLabellingCallback attribute), 22
kg (dicee.read_preprocess_save_load_kg.LoadSaveToDisk attribute), 146
kg (dicee.read_preprocess_save_load_kg.PreprocessKG attribute), 145
kg (dicee.read_preprocess_save_load_kg.preprocess.PreprocessKG attribute), 139
kg (dicee.read_preprocess_save_load_kg.read_from_disk.ReadFromDisk attribute), 140
kg (dicee.read_preprocess_save_load_kg.ReadFromDisk attribute), 146
kg (dicee.read_preprocess_save_load_kg.save_load_disk.LoadSaveToDisk attribute), 141
KGE (class in dicee), 190
KGE (class in dicee.knowledge_graph_embeddings), 46
KGESaveCallback (class in dicee.callbacks), 21
knowledge_graph (dicee.Execute attribute), 194
knowledge_graph (dicee.executer.Execute attribute), 43
KronE (class in dicee.callbacks), 24
KvsAll (class in dicee), 198
KvsAll (class in dicee.dataset_classes), 31
kvsall_score() (dicee.DualE method), 172
kvsall_score() (dicee.models.DualE method), 137
kvsall_score() (dicee.models.dualE.DualE method), 70
KvsSampleDataset (class in dicee), 201
KvsSampleDataset (class in dicee.dataset_classes), 34
label_smoothing_rate (dicee.AllvsAll attribute), 199
label_smoothing_rate (dicee.config.Namespace attribute), 27
label_smoothing_rate (dicee.dataset_classes.AllvsAll attribute), 33
label_smoothing_rate (dicee.dataset_classes.KvsAll attribute), 32
label_smoothing_rate (dicee.dataset_classes.KvsSampleDataset attribute), 35
label_smoothing_rate (dicee.dataset_classes.OnevsSample attribute), 34
label_smoothing_rate (dicee.dataset_classes.TriplePredictionDataset attribute), 36
label_smoothing_rate (dicee.KvsAll attribute), 198
label_smoothing_rate (dicee.KvsSampleDataset attribute), 201
label_smoothing_rate (dicee.OnevsSample attribute), 200
{\tt label\_smoothing\_rate}~(\textit{dicee.TriplePredictionDataset attribute}), 203
LayerNorm (class in dicee.models.transformers), 86
learning_rate (dicee.BaseKGE attribute), 185
learning rate (dicee.models.base model.BaseKGE attribute), 58
learning_rate (dicee.models.BaseKGE attribute), 99, 102, 105, 110, 116, 129, 132
length (dicee.dataset_classes.NegSampleDataset attribute), 36
length (dicee.dataset_classes.TriplePredictionDataset attribute), 36
length (dicee.NegSampleDataset attribute), 202
length (dicee. Triple Prediction Dataset attribute), 203
level (dicee.callbacks.Perturb attribute), 25
LFMult (class in dicee), 180
LFMult (class in dicee.models), 135
LFMult (class in dicee.models.function_space), 74
LFMult1 (class in dicee.models), 135
LFMult1 (class in dicee.models.function_space), 73
linear() (dicee.LFMult method), 181
linear() (dicee.models.function_space.LFMult method), 74
linear() (dicee.models.LFMult method), 136
list2tuple() (dicee.query_generator.QueryGenerator method), 138
list2tuple() (dicee.QueryGenerator method), 207
lm_head (dicee.BytE attribute), 183
lm_head (dicee.models.transformers.BytE attribute), 85
lm_head (dicee.models.transformers.GPT attribute), 90
```

```
1n 1 (dicee.models.transformers.Block attribute), 89
ln_2 (dicee.models.transformers.Block attribute), 89
load() (dicee.read_preprocess_save_load_kg.LoadSaveToDisk method), 146
load() (dicee.read_preprocess_save_load_kg.save_load_disk.LoadSaveToDisk method), 141
load_json() (in module dicee), 188
load_json() (in module dicee.static_funcs), 152
load_model() (in module dicee), 188
load model () (in module dicee.static funcs), 151
load_model_ensemble() (in module dicee), 188
load_model_ensemble() (in module dicee.static_funcs), 151
load_numpy() (in module dicee), 189
load_numpy() (in module dicee.static_funcs), 152
load_numpy_ndarray() (in module dicee.read_preprocess_save_load_kg.util), 144
load_pickle() (in module dicee), 187
load_pickle() (in module dicee.read_preprocess_save_load_kg.util), 145
load_pickle() (in module dicee.static_funcs), 151
load_queries() (dicee.query_generator.QueryGenerator method), 139
load_queries() (dicee.QueryGenerator method), 207
load_queries_and_answers () (dicee.query_generator.QueryGenerator static method), 139
load_queries_and_answers() (dicee.QueryGenerator static method), 208
load_term_mapping() (in module dicee), 188, 195
load_term_mapping() (in module dicee.static_funcs), 151
load_term_mapping() (in module dicee.trainer.dice_trainer), 155
load_with_pandas() (in module dicee.read_preprocess_save_load_kg.util), 144
LoadSaveToDisk (class in dicee.read_preprocess_save_load_kg), 146
LoadSaveToDisk (class in dicee.read_preprocess_save_load_kg.save_load_disk), 141
local_rank (dicee.abstracts.AbstractTrainer attribute), 12
local_rank (dicee.trainer.torch_trainer_ddp.NodeTrainer attribute), 159
loss (dicee.BaseKGE attribute), 185
loss (dicee.models.base_model.BaseKGE attribute), 58
loss (dicee.models.BaseKGE attribute), 99, 102, 106, 110, 116, 129, 132
loss_func (dicee.trainer.torch_trainer_ddp.NodeTrainer attribute), 159
loss_function (dicee.trainer.torch_trainer.TorchTrainer attribute), 157
loss_function() (dicee.BytE method), 183
loss_function() (dicee.models.base_model.BaseKGELightning method), 53
loss_function() (dicee.models.BaseKGELightning method), 94
loss function() (dicee.models.transformers.BytE method), 85
loss_history (dicee.BaseKGE attribute), 186
loss_history (dicee.models.base_model.BaseKGE attribute), 58
loss_history (dicee.models.BaseKGE attribute), 99, 102, 106, 111, 116, 129, 133
loss_history (dicee.models.pykeen_models.PykeenKGE attribute), 78
loss_history (dicee.models.PykeenKGE attribute), 130
loss_history (dicee.PykeenKGE attribute), 182
loss_history (dicee.trainer.torch_trainer_ddp.NodeTrainer attribute), 159
1r (dicee.analyse_experiments.Experiment attribute), 18
1r (dicee.config.Namespace attribute), 26
М
m (dicee.LFMult attribute), 180
m (dicee.models.function_space.LFMult attribute), 74
m (dicee.models.LFMult attribute), 136
main() (in module dicee.scripts.index_serve), 149
main() (in module dicee.scripts.run), 150
make_iterable_verbose() (in module dicee.static_funcs_training), 153
make_iterable_verbose() (in module dicee.trainer.torch_trainer_ddp), 159
mapping_from_first_two_cols_to_third() (in module dicee), 195
mapping_from_first_two_cols_to_third() (in module dicee.static_preprocess_funcs), 154
margin (dicee.models.Pyke attribute), 104
margin (dicee.models.real.Pyke attribute), 83
margin (dicee.models.real.TransE attribute), 83
margin (dicee.models.TransE attribute), 104
margin (dicee. Pyke attribute), 164
margin (dicee. TransE attribute), 168
max_ans_num (dicee.query_generator.QueryGenerator attribute), 138
max_ans_num (dicee.QueryGenerator attribute), 207
max_epochs (dicee.callbacks.KGESaveCallback attribute), 21
max_length_subword_tokens (dicee.BaseKGE attribute), 186
```

```
max_length_subword_tokens (dicee.knowledge_graph.KG attribute), 45
max_length_subword_tokens (dicee.models.base_model.BaseKGE attribute), 58
max_length_subword_tokens (dicee.models.BaseKGE attribute), 99, 102, 106, 111, 117, 129, 133
max_num_of_classes (dicee.dataset_classes.KvsSampleDataset attribute), 35
max_num_of_classes (dicee.KvsSampleDataset attribute), 201
mem_of_model() (dicee.EnsembleKGE method), 187
mem_of_model() (dicee.models.base_model.BaseKGELightning method), 52
mem of model() (dicee.models.BaseKGELightning method), 93
mem_of_model() (dicee.models.ensemble.EnsembleKGE method), 71
method (dicee.callbacks.Perturb attribute), 25
MLP (class in dicee.models.transformers), 87
mlp (dicee.models.transformers.Block attribute), 89
mode (dicee.query_generator.QueryGenerator attribute), 138
mode (dicee.QueryGenerator attribute), 207
model (dicee.config.Namespace attribute), 26
model (dicee.models.pykeen_models.PykeenKGE attribute), 78
model (dicee.models.PykeenKGE attribute), 130
model (dicee.PykeenKGE attribute), 182
model (dicee.trainer.torch_trainer_ddp.NodeTrainer attribute), 159
model (dicee.trainer.torch_trainer.TorchTrainer attribute), 158
model_kwargs (dicee.models.pykeen_models.PykeenKGE attribute), 78
model_kwargs (dicee.models.PykeenKGE attribute), 130
model_kwargs (dicee.PykeenKGE attribute), 181
model_name (dicee.analyse_experiments.Experiment attribute), 18
module
     dicee, 12
     dicee.__main__, 12
     dicee.abstracts, 12
     dicee.analyse_experiments, 17
     dicee.callbacks, 19
     dicee.config, 25
     dicee.dataset_classes, 28
     dicee.eval_static_funcs, 40
     dicee.evaluator, 41
     dicee.executer, 43
     dicee.knowledge_graph,44
     {\tt dicee.knowledge\_graph\_embeddings,46}
     {\tt dicee.models}, 50
     dicee.models.adopt, 50
     dicee.models.base_model, 51
     dicee.models.clifford, 60
     dicee.models.complex, 67
     dicee.models.dualE, 70
     dicee.models.ensemble, 71
     dicee.models.function_space, 72
     {\tt dicee.models.octonion,75}
     dicee.models.pykeen_models, 78
     dicee.models.quaternion, 79
     dicee.models.real, 82
     dicee.models.static_funcs,84
     dicee.models.transformers, 84
     dicee.query_generator, 138
     dicee.read_preprocess_save_load_kg, 139
     dicee.read_preprocess_save_load_kg.preprocess, 139
     dicee.read_preprocess_save_load_kg.read_from_disk, 140
     dicee.read_preprocess_save_load_kg.save_load_disk, 141
     dicee.read_preprocess_save_load_kg.util, 141
     {\tt dicee.sanity\_checkers}, 146
     dicee.scripts, 147
     dicee.scripts.index_serve, 147
     dicee.scripts.run, 149
     dicee.static_funcs, 150
     dicee.static_funcs_training, 153
     dicee.static_preprocess_funcs, 153
     dicee.trainer, 154
     dicee.trainer.dice_trainer, 154
     dicee.trainer.model_parallelism, 156
     dicee.trainer.torch_trainer, 157
```

```
dicee.trainer.torch trainer ddp, 158
modules () (dicee. Ensemble KGE method), 187
modules() (dicee.models.ensemble.EnsembleKGE method), 71
MultiClassClassificationDataset (class in dicee), 197
MultiClassClassificationDataset (class in dicee.dataset_classes), 30
MultiLabelDataset (class in dicee), 196
MultiLabelDataset (class in dicee.dataset_classes), 30
Ν
n (dicee.models.FMult2 attribute), 135
n (dicee.models.function_space.FMult2 attribute), 73
n_embd (dicee.models.transformers.CausalSelfAttention attribute), 87
n_embd (dicee.models.transformers.GPTConfig attribute), 89
n_head (dicee.models.transformers.CausalSelfAttention attribute), 87
n_head (dicee.models.transformers.GPTConfig attribute), 89
n_layer (dicee.models.transformers.GPTConfig attribute), 89
n_layers (dicee.models.FMult2 attribute), 135
n_layers (dicee.models.function_space.FMult2 attribute), 73
name (dicee.abstracts.BaseInteractiveKGE property), 14
name (dicee.AConEx attribute), 173
name (dicee.AConvO attribute), 174
name (dicee.AConvQ attribute), 175
name (dicee.BytE attribute), 183
name (dicee. CKeci attribute), 165
name (dicee.ComplEx attribute), 173
name (dicee.ConEx attribute), 177
name (dicee.ConvO attribute), 176
name (dicee.ConvQ attribute), 175
name (dicee.DeCaL attribute), 169
name (dicee.DistMult attribute), 164
name (dicee.DualE attribute), 172
name (dicee. Ensemble KGE attribute), 187
name (dicee.Keci attribute), 165
name (dicee.LFMult attribute), 180
name (dicee.models.AConEx attribute), 108
name (dicee.models.AConvO attribute), 120
name (dicee.models.AConvQ attribute), 114
name (dicee.models.CKeci attribute), 124
name (dicee.models.clifford.CKeci attribute), 63
name (dicee.models.clifford.DeCaL attribute), 64
name (dicee.models.clifford.Keci attribute), 61
name (dicee.models.ComplEx attribute), 109
name (dicee.models.complex.AConEx attribute), 68
name (dicee.models.complex.ComplEx attribute), 69
name (dicee.models.complex.ConEx attribute), 67
name (dicee.models.ConEx attribute), 107
name (dicee.models.ConvO attribute), 120
name (dicee.models.ConvO attribute), 114
name (dicee.models.DeCaL attribute), 125
name (dicee.models.DistMult attribute), 103
name (dicee.models.DualE attribute), 137
name (dicee.models.dualE.DualE attribute), 70
name (dicee.models.ensemble.EnsembleKGE attribute), 71
name (dicee.models.FMult attribute), 134
name (dicee.models.FMult2 attribute), 135
name (dicee.models.function_space.FMult attribute), 72
name (dicee.models.function_space.FMult2 attribute), 73
name (dicee.models.function_space.GFMult attribute), 72
name (dicee.models.function_space.LFMult attribute), 74
name (dicee.models.function_space.LFMult1 attribute), 73
name (dicee.models.GFMult attribute), 134
name (dicee.models.Keci attribute), 121
name (dicee.models.LFMult attribute), 136
name (dicee.models.LFMult1 attribute), 135
name (dicee.models.octonion.AConvO attribute), 77
name (dicee.models.octonion.ConvO attribute), 77
name (dicee.models.octonion.OMult attribute), 76
```

```
name (dicee.models.OMult attribute), 119
name (dicee.models.Pyke attribute), 104
name (dicee.models.pykeen models.PykeenKGE attribute), 78
name (dicee.models.PykeenKGE attribute), 130
name (dicee.models.QMult attribute), 113
name (dicee.models.quaternion.AConvQ attribute), 82
\verb"name" (\textit{dicee.models.quaternion.ConvQ attribute}), 81
name (dicee.models.quaternion.OMult attribute), 80
name (dicee.models.real.DistMult attribute), 82
name (dicee.models.real.Pyke attribute), 83
name (dicee.models.real.Shallom attribute), 83
name (dicee.models.real.TransE attribute), 83
name (dicee.models.Shallom attribute), 104
name (dicee.models.TransE attribute), 104
name (dicee.models.transformers.BytE attribute), 85
name (dicee.OMult attribute), 180
name (dicee.Pvke attribute), 164
name (dicee.PykeenKGE attribute), 181
name (dicee.QMult attribute), 178
name (dicee.Shallom attribute), 180
name (dicee. TransE attribute), 168
named children() (dicee. Ensemble KGE method), 187
named_children() (dicee.models.ensemble.EnsembleKGE method), 71
Namespace (class in dicee.config), 26
neg_ratio (dicee.BPE_NegativeSamplingDataset attribute), 196
neg_ratio (dicee.config.Namespace attribute), 27
neg_ratio (dicee.dataset_classes.BPE_NegativeSamplingDataset attribute), 30
neg_ratio (dicee.dataset_classes.KvsSampleDataset attribute), 35
neg_ratio (dicee.KvsSampleDataset attribute), 201
neg_sample_ratio (dicee.CVDataModule attribute), 203
neg_sample_ratio (dicee.dataset_classes.CVDataModule attribute), 37
neg sample ratio (dicee.dataset classes.NegSampleDataset attribute), 35
neg_sample_ratio (dicee.dataset_classes.OnevsSample attribute), 33, 34
\verb|neg_sample_ratio| (\textit{dicee.dataset\_classes.TriplePredictionDataset~attribute}), 36
neg_sample_ratio (dicee.NegSampleDataset attribute), 202
neg_sample_ratio (dicee.OnevsSample attribute), 200
neg sample ratio (dicee. TriplePredictionDataset attribute), 203
negnorm() (dicee.KGE method), 193
\verb"negnorm()" (\textit{dicee.knowledge\_graph\_embeddings.KGE method}), 49
NegSampleDataset (class in dicee), 201
NegSampleDataset (class in dicee.dataset_classes), 35
neural_searcher (in module dicee.scripts.index_serve), 148
NeuralSearcher (class in dicee.scripts.index_serve), 148
NodeTrainer (class in dicee.trainer.torch_trainer_ddp), 159
norm_fc1 (dicee.AConEx attribute), 174
norm_fc1 (dicee.AConvO attribute), 174
norm_fc1 (dicee.ConEx attribute), 177
norm_fc1 (dicee.ConvO attribute), 177
norm_fc1 (dicee.models.AConEx attribute), 108
norm_fc1 (dicee.models.AConvO attribute), 121
norm_fc1 (dicee.models.complex.AConEx attribute), 68
norm_fc1 (dicee.models.complex.ConEx attribute), 68
norm_fc1 (dicee.models.ConEx attribute), 107
norm_fc1 (dicee.models.ConvO attribute), 120
norm_fc1 (dicee.models.octonion.AConvO attribute), 78
norm_fc1 (dicee.models.octonion.ConvO attribute), 77
normalization (dicee.analyse_experiments.Experiment attribute), 19
normalization (dicee.config.Namespace attribute), 27
normalize_head_entity_embeddings (dicee.BaseKGE attribute), 186
normalize_head_entity_embeddings (dicee.models.base_model.BaseKGE attribute), 58
normalize_head_entity_embeddings (dicee.models.BaseKGE attribute), 99, 102, 106, 110, 116, 129, 132
normalize_relation_embeddings (dicee.BaseKGE attribute), 186
\verb|normalize_relation_embeddings| \textit{(dicee.models.base\_model.BaseKGE attribute)}, 58
normalize_relation_embeddings (dicee.models.BaseKGE attribute), 99, 102, 106, 110, 116, 129, 132
normalize_tail_entity_embeddings (dicee.BaseKGE attribute), 186
normalize_tail_entity_embeddings (dicee.models.base_model.BaseKGE attribute), 58
normalize_tail_entity_embeddings (dicee.models.BaseKGE attribute), 99, 102, 106, 110, 116, 129, 132
normalizer_class (dicee.BaseKGE attribute), 185
```

```
normalizer class (dicee.models.base model.BaseKGE attribute), 58
normalizer_class (dicee.models.BaseKGE attribute), 99, 102, 106, 110, 116, 129, 132
num_bpe_entities (dicee.BPE_NegativeSamplingDataset attribute), 196
num_bpe_entities (dicee.dataset_classes.BPE_NegativeSamplingDataset attribute), 30
num_bpe_entities (dicee.knowledge_graph.KG attribute), 45
num_core (dicee.config.Namespace attribute), 27
num_datapoints (dicee.BPE_NegativeSamplingDataset attribute), 196
num datapoints (dicee.dataset classes.BPE NegativeSamplingDataset attribute), 30
num_datapoints (dicee.dataset_classes.MultiLabelDataset attribute), 30
num_datapoints (dicee.MultiLabelDataset attribute), 196
num_ent (dicee.DualE attribute), 172
num_ent (dicee.models.DualE attribute), 137
num_ent (dicee.models.dualE.DualE attribute), 70
num_entities (dicee.BaseKGE attribute), 185
num_entities (dicee.CVDataModule attribute), 203
num_entities (dicee.dataset_classes.CVDataModule attribute), 37
num_entities (dicee.dataset_classes.KvsSampleDataset attribute), 35
num_entities (dicee.dataset_classes.NegSampleDataset attribute), 36
num_entities (dicee.dataset_classes.OnevsSample attribute), 33, 34
num_entities (dicee.dataset_classes.TriplePredictionDataset attribute), 36
num_entities (dicee.evaluator.Evaluator attribute), 41
num_entities (dicee.knowledge_graph.KG attribute), 45
num_entities (dicee.KvsSampleDataset attribute), 201
num_entities (dicee.models.base_model.BaseKGE attribute), 58
num_entities (dicee.models.BaseKGE attribute), 98, 102, 105, 110, 116, 128, 132
num_entities (dicee.NegSampleDataset attribute), 202
num_entities (dicee.OnevsSample attribute), 200
num_entities (dicee. TriplePredictionDataset attribute), 203
num_epochs (dicee.abstracts.AbstractPPECallback attribute), 17
num_epochs (dicee.analyse_experiments.Experiment attribute), 18
num_epochs (dicee.callbacks.ASWA attribute), 22
num_epochs (dicee.config.Namespace attribute), 26
num_epochs (dicee.trainer.torch_trainer_ddp.NodeTrainer attribute), 159
num_folds_for_cv (dicee.config.Namespace attribute), 27
num_of_data_points (dicee.dataset_classes.MultiClassClassificationDataset attribute), 31
num_of_data_points (dicee.MultiClassClassificationDataset attribute), 197
num of epochs (dicee.callbacks.PseudoLabellingCallback attribute), 22
num_of_output_channels (dicee.BaseKGE attribute), 185
num_of_output_channels (dicee.config.Namespace attribute), 27
num_of_output_channels (dicee.models.base_model.BaseKGE attribute), 58
num_of_output_channels (dicee.models.BaseKGE attribute), 99, 102, 106, 110, 116, 129, 132
num_params (dicee.analyse_experiments.Experiment attribute), 18
num_relations (dicee.BaseKGE attribute), 185
num_relations (dicee.CVDataModule attribute), 203
num_relations (dicee.dataset_classes.CVDataModule attribute), 37
num_relations (dicee.dataset_classes.NegSampleDataset attribute), 36
num_relations (dicee.dataset_classes.OnevsSample attribute), 33, 34
num_relations (dicee.dataset_classes.TriplePredictionDataset attribute), 36
num_relations (dicee.evaluator.Evaluator attribute), 41
num_relations (dicee.knowledge_graph.KG attribute), 45
num relations (dicee.models.base model.BaseKGE attribute), 58
num_relations (dicee.models.BaseKGE attribute), 98, 102, 105, 110, 116, 128, 132
num_relations (dicee.NegSampleDataset attribute), 202
num_relations (dicee. Onevs Sample attribute), 200
num_relations (dicee. TriplePredictionDataset attribute), 203
num_sample (dicee.models.FMult attribute), 134
num_sample (dicee.models.function_space.FMult attribute), 72
num_sample (dicee.models.function_space.GFMult attribute), 72
num_sample (dicee.models.GFMult attribute), 134
num_tokens (dicee.BaseKGE attribute), 185
num_tokens (dicee.knowledge_graph.KG attribute), 45
num_tokens (dicee.models.base_model.BaseKGE attribute), 58
num_tokens (dicee.models.BaseKGE attribute), 98, 102, 105, 110, 116, 129, 132
num_workers (dicee.CVDataModule attribute), 203
num_workers (dicee.dataset_classes.CVDataModule attribute), 37
numpy_data_type_changer() (in module dicee), 188
numpy_data_type_changer() (in module dicee.static_funcs), 152
```

0 octonion_mul() (in module dicee.models), 118 octonion_mul() (in module dicee.models.octonion), 75 octonion_mul_norm() (in module dicee.models), 118 octonion_mul_norm() (in module dicee.models.octonion), 75 octonion_normalizer() (dicee.AConvO static method), 174 octonion_normalizer() (dicee.ConvO static method), 177 $\verb| octonion_normalizer()| \textit{ (dicee.models. AConvO static method)}, 121$ octonion_normalizer() (dicee.models.ConvO static method), 120 octonion_normalizer() (dicee.models.octonion.AConvO static method), 78 octonion_normalizer() (dicee.models.octonion.ConvO static method), 77 octonion_normalizer() (dicee.models.octonion.OMult static method), 76 $\verb| octonion_normalizer()| \textit{ (dicee.models.OMult static method)}, 119$ octonion_normalizer() (dicee.OMult static method), 180 OMult (class in dicee), 179 OMult (class in dicee.models), 118 OMult (class in dicee.models.octonion), 75 on_epoch_end() (dicee.callbacks.KGESaveCallback method), 22 on_epoch_end() (dicee.callbacks.PseudoLabellingCallback method), 22 $\verb"on_fit_end"()" (\textit{dicee.abstracts.AbstractCallback method}), 16$ on fit end() (dicee.abstracts.AbstractPPECallback method), 17 on_fit_end() (dicee.abstracts.AbstractTrainer method), 13 on_fit_end() (dicee.callbacks.AccumulateEpochLossCallback method), 20 on_fit_end() (dicee.callbacks.ASWA method), 23 on_fit_end() (dicee.callbacks.Eval method), 24 on_fit_end() (dicee.callbacks.KGESaveCallback method), 22 on_fit_end() (dicee.callbacks.PrintCallback method), 20 on_fit_start() (dicee.abstracts.AbstractCallback method), 16 on_fit_start() (dicee.abstracts.AbstractPPECallback method), 17 on_fit_start() (dicee.abstracts.AbstractTrainer method), 12 on_fit_start() (dicee.callbacks.Eval method), 24 $\verb"on_fit_start"() \textit{ (dicee.callbacks.KGES} ave \textit{Callback method}), 21$ on_fit_start() (dicee.callbacks.KronE method), 25 on_fit_start() (dicee.callbacks.PrintCallback method), 20 on_init_end() (dicee.abstracts.AbstractCallback method), 16 on_init_start() (dicee.abstracts.AbstractCallback method), 15 on_train_batch_end() (dicee.abstracts.AbstractCallback method), 16 on_train_batch_end() (dicee.abstracts.AbstractTrainer method), 13 on_train_batch_end() (dicee.callbacks.Eval method), 24 on_train_batch_end() (dicee.callbacks.KGESaveCallback method), 21 $\verb"on_train_batch_end()" (\textit{dicee.callbacks.PrintCallback method}), 20$ on_train_batch_start() (dicee.callbacks.Perturb method), 25 on_train_epoch_end() (dicee.abstracts.AbstractCallback method), 16 on_train_epoch_end() (dicee.abstracts.AbstractTrainer method), 13 on_train_epoch_end() (dicee.callbacks.ASWA method), 23 on_train_epoch_end() (dicee.callbacks.Eval method), 24 on_train_epoch_end() (dicee.callbacks.KGESaveCallback method), 21 on_train_epoch_end() (dicee.callbacks.PrintCallback method), 21 $\verb"on_train_epoch_end"()" (\textit{dicee.models.base_model.BaseKGELightning method}), 53$ on train epoch end() (dicee.models.BaseKGELightning method), 94 OnevsAllDataset (class in dicee), 197 OnevsAllDataset (class in dicee.dataset_classes), 31 OnevsSample (class in dicee), 199 OnevsSample (class in dicee.dataset_classes), 33 optim (dicee.config.Namespace attribute), 26 optimizer (dicee.trainer.torch_trainer_ddp.NodeTrainer attribute), 159 optimizer (dicee.trainer.torch trainer.TorchTrainer attribute), 157 optimizer_name (dicee.BaseKGE attribute), 185 optimizer_name (dicee.models.base_model.BaseKGE attribute), 58 optimizer_name (dicee.models.BaseKGE attribute), 99, 102, 105, 110, 116, 129, 132

Р

p (dicee.config.Namespace attribute), 28

ordered_bpe_entities (dicee.BPE_NegativeSamplingDataset attribute), 196

ordered_bpe_entities (dicee.knowledge_graph.KG attribute), 46 ordered_shaped_bpe_tokens (dicee.knowledge_graph.KG attribute), 45

ordered_bpe_entities (dicee.dataset_classes.BPE_NegativeSamplingDataset attribute), 30

```
p (dicee.DeCaL attribute), 169
p (dicee.Keci attribute), 165
p (dicee.models.clifford.DeCaL attribute), 64
p (dicee.models.clifford.Keci attribute), 61
p (dicee.models.DeCaL attribute), 125
p (dicee.models.Keci attribute), 122
padding (dicee.knowledge_graph.KG attribute), 45
pandas_dataframe_indexer() (in module dicee.read_preprocess_save_load_kg.util), 143
param_init (dicee.BaseKGE attribute), 186
param_init (dicee.models.base_model.BaseKGE attribute), 58
param_init (dicee.models.BaseKGE attribute), 99, 102, 106, 110, 116, 129, 132
parameters () (dicee.abstracts.BaseInteractiveKGE method), 15
parameters () (dicee. Ensemble KGE method), 187
parameters () (dicee.models.ensemble.EnsembleKGE method), 71
path (dicee.abstracts.AbstractPPECallback attribute), 17
path (dicee.callbacks.AccumulateEpochLossCallback attribute), 20
path (dicee.callbacks.ASWA attribute), 22
path (dicee.callbacks.Eval attribute), 23
path (dicee.callbacks.KGESaveCallback attribute), 21
path_dataset_folder (dicee.analyse_experiments.Experiment attribute), 18
path_for_deserialization (dicee.knowledge_graph.KG attribute), 45
path_for_serialization (dicee.knowledge_graph.KG attribute), 45
path_single_kg (dicee.config.Namespace attribute), 26
path_single_kg (dicee.knowledge_graph.KG attribute), 45
path_to_store_single_run (dicee.config.Namespace attribute), 26
Perturb (class in dicee.callbacks), 25
polars_dataframe_indexer() (in module dicee.read_preprocess_save_load_kg.util), 142
poly_NN() (dicee.LFMult method), 180
poly_NN() (dicee.models.function_space.LFMult method), 74
poly_NN() (dicee.models.LFMult method), 136
polynomial() (dicee.LFMult method), 181
polynomial() (dicee.models.function_space.LFMult method), 75
polynomial() (dicee.models.LFMult method), 136
pop () (dicee.LFMult method), 181
pop () (dicee.models.function_space.LFMult method), 75
pop () (dicee.models.LFMult method), 137
pg (dicee.analyse experiments.Experiment attribute), 18
predict() (dicee.KGE method), 192
predict() (dicee.knowledge_graph_embeddings.KGE method), 48
predict_dataloader() (dicee.models.base_model.BaseKGELightning method), 55
\verb|predict_dataloader()| \textit{(dicee.models.BaseKGELightning method)}, 96
predict_missing_head_entity() (dicee.KGE method), 191
predict_missing_head_entity() (dicee.knowledge_graph_embeddings.KGE method), 46
predict_missing_relations() (dicee.KGE method), 191
predict_missing_relations() (dicee.knowledge_graph_embeddings.KGE method), 47
predict_missing_tail_entity() (dicee.KGE method), 191
predict_missing_tail_entity() (dicee.knowledge_graph_embeddings.KGE method), 47
predict_topk() (dicee.KGE method), 192
predict_topk() (dicee.knowledge_graph_embeddings.KGE method), 48
prepare_data() (dicee.CVDataModule method), 205
prepare_data() (dicee.dataset_classes.CVDataModule method), 39
preprocess_with_byte_pair_encoding() (dicee.read_preprocess_save_load_kg.PreprocessKG method), 145
preprocess_with_byte_pair_encoding() (dicee.read_preprocess_save_load_kg.preprocess.PreprocessKG method), 140
preprocess_with_byte_pair_encoding_with_padding() (dicee.read_preprocess_save_load_kg.PreprocessKG method), 145
preprocess_with_byte_pair_encoding_with_padding() (dicee.read_preprocess_save_load_kg.preprocess.PreprocessKG method), 140
preprocess_with_pandas() (dicee.read_preprocess_save_load_kg.PreprocessKG method), 145
preprocess_with_pandas() (dicee.read_preprocess_save_load_kg.preprocess.PreprocessKG method), 140
preprocess_with_polars() (dicee.read_preprocess_save_load_kg.PreprocessKG method), 146
preprocess_with_polars() (dicee.read_preprocess_save_load_kg.preprocess.PreprocessKG method), 140
preprocesses_input_args() (in module dicee.static_preprocess_funcs), 154
PreprocessKG (class in dicee.read_preprocess_save_load_kg), 145
PreprocessKG (class in dicee.read_preprocess_save_load_kg.preprocess), 139
PrintCallback (class in dicee.callbacks), 20
process (dicee.trainer.torch_trainer.TorchTrainer attribute), 158
PseudoLabellingCallback (class in dicee.callbacks), 22
Pyke (class in dicee), 164
Pyke (class in dicee.models), 104
Pyke (class in dicee.models.real), 83
```

```
pykeen_model_kwargs (dicee.config.Namespace attribute), 27
PykeenKGE (class in dicee), 181
PykeenKGE (class in dicee.models), 130
PykeenKGE (class in dicee.models.pykeen_models), 78
Q
q (dicee.config.Namespace attribute), 28
q (dicee.DeCaL attribute), 169
q (dicee.Keci attribute), 165
q (dicee.models.clifford.DeCaL attribute), 64
q (dicee.models.clifford.Keci attribute), 61
q (dicee.models.DeCaL attribute), 125
q (dicee.models.Keci attribute), 122
qdrant_client (dicee.scripts.index_serve.NeuralSearcher attribute), 148
QMult (class in dicee), 177
QMult (class in dicee.models), 112
QMult (class in dicee.models.quaternion), 79
quaternion_mul() (in module dicee.models), 109
quaternion mul() (in module dicee.models.static funcs), 84
quaternion_mul_with_unit_norm() (in module dicee.models), 112
\verb"quaternion_mul_with_unit_norm()" \textit{(in module dicee.models.quaternion)}, 79
quaternion_multiplication_followed_by_inner_product() (dicee.models.QMult method), 113
\verb|quaternion_multiplication_followed_by_inner_product()| \textit{(dicee.models.quaternion.QMult method)}, 80
quaternion_multiplication_followed_by_inner_product() (dicee.QMult method), 178
quaternion_normalizer() (dicee.models.QMult static method), 113
quaternion_normalizer() (dicee.models.quaternion.QMult static method), 80
quaternion_normalizer() (dicee.QMult static method), 178
{\tt queries}~({\it dicee.scripts.index\_serve.StringListRequest~attribute}),~149
query_name_to_struct (dicee.query_generator.QueryGenerator attribute), 138
query_name_to_struct (dicee.QueryGenerator attribute), 207
QueryGenerator (class in dicee), 206
QueryGenerator (class in dicee.query_generator), 138
r (dicee.DeCaL attribute), 169
r (dicee.Keci attribute), 165
r (dicee.models.clifford.DeCaL attribute), 64
r (dicee.models.clifford.Keci attribute), 61
r (dicee.models.DeCaL attribute), 125
r (dicee.models.Keci attribute), 122
random_prediction() (in module dicee), 188
random_prediction() (in module dicee.static_funcs), 152
random_seed (dicee.config.Namespace attribute), 27
ratio (dicee.callbacks.Perturb attribute), 25
re (dicee.DeCaL attribute), 169
re (dicee.models.clifford.DeCaL attribute), 64
re (dicee.models.DeCaL attribute), 125
re_vocab (dicee.evaluator.Evaluator attribute), 41
read_from_disk() (in module dicee.read_preprocess_save_load_kg.util), 144
read_from_triple_store() (in module dicee.read_preprocess_save_load_kg.util), 144
read_only_few (dicee.config.Namespace attribute), 27
read_only_few (dicee.knowledge_graph.KG attribute), 45
read_or_load_kg() (in module dicee), 188
read_or_load_kg() (in module dicee.static_funcs), 152
read_with_pandas() (in module dicee.read_preprocess_save_load_kg.util), 144
read_with_polars() (in module dicee.read_preprocess_save_load_kg.util), 144
ReadFromDisk (class in dicee.read_preprocess_save_load_kg), 146
ReadFromDisk (class in dicee.read_preprocess_save_load_kg.read_from_disk), 140
reducer (dicee.scripts.index_serve.StringListRequest attribute), 149
rel2id (dicee.query_generator.QueryGenerator attribute), 138
rel2id (dicee.QueryGenerator attribute), 207
relation_embeddings (dicee.AConvQ attribute), 175
relation_embeddings (dicee.ConvQ attribute), 175
relation_embeddings (dicee.DeCaL attribute), 169
relation_embeddings (dicee.DualE attribute), 172
relation_embeddings (dicee.LFMult attribute), 180
relation_embeddings (dicee.models.AConvQ attribute), 115
```

```
relation embeddings (dicee.models.clifford.DeCaL attribute), 64
relation_embeddings (dicee.models.ConvQ attribute), 114
relation_embeddings (dicee.models.DeCaL attribute), 125
relation_embeddings (dicee.models.DualE attribute), 137
relation_embeddings (dicee.models.dualE.DualE attribute), 70
relation_embeddings (dicee.models.FMult attribute), 134
relation_embeddings (dicee.models.FMult2 attribute), 135
relation embeddings (dicee.models.function space.FMult attribute), 72
relation_embeddings (dicee.models.function_space.FMult2 attribute), 73
relation_embeddings (dicee.models.function_space.GFMult attribute), 72
relation_embeddings (dicee.models.function_space.LFMult attribute), 74
{\tt relation\_embeddings}~(\textit{dicee.models.function\_space.LFMult1~attribute}), 73
relation_embeddings (dicee.models.GFMult attribute), 134
relation_embeddings (dicee.models.LFMult attribute), 136
relation_embeddings (dicee.models.LFMult1 attribute). 135
relation_embeddings (dicee.models.pykeen_models.PykeenKGE attribute), 78
relation_embeddings (dicee.models.PykeenKGE attribute), 131
relation_embeddings (dicee.models.quaternion.AConvQ attribute), 82
relation_embeddings (dicee.models.quaternion.ConvQ attribute), 81
relation_embeddings (dicee.PykeenKGE attribute), 182
relation_to_idx (dicee.knowledge_graph.KG attribute), 45
relations_str(dicee.knowledge_graph.KG property), 46
reload_dataset() (in module dicee), 195
reload_dataset() (in module dicee.dataset_classes), 29
report (dicee.DICE_Trainer attribute), 189
report (dicee.evaluator.Evaluator attribute), 42
report (dicee. Execute attribute), 194
report (dicee.executer.Execute attribute), 43
report (dicee.trainer.DICE_Trainer attribute), 160
report (dicee.trainer.dice_trainer.DICE_Trainer attribute), 155
reports (dicee.callbacks.Eval attribute), 23
requires_grad_for_interactions (dicee.CKeci attribute), 165
requires_grad_for_interactions (dicee.Keci attribute), 165
requires_grad_for_interactions (dicee.models.CKeci attribute), 124
requires_grad_for_interactions (dicee.models.clifford.CKeci attribute), 63
requires_grad_for_interactions (dicee.models.clifford.Keci attribute), 61
requires grad for interactions (dicee.models.Keci attribute), 122
resid_dropout (dicee.models.transformers.CausalSelfAttention attribute), 87
residual_convolution() (dicee.AConEx method), 174
residual_convolution() (dicee.AConvO method), 174
residual_convolution() (dicee.AConvQ method), 175
residual_convolution() (dicee.ConEx method), 177
residual_convolution() (dicee.ConvO method), 177
residual_convolution() (dicee.ConvQ method), 176
residual_convolution() (dicee.models.AConEx method), 108
residual_convolution() (dicee.models.AConvO method), 121
residual_convolution() (dicee.models.AConvQ method), 115
residual_convolution() (dicee.models.complex.AConEx method), 68
residual_convolution() (dicee.models.complex.ConEx method), 68
residual_convolution() (dicee.models.ConEx method), 107
residual_convolution() (dicee.models.ConvO method), 120
residual_convolution() (dicee.models.ConvQ method), 114
residual_convolution() (dicee.models.octonion.AConvO method), 78
residual_convolution() (dicee.models.octonion.ConvO method), 77
residual_convolution() (dicee.models.quaternion.AConvQ method), 82
residual_convolution() (dicee.models.quaternion.ConvQ method), 81
retrieve_embedding() (dicee.scripts.index_serve.NeuralSearcher method), 148
\verb|retrieve_embeddings()| \textit{(in module dicee.scripts.index\_serve)}, 148
return_multi_hop_query_results() (dicee.KGE method), 193
return_multi_hop_query_results() (dicee.knowledge_graph_embeddings.KGE method), 49
root () (in module dicee.scripts.index_serve), 148
roots (dicee.models.FMult attribute), 134
roots (dicee.models.function_space.FMult attribute), 72
roots (dicee.models.function_space.GFMult attribute), 72
roots (dicee.models.GFMult attribute), 134
runtime (dicee.analyse_experiments.Experiment attribute), 19
```

S

```
sample_counter (dicee.abstracts.AbstractPPECallback attribute), 17
sample_entity() (dicee.abstracts.BaseInteractiveKGE method), 14
sample_relation() (dicee.abstracts.BaseInteractiveKGE method), 14
sample_triples_ratio (dicee.config.Namespace attribute), 27
{\tt sample\_triples\_ratio}~(\textit{dicee.knowledge\_graph.KG attribute}), 45
sanity_checking_with_arguments() (in module dicee.sanity_checkers), 147
save() (dicee.abstracts.BaseInteractiveKGE method), 14
save() (dicee.read_preprocess_save_load_kg.LoadSaveToDisk method), 146
save() (dicee.read_preprocess_save_load_kg.save_load_disk.LoadSaveToDisk method), 141
save_checkpoint() (dicee.abstracts.AbstractTrainer static method), 13
save_checkpoint_model() (in module dicee), 188
{\tt save\_checkpoint\_model()} \ \textit{(in module dicee.static\_funcs)}, 152
save_embeddings() (in module dicee), 188
save_embeddings() (in module dicee.static_funcs), 152
save_embeddings_as_csv (dicee.config.Namespace attribute), 26
save_experiment() (dicee.analyse_experiments.Experiment method), 19
save_model_at_every_epoch (dicee.config.Namespace attribute), 27
save_numpy_ndarray() (in module dicee), 188
save_numpy_ndarray() (in module dicee.read_preprocess_save_load_kg.util), 144
save_numpy_ndarray() (in module dicee.static_funcs), 152
save_pickle() (in module dicee), 187
save_pickle() (in module dicee.read_preprocess_save_load_kg.util), 145
save_pickle() (in module dicee.static_funcs), 151
save_queries() (dicee.query_generator.QueryGenerator method), 139
save_queries() (dicee.QueryGenerator method), 207
save_queries_and_answers() (dicee.query_generator.QueryGenerator static method), 139
save_queries_and_answers() (dicee.QueryGenerator static method), 208
save_trained_model() (dicee.Execute method), 195
save_trained_model() (dicee.executer.Execute method), 43
scalar_batch_NN() (dicee.LFMult method), 181
scalar_batch_NN() (dicee.models.function_space.LFMult method), 74
scalar_batch_NN() (dicee.models.LFMult method), 136
scaler (dicee.callbacks.Perturb attribute), 25
scaler (dicee.trainer.torch_trainer_ddp.NodeTrainer attribute), 159
score () (dicee.ComplEx static method), 173
score() (dicee.DistMult method), 165
score () (dicee. Keci method), 168
score () (dicee.models.clifford.Keci method), 63
score () (dicee.models.ComplEx static method), 109
score () (dicee.models.complex.ComplEx static method), 69
score () (dicee.models.DistMult method), 104
score () (dicee.models.Keci method), 124
score () (dicee.models.octonion.OMult method), 76
score () (dicee.models.OMult method), 119
score () (dicee.models.QMult method), 113
score () (dicee.models.quaternion.QMult method), 81
score() (dicee.models.real.DistMult method), 83
score() (dicee.models.real.TransE method), 83
score () (dicee.models.TransE method), 104
score () (dicee.OMult method), 180
score() (dicee.QMult method), 179
score () (dicee. TransE method), 168
score_func (dicee.models.FMult2 attribute), 135
score_func (dicee.models.function_space.FMult2 attribute), 73
scoring_technique (dicee.analyse_experiments.Experiment attribute), 19
scoring_technique (dicee.config.Namespace attribute), 27
search() (dicee.scripts.index_serve.NeuralSearcher method), 148
search_embeddings() (in module dicee.scripts.index_serve), 148
search_embeddings_batch() (in module dicee.scripts.index_serve), 149
seed (dicee.query_generator.QueryGenerator attribute), 138
seed (dicee. Query Generator attribute), 207
select_model() (in module dicee), 188
select_model() (in module dicee.static_funcs), 151
selected_optimizer (dicee.BaseKGE attribute), 185
\verb|selected_optimizer| (\textit{dicee.models.base\_model.BaseKGE attribute}), 58
selected_optimizer (dicee.models.BaseKGE attribute), 99, 102, 106, 110, 116, 129, 132
separator (dicee.config.Namespace attribute), 27
```

```
separator (dicee.knowledge_graph.KG attribute), 46
sequential_vocabulary_construction() (dicee.read_preprocess_save_load_kg.PreprocessKG method), 146
sequential\_vocabulary\_construction () \ \textit{(dicee.read\_preprocess\_save\_load\_kg.preprocess.PreprocessKG method)}, 140
serve() (in module dicee.scripts.index_serve), 149
set_global_seed() (dicee.query_generator.QueryGenerator method), 138
set_global_seed() (dicee.QueryGenerator method), 207
set_model_eval_mode() (dicee.abstracts.BaseInteractiveKGE method), 14
set model train mode() (dicee.abstracts.BaseInteractiveKGE method), 14
setup() (dicee.CVDataModule method), 204
setup() (dicee.dataset_classes.CVDataModule method), 38
setup_executor() (dicee.Execute method), 194
setup_executor() (dicee.executer.Execute method), 43
Shallom (class in dicee), 180
Shallom (class in dicee.models), 104
Shallom (class in dicee.models.real), 83
shallom (dicee.models.real.Shallom attribute), 83
shallom (dicee.models.Shallom attribute), 104
shallom (dicee.Shallom attribute), 180
\verb|single_hop_query_answering()| \textit{(dicee.KGE method)}, 193
single_hop_query_answering() (dicee.knowledge_graph_embeddings.KGE method), 49
sparql_endpoint (dicee.config.Namespace attribute), 26
sparql_endpoint (dicee.knowledge_graph.KG attribute), 45
start () (dicee.DICE_Trainer method), 190
start () (dicee.Execute method), 195
start () (dicee.executer.Execute method), 44
start() (dicee.read_preprocess_save_load_kg.PreprocessKG method), 145
start() (dicee.read_preprocess_save_load_kg.preprocess.PreprocessKG method), 139
start() (dicee.read_preprocess_save_load_kg.read_from_disk.ReadFromDisk method), 140
start() (dicee.read_preprocess_save_load_kg.ReadFromDisk method), 146
start() (dicee.trainer.DICE_Trainer method), 161
start () (dicee.trainer.dice_trainer.DICE_Trainer method), 156
start time (dicee.callbacks.PrintCallback attribute), 20
start_time (dicee.Execute attribute), 194
start_time (dicee.executer.Execute attribute), 43
step() (dicee.EnsembleKGE method), 187
step() (dicee.models.ADOPT method), 92
step() (dicee.models.adopt.ADOPT method), 51
step() (dicee.models.ensemble.EnsembleKGE method), 71
storage_path (dicee.config.Namespace attribute), 26
storage_path (dicee.DICE_Trainer attribute), 189
storage_path (dicee.trainer.DICE_Trainer attribute), 160
storage_path (dicee.trainer.dice_trainer.DICE_Trainer attribute), 155
store() (in module dicee), 188
store() (in module dicee.static_funcs), 152
store_ensemble() (dicee.abstracts.AbstractPPECallback method), 17
strategy (dicee.abstracts.AbstractTrainer attribute), 12
StringListRequest (class in dicee.scripts.index_serve), 148
swa (dicee.config.Namespace attribute), 28
T() (dicee.DualE method), 172
T() (dicee.models.DualE method), 138
T() (dicee.models.dualE.DualE method), 71
t_conorm() (dicee.KGE method), 193
t_conorm() (dicee.knowledge_graph_embeddings.KGE method), 49
t_norm() (dicee.KGE method), 193
t_norm() (dicee.knowledge_graph_embeddings.KGE method), 49
target_dim (dicee.AllvsAll attribute), 199
target_dim (dicee.dataset_classes.AllvsAll attribute), 33
target_dim (dicee.dataset_classes.MultiLabelDataset attribute), 30
target_dim (dicee.dataset_classes.OnevsAllDataset attribute), 31
target\_dim(dicee.knowledge\_graph.KG attribute), 45
target_dim (dicee.MultiLabelDataset attribute), 196
target_dim (dicee.OnevsAllDataset attribute), 198
temperature (dicee.BytE attribute), 183
temperature (dicee.models.transformers.BytE attribute), 85
tensor_t_norm() (dicee.KGE method), 193
```

```
tensor_t_norm() (dicee.knowledge_graph_embeddings.KGE method), 49
TensorParallel (class in dicee.trainer.model_parallelism), 157
test dataloader() (dicee.models.base model.BaseKGELightning method), 53
test_dataloader() (dicee.models.BaseKGELightning method), 94
test_epoch_end() (dicee.models.base_model.BaseKGELightning method), 53
test_epoch_end() (dicee.models.BaseKGELightning method), 94
test_h1 (dicee.analyse_experiments.Experiment attribute), 19
test h3 (dicee.analyse experiments.Experiment attribute), 19
test_h10 (dicee.analyse_experiments.Experiment attribute), 19
test_mrr (dicee.analyse_experiments.Experiment attribute), 19
test_path (dicee.query_generator.QueryGenerator attribute), 138
test_path (dicee.QueryGenerator attribute), 207
timeit() (in module dicee), 187, 195
timeit() (in module dicee.read_preprocess_save_load_kg.util), 144
timeit() (in module dicee.static_funcs), 151
timeit() (in module dicee.static_preprocess_funcs), 154
to() (dicee.EnsembleKGE method), 187
to() (dicee.KGE method), 190
to() (dicee.knowledge_graph_embeddings.KGE method), 46
to() (dicee.models.ensemble.EnsembleKGE method), 71
to_df() (dicee.analyse_experiments.Experiment method), 19
topk (dicee.BytE attribute), 183
topk (dicee.models.transformers.BytE attribute), 85
topk (dicee.scripts.index_serve.NeuralSearcher attribute), 148
torch_ordered_shaped_bpe_entities (dicee.dataset_classes.MultiLabelDataset attribute), 30
torch_ordered_shaped_bpe_entities (dicee.MultiLabelDataset attribute), 197
TorchDDPTrainer (class in dicee.trainer.torch trainer ddp), 159
TorchTrainer (class in dicee.trainer.torch_trainer), 157
train() (dicee.KGE method), 194
train() (dicee.knowledge_graph_embeddings.KGE method), 50
train() (dicee.trainer.torch_trainer_ddp.NodeTrainer method), 160
train data (dicee, Allys All attribute), 199
train_data (dicee.dataset_classes.AllvsAll attribute), 33
train_data (dicee.dataset_classes.KvsAll attribute), 32
train_data (dicee.dataset_classes.KvsSampleDataset attribute), 35
train_data (dicee.dataset_classes.MultiClassClassificationDataset attribute), 31
train data (dicee.dataset classes.OnevsAllDataset attribute), 31
train_data (dicee.dataset_classes.OnevsSample attribute), 33, 34
train_data (dicee.KvsAll attribute), 198
train_data (dicee.KvsSampleDataset attribute), 201
train_data (dicee.MultiClassClassificationDataset attribute), 197
train_data (dicee.OnevsAllDataset attribute), 197
train_data (dicee. Onevs Sample attribute), 199, 200
train_dataloader() (dicee.CVDataModule method), 203
\verb|train_dataloader()| \textit{(dicee.dataset\_classes.CVDataModule method)}, 37
train_dataloader() (dicee.models.base_model.BaseKGELightning method), 55
train_dataloader() (dicee.models.BaseKGELightning method), 96
train_dataloaders (dicee.trainer.torch_trainer.TorchTrainer attribute), 158
train_dataset_loader (dicee.trainer.torch_trainer_ddp.NodeTrainer attribute), 159
train_h1 (dicee.analyse_experiments.Experiment attribute), 18
train_h3 (dicee.analyse_experiments.Experiment attribute), 18
train_h10 (dicee.analyse_experiments.Experiment attribute), 18
train_indices_target (dicee.dataset_classes.MultiLabelDataset attribute), 30
train_indices_target (dicee.MultiLabelDataset attribute), 196
train_k_vs_all() (dicee.KGE method), 194
{\tt train\_k\_vs\_all()} \ (\textit{dicee.knowledge\_graph\_embeddings.KGE method}), 50
train_mode (dicee.EnsembleKGE attribute), 187
train_mode (dicee.models.ensemble.EnsembleKGE attribute), 71
train_mrr (dicee.analyse_experiments.Experiment attribute), 18
train_path (dicee.query_generator.QueryGenerator attribute), 138
train path (dicee. Ouery Generator attribute), 206
train_set (dicee.BPE_NegativeSamplingDataset attribute), 196
train_set (dicee.dataset_classes.BPE_NegativeSamplingDataset attribute), 29
train_set (dicee.dataset_classes.MultiLabelDataset attribute), 30
train_set (dicee.dataset_classes.NegSampleDataset attribute), 36
train_set (dicee.dataset_classes.TriplePredictionDataset attribute), 36
train_set (dicee.MultiLabelDataset attribute), 196
train_set (dicee.NegSampleDataset attribute), 202
```

```
train set (dicee. TriplePredictionDataset attribute), 203
train_set_idx (dicee.CVDataModule attribute), 203
train_set_idx (dicee.dataset_classes.CVDataModule attribute), 37
train_set_target (dicee.knowledge_graph.KG attribute), 45
train_target (dicee. Allvs All attribute), 199
train_target (dicee.dataset_classes.AllvsAll attribute), 33
train_target (dicee.dataset_classes.KvsAll attribute), 32
train_target (dicee.dataset_classes.KvsSampleDataset attribute), 35
train_target (dicee.KvsAll attribute), 198
train_target (dicee.KvsSampleDataset attribute), 201
train_target_indices (dicee.knowledge_graph.KG attribute), 46
train_triples() (dicee.KGE method), 194
train_triples() (dicee.knowledge_graph_embeddings.KGE method), 50
trained_model (dicee.Execute attribute), 194
trained_model (dicee.executer.Execute attribute), 43
trainer (dicee.config.Namespace attribute), 27
trainer (dicee.DICE_Trainer attribute), 189
trainer (dicee. Execute attribute), 194
trainer (dicee.executer.Execute attribute), 43
trainer (dicee.trainer.DICE_Trainer attribute), 160
trainer (dicee.trainer.dice_trainer.DICE_Trainer attribute), 155
trainer (dicee.trainer.torch_trainer_ddp.NodeTrainer attribute), 159
training_step (dicee.trainer.torch_trainer.TorchTrainer attribute), 158
training_step() (dicee.BytE method), 183
training_step() (dicee.models.base_model.BaseKGELightning method), 52
training_step() (dicee.models.BaseKGELightning method), 93
training_step() (dicee.models.transformers.BytE method), 85
training_step_outputs (dicee.models.base_model.BaseKGELightning attribute), 52
training_step_outputs (dicee.models.BaseKGELightning attribute), 93
training_technique (dicee.knowledge_graph.KG attribute), 45
TransE (class in dicee), 168
TransE (class in dicee.models), 104
TransE (class in dicee.models.real), 83
transfer_batch_to_device() (dicee.CVDataModule method), 204
transfer_batch_to_device() (dicee.dataset_classes.CVDataModule method), 38
transformer (dicee.BytE attribute), 183
transformer (dicee.models.transformers.BytE attribute), 85
transformer (dicee.models.transformers.GPT attribute), 90
trapezoid() (dicee.models.FMult2 method), 135
trapezoid() (dicee.models.function_space.FMult2 method), 73
tri_score() (dicee.LFMult method), 181
tri_score() (dicee.models.function_space.LFMult method), 74
tri_score() (dicee.models.function_space.LFMult1 method), 74
tri_score() (dicee.models.LFMult method), 136
tri_score() (dicee.models.LFMult1 method), 135
triple_score() (dicee.KGE method), 192
triple_score() (dicee.knowledge_graph_embeddings.KGE method), 48
TriplePredictionDataset (class in dicee), 202
TriplePredictionDataset (class in dicee.dataset_classes), 36
tuple2list() (dicee.query_generator.QueryGenerator method), 138
tuple2list() (dicee.QueryGenerator method), 207
unlabelled_size (dicee.callbacks.PseudoLabellingCallback attribute), 22
unmap() (dicee.query_generator.QueryGenerator method), 139
unmap () (dicee. Query Generator method), 207
unmap_query() (dicee.query_generator.QueryGenerator method), 139
unmap_query() (dicee.QueryGenerator method), 207
val_aswa (dicee.callbacks.ASWA attribute), 23
val_dataloader() (dicee.models.base_model.BaseKGELightning method), 54
val_dataloader() (dicee.models.BaseKGELightning method), 95
val_h1 (dicee.analyse_experiments.Experiment attribute), 18
val_h3 (dicee.analyse_experiments.Experiment attribute), 18
val_h10 (dicee.analyse_experiments.Experiment attribute), 18
val_mrr (dicee.analyse_experiments.Experiment attribute), 18
```

```
val_path (dicee.query_generator.QueryGenerator attribute), 138
val_path (dicee.QueryGenerator attribute), 207
validate_knowledge_graph() (in module dicee.sanity_checkers), 146
vocab_preparation() (dicee.evaluator.Evaluator method), 42
vocab_size (dicee.models.transformers.GPTConfig attribute), 89
vocab_to_parquet() (in module dicee), 188
vocab_to_parquet() (in module dicee.static_funcs), 152
vtp_score() (dicee.LFMult method), 181
vtp_score() (dicee.models.function_space.LFMult method), 74
vtp_score() (dicee.models.function_space.LFMult1 method), 74
vtp_score() (dicee.models.LFMult method), 136
vtp_score() (dicee.models.LFMult1 method), 135
W
weight (dicee.models.transformers.LayerNorm attribute), 86
weight_decay (dicee.BaseKGE attribute), 185
weight_decay (dicee.config.Namespace attribute), 27
weight_decay (dicee.models.base_model.BaseKGE attribute), 58
weight_decay (dicee.models.BaseKGE attribute), 99, 102, 106, 110, 116, 129, 132
weights (dicee.models.FMult attribute), 134
{\tt weights}~(\textit{dicee.models.function\_space.FMult~attribute}), 72
weights (dicee.models.function_space.GFMult attribute), 73
weights (dicee.models.GFMult attribute), 134
write_csv_from_model_parallel() (in module dicee), 189
write_csv_from_model_parallel() (in module dicee.static_funcs), 153
write_links() (dicee.query_generator.QueryGenerator method), 139
write_links() (dicee.QueryGenerator method), 207
write_report() (dicee.Execute method), 195
write_report() (dicee.executer.Execute method), 44
Χ
x_values (dicee.LFMult attribute), 180
x_values (dicee.models.function_space.LFMult attribute), 74
```

x_values (dicee.models.LFMult attribute), 136