DICE Embeddings

Release 0.1.3.2

Caglar Demir

Jul 22, 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 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 12 166 167 168 169
Py	thon Module Index	216

Index 217

DICE Embeddings¹: Hardware-agnostic Framework for Large-scale Knowledge Graph Embeddings:

1 Dicee Manual

Version: dicee 0.2.0

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

Publisher and maintainer: Caglar Demir²

Contact: caglar.demir@upb.de

License: OSI Approved :: MIT License

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
```

(continues on next page)

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

For more, please refer to examples/multi_hop_query_answering.

8 Predicting Missing Links

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

9 Downloading Pretrained Models

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

• For more please look at dice-research.org/projects/DiceEmbeddings/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/ init .py	7	0	100%	
dicee/abstracts.py	338	115	66%	112-113,_
			(con	tinues on next page)

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

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

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

→ 114, 261-356, 363-414, 442, 465-468

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

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

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

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

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

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

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

(continues on next page)

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

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

→452, 470-474, 491-494, 498-503, 507-511, 515-516, 522-524, 539-553, 558-561, 566-
\hookrightarrow 569, 578-629, 634-646, 663-680, 683-691, 695-713, 724
dicee/static_funcs_training.py
                                                              155
                                                                       66
                                                                             57%
                                                                                    7-10, _
⇔222-319, 327-328
dicee/static_preprocess_funcs.py
                                                               98
                                                                       43
                                                                             56%
                                                                                    17-25, _
\hookrightarrow 50, 57, 59, 70, 83-107, 112-115, 120-123, 128-131
                                                                        0
                                                                            100%
dicee/trainer/__init__.py
                                                                                    22, 30-
dicee/trainer/dice_trainer.py
                                                              151
                                                                       18
                                                                             88%
\Rightarrow31, 33-35, 97, 104, 109-114, 152, 237, 280-283
dicee/trainer/model_parallelism.py
                                                               99
                                                                       87
                                                                             12%
                                                                                    10-25, _
\hookrightarrow 30-116, 121-132, 136, 141-197
                                                                                    31, 102, _
dicee/trainer/torch_trainer.py
                                                               77
                                                                        6
                                                                             92%
→168, 179-181
dicee/trainer/torch_trainer_ddp.py
                                                               89
                                                                       71
                                                                             20%
                                                                                    11-14, _
\hookrightarrow 43, 47-67, 78-94, 113-122, 126-136, 151-158, 168-191
TOTAL
                                                             6948
                                                                    3169
                                                                             54%
```

13 How to cite

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

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

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

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

(continues on next page)

```
@inproceedings{demir2021convolutional,
title={Convolutional Complex Knowledge Graph Embeddings},
author={Caglar Demir and Axel-Cyrille Ngonga Ngomo},
booktitle={Eighteenth Extended Semantic Web Conference - Research Track},
year={2021},
url={https://openreview.net/forum?id=6T45-4TFqaX}}
# Shallom
@inproceedings{demir2021shallow,
   title={A shallow neural model for relation prediction},
   author={Demir, Caglar and Moussallem, Diego and Ngomo, Axel-Cyrille Ngonga},
   booktitle={2021 IEEE 15th International Conference on Semantic Computing (ICSC)},
   pages={179-182},
   year={2021},
   organization={IEEE}
```

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

14 dicee

14.1 Submodules

dicee. main

dicee.abstracts

Classes

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

Module Contents

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

Abstract class for Trainer class for knowledge graph embedding models

Parameter

```
args
[str] ?
callbacks: list
?
```

```
attributes
callbacks
is_global_zero = True
global_rank = 0
local_rank = 0
strategy = None
on_fit_start(*args, **kwargs)
     A function to call callbacks before the training starts.
     Parameter
     args
     kwargs
         rtype
             None
on_fit_end(*args, **kwargs)
     A function to call callbacks at the ned of the training.
     Parameter
     args
     kwargs
         rtype
             None
on_train_epoch_end(*args, **kwargs)
     A function to call callbacks at the end of an epoch.
     Parameter
     args
     kwargs
         rtype
             None
on_train_batch_end(*args, **kwargs)
     A function to call callbacks at the end of each mini-batch during training.
     Parameter
     args
     kwargs
         rtype
             None
```

```
static save_checkpoint (full\_path: str, model) \rightarrow None
            A static function to save a model into disk
            Parameter
           full_path: str
            model:
                rtype
                     None
class dicee.abstracts.BaseInteractiveKGE (path: str = None, url: str = None,
             construct\_ensemble: bool = False, model\_name: str = None,
             apply_semantic_constraint: bool = False)
      Abstract/base class for using knowledge graph embedding models interactively.
      Parameter
      path_of_pretrained_model_dir
           [str]?
      construct_ensemble: boolean
           ?
      model_name: str apply_semantic_constraint : boolean
      construct_ensemble = False
      apply_semantic_constraint = False
      configs
      \texttt{get\_eval\_report}() \rightarrow dict
      \texttt{get\_bpe\_token\_representation} (\textit{str\_entity\_or\_relation: List[str]} \mid \textit{str}) \rightarrow \texttt{List[List[int]]} \mid \texttt{List[int]}
                     str_entity_or_relation(corresponds to a str or a list of strings to
                    be tokenized via BPE and shaped.)
                Return type
                     A list integer(s) or a list of lists containing integer(s)
      \verb|get_padded_bpe_triple_representation| (\textit{triples: List[List[str]]}) \rightarrow Tuple[List, List, List]
                Parameters
                    triples
      \verb"set_model_train_mode"() \to None
            Setting the model into training mode
            Parameter
      \verb"set_model_eval_mode"() \to None
            Setting the model into eval mode
```

Parameter

```
property name
sample\_entity(n:int) \rightarrow List[str]
sample\_relation(n:int) \rightarrow List[str]
is\_seen(entity: str = None, relation: str = None) \rightarrow bool
save() \rightarrow None
get_entity_index(x: str)
get_relation_index(x: str)
index_triple (head_entity: List[str], relation: List[str], tail_entity: List[str])
              \rightarrow Tuple[torch.LongTensor, torch.LongTensor, torch.LongTensor]
     Index Triple
     Parameter
     head_entity: List[str]
     String representation of selected entities.
     relation: List[str]
     String representation of selected relations.
     tail_entity: List[str]
     String representation of selected entities.
     Returns: Tuple
     pytorch tensor of triple score
add_new_entity_embeddings (entity_name: str = None, embeddings: torch.FloatTensor = None)
get_entity_embeddings (items: List[str])
     Return embedding of an entity given its string representation
     Parameter
     items:
          entities
get_relation_embeddings (items: List[str])
     Return embedding of a relation given its string representation
     Parameter
     items:
          relations
construct_input_and_output (head_entity: List[str], relation: List[str], tail_entity: List[str], labels)
     Construct a data point :param head_entity: :param relation: :param tail_entity: :param labels: :return:
```

```
parameters()
class dicee.abstracts.InteractiveQueryDecomposition
     t_norm(tens_1: torch.Tensor, tens_2: torch.Tensor, tnorm: str = 'min') \rightarrow torch.Tensor
     tensor_t_norm (subquery_scores: torch.FloatTensor, tnorm: str = 'min') \rightarrow torch.FloatTensor
           Compute T-norm over [0,1] ^{n imes d} where n denotes the number of hops and d denotes number of
           entities
     t\_conorm (tens_1: torch.Tensor, tens_2: torch.Tensor, tconorm: str = 'min') \rightarrow torch.Tensor
     negnorm(tens\_1: torch.Tensor, lambda\_: float, neg\_norm: str = 'standard') \rightarrow torch.Tensor
class dicee.abstracts.AbstractCallback
     Bases: abc.ABC, lightning.pytorch.callbacks.Callback
     Abstract class for Callback class for knowledge graph embedding models
     Parameter
     on_init_start(*args, **kwargs)
           Parameter
           trainer:
           model:
               rtype
                   None
     on_init_end(*args, **kwargs)
           Call at the beginning of the training.
           Parameter
           trainer:
           model:
               rtype
                   None
     on_fit_start (trainer, model)
           Call at the beginning of the training.
           Parameter
           trainer:
           model:
               rtype
                   None
     on_train_epoch_end(trainer, model)
           Call at the end of each epoch during training.
```

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

model:

rtvpe

None

on_fit_end(trainer, model)

Call at the end of the training.

Parameter

trainer:

model:

rtype

None

 $store_ensemble (param_ensemble) \rightarrow None$

class dicee.abstracts.BaseInteractiveTrainKGE

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

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

```
train_k_vs_all(h, r, iteration=1, lr=0.001)
```

Train k vs all :param head_entity: :param relation: :param iteration: :param lr: :return:

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

train_literals (train_file_path: str = None, num_epochs: int = 100, lit_lr: float = 0.001, lit_normalization_type: str = 'z-norm', batch_size: int = 1024, sampling_ratio: float = None, random_seed=1, loader_backend: str = 'pandas', freeze_entity_embeddings: bool = True, gate_residual: bool = True, device: str = None, suffle_data: bool = True)

Trains the Literal Embeddings model using literal data.

Parameters

- train_file_path (str) Path to the training data file.
- num_epochs (int) Number of training epochs.
- lit_lr (float) Learning rate for the literal model.
- norm type (str) Normalization type to use ('z-norm', 'min-max', or None).
- batch_size (int) Batch size for training.
- sampling_ratio (float) Ratio of training triples to use.
- loader_backend (str) Backend for loading the dataset ('pandas' or 'rdflib').
- **freeze_entity_embeddings** (bool) If True, freeze the entity embeddings during training.
- gate_residual (bool) If True, use gate residual connections in the model.
- device (str) Device to use for training ('cuda' or 'cpu'). If None, will use available GPU or CPU.
- **suffle_data** (bool) If True, shuffle the dataset before training.

dicee.analyse experiments

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

Classes

```
Experiment
```

Functions

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

Module Contents

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

```
val_mrr = []
val_h1 = []
val_h3 = []
val_h10 = []
test_mrr = []
test_h1 = []
test_h3 = []
test_h10 = []
runtime = []
normalization = []
scoring_technique = []
save_experiment(x)
to_df()
dicee.analyse_experiments.analyse(args)
```

dicee.callbacks

Classes

AccumulateEpochLossCallback	Abstract class for Callback class for knowledge graph embedding models
PrintCallback	Abstract class for Callback class for knowledge graph embedding models
KGESaveCallback	Abstract class for Callback class for knowledge graph embedding models
PseudoLabellingCallback	Abstract class for Callback class for knowledge graph embedding models
ASWA	Adaptive stochastic weight averaging
Eval	Abstract class for Callback class for knowledge graph embedding models
KronE	Abstract class for Callback class for knowledge graph embedding models
Perturb	A callback for a three-Level Perturbation
PeriodicEvalCallback	Callback to periodically evaluate the model and optionally save checkpoints during training.

Functions

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

Module Contents

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

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

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

```
num_epochs
     initial_eval_setting = None
     epoch_count = 0
     alphas = []
     val_aswa = -1
     on_fit_end(trainer, model)
          Call at the end of the training.
          Parameter
          trainer:
          model:
              rtype
                  None
     \verb|static compute_mrr|(trainer, model)| \rightarrow \verb|float|
     {\tt get\_aswa\_state\_dict} \ (model)
     decide (running_model_state_dict, ensemble_state_dict, val_running_model,
                 mrr_updated_ensemble_model)
          Perform Hard Update, software or rejection
              Parameters
                   • running_model_state_dict
                   • ensemble_state_dict
                   • val_running_model
                   • mrr_updated_ensemble_model
     on_train_epoch_end(trainer, model)
          Call at the end of each epoch during training.
          Parameter
          trainer:
          model:
              rtype
                  None
class dicee.callbacks.Eval (path, epoch_ratio: int = None)
     Bases: dicee.abstracts.AbstractCallback
```

Abstract class for Callback class for knowledge graph embedding models

Parameter

```
path
reports = []
epoch_ratio = None
epoch_counter = 0
on_fit_start(trainer, model)
     Call at the beginning of the training.
     Parameter
     trainer:
     model:
         rtype
             None
on_fit_end(trainer, model)
     Call at the end of the training.
     Parameter
     trainer:
     model:
         rtype
             None
on_train_epoch_end(trainer, model)
     Call at the end of each epoch during training.
     Parameter
     trainer:
     model:
         rtype
             None
on_train_batch_end(*args, **kwargs)
     Call at the end of each mini-batch during the training.
     Parameter
     trainer:
     model:
         rtype
             None
```

```
class dicee.callbacks.KronE
     Bases: dicee.abstracts.AbstractCallback
     Abstract class for Callback class for knowledge graph embedding models
     Parameter
     f = None
     static batch_kronecker_product(a, b)
           Kronecker product of matrices a and b with leading batch dimensions. Batch dimensions are broadcast. The
           number of them mush :type a: torch.Tensor :type b: torch.Tensor :rtype: torch.Tensor
     get_kronecker_triple_representation (indexed_triple: torch.LongTensor)
           Get kronecker embeddings
     on_fit_start(trainer, model)
           Call at the beginning of the training.
           Parameter
           trainer:
           model:
               rtype
                   None
class dicee.callbacks.Perturb (level: str = linput', 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'
```

```
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.

class dicee.callbacks.PeriodicEvalCallback (experiment_path: str, max_epochs: int, eval_every_n_epoch: int = 0, eval_at_epochs: list = None, save_model_every_n_epoch: bool = True, n_epochs_eval_model: str = 'val_test')
```

Bases: dicee.abstracts.AbstractCallback

Callback to periodically evaluate the model and optionally save checkpoints during training.

Evaluates at regular intervals (every N epochs) or at explicitly specified epochs. Stores evaluation reports and model checkpoints.

```
experiment_dir
max_epochs
epoch_counter = 0
save_model_every_n_epoch = True
reports
n_epochs_eval_model = 'val_test'
default eval model = None
eval_epochs
on_fit_end(trainer, model)
     Called at the end of training. Saves final evaluation report.
\verb"on_train_epoch_end" (\textit{trainer}, model")
```

Called at the end of each training epoch. Performs evaluation and checkpointing if scheduled.

Parameters

- trainer (object) The training controller.
- model (torch.nn.Module) The model being trained.

dicee.config

Classes

Namespace

Simple object for storing attributes.

Module Contents

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

Bases: argparse.Namespace

Simple object for storing attributes.

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

```
dataset_dir: str = None
```

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

```
save_embeddings_as_csv: bool = False
```

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

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

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

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

```
normalization: str = 'None'
    LayerNorm, BatchNorm1d, or None
init_param: str = None
    xavier_normal or None
gradient_accumulation_steps: int = 0
    Not tested e
num_folds_for_cv: int = 0
    Number of folds for CV
eval_model: str = 'train_val_test'
    ["None", "train", "train_val", "train_val_test", "test"]
        Type
            Evaluate trained model choices
save_model_at_every_epoch: int = None
    Not tested
label_smoothing_rate: float = 0.0
num core: int = 0
    Number of CPUs to be used in the mini-batch loading process
random_seed: int = 0
    Random Seed
sample_triples_ratio: float = None
    Read some triples that are uniformly at random sampled. Ratio being between 0 and 1
read_only_few: int = None
    Read only first few triples
pykeen_model_kwargs
    Additional keyword arguments for pykeen models
kernel size: int = 3
    Size of a square kernel in a convolution operation
num_of_output_channels: int = 32
    Number of slices in the generated feature map by convolution.
p: int = 0
    P parameter of Clifford Embeddings
q: int = 1
    Q parameter of Clifford Embeddings
input_dropout_rate: float = 0.0
    Dropout rate on embeddings of input triples
hidden_dropout_rate: float = 0.0
    Dropout rate on hidden representations of input triples
feature_map_dropout_rate: float = 0.0
    Dropout rate on a feature map generated by a convolution operation
```

byte_pair_encoding: bool = False

Byte pair encoding

Type WIP

adaptive_swa: bool = False

Adaptive stochastic weight averaging

swa: bool = False

Stochastic weight averaging

block_size: int = None

block size of LLM

continual_learning = None

Path of a pretrained model size of LLM

auto_batch_finding = False

A flag for using auto batch finding

eval_every_n_epochs: int = 0

Evaluate model every n epochs. If 0, no evaluation is applied.

save_every_n_epochs: bool = False

Save model every n epochs. If True, save model at every epoch.

eval_at_epochs: list = None

List of epoch numbers at which to evaluate the model (e.g., 1 5 10).

n_epochs_eval_model: str = 'val_test'

Evaluating link prediction performance on data splits while performing periodic evaluation.

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

Functions

```
reload_dataset(path, form_of_labelling, ...)
construct_dataset(→ torch.utils.data.Dataset)
```

Reload the files from disk to construct the Pytorch 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.

```
train_set
     train_indices_target
     target_dim
     num datapoints
     torch_ordered_shaped_bpe_entities
     collate_fn = None
     __len__()
     \__getitem_(idx)
class dicee.dataset_classes.MultiClassClassificationDataset(
           subword_units: numpy.ndarray, block_size: int = 8)
     Bases: torch.utils.data.Dataset
     Dataset for the 1vsALL training strategy
          Parameters
                • train_set_idx - Indexed triples for the training.
                • entity_idxs - mapping.
                • relation_idxs - mapping.
                • form - ?
                                               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__()
__getitem__(idx)
```

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

Bases: torch.utils.data.Dataset

Dataset for the 1vsALL training strategy

Parameters

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

Return type

torch.utils.data.Dataset

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

Bases: torch.utils.data.Dataset

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

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

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



train_set_idx

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

entity_idxs

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

relation_idxs

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

self: torch.utils.data.Dataset

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

```
train_data = None
train_target = None
label_smoothing_rate
collate_fn = None
__len__()
\__getitem\__(idx)
```

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

Bases: torch.utils.data.Dataset

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

Let D denote a dataset for AllvsAll training and be defined as $D := \{(x,y)_i\}_i ^n N$, 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, $label_smoothing_rate$: float = 0.0)

Bases: torch.utils.data.Dataset

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

Parameters

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

train_data

The input data converted into a PyTorch tensor.

Type

torch.Tensor

num_entities

Number of entities in the dataset.

Type int

num_relations

Number of relations in the dataset.

```
Type int
```

neg_sample_ratio

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

```
Type int
```

label_smoothing_rate

The smoothing factor applied to the labels.

Type

torch.Tensor

```
collate_fn
```

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

Type

function, optional

```
train_data
num_entities
num_relations
neg_sample_ratio = None
label_smoothing_rate
collate_fn = None
__len__()
    Returns the number of samples in the dataset.
```

. .

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

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

Parameters

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

Returns

A tuple consisting of:

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

Return type

tuple

KvsSample a Dataset:

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

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

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

At each mini-batch construction, we subsample(y), hence n

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__()
     \__{getitem}_{\_}(idx)
class dicee.dataset_classes.NegSampleDataset(train_set: numpy.ndarray, num_entities: int,
           num_relations: int, neg_sample_ratio: int = 1)
     Bases: torch.utils.data.Dataset
```

An abstract class representing a Dataset.

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

1 Note

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

```
neg_sample_ratio
train_set
length
num_entities
num_relations
```

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

Parameters

- train_set_idx Indexed triples for the training.
- num_entities entity to index mapping.
- num_relations relation to index mapping.
- batch_size int
- form ?
- num_workers https://pytorch.org/docs/stable/data.html#torch.utils.data. int for DataLoader

Return type

?

train_set_idx

num_entities num_relations

neg_sample_ratio

batch_size

num_workers

train_dataloader() → torch.utils.data.DataLoader

An iterable or collection of iterables specifying training samples.

For more information about multiple dataloaders, see this section.

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

For data processing use the following pattern:

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

However, the above are only necessary for distributed processing.

Warning

do not assign state in prepare_data

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

1 Note

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

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

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

Parameters

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

Example:

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

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

# don't do this
        self.something = else

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

transfer_batch_to_device(*args, **kwargs)

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

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

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

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

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_
\hookrightarrow i dx)
   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()
```

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

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

train_file_path

Path to the training data file.

```
Type
st
```

normalization

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

```
Type
str
```

normalization_params

Parameters used for normalization.

```
Type
dict
```

sampling_ratio

Fraction of the training set to use for ablations.

```
Type float
```

```
entity_to_idx
     Mapping of entities to their indices.
         Type
             dict
num_entities
     Total number of entities.
         Type
             int
data_property_to_idx
     Mapping of data properties to their indices.
         Type
             dict
num_data_properties
     Total number of data properties.
         Type
loader_backend
     Backend to use for loading data ('pandas' or 'rdflib').
         Type
train_file_path
loader_backend = 'pandas'
normalization_type = 'z-norm'
normalization_params
sampling_ratio = None
entity_to_idx = None
num_entities
__getitem__(index)
__len__()
static load_and_validate_literal_data (file_path: str = None, loader_backend: str = 'pandas')
             \rightarrow pandas.DataFrame
     Loads and validates the literal data file. :param file_path: Path to the literal data file. :type file_path: str
             DataFrame containing the loaded and validated data.
         Return type
             pd.DataFrame
```

 ${\tt static \ denormalize}\ (preds_norm,\ attributes,\ normalization_params) \ o \ numpy.ndarray$

Denormalizes the predictions based on the normalization type.

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

Returns

Denormalized predictions.

Return type

np.ndarray

dicee.eval static funcs

Functions

```
evaluate_link_prediction_performance(→
Dict)
evaluate_link_prediction_performance_with_.

evaluate_link_prediction_performance_with_;

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

Module Contents

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

Parameters

- model
- triples
- er_vocab
- re_vocab

Parameters

- model
- triples
- within_entities
- er_vocab
- re_vocab

```
dicee.eval_static_funcs.evaluate_literal_prediction(
    kge_model: dicee.knowledge_graph_embeddings.KGE, eval_file_path: str = None,
    store_lit_preds: bool = True, eval_literals: bool = True, loader_backend: str = 'pandas',
    return_attr_error_metrics: bool = False)
```

Evaluates the trained literal prediction model on a test file.

Parameters

- eval_file_path (str) Path to the evaluation file.
- **store_lit_preds** (bool) If True, stores the predictions in a CSV file.
- eval_literals (bool) If True, evaluates the literal predictions and prints error metrics.
- loader_backend (str) Backend for loading the dataset ('pandas' or 'rdflib').

Returns

DataFrame containing error metrics for each attribute if return_attr_error_metrics is True.

Return type

pd.DataFrame

Raises

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

dicee.evaluator

Classes

Evaluator 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
save_trained_model() → None
```

Save a knowledge graph embedding model

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

Parameter

rtypeNone

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

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

Start training

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

Parameter

rtype

A dict containing information about the training and/or evaluation

class dicee.executer.ContinuousExecute(args)

Bases: Execute

A subclass of Execute Class for retraining

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

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

 $continual_start() \rightarrow dict$

Start Continual Training

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

Parameter

rtype

A dict containing information about the training and/or evaluation

KG Knowledge Graph

Module Contents

num_tokens

```
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_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

Module Contents

```
create_vector_database (collection_name: str, distance: str, location: str = 'localhost',
             port: int = 6333)
generate (h=", r=")
eval_lp_performance(dataset=List[Tuple[str, str, str]], filtered=True)
predict_missing_head_entity (relation: List[str] | str, tail_entity: List[str] | str, within=None,
              batch\_size=2, topk=1, return\_indices=False) \rightarrow Tuple
     Given a relation and a tail entity, return top k ranked head entity.
     argmax_{e in E } f(e,r,t), where r in R, t in E.
     Parameter
     relation: Union[List[str], str]
     String representation of selected relations.
     tail entity: Union[List[str], str]
     String representation of selected entities.
     k: int
     Highest ranked k entities.
     Returns: Tuple
     Highest K scores and entities
predict_missing_relations (head_entity: List[str] | str, tail_entity: List[str] | str, within=None,
             batch size=2, topk=1, return\ indices=False) <math>\rightarrow Tuple
     Given a head entity and a tail entity, return top k ranked relations.
     argmax_{r} in R \} f(h,r,t), where h, t in E.
     Parameter
     head_entity: List[str]
     String representation of selected entities.
     tail_entity: List[str]
     String representation of selected entities.
     k: int
     Highest ranked k entities.
     Returns: Tuple
     Highest K scores and entities
predict_missing_tail_entity (head_entity: List[str] | str, relation: List[str] | str,
              within: List[str] = None, batch_size=2, topk=1, return_indices=False) \rightarrow torch.FloatTensor
     Given a head entity and a relation, return top k ranked entities
     argmax_{e} = in E  f(h,r,e), where h in E and r in R.
```

Parameter

```
head_entity: List[str]
```

String representation of selected entities.

```
tail_entity: List[str]
```

String representation of selected entities.

Returns: Tuple

scores

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

Parameters

- logits
- h
- r
- t
- within

Predict missing item in a given triple.

Returns

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

Predict triple score

Parameter

head_entity: List[str]

String representation of selected entities.

relation: List[str]

String representation of selected relations.

tail_entity: List[str]

String representation of selected entities.

logits: bool

If logits is True, unnormalized score returned

Returns: Tuple

```
pytorch tensor of triple score
return_multi_hop_query_results (aggregated_query_for_all_entities, k: int, only_scores)
single_hop_query_answering(query: tuple, only_scores: bool = True, k: int = None)
answer_multi_hop_query (query_type: str = None, query: Tuple[str | Tuple[str, str], Ellipsis] = None,
             queries: List[Tuple[str | Tuple[str, str], Ellipsis]] = None, tnorm: str = 'prod',
             neg norm: str = 'standard', lambda : float = 0.0, k: int = 10, only scores=False)
              \rightarrow List[Tuple[str, torch.Tensor]]
     # @TODO: Refactoring is needed # @TODO: Score computation for each query type should be done in a
     static function
     Find an answer set for EPFO queries including negation and disjunction
     Parameter
     query_type: str The type of the query, e.g., "2p".
     query: Union[str, Tuple[str, Tuple[str, str]]] The query itself, either a string or a nested tuple.
     queries: List of Tuple[Union[str, Tuple[str, str]], ...]
     tnorm: str The t-norm operator.
     neg_norm: str The negation norm.
     lambda_: float lambda parameter for sugeno and yager negation norms
     k: int The top-k substitutions for intermediate variables.
          returns
               • List[Tuple[str, torch.Tensor]]
               • Entities and corresponding scores sorted in the descening order of scores
find missing triples (confidence: float, entities: List[str] = None, relations: List[str] = None,
             topk: int = 10, at most: int = sys.maxsize) \rightarrow Set
          Find missing triples
          Iterative over a set of entities E and a set of relation R:
     orall e in E and orall r in R f(e.r.x)
          Return (e,r,x)
     otin G and f(e,r,x) > confidence
          confidence: float
```

A threshold for an output of a sigmoid function given a triple.

Stop after finding at_most missing triples $\{(e,r,x) \mid f(e,r,x) > \text{confidence land } (e,r,x)\}$

Highest ranked k item to select triples with f(e,r,x) > confidence.

topk: int

otin G

at most: int

```
deploy(share: bool = False, top\_k: int = 10)
```

```
predict_literals (entity: List[str] | str = None, attribute: List[str] | str = None,
              denormalize\_preds: bool = True) \rightarrow numpy.ndarray
```

Predicts literal values for given entities and attributes.

Parameters

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

Returns

Predictions for the given entities and attributes.

Return type

numpy ndarray

dicee.models

Submodules

dicee.models.adopt

Classes

ADOPT

Base class for all optimizers.

Functions

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

Module Contents

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

Bases: torch.optim.optimizer.Optimizer

Base class for all optimizers.



🔔 Warning

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

Parameters

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

clip lambda

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

Perform a single optimization step.

Parameters

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

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

(continues on next page)

(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.



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

Variables

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

```
training_step_outputs = []
mem_of_model() -> 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 dataloader you return will not be unless you :paramref: `~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
```

(continues on next 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.

1 Note

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

Variables

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

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

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

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

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

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

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

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

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

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

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

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

returns

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

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

requires_grad_for_interactions = False

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

Base class for all neural network modules.

Your models should also subclass this class.

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

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

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

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

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

1 Note

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

Variables

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

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

Parameter

x: torch.LongTensor with (n,) shape

rtype

torch.FloatTensor with (n) shape

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

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

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

compute_sigmas_single (list_h_emb, list_r_emb, list_t_emb)

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

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

and return:

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

compute_sigmas_multivect(list_h_emb, list_r_emb)

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

For same bases vectors interaction we have

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

For different base vector interactions, we have

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

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

Kvsall training

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

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

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

Multiplying a base vector with its scalar coefficient

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

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

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

Parameter

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

returns

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

$compute_sigma_pp(hp, rp)$

Compute .. math:

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

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

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

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

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

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

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

$compute_sigma_qq(hq, rq)$

Compute

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

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

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

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

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

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

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

$compute_sigma_rr(hk, rk)$

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

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

Compute

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

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

for j in range(q):

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

print(sigma_pq.shape)

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

Compute

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

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

for j in range(q):

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

print(sigma_pq.shape)

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

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

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

for j in range(q):

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

print(sigma_pq.shape)

dicee.models.complex

Classes

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

Module Contents

class dicee.models.complex.ConEx(args)

Bases: dicee.models.base_model.BaseKGE

Convolutional ComplEx Knowledge Graph Embeddings

name = 'ConEx'

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

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

Base class for all neural network modules.

Your models should also subclass this class.

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

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

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

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

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

1 Note

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

Variables

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

Parameters

- emb_h
- emb_r
- emb E

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

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

```
torch.FloatTensor with (n) shape

T (x: torch.tensor) → torch.tensor

Transpose function

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

dicee.models.ensemble

Classes

EnsembleKGE

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

dicee.models.function space

Classes

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

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

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

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

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

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

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

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

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

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

pop(coeff, x, degree)

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

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

dicee.models.literal

Classes

LiteralEmbeddings

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

Module Contents

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

Bases: torch.nn.Module

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

num_of_data_properties

Number of data properties (attributes).

Type int

embedding_dims

Dimension of the embeddings.

Type int

entity_embeddings

Pre-trained entity embeddings.

Type

torch.tensor

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

property device

dicee.models.octonion

Classes

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

Functions

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

Module Contents

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

Base class for all neural network modules.

Your models should also subclass this class.

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

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

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

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

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

1 Note

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

Variables

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

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

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

Base class for all neural network modules.

Your models should also subclass this class.

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

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

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

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

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

1 Note

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

Variables

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

```
name = 'ConvO'
conv2d
```

```
fc_num_input
     fc1
     bn_conv2d
     norm_fc1
     feature_map_dropout
     static octonion_normalizer(emb_rel_e0, emb_rel_e1, emb_rel_e2, emb_rel_e3, emb_rel_e4,
                  emb_rel_e5, emb_rel_e6, emb_rel_e7)
     residual\_convolution(O\_1, O\_2)
     forward\_triples(x: torch.Tensor) \rightarrow torch.Tensor
               Parameters
     forward_k_vs_all (x: torch.Tensor)
           Given a head entity and a relation (h,r), we compute scores for all entities. [score(h,r,x)|x in Entities] =>
           [0.0,0.1,...,0.8], shape=> (1, |Entities|) Given a batch of head entities and relations => shape (size of batch,|
           Entities|)
class dicee.models.octonion.AConvO(args: dict)
     Bases: dicee.models.base_model.BaseKGE
     Additive Convolutional Octonion Knowledge Graph Embeddings
     name = 'AConvO'
     conv2d
     fc_num_input
     fc1
     bn_conv2d
     norm_fc1
     feature_map_dropout
     static octonion_normalizer(emb_rel_e0, emb_rel_e1, emb_rel_e2, emb_rel_e3, emb_rel_e4,
                  emb_rel_e5, emb_rel_e6, emb_rel_e7)
     residual_convolution (O_1, O_2)
     forward_triples (x: torch.Tensor) \rightarrow torch.Tensor
               Parameters
                   x
     forward_k_vs_all (x: torch.Tensor)
           Given a head entity and a relation (h,r), we compute scores for all entities. [score(h,r,x)|x in Entities] =>
           [0.0,0.1,...,0.8], shape=> (1, |Entities|) Given a batch of head entities and relations => shape (size of batch,|
           Entities l)
```

dicee.models.pykeen_models

Classes

PykeenKGE	A class for using knowledge graph embedding models im-
	plemented in Pykeen

Module Contents

```
class dicee.models.pykeen_models.PykeenKGE (args: dict)
     Bases: dicee.models.base model.BaseKGE
     A class for using knowledge graph embedding models implemented in Pykeen
     Notes: Pykeen_DistMult: C Pykeen_ComplEx: Pykeen_QuatE: Pykeen_MuRE: Pykeen_CP: Pykeen_HolE: Py-
     keen_HolE: Pykeen_TransD: Pykeen_TransE: Pykeen_TransF: Pykeen_TransH: Pykeen_TransR:
     model_kwargs
     name
     model
     loss_history = []
     args
     entity_embeddings = None
     relation embeddings = None
     forward_k_vs_all (x: torch.LongTensor)
           # => Explicit version by this we can apply bn and dropout
           # (1) Retrieve embeddings of heads and relations + apply Dropout & Normalization if given. h, r =
           self.get head relation representation(x) # (2) Reshape (1). if self.last dim > 0:
               h = h.reshape(len(x), self.embedding_dim, self.last_dim) r = r.reshape(len(x), self.embedding_dim,
               self.last dim)
           \# (3) Reshape all entities. if self.last dim > 0:
               t = self.entity embeddings.weight.reshape(self.num entities, self.embedding dim, self.last dim)
           else:
               t = self.entity_embeddings.weight
           # (4) Call the score_t from interactions to generate triple scores. return self.interaction.score_t(h=h, r=r,
           all_entities=t, slice_size=1)
     forward\_triples (x: torch.LongTensor) \rightarrow torch.FloatTensor
           # => Explicit version by this we can apply bn and dropout
           # (1) Retrieve embeddings of heads, relations and tails and apply Dropout & Normalization if given. h, r, t =
```

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

 $self.get_triple_representation(x) \# (2) Reshape (1). if <math>self.last_dim > 0$:

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

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

abstract forward_k_vs_sample (x: torch.LongTensor, target_entity_idx)

dicee.models.quaternion

Classes

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

Functions

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

Module Contents

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

class dicee.models.quaternion.QMult(args)

Bases: dicee.models.base\_model.BaseKGE
```

Base class for all neural network modules.

Your models should also subclass this class.

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

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

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

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

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



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

Variables

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

name = 'QMult'

explicit = True

 $quaternion_multiplication_followed_by_inner_product(h, r, t)$

Parameters

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

Returns

Triple scores.

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

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

Absolute value of a quaternion

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

L2 norm of quaternion vector:

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

Parameters

 \mathbf{x} – The vector.

Returns

The normalized vector.

 $\verb+k_vs_all_score+ (bpe_head_ent_emb, bpe_rel_ent_emb, E)$

Parameters

- bpe_head_ent_emb
- bpe_rel_ent_emb
- E

 $forward_k_vs_all(x)$

Parameters

x

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

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

forward_k_vs_sample (x, target_entity_idx)

```
\label{lem:convolution} \begin{tabular}{ll} \textbf{feature\_map\_dropout} \\ \textbf{residual\_convolution} \ (Q\_1,Q\_2) \\ \end{tabular} \begin{tabular}{ll} \textbf{forward\_triples} \ (\textit{indexed\_triple: torch.Tensor}) \ \to \ \text{torch.Tensor} \\ \end{tabular}
```

Parameters

x

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

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

dicee.models.real

Classes

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

Module Contents

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

Bases: dicee.models.base_model.BaseKGE

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

```
name = 'DistMult'
```

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

Parameters

- emb_h
- emb_r
- emb_E

forward_k_vs_all (x: torch.LongTensor)

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

score(h, r, t)

class dicee.models.real.TransE(args)

Bases: dicee.models.base_model.BaseKGE

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

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

dicee.models.static_funcs

Functions

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

```
\label{eq:dicee.models.static_funcs.quaternion_mul} (*, Q\_1, Q\_2) \\ \rightarrow Tuple[torch.Tensor, torch.Tensor, torch.Tensor, torch.Tensor] \\ Perform quaternion multiplication :param Q\_1: :param Q\_2: :return:
```

dicee.models.transformers

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

Classes

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

Module Contents

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

Base class for all neural network modules.

Your models should also subclass this class.

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

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

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

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

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

1 Note

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

Variables

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

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

Parameters

- yhat_batch
- y_batch

loss_function(yhat_batch, y_batch)

forward (x: torch.LongTensor)

Parameters

```
\mathbf{x} (B by T tensor)
```

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

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

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

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

Parameters

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

Returns

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

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

Example:

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

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

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

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

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

1 Note

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

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

Bases: torch.nn.Module

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

weight

bias

forward(input)

class dicee.models.transformers.CausalSelfAttention(config)

Bases: torch.nn.Module

Base class for all neural network modules.

Your models should also subclass this class.

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

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

class Model (nn.Module):
```

(continues on next page)

(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.

```
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)
```

(continues on next page)

(continued from previous page)

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

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

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

1 Note

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

Variables

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

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

Base class for all neural network modules.

Your models should also subclass this class.

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

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

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

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

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

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

Variables

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

```
ln_1
attn
ln_2
mlp
forward(x)

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

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

Base class for all neural network modules.

Your models should also subclass this class.

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

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

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

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

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



1 Note

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

Variables

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

config

transformer

lm_head

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

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

```
forward(idx, targets=None)
crop_block_size(block_size)
classmethod from_pretrained(model_type, override_args=None)
configure_optimizers (weight_decay, learning_rate, betas, device_type)
estimate_mfu(fwdbwd_per_iter, dt)
```

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

Classes

ADOPT	Base class for all optimizers.
BaseKGELightning	Base class for all neural network modules.
BaseKGE	Base class for all neural network modules.
IdentityClass	Base class for all neural network modules.
BaseKGE	Base class for all neural network modules.
DistMult	Embedding Entities and Relations for Learning and Infer-
	ence in Knowledge Bases
TransE	Translating Embeddings for Modeling
Shallom	A shallow neural model for relation prediction (https:
	//arxiv.org/abs/2101.09090)
Pyke	A Physical Embedding Model for Knowledge Graphs
BaseKGE	Base class for all neural network modules.
ConEx	Convolutional ComplEx Knowledge Graph Embeddings
AConEx	Additive Convolutional ComplEx Knowledge Graph Em-
	beddings
ComplEx	Base class for all neural network modules.
BaseKGE	Base class for all neural network modules.
IdentityClass	Base class for all neural network modules.

continues on next page

Table 1 - continued from previous page

QMult	Base class for all neural network modules.
ConvQ	Convolutional Quaternion Knowledge Graph Embed-
	dings
AConvQ	Additive Convolutional Quaternion Knowledge Graph
	Embeddings
BaseKGE	Base class for all neural network modules.
IdentityClass	Base class for all neural network modules.
OMult	Base class for all neural network modules.
Conv0	Base class for all neural network modules.
AConvO	Additive Convolutional Octonion Knowledge Graph Em-
	beddings
Keci	Base class for all neural network modules.
CKeci	Without learning dimension scaling
DeCaL	Base class for all neural network modules.
BaseKGE	Base class for all neural network modules.
PykeenKGE	A class for using knowledge graph embedding models im-
	plemented in Pykeen
BaseKGE	Base class for all neural network modules.
FMult	Learning Knowledge Neural Graphs
GFMult	Learning Knowledge Neural Graphs
FMult2	Learning Knowledge Neural Graphs
LFMult1	Embedding with trigonometric functions. We represent
	all entities and relations in the complex number space as:
LFMult	Embedding with polynomial functions. We represent all
	entities and relations in the polynomial space as:
DualE	Dual Quaternion Knowledge Graph Embeddings
	(https://ojs.aaai.org/index.php/AAAI/article/download/
	16850/16657)

Functions

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

Package Contents

Base class for all optimizers.

Warning

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

Parameters

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

clip_lambda

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

Perform a single optimization step.

Parameters

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

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

Bases: lightning.LightningModule

Base class for all neural network modules.

Your models should also subclass this class.

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

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

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



1 Note

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

Variables

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

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

Size of model in MB and number of params

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

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

Parameters

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

Returns

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

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

Example:

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

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

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

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

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

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

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

Parameters

- yhat_batch
- y_batch

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

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

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

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

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

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

test_epoch_end(outputs: List[Any])

$\texttt{test_dataloader}\,()\,\to None$

An iterable or collection of iterables specifying test samples.

For more information about multiple dataloaders, see this section.

For data processing use the following pattern:

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

However, the above are only necessary for distributed processing.

Λ

Warning

do not assign state in prepare_data

• test()

- prepare_data()
- setup()

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

1 Note

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

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

An iterable or collection of iterables specifying validation samples.

For more information about multiple dataloaders, see this section.

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

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

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

1 Note

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

1 Note

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

$\texttt{predict_dataloader}\,() \, \to None$

An iterable or collection of iterables specifying prediction samples.

For more information about multiple dataloaders, see this section.

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

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

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

Returns

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

$train_dataloader() \rightarrow None$

An iterable or collection of iterables specifying training samples.

For more information about multiple dataloaders, see this section.

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

For data processing use the following pattern:

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

However, the above are only necessary for distributed processing.

🛕 Warning

do not assign state in prepare_data

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

1 Note

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

configure_optimizers (parameters=None)

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

Returns

Any of these 6 options.

- · Single optimizer.
- List or Tuple of optimizers.
- Two lists The first list has multiple optimizers, and the second has multiple LR schedulers (or multiple lr_scheduler_config).

- Dictionary, with an "optimizer" key, and (optionally) a "lr_scheduler" key whose value is a single LR scheduler or lr_scheduler_config.
- None Fit will run without any optimizer.

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

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

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

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

1 Note

Some things to know:

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

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

Bases: BaseKGELightning

Base class for all neural network modules.

Your models should also subclass this class.

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

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

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

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

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

1 Note

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

Variables

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

args

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

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

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

Base class for all neural network modules.

Your models should also subclass this class.

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

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

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

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

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

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

Variables

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

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

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

Base class for all neural network modules.

Your models should also subclass this class.

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

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

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

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

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

1 Note

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

Variables

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

```
args
embedding_dim = None
num entities = None
```

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

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

```
forward_k_vs_sample (x: torch.LongTensor, target_entity_idx: torch.LongTensor)
     \mathtt{score}\,(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
     get_embeddings() → Tuple[numpy.ndarray, None]
     forward_k_vs_all (x) \rightarrow \text{torch.FloatTensor}
     forward\_triples(x) \rightarrow torch.FloatTensor
              Parameters
                  x
              Returns
class dicee.models.Pyke(args)
     Bases: dicee.models.base model.BaseKGE
     A Physical Embedding Model for Knowledge Graphs
     name = 'Pyke'
     dist_func
     margin = 1.0
     forward_triples (x: torch.LongTensor)
              Parameters
                  x
class dicee.models.BaseKGE(args: dict)
     Bases: BaseKGELightning
     Base class for all neural network modules.
```

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

Your models should also subclass this class.

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

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

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

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

1 Note

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

Variables

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

args

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

```
normalizer_class = None
normalize_head_entity_embeddings
normalize_relation_embeddings
normalize_tail_entity_embeddings
hidden_normalizer
param_init
input_dp_ent_real
input_dp_rel_real
hidden_dropout
loss_history = []
byte_pair_encoding
max_length_subword_tokens
block_size
forward_byte_pair_encoded_k_vs_all (x: torch.LongTensor)
        Parameters
            x (B x 2 x T)
forward_byte_pair_encoded_triple (x: Tuple[torch.LongTensor, torch.LongTensor])
    byte pair encoded neural link predictors
        Parameters
init_params_with_sanity_checking()
forward(x: torch.LongTensor | Tuple[torch.LongTensor, torch.LongTensor],
           y_idx: torch.LongTensor = None)
        Parameters
            • x
            • y_idx
            • ordered_bpe_entities
forward\_triples(x: torch.LongTensor) \rightarrow torch.Tensor
        Parameters
forward_k_vs_all(*args, **kwargs)
forward_k_vs_sample(*args, **kwargs)
get_triple_representation(idx_hrt)
{\tt get\_head\_relation\_representation}\ (indexed\_triple)
```

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

```
fc1
```

norm_fc1

bn_conv2d

feature_map_dropout

```
residual_convolution (C_1: Tuple[torch.Tensor, torch.Tensor], C_2: Tuple[torch.Tensor, torch.Tensor]) \rightarrow torch.FloatTensor
```

Compute residual score of two complex-valued embeddings. :param C_1 : a tuple of two pytorch tensors that corresponds complex-valued embeddings :param C_2 : a tuple of two pytorch tensors that corresponds complex-valued embeddings :return:

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

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

Parameters

x

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

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

Bases: dicee.models.base_model.BaseKGE

Base class for all neural network modules.

Your models should also subclass this class.

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

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

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

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

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

1 Note

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

Variables

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

```
name = 'ComplEx'
     static score (head_ent_emb: torch.FloatTensor, rel_ent_emb: torch.FloatTensor,
                 tail ent emb: torch.FloatTensor)
     static k_vs_all_score (emb_h: torch.FloatTensor, emb_r: torch.FloatTensor,
                 emb E: torch.FloatTensor)
              Parameters
                   • emb h
                   • emb_r
                   • emb E
     forward_k_vs_all(x: torch.LongTensor) \rightarrow torch.FloatTensor
     forward_k_vs_sample (x: torch.LongTensor, target_entity_idx: torch.LongTensor)
dicee.models.quaternion_mul(*, Q_1, Q_2)
             → Tuple[torch.Tensor, torch.Tensor, torch.Tensor]
     Perform quaternion multiplication :param Q_1: :param Q_2: :return:
class dicee.models.BaseKGE (args: dict)
     Bases: BaseKGELightning
```

Base class for all neural network modules.

Your models should also subclass this class.

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

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

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

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

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

1 Note

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

Variables

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

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

```
forward_byte_pair_encoded_triple(x: Tuple[torch.LongTensor, torch.LongTensor])
          byte pair encoded neural link predictors
              Parameters
     init_params_with_sanity_checking()
     forward(x: torch.LongTensor | Tuple[torch.LongTensor, torch.LongTensor],
                 y idx: torch.LongTensor = None
              Parameters
                  • x
                  • y_idx
                  • ordered_bpe_entities
     forward\_triples(x: torch.LongTensor) \rightarrow torch.Tensor
              Parameters
     forward_k_vs_all(*args, **kwargs)
     forward_k_vs_sample(*args, **kwargs)
     get triple representation(idx hrt)
     get_head_relation_representation(indexed_triple)
     get_sentence_representation(x: torch.LongTensor)
              Parameters
                  • (b (x shape)
                  • 3
                  • t)
     get_bpe_head_and_relation_representation(x: torch.LongTensor)
                  \rightarrow Tuple[torch.FloatTensor, torch.FloatTensor]
              Parameters
                  x (B x 2 x T)
     \mathtt{get\_embeddings}() \rightarrow Tuple[numpy.ndarray, numpy.ndarray]
class dicee.models.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.quaternion_mul_with_unit_norm(*, Q_1, Q_2)

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

Base class for all neural network modules.

Your models should also subclass this class.

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

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

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

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

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

1 Note

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

Variables

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

name = 'OMult'

explicit = True

 $quaternion_multiplication_followed_by_inner_product(h, r, t)$

Parameters

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

Returns

Triple scores.

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

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

Absolute value of a quaternion

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

L2 norm of quaternion vector:

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

Parameters

 \mathbf{x} – The vector.

Returns

The normalized vector.

score (head_ent_emb: torch.FloatTensor, rel_ent_emb: torch.FloatTensor, tail ent emb: torch.FloatTensor)

 $k_vs_all_score$ (bpe_head_ent_emb, bpe_rel_ent_emb, E)

Parameters

- bpe_head_ent_emb
- bpe_rel_ent_emb
- E

```
forward_k_vs_all(x)
               Parameters
                  x
     forward_k_vs_sample (x, target_entity_idx)
          Completed. Given a head entity and a relation (h,r), we compute scores for all possible triples, i.e.,
          [score(h,r,x)|x in Entities] => [0.0,0.1,...,0.8], shape=> (1, |Entities|) Given a batch of head entities and
          relations => shape (size of batch, | Entities|)
class dicee.models.ConvQ(args)
     Bases: dicee.models.base_model.BaseKGE
     Convolutional Quaternion Knowledge Graph Embeddings
     name = 'ConvQ'
     entity_embeddings
     relation_embeddings
     conv2d
     fc_num_input
     fc1
     bn_conv1
     bn_conv2
     feature_map_dropout
     {\tt residual\_convolution}\,(Q\_1,\,Q\_2)
     forward_triples (indexed_triple: torch.Tensor) → torch.Tensor
               Parameters
                  x
     forward_k_vs_all (x: torch.Tensor)
          Given a head entity and a relation (h,r), we compute scores for all entities. [score(h,r,x)|x in Entities] =>
          [0.0,0.1,...,0.8], shape=> (1, |Entities|) Given a batch of head entities and relations => shape (size of batch,|
          Entities()
class dicee.models.AConvQ(args)
     Bases: dicee.models.base_model.BaseKGE
     Additive Convolutional Quaternion Knowledge Graph Embeddings
     name = 'AConvQ'
     entity_embeddings
     relation_embeddings
     conv2d
     fc_num_input
     fc1
```

```
\begin{tabular}{l} bn\_conv1 \\ bn\_conv2 \\ feature\_map\_dropout \\ residual\_convolution (Q\_1, Q\_2) \\ forward\_triples (indexed\_triple: torch.Tensor) $\rightarrow$ torch.Tensor \\ \hline \end{tabular}
```

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 <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.

args

embedding_dim = None

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

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

Base class for all neural network modules.

Your models should also subclass this class.

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

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

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

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

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

1 Note

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

Variables

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

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

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

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

class dicee.models.OMult(args)

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

Base class for all neural network modules.

Your models should also subclass this class.

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

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

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

def forward(self, x):
```

(continues on next page)

(continued from previous page)

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

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



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

Variables

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

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

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

Bases: dicee.models.base_model.BaseKGE

Base class for all neural network modules.

Your models should also subclass this class.

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

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

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

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

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

1 Note

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

Variables

name = 'ConvO'

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

```
conv2d
     fc_num_input
     fc1
     bn conv2d
     norm_fc1
     feature_map_dropout
     static octonion normalizer (emb rel e0, emb rel e1, emb rel e2, emb rel e3, emb rel e4,
                 emb_rel_e5, emb_rel_e6, emb_rel_e7)
     residual\_convolution(O\_1, O\_2)
     forward\_triples(x: torch.Tensor) \rightarrow torch.Tensor
              Parameters
                  x
     forward_k_vs_all (x: torch.Tensor)
          Given a head entity and a relation (h,r), we compute scores for all entities. [score(h,r,x)|x in Entities] =>
          [0.0,0.1,...,0.8], shape=> (1, |Entities|) Given a batch of head entities and relations => shape (size of batch,|
          Entities|)
class dicee.models.AConvO(args: dict)
     Bases: dicee.models.base_model.BaseKGE
     Additive Convolutional Octonion Knowledge Graph Embeddings
     name = 'AConvO'
     conv2d
     fc_num_input
     fc1
     bn_conv2d
     norm_fc1
     feature_map_dropout
     static octonion_normalizer(emb_rel_e0, emb_rel_e1, emb_rel_e2, emb_rel_e3, emb_rel_e4,
                 emb_rel_e5, emb_rel_e6, emb_rel_e7)
```

```
\label{eq:convolution} \textbf{residual\_convolution} \ (O\_1,O\_2) \label{eq:convolution} \textbf{forward\_triples} \ (x: torch.Tensor) \ \to \textbf{torch}.\textbf{Tensor} \label{eq:convolution} \textbf{Parameters}  \textbf{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|)

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

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

Base class for all neural network modules.

forward_k_vs_all (x: torch.Tensor)

Your models should also subclass this class.

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

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

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

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

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

1 Note

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

Variables

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

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

```
compute\_sigma\_pp(hp, rp)
          Compute sigma_{pp} = sum_{i=1}^{p-1} sum_{k=i+1}^p (h_i r_k - h_k r_i) e_i e_k
          sigma {pp} captures the interactions between along p bases For instance, let p e 1, e 2, e 3, we compute
          interactions between e 1 e 2, e 1 e 3, and e 2 e 3 This can be implemented with a nested two for loops
                  results = [] for i in range(p - 1):
                         for k in range(i + 1, p):
                              results.append(hp[:, :, i] * rp[:, :, k] - hp[:, :, k] * rp[:, :, i])
                  sigma_pp = torch.stack(results, dim=2) assert sigma_pp.shape == (b, r, int((p * (p - 1)) / 2))
          Yet, this computation would be quite inefficient. Instead, we compute interactions along all p, e.g., e1e1,
          e1e2, e1e3,
                  e2e1, e2e2, e2e3, e3e1, e3e2, e3e3
          Then select the triangular matrix without diagonals: e1e2, e1e3, e2e3.
compute\_sigma\_qq(hq, rq)
          Compute sigma_{qq} = sum_{j=1}^{p+q-1} sum_{k=j+1}^{p+q} (h_j r_k - h_k r_j) e_j e_k sigma_{q}
          captures the interactions between along q bases For instance, let q e_1, e_2, e_3, we compute interactions
          between e_1 e_2, e_1 e_3, and e_2 e_3 This can be implemented with a nested two for loops
                  results = [] for j in range(q - 1):
                         for k in range(j + 1, q):
                              results.append(hq[:, :, j] * rq[:, :, k] - hq[:, :, k] * rq[:, :, j])
                  sigma_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 j in range(q):
                         sigma_pq[:, :, i, j] = hp[:, :, i] * rq[:, :, j] - hq[:, :, j] * rp[:, :, i]
          print(sigma_pq.shape)
apply_coefficients(hp, hq, rp, rq)
          Multiplying a base vector with its scalar coefficient
clifford_multiplication (h0, hp, hq, r0, rp, rq)
          Compute our CL multiplication
                  sum_{j=p+1}^{p+q} r_j e_j
                  ei ^2 = +1 for i = < i = < p ej ^2 = -1 for p < j = < p+q ei ej = -eje1 for i
          eq j
                  h r = sigma_0 + sigma_p + sigma_q + sigma_{pp} + sigma_{q} + sig
                  (1) sigma_0 = h_0 r_0 + sum_{i=1}^p (h_0 r_i) e_i - sum_{j=p+1}^{p+q} (h_j r_j) e_j
```

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

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

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

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

Parameter

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

returns

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

forward_k_vs_with_explicit(x: torch.Tensor)

k_vs_all_score(bpe_head_ent_emb, bpe_rel_ent_emb, E)

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

Kvsall training

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

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

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

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

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

Parameter

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

returns

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

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

Parameter

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

Base class for all neural network modules.

Your models should also subclass this class.

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

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

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

1 Note

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

Variables

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

name = 'DeCaL'

entity_embeddings

relation embeddings

p

q

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))

 $\verb|compute_sigmas_single| (\textit{list}_h_\textit{emb}, \textit{list}_r_\textit{emb}, \textit{list}_t_\textit{emb})$

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

$$s0 = h_0 r_0 t_0 s1 = \sum_{i=1}^{p} h_i r_i t_0 s2 = \sum_{j=p+1}^{p+q} h_j r_j t_0 s3 = \sum_{i=1}^{q} (h_0 r_i t_i + h_i r_0 t_i) s4 = \sum_{i=p+1}^{p+q} (h_0 r_i t_i + h_i r_0 t_i) s5 = \sum_{i=p+q+1}^{p+q+r} (h_0 r_i t_i + h_i r_0 t_i) s5 = \sum_{i=p+q+1}^{p+q+r} (h_0 r_i t_i + h_i r_0 t_i) s6 = \sum_{i=p+q+r}^{p+q+r} (h_0 r_i t_i + h_i r_0 t_i) s6 = \sum_{i=p+q+r}^{p+q+r} (h_0 r_i t_i + h_i r_0 t_i) s6 = \sum_{i=p+q+r}^{p+q+r} (h_0 r_i t_i + h_i r_0 t_i) s6 = \sum_{i=p+q+r}^{p+q+r} (h_0 r_i t_i + h_i r_0 t_i) s6 = \sum_{i=p+q+r}^{p+q+r} (h_0 r_i t_i + h_i r_0 t_i) s6 = \sum_{i=p+q+r}^{p+q+r} (h_0 r_i t_i + h_i r_0 t_i) s6 = \sum_{i=p+q+r}^{p+q+r} (h_0 r_i t_i + h_i r_0 t_i) s6 = \sum_{i=p+q+r}^{p+q+r} (h_0 r_i t_i + h_i r_0 t_i) s6 = \sum_{i=p+q+r}^{p+q+r} (h_0 r_i t_i + h_i r_0 t_i) s6 = \sum_{i=p+q+r}^{p+q+r} (h_0 r_i t_i + h_i r_0 t_i) s6 = \sum_{i=p+q+r}^{p+q+r} (h_0 r_i t_i + h_i r_0 t_i) s6 = \sum_{i=p+q+r}^{p+q+r} (h_0 r_i t_i + h_i r_0 t_i) s6 = \sum_{i=p+q+r}$$

and return:

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

compute_sigmas_multivect (list_h_emb, list_r_emb)

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

For same bases vectors interaction we have

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

For different base vector interactions, we have

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

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

Kvsall training

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

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

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

Multiplying a base vector with its scalar coefficient

 $\verb|construct_cl_multivector||(x: torch.FloatTensor, re: int, p: int, q: int, r: int)|$

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

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

Parameter

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

returns

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

 $compute_sigma_pp(hp, rp)$

Compute .. math:

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

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

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

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

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

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

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

 $\texttt{compute_sigma_qq}\,(hq,rq)$

Compute

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

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

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

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

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

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)

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

Compute

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

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

for j in range(q):

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

print(sigma_pq.shape)

 $\texttt{compute_sigma_qr} \ (*, hq, hk, rq, rk)$

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

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

for j in range(q):

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

print(sigma_pq.shape)

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

Bases: BaseKGELightning

Base class for all neural network modules.

Your models should also subclass this class.

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

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

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

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

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

1 Note

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

Variables

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

args

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

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

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

t = self.entity_embeddings.weight.reshape(self.num_entities, self.embedding_dim, self.last_dim)

else:

t = self.entity_embeddings.weight

(4) Call the score_t from interactions to generate triple scores. return self.interaction.score_t(h=h, r=r, all entities=t, slice size=1)

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

- # => Explicit version by this we can apply bn and dropout
- # (1) Retrieve embeddings of heads, relations and tails and apply Dropout & Normalization if given. h, r, t = self.get_triple_representation(x) # (2) Reshape (1). if self.last_dim > 0:
 - $\label{eq:hammed} h = h.reshape(len(x), self.embedding_dim, self.last_dim) \\ r = r.reshape(len(x), self.embedding_dim, self.last_dim) \\ t = t.reshape(len(x), self.embedding_dim, self.last_dim) \\ t = t.t. \\ t = t.$
- # (3) Compute the triple score return self.interaction.score(h=h, r=r, t=t, slice_size=None, slice_dim=0)

abstract forward_k_vs_sample (x: torch.LongTensor, target_entity_idx)

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

Bases: BaseKGELightning

Base class for all neural network modules.

Your models should also subclass this class.

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

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

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

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

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

1 Note

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

Variables

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

args

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

```
forward_byte_pair_encoded_triple (x: Tuple[torch.LongTensor, torch.LongTensor])
          byte pair encoded neural link predictors
              Parameters
     init_params_with_sanity_checking()
     forward(x: torch.LongTensor | Tuple[torch.LongTensor, torch.LongTensor],
                 y_idx: torch.LongTensor = None
              Parameters
                  • x
                  • y_idx
                  • ordered_bpe_entities
     forward\_triples(x: torch.LongTensor) \rightarrow torch.Tensor
              Parameters
     forward_k_vs_all(*args, **kwargs)
     forward_k_vs_sample(*args, **kwargs)
     get_triple_representation(idx_hrt)
     get_head_relation_representation(indexed_triple)
     get_sentence_representation(x: torch.LongTensor)
              Parameters
                  • (b (x shape)
                  • 3
                  • t)
     get_bpe_head_and_relation_representation(x: torch.LongTensor)
                  \rightarrow Tuple[torch.FloatTensor, torch.FloatTensor]
              Parameters
                  x (B x 2 x T)
     \mathtt{get\_embeddings}() \rightarrow Tuple[numpy.ndarray, numpy.ndarray]
class dicee.models.FMult(args)
     Bases: dicee.models.base_model.BaseKGE
     Learning Knowledge Neural Graphs
     name = 'FMult'
     entity_embeddings
     relation_embeddings
     k
```

```
num_sample = 50
      gamma
      roots
      weights
      compute\_func(weights: torch.FloatTensor, x) \rightarrow torch.FloatTensor
      chain_func (weights, x: torch.FloatTensor)
      forward\_triples(idx\_triple: torch.Tensor) \rightarrow torch.Tensor
                Parameters
class dicee.models.GFMult(args)
      Bases: dicee.models.base_model.BaseKGE
      Learning Knowledge Neural Graphs
      name = 'GFMult'
      entity_embeddings
      relation_embeddings
      num_sample = 250
      roots
      weights
      \verb|compute_func| (\textit{weights: torch.FloatTensor}, \textit{x}) \rightarrow \textit{torch.FloatTensor}
      chain_func(weights, x: torch.FloatTensor)
      \textbf{forward\_triples} (\textit{idx\_triple: torch.Tensor}) \rightarrow \text{torch.Tensor}
                Parameters
class dicee.models.FMult2(args)
      Bases: dicee.models.base_model.BaseKGE
      Learning Knowledge Neural Graphs
      name = 'FMult2'
      n_{\text{layers}} = 3
      n = 50
      score_func = 'compositional'
      discrete_points
```

```
entity_embeddings
     relation_embeddings
     build_func(Vec)
     build_chain_funcs (list_Vec)
     compute_func (W, b, x) \rightarrow \text{torch.FloatTensor}
     function(list_W, list_b)
     trapezoid(list_W, list_b)
     forward\_triples(idx\_triple: torch.Tensor) \rightarrow torch.Tensor
               Parameters
class dicee.models.LFMult1(args)
     Bases: dicee.models.base_model.BaseKGE
     Embedding with trigonometric functions. We represent all entities and relations in the complex number space as:
     f(x) = sum_{k=0}^{k=0}^{k=d-1}wk e^{kix}, and use the three differents scoring function as in the paper to evaluate
     the score
     name = 'LFMult1'
     entity_embeddings
     relation_embeddings
     forward_triples (idx_triple)
               Parameters
     tri_score(h, r, t)
     \mathtt{vtp\_score}(h, r, t)
class dicee.models.LFMult(args)
     Bases: dicee.models.base_model.BaseKGE
     Embedding with polynomial functions. We represent all entities and relations in the polynomial space as: f(x) =
     sum \{i=0\}^{d-1} a k x^{i} and use the three differents scoring function as in the paper to evaluate the score.
     We also consider combining with Neural Networks.
     name = 'LFMult'
     entity_embeddings
     relation_embeddings
     degree
     x_values
```

forward_triples (idx_triple)

Parameters

x

construct_multi_coeff(X)

poly NN (x, coefh, coefr, coeft)

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

linear (x, w, b)

$scalar_batch_NN(a, b, c)$

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

tri_score (coeff_h, coeff_r, coeff_t)

this part implement the trilinear scoring techniques:

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

$\mathtt{vtp_score}(h, r, t)$

this part implement the vector triple product scoring techniques:

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

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

 $comp_func(h, r, t)$

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

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

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

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

pop (coeff, x, degree)

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

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

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

class dicee.models.DualE(args)

Bases: dicee.models.base_model.BaseKGE

Dual Quaternion Knowledge Graph Embeddings (https://ojs.aaai.org/index.php/AAAI/article/download/16850/16657)

```
name = 'DualE'
entity_embeddings
relation_embeddings
num_ent = None
kvsall_score (e_1_h, e_2_h, e_3_h, e_4_h, e_5_h, e_6_h, e_7_h, e_8_h, e_1_t, e_2_t, e_3_t, e_4_t,
             e_5_t, e_6_t, e_7_t, e_8_t, r_1, r_2, r_3, r_4, r_5, r_6, r_7, r_8) \rightarrow \text{torch.tensor}
     KvsAll scoring function
     Input
     x: torch.LongTensor with (n, ) shape
     Output
     torch.FloatTensor with (n) shape
forward\_triples(idx\_triple: torch.tensor) \rightarrow torch.tensor
     Negative Sampling forward pass:
     Input
     x: torch.LongTensor with (n, ) shape
     Output
     torch.FloatTensor with (n) shape
{\tt forward\_k\_vs\_all}\;(\mathcal{X})
     KvsAll forward pass
     Input
     x: torch.LongTensor with (n, ) shape
     Output
     torch.FloatTensor with (n) shape
T (x: torch.tensor) \rightarrow torch.tensor
     Transpose function
     Input: Tensor with shape (nxm) Output: Tensor with shape (mxn)
```

dicee.query_generator

Classes

QueryGenerator

Module Contents

```
class dicee.query_generator.QueryGenerator(train_path, val_path: str, test_path: str,
             ent2id: Dict = None, rel2id: Dict = None, seed: int = 1, gen_valid: bool = False,
             gen\_test: bool = True)
      train_path
      val_path
      test_path
      gen_valid = False
      gen_test = True
      seed = 1
      max_ans_num = 1000000.0
      mode
      ent2id = None
      rel2id: Dict = None
      ent_in: Dict
      ent_out: Dict
      query_name_to_struct
      list2tuple(list_data)
      tuple2list(x: List | Tuple) \rightarrow List | Tuple
           Convert a nested tuple to a nested list.
      set_global_seed (seed: int)
           Set seed
      construct\_graph(paths: List[str]) \rightarrow Tuple[Dict, Dict]
           Construct graph from triples Returns dicts with incoming and outgoing edges
      fill_query(query\_structure: List[str | List], ent_in: Dict, ent_out: Dict, answer: int) \rightarrow bool
           Private method for fill_query logic.
      achieve\_answer(query: List[str | List], ent\_in: Dict, ent\_out: Dict) \rightarrow set
           Private method for achieve_answer logic. @TODO: Document the code
      write_links (ent_out, small_ent_out)
      ground queries (query structure: List[str | List], ent in: Dict, ent out: Dict, small ent in: Dict,
                   small_ent_out: Dict, gen_num: int, query_name: str)
           Generating queries and achieving answers
      unmap (query_type, queries, tp_answers, fp_answers, fn_answers)
      unmap_query (query_structure, query, id2ent, id2rel)
```

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

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

abstract load_queries (path)

get_queries (query_type: str, gen_num: int)

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

→ None

Save Queries into Disk

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

Load Queries from Disk to Memory

dicee.read_preprocess_save_load_kg

Submodules

dicee.read_preprocess_save_load_kg.preprocess

Classes
```

PreprocessKG

Preprocess the data in memory

Module Contents

(2) Construct vocabulary

(3) Index datasets

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

Preprocess the data in memory

kg

start() → None

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

Parameter

rtype

None

preprocess_with_byte_pair_encoding()

preprocess_with_byte_pair_encoding_with_padding() → None

preprocess_with_pandas() → None

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

(1) Add recipriocal or noisy triples
```

Parameter

rtype

None

 $\label{eq:preprocess_with_polars()} \textbf{\rightarrow None}$ $\mbox{sequential_vocabulary_construction()} \rightarrow \mbox{None}$

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

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

dicee.read_preprocess_save_load_kg.read_from_disk

Classes

ReadFromDisk

Read the data from disk into memory

Module Contents

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

Read the data from disk into memory

kg

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

Read a knowledge graph from disk into memory

Data will be available at the train_set, test_set, valid_set attributes.

Parameter

None

rtype

None

add_noisy_triples_into_training()

dicee.read_preprocess_save_load_kg.save_load_disk

Classes

LoadSaveToDisk

Module Contents

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

dicee.read_preprocess_save_load_kg.util

Functions

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

Module Contents

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

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

Parameters:

df_polars

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

idx entity

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

idx relation

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

Returns:

polars.DataFrame

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

Example Usage:

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

Steps:

- 1. Join the input DataFrame *df_polars* on the 'relation' column with *idx_relation* to replace the relations with their indices.
- 2. Join on 'subject' to replace it with the corresponding entity index using a left join on idx_entity.
- 3. Join on 'object' to replace it with the corresponding entity index using a left join on idx_entity.

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

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

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

Parameters:

df pandas

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

idx_entity

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

idx_relation

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

Returns:

pd.DataFrame

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

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

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

Load and Preprocess via Polars

```
dicee.read_preprocess_save_load_kg.util.get_er_vocab(data, file_path: str = None)
dicee.read_preprocess_save_load_kg.util.get_re_vocab(data, file_path: str = None)
dicee.read_preprocess_save_load_kg.util.get_ee_vocab(data, file_path: str = None)
dicee.read_preprocess_save_load_kg.util.create_constraints(triples, file_path: str = None)
```

(1) Extract domains and ranges of relations

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

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

Classes

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

Package Contents

```
Preprocess train, valid and test datasets stored in knowledge graph instance with pandas
           (1) Add recipriocal or noisy triples
           (2) Construct vocabulary
           (3) Index datasets
           Parameter
               rtype
                   None
     {\tt preprocess\_with\_polars}\,() \,\to None
     \verb|sequential_vocabulary_construction|()| \to None
           (1) Read input data into memory
           (2) Remove triples with a condition
           (3) Serialize vocabularies in a pandas dataframe where
                   => the index is integer and => a single column is string (e.g. URI)
class dicee.read_preprocess_save_load_kg.LoadSaveToDisk(kg)
     kg
     save()
     load()
\verb"class" dicee.read_preprocess_save_load_kg. \verb"ReadFromDisk" ($kg$)
     Read the data from disk into memory
     kg
     \mathtt{start}() \to None
           Read a knowledge graph from disk into memory
           Data will be available at the train_set, test_set, valid_set attributes.
           Parameter
           None
               rtype
                   None
     add_noisy_triples_into_training()
dicee.sanity checkers
```

 $preprocess_with_pandas() \rightarrow None$

Functions

Module Contents

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

dicee.scripts

Submodules

dicee.scripts.index_serve

\$ docker pull qdrant/qdrant && docker run -p 6333:6333 -p 6334:6334 -v \$(pwd)/qdrant_storage:/qdrant/storage:z qdrant/qdrant \$ dicee_vector_db -index -serve -path CountryEmbeddings -collection "countries_vdb"

Attributes

```
app
neural_searcher
```

Classes

NeuralSearcher	
StringListRequest	!!! abstract "Usage Documentation"

Functions

```
get_default_arguments()
index(args)

root()

search_embeddings(q)

retrieve_embeddings(q)

search_embeddings_batch(request)

serve(args)

main()
```

Module Contents

```
dicee.scripts.index_serve.get_default_arguments()
dicee.scripts.index_serve.index(args)
dicee.scripts.index_serve.app
dicee.scripts.index_serve.neural_searcher = None
class dicee.scripts.index_serve.NeuralSearcher(args)
     collection_name
     entity_to_idx = None
     qdrant_client
     topk = 5
     retrieve_embedding (entity: str = None, entities: List[str] = None) \rightarrow List
     search (entity: str)
async dicee.scripts.index_serve.root()
async dicee.scripts.index_serve.search_embeddings(q: str)
async dicee.scripts.index_serve.retrieve_embeddings(q: str)
class dicee.scripts.index_serve.StringListRequest(/, **data: Any)
     Bases: {\tt pydantic.BaseModel}
     !!! abstract "Usage Documentation"
         [Models](../concepts/models.md)
     A base class for creating Pydantic models.
```

```
__class_vars__
     The names of the class variables defined on the model.
__private_attributes__
     Metadata about the private attributes of the model.
     The synthesized __init__ [Signature][inspect.Signature] of the model.
pydantic_complete_
     Whether model building is completed, or if there are still undefined fields.
pydantic core schema
     The core schema of the model.
__pydantic_custom_init__
     Whether the model has a custom __init__ function.
__pydantic_decorators__
     Metadata containing the decorators defined on the model. This replaces Model. validators and
     Model.__root_validators__ from Pydantic V1.
__pydantic_generic_metadata__
     Metadata for generic models; contains data used for a similar purpose to __args__, __origin__, __parame-
     ters__ in typing-module generics. May eventually be replaced by these.
__pydantic_parent_namespace__
     Parent namespace of the model, used for automatic rebuilding of models.
__pydantic_post_init__
     The name of the post-init method for the model, if defined.
__pydantic_root_model__
     Whether the model is a [RootModel][pydantic.root_model.RootModel].
__pydantic_serializer__
     The pydantic-core SchemaSerializer used to dump instances of the model.
pydantic_validator_
     The pydantic-core Schema Validator used to validate instances of the model.
__pydantic_fields__
     A dictionary of field names and their corresponding [FieldInfo][pydantic.fields.FieldInfo] objects.
__pydantic_computed_fields__
          dictionary
                      of
                            computed
                                         field
                                                                their
                                                                        corresponding
                                                                                        [ComputedField-
     Α
                                                names
                                                         and
     Info][pydantic.fields.ComputedFieldInfo] objects.
__pydantic_extra__
     A dictionary containing extra values, if [extra][pydantic.config.ConfigDict.extra] is set to 'allow'.
__pydantic_fields_set__
     The names of fields explicitly set during instantiation.
__pydantic_private__
     Values of private attributes set on the model instance.
```

queries: List[str]

```
reducer: str | None = None
async dicee.scripts.index_serve.search_embeddings_batch(request: StringListRequest)
dicee.scripts.index_serve.serve(args)
dicee.scripts.index_serve.main()
```

dicee.scripts.run

Functions

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

Module Contents

dicee.static_funcs

Functions

anasta raginniagal triplag(v)	Add inverse triples into deek detefreme
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>	
+ (1.4.f. C14.l)	
<pre>get_ee_vocab(data[, file_path])</pre>	
(0)	
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-</pre>	
age_path])	
$load_model(\rightarrow Tuple[object, Tuple[dict, dict]])$	Load weights and initialize pytorch module from names-
	pace arguments
load_model_ensemble()	Construct Ensemble Of weights and initialize pytorch
	module from namespace arguments
save_numpy_ndarray(*, data, file_path)	
- · ·	
numpy_data_type_changer(→ numpy.ndarray)	Detect most efficient data type for a given triples
	continues on next page

continues on next page

Table 2 - continued from previous page

```
save\_checkpoint\_model(\rightarrow None)
                                                        Store Pytorch model into disk
store(\rightarrow None)
                                                        Add randomly constructed triples
add\_noisy\_triples(\rightarrow pandas.DataFrame)
read_or_load_kg(args, cls)
intialize\_model(\rightarrow Tuple[object, str])
load_json(\rightarrow dict)
                                                        Save it as CSV if memory allows.
save\_embeddings(\rightarrow None)
random_prediction(pre_trained_kge)
deploy_triple_prediction(pre_trained_kge,
str_subject, ...)
deploy_tail_entity_prediction(pre_trained_kge,
deploy_head_entity_prediction(pre_trained_kge,
deploy_relation_prediction(pre_trained_kge,
vocab_to_parquet(vocab_to_idx, name, ...)
create_experiment_folder([folder_name])
continual\_training\_setup\_executor(\rightarrow None)
exponential\_function(\rightarrow torch.FloatTensor)
load_numpy(→ numpy.ndarray)
                                                        # @TODO: CD: Renamed this function
evaluate(entity_to_idx,
                             scores,
                                        easy answers,
hard answers)
download_file(url[, destination_folder])
download\_files\_from\_url(\rightarrow None)
download\_pretrained\_model(\rightarrow str)
write_csv_from_model_parallel(path)
                                                        Create
from_pretrained_model_write_embeddings_int
None)
```

Module Contents

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

```
dicee.static_funcs.timeit(func)
dicee.static_funcs.save_pickle(*, data: object = None, file_path=str)
dicee.static_funcs.load_pickle(file_path=str)
dicee.static_funcs.load_term_mapping(file_path=str)
dicee.static_funcs.select_model(args: dict, is_continual_training: bool = None,
            storage path: str = None
dicee.static_funcs.load_model(path_of_experiment_folder: str, model_name='model.pt', verbose=0)
             → Tuple[object, Tuple[dict, dict]]
     Load weights and initialize pytorch module from namespace arguments
dicee.static_funcs.load_model_ensemble(path_of_experiment_folder: str)
             → Tuple[dicee.models.base_model.BaseKGE, Tuple[pandas.DataFrame, pandas.DataFrame]]
     Construct Ensemble Of weights and initialize pytorch module from namespace arguments
       (1) Detect models under given path
      (2) Accumulate parameters of detected models
       (3) Normalize parameters
       (4) Insert (3) into model.
dicee.static_funcs.save_numpy_ndarray(*, data: numpy.ndarray, file_path: str)
dicee.static_funcs.numpy_data_type_changer(train_set: numpy.ndarray, num: int)
             \rightarrow numpy.ndarray
     Detect most efficient data type for a given triples :param train_set: :param num: :return:
dicee.static_funcs.save_checkpoint_model(model, path: str) \rightarrow None
     Store Pytorch model into disk
dicee.static_funcs.store(trained model, model name: str = 'model', full storage path: str = None,
            save\_embeddings\_as\_csv=False) \rightarrow None
dicee.static_funcs.add_noisy_triples(train_set: pandas.DataFrame, add_noise_rate: float)
             \rightarrow pandas.DataFrame
     Add randomly constructed triples :param train_set: :param add_noise_rate: :return:
dicee.static_funcs.read_or_load_kg(args, cls)
dicee.static_funcs.intialize model(args: dict, verbose=0) \rightarrow Tuple[object, str]
dicee.static_funcs.load_json(p: str) \rightarrow dict
dicee.static_funcs.save_embeddings (embeddings: numpy.ndarray, indexes, path: str) \rightarrow None
     Save it as CSV if memory allows. :param embeddings: :param indexes: :param path: :return:
dicee.static_funcs.random_prediction(pre_trained_kge)
dicee.static_funcs.deploy_triple_prediction(pre_trained_kge, str_subject, str_predicate,
            str_object)
dicee.static_funcs.deploy_tail_entity_prediction(pre_trained_kge, str_subject, str_predicate,
            top_k)
```

```
dicee.static_funcs.deploy_head_entity_prediction(pre_trained_kge, str_object, str_predicate,
           top_k)
dicee.static_funcs.deploy_relation_prediction(pre_trained_kge, str_subject, str_object, top_k)
dicee.static_funcs.vocab_to_parquet(vocab_to_idx, name, path_for_serialization, print_into)
dicee.static_funcs.create_experiment_folder(folder_name='Experiments')
dicee.static_funcs.continual_training_setup_executor(executor) \rightarrow None
dicee.static_funcs.exponential function (x: numpy.ndarray, lam: float, ascending order=True)
            → torch.FloatTensor
dicee.static_funcs.load_numpy(path) \rightarrow numpy.ndarray
dicee.static_funcs.evaluate(entity_to_idx, scores, easy_answers, hard_answers)
     # @TODO: CD: Renamed this function Evaluate multi hop query answering on different query types
dicee.static_funcs.download_file(url, destination_folder='.')
dicee.static_funcs.download_files_from_url(base\_url: str, destination\_folder='.') \rightarrow None
          Parameters
                                                "https://files.dice-research.org/projects/DiceEmbeddings/
                • base_url
                                (e.g.
                  KINSHIP-Keci-dim128-epoch256-KvsAll")
                • destination_folder (e.g. "KINSHIP-Keci-dim128-epoch256-KvsA11")
dicee.static_funcs.download_pretrained_model(url: str) \rightarrow str
dicee.static_funcs.write_csv_from_model_parallel(path: str)
     Create
dicee.static_funcs.from_pretrained_model_write_embeddings_into_csv(path: str) \rightarrow None
```

dicee.static funcs training

Functions

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

Module Contents

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

dicee.static_preprocess_funcs

Attributes

enable_log

Functions

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

Module Contents

- (1) Extract domains and ranges of relations
- (2) Store a mapping from relations to entities that are outside of the domain and range. Create constraints entities based on the range of relations :param triples: :return:

```
dicee.static_preprocess_funcs.get_er_vocab(data)
dicee.static_preprocess_funcs.get_re_vocab(data)
```

```
dicee.static_preprocess_funcs.get_ee_vocab(data)
dicee.static_preprocess_funcs.mapping_from_first_two_cols_to_third(train_set_idx)
```

dicee.trainer

Submodules

dicee.trainer.dice_trainer

Classes

```
DICE_Trainer implement
```

Functions

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

Module Contents

```
dicee.trainer.dice_trainer.load_term_mapping(file_path=str)
dicee.trainer.dice_trainer.initialize_trainer(args, callbacks)
             \rightarrow dicee.trainer.torch_trainer.TorchTrainer | dicee.trainer.model_parallelism.TensorParallel | dicee.trainer.torch_trainer_ddp
\verb|dicee.trainer.dice_trainer.get_callbacks|| (args)
class dicee.trainer.dice_trainer.DICE_Trainer (args, is_continual_training: bool, storage_path,
            evaluator=None)
     DICE_Trainer implement
           1- Pytorch Lightning trainer (https://pytorch-lightning.readthedocs.io/en/stable/common/trainer.html)
           2- Multi-GPU Trainer(https://pytorch.org/docs/stable/generated/torch.nn.parallel.DistributedDataParallel.
           html) 3- CPU Trainer
           args
           is_continual_training:bool
           storage_path:str
           evaluator:
           report:dict
     report
     args
     trainer = None
```

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

    model

                                    • form of labelling (str)
initialize_trainer(callbacks: List)
                                  → lightning.Trainer | dicee.trainer.model_parallelism.TensorParallel | dicee.trainer.torch_trainer.TorchTrainer | dicee.trainer.torch_trainer.TorchTrainer | dicee.trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_traine
             Initialize Trainer from input arguments
initialize_or_load_model()
\verb"init_dataloader" (\textit{dataset: torch.utils.data.Dataset}) \rightarrow torch.utils.data.DataLoader
init\_dataset() \rightarrow torch.utils.data.Dataset
start (knowledge_graph: dicee.knowledge_graph.KG | numpy.memmap)
                                  → Tuple[dicee.models.base_model.BaseKGE, str]
             Start the training
              (1) Initialize Trainer
              (2) Initialize or load a pretrained KGE model
             in DDP setup, we need to load the memory map of already read/index KG.
k\_fold\_cross\_validation(dataset) \rightarrow Tuple[dicee.models.base\_model.BaseKGE, str]
             Perform K-fold Cross-Validation
                 1. Obtain K train and test splits.
                 2. For each split,
                                   2.1 initialize trainer and model 2.2. Train model with configuration provided in args. 2.3. Compute
                                   the mean reciprocal rank (MRR) score of the model on the test respective split.
                 3. Report the mean and average MRR.
                        Parameters

    self

                                   • dataset
                        Returns
```

model

dicee.trainer.model_parallelism

Classes

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

Functions

```
extract_input_outputs(z[, device])

find_good_batch_size(train_loader,

tp_ensemble_model)

forward_backward_update_loss(→ float)
```

Module Contents

dicee.trainer.torch_trainer

fit (*args, **kwargs)
Train model

Classes

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

Module Contents

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

dicee.trainer.torch_trainer_ddp

Classes

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

Functions

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

Module Contents

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

```
optimizer

train_dataset_loader

loss_func

callbacks

model

num_epochs

loss_history = []

ctx

scaler

extract_input_outputs(z: list)

train()

Training loop for DDP
```

Classes

DICE_Trainer

DICE_Trainer implement

Package Contents

class dicee.trainer.DICE_Trainer(args, is_continual_training: bool, storage_path, evaluator=None)

DICE_Trainer implement

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

args

is_continual_training:bool

storage_path:str

evaluator:

report:dict

report

args

trainer = None

is_continual_training

storage_path

evaluator = None

form_of_labelling = None

```
continual_start (knowledge_graph)
                  (1) Initialize training.
                  (2) Load model
                (3) Load trainer (3) Fit model
                Parameter
                              returns

    model

                                            • form_of_labelling (str)
initialize_trainer(callbacks: List)
                                           → lightning.Trainer | dicee.trainer.model_parallelism.TensorParallel | dicee.trainer.torch_trainer.TorchTrainer | dicee.trainer.torch_trainer.TorchTrainer | dicee.trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_traine
                Initialize Trainer from input arguments
initialize_or_load_model()
\verb"init_dataloader" (dataset: torch.utils.data.Dataset") 	o torch.utils.data.DataLoader
\verb"init_dataset"() \rightarrow torch.utils.data.Dataset"
start (knowledge_graph: dicee.knowledge_graph.KG | numpy.memmap)
                                           → Tuple[dicee.models.base_model.BaseKGE, str]
                Start the training
                  (1) Initialize Trainer
                  (2) Initialize or load a pretrained KGE model
                in DDP setup, we need to load the memory map of already read/index KG.
k\_fold\_cross\_validation(dataset) \rightarrow Tuple[dicee.models.base\_model.BaseKGE, str]
                Perform K-fold Cross-Validation
                     1. Obtain K train and test splits.
```

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

Parameters

- self
- dataset

Returns

model

14.2 Attributes

__version__

14.3 Classes

Duko	A Physical Embedding Model for Knowledge Graphs
Pyke	• • • • • • • • • • • • • • • • • • • •
DistMult	Embedding Entities and Relations for Learning and Inference in Knowledge Bases
CV	•
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.
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 Em-
	beddings
AConvQ	Additive Convolutional Quaternion Knowledge Graph Embeddings
ConvQ	Convolutional Quaternion Knowledge Graph Embed-
	dings
Conv0	Base class for all neural network modules.
ConEx	Convolutional ComplEx Knowledge Graph Embeddings
QMult	Base class for all neural network modules.
OMult	Base class for all neural network modules.
Shallom	A shallow neural model for relation prediction (https:
	//arxiv.org/abs/2101.09090)
LFMult	Embedding with polynomial functions. We represent all
	entities and relations in the polynomial space as:
PykeenKGE	A class for using knowledge graph embedding models 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
KvsA11	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
	continues on next page

continues on next page

Table 3 - continued from previous page

CVDataModule	Create a Dataset for cross validation
LiteralDataset	Dataset for loading and processing literal data for training Literal Embedding model.
QueryGenerator	

14.4 Functions

<pre>create_recipriocal_triples(x)</pre>	Add inverse triples into dask dataframe
<pre>get_er_vocab(data[, file_path])</pre>	
<pre>get_re_vocab(data[, file_path])</pre>	
get_re_vocab(data[, inc_patii])	
<pre>get_ee_vocab(data[, file_path])</pre>	
timeit(func)	
timert(tunc)	
<pre>save_pickle(*[, data, file_path])</pre>	
(10)	
load_pickle([file_path])	
<pre>load_term_mapping([file_path])</pre>	
_	
select_model(args[, is_continual_training, stor-	
age_path])	
$load_model(\rightarrow Tuple[object, Tuple[dict, dict]])$	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(→ None)	Store Pytorch model into disk
store(→ None)	·
add_noisy_triples(→ pandas.DataFrame)	Add randomly constructed triples
read_or_load_kg(args, cls)	
intialize_model(→ Tuple[object, str])	
$load_{json}(\rightarrow dict)$	
$save_embeddings(\rightarrow None)$	Save it as CSV if memory allows.
random_prediction(pre_trained_kge)	
deploy_triple_prediction(pre_trained_kge,	
str_subject,)	
<pre>deploy_tail_entity_prediction(pre_trained_kge,)</pre>	
)	continues on next nage

continues on next page

Table 4 - 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(\rightarrow None)
exponential\_function(\rightarrow torch.FloatTensor)
load_numpy(→ numpy.ndarray)
                                                      # @TODO: CD: Renamed this function
evaluate(entity_to_idx,
                            scores,
                                      easy answers,
hard answers)
download_file(url[, destination_folder])
download\_files\_from\_url(\rightarrow None)
download_pretrained_model(\rightarrow str)
write_csv_from_model_parallel(path)
                                                      Create
from_pretrained_model_write_embeddings_int
None)
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
        x
```

```
Embedding Entities and Relations for Learning and Inference in Knowledge Bases https://arxiv.org/abs/1412.6575
     name = 'DistMult'
     k_vs_all_score (emb_h: torch.FloatTensor, emb_r: torch.FloatTensor, emb_E: torch.FloatTensor)
               Parameters
                   • emb h
                   • emb_r
                   • emb_E
     forward_k_vs_all (x: torch.LongTensor)
     forward_k_vs_sample (x: torch.LongTensor, target_entity_idx: torch.LongTensor)
     \mathtt{score}\left(h,r,t\right)
class dicee.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 dicee.DistMult(args)

class Model(nn.Module):

to(), etc.

def __init__(self) -> None:
 super().__init__()

def forward(self, x):

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

Bases: dicee.models.base_model.BaseKGE

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

1 Note

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

Variables

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

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

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

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

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

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

```
\begin{split} & \texttt{compute\_sigma\_pq} \ (*, hp, hq, rp, rq) \\ & sum\_\{i=1\}^{p} \ sum\_\{j=p+1\}^{p+q} \ (h_i \ r_j - h_j \ r_i) \ e_i \ e_j \\ & results = [] \ sigma\_pq = torch.zeros(b, r, p, q) \ for \ i \ in \ range(p): \end{split}
```

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

eq j

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

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

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

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

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

Parameter

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

returns

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

forward_k_vs_with_explicit(x: torch.Tensor)

 $k_vs_all_score$ (bpe_head_ent_emb, bpe_rel_ent_emb, E)

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

Kvsall training

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

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

```
construct_batch_selected_cl_multivector(x: torch.FloatTensor, r: int, p: int, q: int)
                    → tuple[torch.FloatTensor, torch.FloatTensor, torch.FloatTensor]
           Construct a batch of batchs multivectors Cl_{p,q}(mathbb\{R\}^d)
           Parameter
           x: torch.FloatTensor with (n,k, d) shape
                returns
                    • a0 (torch.FloatTensor with (n,k, m) shape)
                    • ap (torch.FloatTensor with (n,k, m, p) shape)
                    • aq (torch.FloatTensor with (n,k, m, q) shape)
      \textbf{forward\_k\_vs\_sample} \ (x: torch.LongTensor, target\_entity\_idx: torch.LongTensor) \ \rightarrow \textbf{torch}.FloatTensor
           Parameter
           x: torch.LongTensor with (n,2) shape
           target_entity_idx: torch.LongTensor with (n, k) shape k denotes the selected number of examples.
                rtype
                    torch.FloatTensor with (n, k) shape
      score(h, r, t)
      forward\_triples(x: torch.Tensor) \rightarrow torch.FloatTensor
           Parameter
           x: torch.LongTensor with (n,3) shape
                rtype
                    torch.FloatTensor with (n) shape
class dicee.TransE(args)
      Bases: dicee.models.base_model.BaseKGE
      Translating Embeddings for Modeling Multi-relational Data https://proceedings.neurips.cc/paper/2013/file/
      1cecc7a77928ca8133fa24680a88d2f9-Paper.pdf
      name = 'TransE'
      margin = 4
      score (head_ent_emb, rel_ent_emb, tail_ent_emb)
      forward_k_vs_all(x: torch.Tensor) \rightarrow torch.FloatTensor
class dicee.DeCaL(args)
      Bases: dicee.models.base_model.BaseKGE
```

Base class for all neural network modules.

Your models should also subclass this class.

Modules can also contain other Modules, allowing 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
p
q
r
re
forward_triples (x: torch.Tensor) → torch.FloatTensor
```

Parameter

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

rtype

torch.FloatTensor with (n) shape

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

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

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

compute_sigmas_single(list_h_emb, list_r_emb, list_t_emb)

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

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

and return:

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

compute_sigmas_multivect(list_h_emb, list_r_emb)

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

For same bases vectors interaction we have

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

For different base vector interactions, we have

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

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

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 $\{R\}^{\wedge}d$).
- (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):

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

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

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

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

compute sigma rr(hk, rk)

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

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

Compute

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

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

for j in range(q):

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

print(sigma_pq.shape)

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

Compute

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

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

for j in range(q):

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

print(sigma_pq.shape)

 $\texttt{compute_sigma_qr} \ (*, hq, hk, rq, rk)$

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

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

for j in range(q):

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

print(sigma_pq.shape)

class dicee.DualE(args)

Bases: dicee.models.base_model.BaseKGE

Dual Quaternion Knowledge Graph Embeddings (https://ojs.aaai.org/index.php/AAAI/article/download/16850/16657)

name = 'DualE'

entity_embeddings

relation_embeddings

num_ent = None

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

KvsAll scoring function

Input

x: torch.LongTensor with (n,) shape

Output

torch.FloatTensor with (n) shape

 $forward_triples(idx_triple: torch.tensor) \rightarrow torch.tensor$

Negative Sampling forward pass:

Input

x: torch.LongTensor with (n,) shape

Output

torch.FloatTensor with (n) shape

```
forward_k_vs_all(x)
```

KvsAll forward pass

Input

x: torch.LongTensor with (n,) shape

Output

torch.FloatTensor with (n) shape

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

Transpose function

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

```
class dicee.ComplEx(args)
```

Bases: dicee.models.base_model.BaseKGE

Base class for all neural network modules.

Your models should also subclass this class.

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

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

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

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

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

1 Note

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

Variables

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

```
name = 'ComplEx'
     static score (head_ent_emb: torch.FloatTensor, rel_ent_emb: torch.FloatTensor,
                  tail ent emb: torch.FloatTensor)
     static k_vs_all_score (emb_h: torch.FloatTensor, emb_r: torch.FloatTensor,
                  emb E: torch.FloatTensor)
               Parameters
                   • emb h
                   • emb_r
                   • emb E
     forward_k_vs_all(x: torch.LongTensor) \rightarrow torch.FloatTensor
     forward_k_vs_sample (x: torch.LongTensor, target_entity_idx: torch.LongTensor)
class dicee.AConEx(args)
     Bases: dicee.models.base_model.BaseKGE
     Additive Convolutional ComplEx Knowledge Graph Embeddings
     name = 'AConEx'
     conv2d
     fc_num_input
     fc1
     norm_fc1
     bn_conv2d
     feature_map_dropout
     residual_convolution (C_1: Tuple[torch.Tensor, torch.Tensor],
                  C_2: Tuple[torch.Tensor, torch.Tensor]) \rightarrow torch.FloatTensor
           Compute residual score of two complex-valued embeddings. :param C_1: a tuple of two pytorch tensors
           that corresponds complex-valued embeddings :param C_2: a tuple of two pytorch tensors that corresponds
           complex-valued embeddings :return:
     forward_k_vs_all(x: torch.Tensor) \rightarrow torch.FloatTensor
     forward\_triples(x: torch.Tensor) \rightarrow torch.FloatTensor
               Parameters
                   x
     forward k vs sample (x: torch. Tensor, target entity idx: torch. Tensor)
class dicee.AConvO(args: dict)
     Bases: dicee.models.base_model.BaseKGE
     Additive Convolutional Octonion Knowledge Graph Embeddings
     name = 'AConvO'
     conv2d
```

```
fc_num_input
     fc1
     bn_conv2d
     norm_fc1
     feature_map_dropout
     static octonion_normalizer(emb_rel_e0, emb_rel_e1, emb_rel_e2, emb_rel_e3, emb_rel_e4,
                  emb_rel_e5, emb_rel_e6, emb_rel_e7)
     residual\_convolution(O\_1, O\_2)
     forward\_triples(x: torch.Tensor) \rightarrow torch.Tensor
               Parameters
     forward_k_vs_all (x: torch.Tensor)
           Given a head entity and a relation (h,r), we compute scores for all entities. [score(h,r,x)|x in Entities] =>
           [0.0,0.1,...,0.8], shape=> (1, |Entities|) Given a batch of head entities and relations => shape (size of batch,|
           Entities|)
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,|
           Entitiesl)
```

```
class dicee.ConvQ(args)
     Bases: dicee.models.base_model.BaseKGE
     Convolutional Quaternion Knowledge Graph Embeddings
     name = 'ConvQ'
     entity_embeddings
     relation embeddings
     conv2d
     fc_num_input
     fc1
     bn_conv1
     bn_conv2
     feature_map_dropout
     residual\_convolution(Q_1, Q_2)
     forward\_triples (indexed\_triple: torch.Tensor) \rightarrow torch.Tensor
               Parameters
     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
```

Dases. dicee.models.base_model.ba

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

feature_map_dropout

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

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

```
residual_convolution (C_1: Tuple[torch.Tensor, torch.Tensor], C_2: Tuple[torch.Tensor, torch.Tensor]) \rightarrow torch.FloatTensor
```

Compute residual score of two complex-valued embeddings. :param C_1: a tuple of two pytorch tensors that corresponds complex-valued embeddings :param C_2: a tuple of two pytorch tensors that corresponds complex-valued embeddings :return:

class dicee.QMult(args)

Bases: dicee.models.base_model.BaseKGE

Base class for all neural network modules.

Your models should also subclass this class.

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

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

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

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

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

1 Note

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

Variables

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

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

Parameters

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

Returns

Triple scores.

$\mathtt{static}\ \mathtt{quaternion_normalizer}\ (x:\ torch.FloatTensor) \ o \ torch.FloatTensor$

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

Absolute value of a quaternion

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

L2 norm of quaternion vector:

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

Parameters

 \mathbf{x} – The vector.

Returns

The normalized vector.

k_vs_all_score (bpe_head_ent_emb, bpe_rel_ent_emb, E)

Parameters

- bpe_head_ent_emb
- bpe rel ent emb
- E

 ${\tt forward_k_vs_all}\;(\mathcal{X})$

Parameters

x

forward_k_vs_sample (x, target_entity_idx)

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

class dicee.OMult(args)

Bases: dicee.models.base_model.BaseKGE

Base class for all neural network modules.

Your models should also subclass this class.

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

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

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

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

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

1 Note

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

Variables

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

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

```
class dicee.Shallom(args)
```

Bases: dicee.models.base_model.BaseKGE

A shallow neural model for relation prediction (https://arxiv.org/abs/2101.09090)

```
name = 'Shallom'
shallom
get_embeddings() \rightarrow Tuple[numpy.ndarray, None]
forward_k_vs_all(x) \rightarrow torch.FloatTensor
forward_triples(x) \rightarrow torch.FloatTensor
```

Parameters

x

Returns

class dicee.LFMult(args)

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

4. take the sum over each batch

```
comp\_func(h, r, t)
```

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

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

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

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

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

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

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

```
\operatorname{coeff}[1][0] + \operatorname{coeff}[1][1]x + ... + \operatorname{coeff}[1][d]x^{\wedge}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, $r = self.get_head_relation_representation(x) # (2) Reshape (1). if <math>self.last_dim > 0$:

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

(3) Reshape all entities. if self.last_dim > 0:

t = self.entity_embeddings.weight.reshape(self.num_entities, self.embedding_dim, self.last_dim)

else:

t = self.entity_embeddings.weight

(4) Call the score_t from interactions to generate triple scores. return self.interaction.score_t(h=h, r=r, all_entities=t, slice_size=1)

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

=> Explicit version by this we can apply bn and dropout

(1) Retrieve embeddings of heads, relations and tails and apply Dropout & Normalization if given. h, r, t = self.get_triple_representation(x) # (2) Reshape (1). if self.last_dim > 0:

```
h = h.reshape(len(x), self.embedding\_dim, self.last\_dim) r = r.reshape(len(x), self.embedding\_dim, self.last\_dim) t = t.reshape(len(x), self.embedding\_dim, self.last\_dim)
```

(3) Compute the triple score return self.interaction.score(h=h, r=r, t=t, slice size=None, slice dim=0)

abstract forward_k_vs_sample (x: torch.LongTensor, target_entity_idx)

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

Bases: dicee.models.base_model.BaseKGE

Base class for all neural network modules.

Your models should also subclass this class.

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

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

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

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

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

1 Note

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

Variables

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

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

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
```

(continues on next page)

(continued from previous page)

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

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

1 Note

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

class dicee.BaseKGE(args: dict)

Bases: BaseKGELightning

Base class for all neural network modules.

Your models should also subclass this class.

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

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

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

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

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

1 Note

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

Variables

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

args

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

```
forward_byte_pair_encoded_triple (x: Tuple[torch.LongTensor, torch.LongTensor])
          byte pair encoded neural link predictors
              Parameters
     init_params_with_sanity_checking()
     forward(x: torch.LongTensor | Tuple[torch.LongTensor, torch.LongTensor],
                 y_idx: torch.LongTensor = None
              Parameters
                  • x
                  • y_idx
                  • ordered_bpe_entities
     forward_triples (x: torch.LongTensor) \rightarrow torch.Tensor
              Parameters
     forward_k_vs_all(*args, **kwargs)
     forward_k_vs_sample(*args, **kwargs)
     get_triple_representation(idx_hrt)
     get_head_relation_representation(indexed_triple)
     get_sentence_representation(x: torch.LongTensor)
              Parameters
                  • (b (x shape)
                  • 3
                  • t)
     get_bpe_head_and_relation_representation(x: torch.LongTensor)
                  \rightarrow Tuple[torch.FloatTensor, torch.FloatTensor]
              Parameters
                  x (B x 2 x T)
     \mathtt{get\_embeddings}() \rightarrow Tuple[numpy.ndarray, numpy.ndarray]
class dicee.EnsembleKGE (seed_model=None, pretrained_models: List = None)
     name
     train_mode = True
     named_children()
     property example_input_array
     parameters()
     modules()
```

```
__iter__()
      __len__()
     eval()
     to (device)
     mem_of_model()
     __call__(x_batch)
     step()
     get_embeddings()
     __str__()
dicee.create_recipriocal_triples(x)
     Add inverse triples into dask dataframe :param x: :return:
dicee.get_er_vocab(data, file_path: str = None)
dicee.get_re_vocab(data, file_path: str = None)
dicee.get_ee_vocab(data, file_path: str = None)
dicee.timeit(func)
dicee.save_pickle(*, data: object = None, file_path=str)
dicee.load_pickle(file_path=str)
dicee.load_term_mapping(file_path=str)
dicee.select_model(args: dict, is_continual_training: bool = None, storage_path: str = None)
dicee.load_model(path_of_experiment_folder: str, model_name='model.pt', verbose=0)
             → Tuple[object, Tuple[dict, dict]]
     Load weights and initialize pytorch module from namespace arguments
dicee.load_model_ensemble(path_of_experiment_folder: str)
             → Tuple[dicee.models.base_model.BaseKGE, Tuple[pandas.DataFrame, pandas.DataFrame]]
     Construct Ensemble Of weights and initialize pytorch module from namespace arguments
       (1) Detect models under given path
       (2) Accumulate parameters of detected models
       (3) Normalize parameters
       (4) Insert (3) into model.
dicee.save_numpy_ndarray(*, data: numpy.ndarray, file_path: str)
dicee.numpy_data_type_changer(train\_set: numpy.ndarray, num: int) \rightarrow numpy.ndarray
     Detect most efficient data type for a given triples :param train_set: :param num: :return:
\texttt{dicee.save\_checkpoint\_model} \ (\textit{model}, \textit{path: str}) \ \rightarrow None
     Store Pytorch model into disk
```

```
dicee.store(trained_model, model_name: str = 'model', full_storage_path: str = None,
            save\_embeddings\_as\_csv=False) \rightarrow None
dicee.add\_noisy\_triples (train_set: pandas.DataFrame, add_noise_rate: float) \rightarrow pandas.DataFrame
     Add randomly constructed triples :param train_set: :param add_noise_rate: :return:
dicee.read_or_load_kg(args, cls)
dicee.intialize_model(args: dict, verbose=0) \rightarrow Tuple[object, str]
dicee.load_json(p: str) \rightarrow dict
dicee.save_embeddings(embeddings: numpy.ndarray, indexes, path: str) \rightarrow None
     Save it as CSV if memory allows. :param embeddings: :param indexes: :param path: :return:
dicee.random_prediction(pre_trained_kge)
dicee.deploy_triple_prediction(pre_trained_kge, str_subject, str_predicate, str_object)
dicee.deploy_tail_entity_prediction(pre_trained_kge, str_subject, str_predicate, top_k)
dicee.deploy_head_entity_prediction(pre_trained_kge, str_object, str_predicate, top_k)
dicee.deploy_relation_prediction(pre_trained_kge, str_subject, str_object, top_k)
dicee.vocab_to_parquet(vocab_to_idx, name, path_for_serialization, print_into)
dicee.create_experiment_folder(folder_name='Experiments')
dicee.continual\_training\_setup\_executor(executor) \rightarrow None
dicee.exponential_function (x: numpy.ndarray, lam: float, ascending\_order=True) \rightarrow torch.FloatTensor
dicee.load_numpy(path) \rightarrow numpy.ndarray
dicee.evaluate(entity_to_idx, scores, easy_answers, hard_answers)
     # @TODO: CD: Renamed this function Evaluate multi hop query answering on different query types
dicee.download_file (url, destination_folder='.')
dicee.download_files_from_url(base_url: str, destination_folder='.') \rightarrow None
           Parameters
                                                   "https://files.dice-research.org/projects/DiceEmbeddings/

    base_url

                                  (e.g.
                   KINSHIP-Keci-dim128-epoch256-KvsAll")
                 • destination_folder (e.g. "KINSHIP-Keci-dim128-epoch256-KvsA11")
dicee.download\_pretrained\_model(url:str) \rightarrow str
dicee.write_csv_from_model_parallel(path: str)
dicee.from_pretrained_model_write_embeddings_into_csv(path:str) \rightarrow None
```

```
DICE_Trainer implement
              1- Pytorch Lightning trainer (https://pytorch-lightning.readthedocs.io/en/stable/common/trainer.html)
              2- Multi-GPU Trainer(https://pytorch.org/docs/stable/generated/torch.nn.parallel.DistributedDataParallel.
              html) 3- CPU Trainer
              args
              is_continual_training:bool
              storage_path:str
              evaluator:
              report:dict
report
args
trainer = None
is_continual_training
storage path
evaluator = None
form_of_labelling = None
continual_start (knowledge_graph)
               (1) Initialize training.
               (2) Load model
              (3) Load trainer (3) Fit model
              Parameter
                          returns

    model

                                       • form_of_labelling (str)
initialize_trainer(callbacks: List)
                                     \rightarrow lightning.Trainer | dicee.trainer.model_parallelism.TensorParallel | dicee.trainer.torch_trainer.TorchTrainer | dicee.trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_trainer.torch_train
              Initialize Trainer from input arguments
initialize_or_load_model()
init\_dataloader (dataset: torch.utils.data.Dataset) \rightarrow torch.utils.data.DataLoader
init_dataset() \rightarrow torch.utils.data.Dataset
start (knowledge_graph: dicee.knowledge_graph.KG | numpy.memmap)
                                     → Tuple[dicee.models.base_model.BaseKGE, str]
              Start the training
               (1) Initialize Trainer
```

(2) Initialize or load a pretrained KGE model

in DDP setup, we need to load the memory map of already read/index KG.

 $k_fold_cross_validation(dataset) \rightarrow Tuple[dicee.models.base_model.BaseKGE, str]$

Perform K-fold Cross-Validation

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

Parameters

- self
- dataset

Returns

model

```
class dicee.KGE (path=None, url=None, construct_ensemble=False, model_name=None)
```

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

Interactive QueryDecomposition, dicee.abstracts.BaseInteractiveTrainKGE

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

```
__str__()
```

to (device: str) \rightarrow None

 $\begin{tabular}{ll} \tt get_transductive_entity_embeddings (indices: torch.LongTensor \mid List[str], as_pytorch=False, \\ as_numpy=False, as_list=True) \rightarrow {\tt torch.FloatTensor \mid numpy.ndarray \mid List[float]} \end{tabular}$

 $create_vector_database$ (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)

 $\label{limitsing_head_entity} $$predict_missing_head_entity$ (relation: List[str] | str, tail_entity$: List[str] | str, within=None, \\ batch_size=2$, topk=1$, return_indices=False$) $\to $$Tuple$

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

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

Parameter

relation: Union[List[str], str]

String representation of selected relations.

tail_entity: Union[List[str], str]

String representation of selected entities.

k: int

Highest ranked k entities.

Returns: Tuple

```
Highest K scores and entities
```

```
predict_missing_relations (head_entity: List[str] | str, tail_entity: List[str] | str, within=None, batch_size=2, topk=1, return_indices=False) \rightarrow Tuple
```

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

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

Parameter

head_entity: List[str]

String representation of selected entities.

tail_entity: List[str]

String representation of selected entities.

k: int

Highest ranked k entities.

Returns: Tuple

Highest K scores and entities

```
predict_missing_tail_entity (head_entity: List[str] | str, relation: List[str] | str, within: List[str] = None, batch_size=2, topk=1, return_indices=False) \rightarrow torch.FloatTensor Given a head entity and a relation, return top k ranked entities
```

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

Parameter

head_entity: List[str]

String representation of selected entities.

tail_entity: List[str]

String representation of selected entities.

Returns: Tuple

scores

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

Parameters

- logits
- h
- r
- t
- within

Predict missing item in a given triple.

Returns

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

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

Predict triple score

Parameter

head_entity: List[str]

String representation of selected entities.

relation: List[str]

String representation of selected relations.

tail_entity: List[str]

String representation of selected entities.

logits: bool

If logits is True, unnormalized score returned

Returns: Tuple

pytorch tensor of triple score

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

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

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

→ List[Tuple[str, torch.Tensor]]
```

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

Find an answer set for EPFO queries including negation and disjunction

Parameter

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

query: Union[str, Tuple[str, 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

otin G $deploy (share: bool = False, top \ k: int = 10)$

predict literals (entity: List[str] | str = None, attribute: List[str] | str = None,

 $denormalize_preds: bool = True) \rightarrow numpy.ndarray$

Predicts literal values for given entities and attributes.

Stop after finding at_most missing triples $\{(e,r,x) \mid f(e,r,x) > \text{confidence land } (e,r,x)\}$

Parameters

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

Returns

Predictions for the given entities and attributes.

Return type

numpy ndarray

 $\verb"class" dicee.Execute" (args, continuous_training=False)$

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
\texttt{setup\_executor}\,(\,)\,\to 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
```

A dict containing information about the training and/or evaluation

rtype

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.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__()
     \__{\texttt{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

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

 $\verb"class" dicee.KvsAll" (\textit{train_set_idx: numpy.ndarray, entity_idxs, relation_idxs, form, store=None, and the context of the$

 $label_smoothing_rate: float = 0.0$)

Bases: torch.utils.data.Dataset

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

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

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



train set idx

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

entity_idxs

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

relation_idxs

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

self: torch.utils.data.Dataset

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

```
train_data = None
train_target = None
label_smoothing_rate
collate_fn = None
__len__()
\__getitem\__(idx)
```

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

Bases: torch.utils.data.Dataset

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

Let D denote a dataset for AllvsAll training and be defined as $D := \{(x,y)_i\}_i ^n N$, 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.

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.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.

Туре

torch.Tensor

collate_fn

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

Type

function, optional

train_data

num_entities

```
num_relations
      neg_sample_ratio = None
      label_smoothing_rate
      collate_fn = None
      __len__()
           Returns the number of samples in the dataset.
      \__getitem\__(idx)
           Retrieves a single data sample from the dataset at the given index.
                    idx (int) – The index of the sample to retrieve.
                Returns
                    A tuple consisting of:
                      • x (torch.Tensor): The head and relation part of the triple.
                      • y_idx (torch.Tensor): The concatenated indices of the true object (tail entity) and the
                         indices of the negative samples.
                      • y_vec (torch.Tensor): A vector containing the labels for the positive and negative samples,
                         with label smoothing applied.
                Return type
                    tuple
class dicee.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
                    |new_y| << |E| new_y contains all 1's if sum(y)< neg_sample ratio new_y contains</pre>
           train_set_idx
                Indexed triples for the training.
           entity_idxs
                mapping.
           relation_idxs
                mapping.
           form
           store
           label_smoothing_rate
```

torch.utils.data.Dataset

```
train_data = None

train_target = None

neg_ratio = None

num_entities

label_smoothing_rate

collate_fn = None

max_num_of_classes

__len__()

__getitem__(idx)

class dicee.NegSampleDataset(train_set: numpy.ndarray, num_entities: int, num_relations: int, neg_sample_ratio: int = 1)
```

Bases: torch.utils.data.Dataset

An abstract class representing a Dataset.

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

1 Note

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

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

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

• num workers int for https://pytorch.org/docs/stable/data.html#torch.utils.data. DataLoader

Return type

train set idx

num_entities

num_relations

neg_sample_ratio

batch_size

num_workers

train_dataloader() → torch.utils.data.DataLoader

An iterable or collection of iterables specifying training samples.

For more information about multiple dataloaders, see this section.

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

For data processing use the following pattern:

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

However, the above are only necessary for distributed processing.

🛕 Warning

do not assign state in prepare_data

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

1 Note

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

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

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

Parameters

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

Example:

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

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

# don't do this
        self.something = else

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

transfer_batch_to_device(*args, **kwargs)

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

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

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

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

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)
        (continues on next page)
```

(continued from previous page)

```
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.

A 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
```

(continues on next page)

(continued from previous page)

```
# 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()
```

```
\label{eq:class} \begin{tabular}{ll} \verb|class| & dicee.LiteralDataset| & (file\_path: str, ent\_idx: dict = None, normalization\_type: str = 'z-norm', \\ & sampling\_ratio: & float = None, loader\_backend: str = 'pandas') \\ \end{tabular}
```

```
Bases: torch.utils.data.Dataset
```

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

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

train_file_path

Path to the training data file.

```
Type
```

normalization

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

```
Type str
```

normalization_params

Parameters used for normalization.

```
Type
dict
```

sampling_ratio

Fraction of the training set to use for ablations.

```
Type
float
```

entity_to_idx

Mapping of entities to their indices.

```
Type dict
```

num_entities

Total number of entities.

```
Type
             int
data_property_to_idx
     Mapping of data properties to their indices.
         Type
             dict
num_data_properties
     Total number of data properties.
         Type
             int
loader_backend
     Backend to use for loading data ('pandas' or 'rdflib').
             str
train_file_path
loader_backend = 'pandas'
normalization_type = 'z-norm'
normalization_params
sampling_ratio = None
entity_to_idx = None
num_entities
__getitem__(index)
__len__()
static load_and_validate_literal_data(file_path: str = None, loader_backend: str = 'pandas')
             \rightarrow pandas.DataFrame
     Loads and validates the literal data file. :param file_path: Path to the literal data file. :type file_path: str
         Returns
             DataFrame containing the loaded and validated data.
         Return type
             pd.DataFrame
```

 ${\tt static}$ denormalize (preds_norm, attributes, normalization_params) \to numpy.ndarray

Denormalizes the predictions based on the normalization type.

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

Returns

Denormalized predictions.

Return type

np.ndarray

```
class dicee. QueryGenerator (train_path, val_path: str, test_path: str, ent2id: Dict = None,
             rel2id: Dict = None, seed: int = 1, gen\_valid: bool = False, gen\_test: bool = True)
      train_path
      val_path
      test path
      gen valid = False
      gen test = True
      seed = 1
      max_ans_num = 1000000.0
      mode
      ent2id = None
      rel2id: Dict = None
      ent_in: Dict
      ent_out: Dict
      query_name_to_struct
      list2tuple(list_data)
      tuple2list(x: List | Tuple) \rightarrow List | Tuple
           Convert a nested tuple to a nested list.
      set_global_seed (seed: int)
           Set seed
      construct\_graph(paths: List[str]) \rightarrow Tuple[Dict, Dict]
           Construct graph from triples Returns dicts with incoming and outgoing edges
      fill_query(query\_structure: List[str | List], ent_in: Dict, ent_out: Dict, answer: int) \rightarrow bool
           Private method for fill_query logic.
      achieve\_answer(query: List[str | List], ent\_in: Dict, ent\_out: Dict) \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]]])

→ None
Save Queries into Disk

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

Load Queries from Disk to Memory

dicee.__version__ = '0.1.5'
```

Python Module Index

d

```
dicee, 12
dicee.__main__,12
dicee.abstracts, 12
dicee.analyse_experiments, 19
dicee.callbacks, 20
dicee.config, 27
dicee.dataset_classes, 30
dicee.eval_static_funcs, 44
dicee.evaluator, 45
dicee.executer, 47
dicee.knowledge_graph, 49
dicee.knowledge_graph_embeddings, 50
dicee.models, 54
dicee.models.adopt, 54
dicee.models.base_model, 55
dicee.models.clifford, 64
dicee.models.complex, 71
dicee.models.dualE, 74
dicee.models.ensemble, 75
dicee.models.function_space, 76
dicee.models.literal, 79
dicee.models.octonion, 81
dicee.models.pykeen_models, 84
dicee.models.quaternion, 85
dicee.models.real.88
dicee.models.static_funcs, 89
dicee.models.transformers, 90
dicee.query_generator, 143
dicee.read_preprocess_save_load_kg, 145
dicee.read_preprocess_save_load_kg.preprocess,
dicee.read_preprocess_save_load_kg.read_from_disk,
        146
dicee.read_preprocess_save_load_kg.save_load_disk,
dicee.read_preprocess_save_load_kg.util,
       147
dicee.sanity_checkers, 151
dicee.scripts, 152
dicee.scripts.index_serve, 152
dicee.scripts.run, 155
dicee.static_funcs, 155
dicee.static_funcs_training, 158
dicee.static_preprocess_funcs, 159
dicee.trainer, 160
dicee.trainer.dice_trainer, 160
dicee.trainer.model_parallelism, 162
dicee.trainer.torch_trainer, 162
dicee.trainer.torch_trainer_ddp, 164
```

Index

Non-alphabetical

```
__call__() (dicee.EnsembleKGE method), 193
 _call__() (dicee.models.base_model.IdentityClass method), 64
__call__() (dicee.models.ensemble.EnsembleKGE method), 75
__call__() (dicee.models.IdentityClass method), 107, 118, 124
__class_vars__ (dicee.scripts.index_serve.StringListRequest attribute), 153
__getitem__() (dicee.AllvsAll method), 204
__getitem__() (dicee.BPE_NegativeSamplingDataset method), 201
__getitem__() (dicee.dataset_classes.AllvsAll method), 35
__getitem__() (dicee.dataset_classes.BPE_NegativeSamplingDataset method), 31
__getitem__() (dicee.dataset_classes.KvsAll method), 34
__getitem__() (dicee.dataset_classes.KvsSampleDataset method), 37
__getitem__() (dicee.dataset_classes.LiteralDataset method), 43
__getitem__() (dicee.dataset_classes.MultiClassClassificationDataset method), 33
__getitem__() (dicee.dataset_classes.MultiLabelDataset method), 32
__getitem__() (dicee.dataset_classes.NegSampleDataset method), 38
__getitem__() (dicee.dataset_classes.OnevsAllDataset method), 33
__getitem__() (dicee.dataset_classes.OnevsSample method), 36
__getitem__() (dicee.dataset_classes.TriplePredictionDataset method), 38
__getitem__() (dicee.KvsAll method), 204
__getitem__() (dicee.KvsSampleDataset method), 207
__getitem__() (dicee.LiteralDataset method), 213
__getitem__() (dicee.MultiClassClassificationDataset method), 202
__getitem__() (dicee.MultiLabelDataset method), 202
__getitem__() (dicee.NegSampleDataset method), 207
__getitem__() (dicee.OnevsAllDataset method), 203
__getitem__() (dicee.OnevsSample method), 206
__getitem__() (dicee.TriplePredictionDataset method), 208
__iter__() (dicee.config.Namespace method), 30
__iter__() (dicee.EnsembleKGE method), 192
__iter__() (dicee.knowledge_graph.KG method), 50
__iter__() (dicee.models.ensemble.EnsembleKGE method), 75
__len__() (dicee.AllvsAll method), 204
__len__() (dicee.BPE_NegativeSamplingDataset method), 201
__len__() (dicee.dataset_classes.AllvsAll method), 35
__len__() (dicee.dataset_classes.BPE_NegativeSamplingDataset method), 31
__len__() (dicee.dataset_classes.KvsAll method), 34
__len__() (dicee.dataset_classes.KvsSampleDataset method), 37
__len__() (dicee.dataset_classes.LiteralDataset method), 43
__len__() (dicee.dataset_classes.MultiClassClassificationDataset method), 33
__len__() (dicee.dataset_classes.MultiLabelDataset method), 32
__len__() (dicee.dataset_classes.NegSampleDataset method), 37
__len__() (dicee.dataset_classes.OnevsAllDataset method), 33
__len__() (dicee.dataset_classes.OnevsSample method), 36
__len__() (dicee.dataset_classes.TriplePredictionDataset method), 38
  _len__() (dicee.EnsembleKGE method), 193
__len__() (dicee.knowledge_graph.KG method), 50
__len__() (dicee.KvsAll method), 204
__len__() (dicee.KvsSampleDataset method), 207
__len__() (dicee.LiteralDataset method), 213
__len__() (dicee.models.ensemble.EnsembleKGE method), 75
__len__() (dicee.MultiClassClassificationDataset method), 202
__len__() (dicee.MultiLabelDataset method), 202
__len__() (dicee.NegSampleDataset method), 207
__len__() (dicee.OnevsAllDataset method), 203
  _len__() (dicee.OnevsSample method), 206
__len__() (dicee.TriplePredictionDataset method), 208
__private_attributes__ (dicee.scripts.index_serve.StringListRequest attribute), 154
__pydantic_complete__(dicee.scripts.index_serve.StringListRequest attribute), 154
__pydantic_computed_fields__ (dicee.scripts.index_serve.StringListRequest attribute), 154
__pydantic_core_schema__ (dicee.scripts.index_serve.StringListRequest attribute), 154
__pydantic_custom_init__ (dicee.scripts.index_serve.StringListRequest attribute), 154
__pydantic_decorators__ (dicee.scripts.index_serve.StringListRequest attribute), 154
__pydantic_extra__ (dicee.scripts.index_serve.StringListRequest attribute), 154
__pydantic_fields__ (dicee.scripts.index_serve.StringListRequest attribute), 154
```

```
__pydantic_fields_set__ (dicee.scripts.index_serve.StringListRequest attribute), 154
__pydantic_generic_metadata__ (dicee.scripts.index_serve.StringListRequest attribute), 154
__pydantic_parent_namespace__ (dicee.scripts.index_serve.StringListRequest attribute), 154
__pydantic_post_init__ (dicee.scripts.index_serve.StringListRequest attribute), 154
__pydantic_private__ (dicee.scripts.index_serve.StringListRequest attribute), 154
__pydantic_root_model__(dicee.scripts.index_serve.StringListRequest attribute), 154
__pydantic_serializer__ (dicee.scripts.index_serve.StringListRequest attribute), 154
__pydantic_validator__ (dicee.scripts.index_serve.StringListRequest attribute), 154
__setstate__() (dicee.models.ADOPT method), 98
__setstate__() (dicee.models.adopt.ADOPT method), 55
__signature__(dicee.scripts.index_serve.StringListRequest attribute), 154
__str__() (dicee.EnsembleKGE method), 193
__str__() (dicee.KGE method), 196
__str__() (dicee.knowledge_graph_embeddings.KGE method), 50
__str__() (dicee.models.ensemble.EnsembleKGE method), 75
__version__ (in module dicee), 215
Α
AbstractCallback (class in dicee.abstracts), 16
AbstractPPECallback (class in dicee.abstracts), 17
AbstractTrainer (class in dicee.abstracts), 12
AccumulateEpochLossCallback (class in dicee.callbacks), 21
achieve_answer() (dicee.query_generator.QueryGenerator method), 144
achieve_answer() (dicee.QueryGenerator method), 214
AConEx (class in dicee), 179
AConEx (class in dicee.models), 113
AConEx (class in dicee.models.complex), 72
AConvo (class in dicee), 179
AConvo (class in dicee.models), 126
AConvO (class in dicee.models.octonion), 83
AConvQ (class in dicee), 180
AConvQ (class in dicee.models), 120
AConvQ (class in dicee.models.quaternion), 87
adaptive_swa (dicee.config.Namespace attribute), 30
add_new_entity_embeddings() (dicee.abstracts.BaseInteractiveKGE method), 15
add_noise_rate (dicee.config.Namespace attribute), 28
add_noise_rate (dicee.knowledge_graph.KG attribute), 49
add_noisy_triples() (in module dicee), 194
add_noisy_triples() (in module dicee.static_funcs), 157
add_noisy_triples_into_training() (dicee.read_preprocess_save_load_kg.read_from_disk.ReadFromDisk method), 146
add_noisy_triples_into_training() (dicee.read_preprocess_save_load_kg.ReadFromDisk method), 151
add_reciprocal (dicee.knowledge_graph.KG attribute), 49
ADOPT (class in dicee.models), 97
ADOPT (class in dicee.models.adopt), 54
adopt () (in module dicee.models.adopt), 55
AllvsAll (class in dicee), 204
AllvsAll (class in dicee.dataset_classes), 34
alphas (dicee.abstracts.AbstractPPECallback attribute), 17
alphas (dicee.callbacks.ASWA attribute), 24
analyse() (in module dicee.analyse_experiments), 20
answer_multi_hop_query() (dicee.KGE method), 198
answer_multi_hop_query() (dicee.knowledge_graph_embeddings.KGE method), 53
app (in module dicee.scripts.index_serve), 153
apply_coefficients() (dicee.DeCaL method), 175
apply_coefficients() (dicee.Keci method), 172
apply_coefficients() (dicee.models.clifford.DeCaL method), 69
apply_coefficients() (dicee.models.clifford.Keci method), 66
apply_coefficients() (dicee.models.DeCaL method), 132
apply_coefficients() (dicee.models.Keci method), 128
apply_reciprical_or_noise() (in module dicee.read_preprocess_save_load_kg.util), 149
apply_semantic_constraint (dicee.abstracts.BaseInteractiveKGE attribute), 14
apply_unit_norm (dicee.BaseKGE attribute), 191
apply_unit_norm (dicee.models.base_model.BaseKGE attribute), 62
apply_unit_norm (dicee.models.BaseKGE attribute), 104, 108, 111, 116, 122, 134, 138
args (dicee.BaseKGE attribute), 190
args (dicee.DICE_Trainer attribute), 195
args (dicee.evaluator.Evaluator attribute), 46
```

```
args (dicee.Execute attribute), 199
args (dicee.executer.Execute attribute), 47
args (dicee.models.base model.BaseKGE attribute), 61
args (dicee.models.base_model.IdentityClass attribute), 64
args (dicee.models.BaseKGE attribute), 104, 107, 111, 115, 121, 134, 137
args (dicee.models.IdentityClass attribute), 107, 118, 124
args (dicee.models.pykeen_models.PykeenKGE attribute), 84
args (dicee.models.PykeenKGE attribute), 136
args (dicee.PykeenKGE attribute), 187
args (dicee.trainer.DICE_Trainer attribute), 165
args (dicee.trainer.dice_trainer.DICE_Trainer attribute), 160
ASWA (class in dicee.callbacks), 23
aswa (dicee.analyse_experiments.Experiment attribute), 19
attn (dicee.models.transformers.Block attribute), 95
attn_dropout (dicee.models.transformers.CausalSelfAttention attribute), 93
attributes (dicee.abstracts.AbstractTrainer attribute), 13
auto_batch_finding (dicee.config.Namespace attribute), 30
В
backend (dicee.config.Namespace attribute), 28
backend (dicee.knowledge_graph.KG attribute), 49
BaseInteractiveKGE (class in dicee.abstracts), 14
BaseInteractiveTrainKGE (class in dicee.abstracts), 18
BaseKGE (class in dicee), 190
BaseKGE (class in dicee.models), 103, 107, 110, 115, 121, 133, 137
BaseKGE (class in dicee.models.base_model), 61
BaseKGELightning (class in dicee.models), 98
BaseKGELightning (class in dicee.models.base_model), 55
batch_kronecker_product() (dicee.callbacks.KronE static method), 26
batch_size (dicee.analyse_experiments.Experiment attribute), 19
batch_size (dicee.callbacks.PseudoLabellingCallback attribute), 23
batch_size (dicee.config.Namespace attribute), 28
batch_size (dicee.CVDataModule attribute), 209
batch_size (dicee.dataset_classes.CVDataModule attribute), 39
bias (dicee.models.transformers.GPTConfig attribute), 95
bias (dicee.models.transformers.LayerNorm attribute), 92
Block (class in dicee.models.transformers), 94
block_size (dicee.BaseKGE attribute), 191
block_size (dicee.config.Namespace attribute), 30
\verb|block_size| (\textit{dicee.dataset\_classes}. \textit{MultiClassClassificationDataset attribute}), 32
block size (dicee.models.base model.BaseKGE attribute), 62
block_size (dicee.models.BaseKGE attribute), 105, 108, 112, 116, 122, 135, 138
block_size (dicee.models.transformers.GPTConfig attribute), 95
block_size (dicee.MultiClassClassificationDataset attribute), 202
bn_conv1 (dicee.AConvQ attribute), 180
bn_conv1 (dicee.ConvQ attribute), 181
bn_conv1 (dicee.models.AConvQ attribute), 120
bn_conv1 (dicee.models.ConvQ attribute), 120
bn_conv1 (dicee.models.quaternion.AConvQ attribute), 87
bn_conv1 (dicee.models.quaternion.ConvQ attribute), 87
bn_conv2 (dicee.AConvQ attribute), 180
bn_conv2 (dicee.ConvQ attribute), 181
bn_conv2 (dicee.models.AConvQ attribute), 121
bn_conv2 (dicee.models.ConvQ attribute), 120
bn_conv2 (dicee.models.quaternion.AConvQ attribute), 87
bn_conv2 (dicee.models.quaternion.ConvQ attribute), 87
bn_conv2d (dicee.AConEx attribute), 179
bn_conv2d (dicee.AConvO attribute), 180
bn_conv2d (dicee.ConEx attribute), 182
bn_conv2d (dicee.ConvO attribute), 182
bn_conv2d (dicee.models.AConEx attribute), 114
bn_conv2d (dicee.models.AConvO attribute), 126
bn_conv2d (dicee.models.complex.AConEx attribute), 72
bn_conv2d (dicee.models.complex.ConEx attribute), 72
bn_conv2d (dicee.models.ConEx attribute), 113
bn_conv2d (dicee.models.ConvO attribute), 126
bn_conv2d (dicee.models.octonion.AConvO attribute), 83
```

```
bn conv2d (dicee.models.octonion.ConvO attribute), 83
BPE_NegativeSamplingDataset (class in dicee), 201
BPE_NegativeSamplingDataset (class in dicee.dataset_classes), 31
build_chain_funcs() (dicee.models.FMult2 method), 141
build_chain_funcs() (dicee.models.function_space.FMult2 method), 77
build_func() (dicee.models.FMult2 method), 141
build_func() (dicee.models.function_space.FMult2 method), 77
BytE (class in dicee), 188
BytE (class in dicee.models.transformers), 90
byte_pair_encoding (dicee.analyse_experiments.Experiment attribute), 19
byte_pair_encoding (dicee.BaseKGE attribute), 191
byte_pair_encoding (dicee.config.Namespace attribute), 29
byte_pair_encoding (dicee.knowledge_graph.KG attribute), 49
byte_pair_encoding (dicee.models.base_model.BaseKGE attribute), 62
byte_pair_encoding (dicee.models.BaseKGE attribute), 105, 108, 112, 116, 122, 135, 138
c_attn (dicee.models.transformers.CausalSelfAttention attribute), 93
c fc (dicee.models.transformers.MLP attribute), 94
c_proj (dicee.models.transformers.CausalSelfAttention attribute), 93
c_proj (dicee.models.transformers.MLP attribute), 94
callbacks (dicee.abstracts.AbstractTrainer attribute), 13
callbacks (dicee.analyse_experiments.Experiment attribute), 19
callbacks (dicee.config.Namespace attribute), 28
callbacks (dicee.trainer.torch_trainer_ddp.NodeTrainer attribute), 165
CausalSelfAttention (class in dicee.models.transformers), 92
chain_func() (dicee.models.FMult method), 140
\verb|chain_func()| \textit{ (dicee.models.function\_space.FMult method)}, 76
chain_func() (dicee.models.function_space.GFMult method), 77
chain_func() (dicee.models.GFMult method), 140
CKeci (class in dicee), 170
CKeci (class in dicee.models), 130
CKeci (class in dicee.models.clifford), 67
cl_pgr() (dicee.DeCaL method), 174
cl_pqr() (dicee.models.clifford.DeCaL method), 69
cl_pqr() (dicee.models.DeCaL method), 131
clifford_multiplication() (dicee.Keci method), 172
clifford_multiplication() (dicee.models.clifford.Keci method), 66
clifford_multiplication() (dicee.models.Keci method), 128
clip_lambda (dicee.models.ADOPT attribute), 98
clip lambda (dicee.models.adopt.ADOPT attribute), 55
collate_fn (dicee.AllvsAll attribute), 204
collate_fn (dicee.dataset_classes.AllvsAll attribute), 34
collate_fn (dicee.dataset_classes.KvsAll attribute), 34
collate_fn (dicee.dataset_classes.KvsSampleDataset attribute), 37
collate_fn (dicee.dataset_classes.MultiClassClassificationDataset attribute), 32
collate_fn (dicee.dataset_classes.MultiLabelDataset attribute), 32
collate fn (dicee.dataset classes.OnevsAllDataset attribute), 33
collate_fn (dicee.dataset_classes.OnevsSample attribute), 35, 36
collate_fn (dicee.KvsAll attribute), 204
collate_fn (dicee.KvsSampleDataset attribute), 207
\verb|collate_fn| (\textit{dicee.MultiClassClassificationDataset attribute}), 202
collate_fn (dicee.MultiLabelDataset attribute), 202
collate_fn (dicee.OnevsAllDataset attribute), 203
collate_fn (dicee.OnevsSample attribute), 205, 206
collate_fn() (dicee.BPE_NegativeSamplingDataset method), 201
collate_fn() (dicee.dataset_classes.BPE_NegativeSamplingDataset method), 31
collate_fn() (dicee.dataset_classes.TriplePredictionDataset method), 38
collate_fn() (dicee.TriplePredictionDataset method), 208
collection_name (dicee.scripts.index_serve.NeuralSearcher attribute), 153
comp_func() (dicee.LFMult method), 186
\verb|comp_func()| \textit{ (dicee.models.function\_space.LFMult method)}, 79
comp_func() (dicee.models.LFMult method), 142
Complex (class in dicee), 178
Complex (class in dicee.models), 114
Complex (class in dicee.models.complex), 72
compute_convergence() (in module dicee.callbacks), 23
```

```
compute func () (dicee.models.FMult method), 140
compute_func() (dicee.models.FMult2 method), 141
compute func() (dicee.models.function space.FMult method), 76
compute_func() (dicee.models.function_space.FMult2 method), 77
compute_func() (dicee.models.function_space.GFMult method), 77
compute_func() (dicee.models.GFMult method), 140
compute_mrr() (dicee.callbacks.ASWA static method), 24
compute_sigma_pp() (dicee.DeCaL method), 175
compute_sigma_pp() (dicee.Keci method), 171
\verb|compute_sigma_pp()| \textit{(dicee.models.clifford.DeCaL method)}, 70
compute_sigma_pp() (dicee.models.clifford.Keci method), 65
compute_sigma_pp() (dicee.models.DeCaL method), 132
compute_sigma_pp() (dicee.models.Keci method), 127
compute_sigma_pq() (dicee.DeCaL method), 176
compute_sigma_pq() (dicee.Keci method), 171
compute_sigma_pq() (dicee.models.clifford.DeCaL method), 71
compute_sigma_pq() (dicee.models.clifford.Keci method). 66
compute_sigma_pq() (dicee.models.DeCaL method), 133
compute_sigma_pq() (dicee.models.Keci method), 128
compute_sigma_pr() (dicee.DeCaL method), 177
compute_sigma_pr() (dicee.models.clifford.DeCaL method), 71
compute_sigma_pr() (dicee.models.DeCaL method), 133
compute_sigma_gq() (dicee.DeCaL method), 176
compute_sigma_qq() (dicee.Keci method), 171
compute_sigma_gg() (dicee.models.clifford.DeCaL method), 70
compute_sigma_qq() (dicee.models.clifford.Keci method), 65
compute_sigma_qq() (dicee.models.DeCaL method), 132
compute_sigma_qq() (dicee.models.Keci method), 128
compute_sigma_qr() (dicee.DeCaL method), 177
compute_sigma_gr() (dicee.models.clifford.DeCaL method), 71
compute_sigma_qr() (dicee.models.DeCaL method), 133
compute_sigma_rr() (dicee.DeCaL method), 176
compute_sigma_rr() (dicee.models.clifford.DeCaL method), 70
compute_sigma_rr() (dicee.models.DeCaL method), 133
compute_sigmas_multivect() (dicee.DeCaL method), 175
compute_sigmas_multivect() (dicee.models.clifford.DeCaL method), 69
compute sigmas multivect() (dicee.models.DeCaL method), 131
compute_sigmas_single() (dicee.DeCaL method), 174
compute_sigmas_single() (dicee.models.clifford.DeCaL method).69
compute_sigmas_single() (dicee.models.DeCaL method), 131
ConEx (class in dicee), 182
ConEx (class in dicee.models), 113
ConEx (class in dicee.models.complex), 71
config (dicee.BytE attribute), 188
config (dicee.models.transformers.BytE attribute), 91
config (dicee.models.transformers.GPT attribute), 96
configs (dicee.abstracts.BaseInteractiveKGE attribute), 14
configure_optimizers() (dicee.models.base_model.BaseKGELightning method), 60
configure_optimizers() (dicee.models.BaseKGELightning method), 102
configure_optimizers() (dicee.models.transformers.GPT method), 96
construct batch selected cl multivector() (dicee. Keci method), 172
construct_batch_selected_cl_multivector() (dicee.models.clifford.Keci method), 67
construct_batch_selected_cl_multivector() (dicee.models.Keci method), 129
construct_cl_multivector() (dicee.DeCaL method), 175
construct_cl_multivector() (dicee.Keci method), 172
construct_cl_multivector() (dicee.models.clifford.DeCaL method), 69
construct_cl_multivector() (dicee.models.clifford.Keci method), 66
construct_cl_multivector() (dicee.models.DeCaL method), 132
construct_cl_multivector() (dicee.models.Keci method), 129
construct_dataset() (in module dicee), 201
construct dataset () (in module dicee.dataset classes), 31
construct_ensemble (dicee.abstracts.BaseInteractiveKGE attribute), 14
construct_graph() (dicee.query_generator.QueryGenerator method), 144
construct_graph() (dicee.QueryGenerator method), 214
construct_input_and_output() (dicee.abstracts.BaseInteractiveKGE method), 15
construct_multi_coeff() (dicee.LFMult method), 186
construct_multi_coeff() (dicee.models.function_space.LFMult method), 78
construct_multi_coeff() (dicee.models.LFMult method), 142
```

```
continual_learning (dicee.config.Namespace attribute), 30
continual_start() (dicee.DICE_Trainer method), 195
continual_start() (dicee.executer.ContinuousExecute method), 48
continual_start() (dicee.trainer.DICE_Trainer method), 165
continual_start() (dicee.trainer.dice_trainer.DICE_Trainer method), 161
continual_training_setup_executor() (in module dicee), 194
continual_training_setup_executor() (in module dicee.static_funcs), 158
Continuous Execute (class in dicee.executer), 48
conv2d (dicee.AConEx attribute), 179
conv2d (dicee.AConvO attribute), 179
conv2d (dicee.AConvQ attribute), 180
conv2d (dicee.ConEx attribute), 182
conv2d (dicee.ConvO attribute), 182
conv2d (dicee.ConvQ attribute), 181
conv2d (dicee.models.AConEx attribute), 113
conv2d (dicee.models.AConvO attribute), 126
conv2d (dicee.models.AConvQ attribute), 120
conv2d (dicee.models.complex.AConEx attribute), 72
conv2d (dicee.models.complex.ConEx attribute), 71
conv2d (dicee.models.ConEx attribute), 113
conv2d (dicee.models.ConvO attribute), 126
conv2d (dicee.models.ConvO attribute), 120
conv2d (dicee.models.octonion.AConvO attribute), 83
conv2d (dicee.models.octonion.ConvO attribute), 82
conv2d (dicee.models.quaternion.AConvQ attribute), 87
conv2d (dicee.models.quaternion.ConvQ attribute), 87
ConvO (class in dicee), 181
ConvO (class in dicee.models), 125
ConvO (class in dicee.models.octonion), 82
ConvQ (class in dicee), 180
ConvQ (class in dicee.models), 120
ConvO (class in dicee.models.auaternion), 87
create_constraints() (in module dicee.read_preprocess_save_load_kg.util), 149
create_constraints() (in module dicee.static_preprocess_funcs), 159
create_experiment_folder() (in module dicee), 194
create_experiment_folder() (in module dicee.static_funcs), 158
create random data() (dicee.callbacks.PseudoLabellingCallback method), 23
create_recipriocal_triples() (in module dicee), 193
create_recipriocal_triples() (in module dicee.read_preprocess_save_load_kg.util), 150
create_recipriocal_triples() (in module dicee.static_funcs), 156
create_vector_database() (dicee.KGE method), 196
create_vector_database() (dicee.knowledge_graph_embeddings.KGE method), 50
crop_block_size() (dicee.models.transformers.GPT method), 96
ctx (dicee.trainer.torch_trainer_ddp.NodeTrainer attribute), 165
CVDataModule (class in dicee), 208
CVDataModule (class in dicee.dataset_classes), 38
D
data_module (dicee.callbacks.PseudoLabellingCallback attribute), 23
data_property_embeddings (dicee.models.literal.LiteralEmbeddings attribute), 80
data_property_to_idx (dicee.dataset_classes.LiteralDataset attribute), 43
data_property_to_idx (dicee.LiteralDataset attribute), 213
dataset_dir (dicee.config.Namespace attribute), 27
{\tt dataset\_dir}~(\textit{dicee.knowledge\_graph.KG}~\textit{attribute}), 49
dataset_sanity_checking() (in module dicee.read_preprocess_save_load_kg.util), 150
DeCaL (class in dicee), 173
DeCaL (class in dicee.models), 130
DeCal (class in dicee.models.clifford), 68
decide() (dicee.callbacks.ASWA method), 24
default_eval_model (dicee.callbacks.PeriodicEvalCallback attribute), 27
degree (dicee.LFMult attribute), 186
degree (dicee.models.function_space.LFMult attribute), 78
degree (dicee.models.LFMult attribute), 141
denormalize() (dicee.dataset_classes.LiteralDataset static method), 43
denormalize() (dicee.LiteralDataset static method), 213
deploy() (dicee.KGE method), 199
{\tt deploy()} \ ({\it dicee.knowledge\_graph\_embeddings.KGE\ method}), 53
```

```
deploy_head_entity_prediction() (in module dicee), 194
deploy_head_entity_prediction() (in module dicee.static_funcs), 157
{\tt deploy\_relation\_prediction()} \ \textit{(in module dicee)}, 194
deploy_relation_prediction() (in module dicee.static_funcs), 158
deploy_tail_entity_prediction() (in module dicee), 194
deploy_tail_entity_prediction() (in module dicee.static_funcs), 157
deploy_triple_prediction() (in module dicee), 194
deploy_triple_prediction() (in module dicee.static_funcs), 157
describe() (dicee.knowledge_graph.KG method), 50
{\tt description\_of\_input}~(\textit{dicee.knowledge\_graph.KG attribute}), 50
device (dicee.models.literal.LiteralEmbeddings property), 80
DICE_Trainer (class in dicee), 194
DICE_Trainer (class in dicee.trainer), 165
DICE_Trainer (class in dicee.trainer.dice_trainer), 160
dicee
     module, 12
dicee.___main_
    module, 12
dicee.abstracts
     module, 12
dicee.analyse_experiments
     module, 19
dicee.callbacks
    module, 20
dicee.config
     module, 27
dicee.dataset_classes
     module, 30
dicee.eval_static_funcs
     module, 44
dicee.evaluator
    module, 45
dicee.executer
    module, 47
dicee.knowledge_graph
     module, 49
dicee.knowledge_graph_embeddings
     module, 50
dicee.models
     module, 54
dicee.models.adopt
     module, 54
dicee.models.base_model
     module, 55
dicee.models.clifford
    module, 64
dicee.models.complex
     module, 71
dicee.models.dualE
     module, 74
dicee.models.ensemble
     module, 75
dicee.models.function_space
     module, 76
dicee.models.literal
    module, 79
dicee.models.octonion
     module, 81
dicee.models.pykeen_models
     module, 84
dicee.models.quaternion
     module, 85
dicee.models.real
     module, 88
dicee.models.static_funcs
    module, 89
dicee.models.transformers
     module, 90
```

```
dicee.query_generator
     module, 143
dicee.read_preprocess_save_load_kg
     module, 145
dicee.read_preprocess_save_load_kg.preprocess
     module, 145
dicee.read_preprocess_save_load_kg.read_from_disk
    module, 146
dicee.read_preprocess_save_load_kg.save_load_disk
     module, 146
dicee.read_preprocess_save_load_kg.util
     module, 147
dicee.sanity_checkers
    module, 151
dicee.scripts
    module, 152
dicee.scripts.index_serve
    module, 152
dicee.scripts.run
     module, 155
dicee.static_funcs
    module, 155
dicee.static_funcs_training
    module, 158
dicee.static_preprocess_funcs
    module, 159
dicee.trainer
    module, 160
dicee.trainer.dice_trainer
     module, 160
dicee.trainer.model_parallelism
    module, 162
dicee.trainer.torch_trainer
    module, 162
dicee.trainer.torch_trainer_ddp
     module, 164
discrete_points (dicee.models.FMult2 attribute), 140
discrete_points (dicee.models.function_space.FMult2 attribute), 77
dist_func (dicee.models.Pyke attribute), 110
dist_func (dicee.models.real.Pyke attribute), 89
dist_func (dicee.Pyke attribute), 169
DistMult (class in dicee), 169
DistMult (class in dicee.models), 109
DistMult (class in dicee.models.real), 88
download_file() (in module dicee), 194
download_file() (in module dicee.static_funcs), 158
download_files_from_url() (in module dicee), 194
download_files_from_url() (in module dicee.static_funcs), 158
download_pretrained_model() (in module dicee), 194
download_pretrained_model() (in module dicee.static_funcs), 158
dropout (dicee.models.literal.LiteralEmbeddings attribute), 79, 80
dropout (dicee.models.transformers.CausalSelfAttention attribute), 93
dropout (dicee.models.transformers.GPTConfig attribute), 95
dropout (dicee.models.transformers.MLP attribute), 94
DualE (class in dicee), 177
DualE (class in dicee.models), 142
DualE (class in dicee.models.dualE), 74
dummy_eval() (dicee.evaluator.Evaluator method), 46
dummy_id (dicee.knowledge_graph.KG attribute), 50
during_training (dicee.evaluator.Evaluator attribute), 46
Ε
ee_vocab (dicee.evaluator.Evaluator attribute), 45
efficient_zero_grad() (in module dicee.static_funcs_training), 159
embedding_dim (dicee.analyse_experiments.Experiment attribute), 19
embedding_dim (dicee.BaseKGE attribute), 190
embedding_dim (dicee.config.Namespace attribute), 28
```

```
embedding dim (dicee.models.base model.BaseKGE attribute), 62
embedding_dim (dicee.models.BaseKGE attribute), 104, 107, 111, 116, 121, 134, 137
embedding dim (dicee.models.literal.LiteralEmbeddings attribute), 80
embedding_dims (dicee.models.literal.LiteralEmbeddings attribute), 79
enable_log (in module dicee.static_preprocess_funcs), 159
enc (dicee.knowledge_graph.KG attribute), 49
end() (dicee.Execute method), 200
end() (dicee.executer.Execute method), 47
EnsembleKGE (class in dicee), 192
EnsembleKGE (class in dicee.models.ensemble), 75
ent2id (dicee.query_generator.QueryGenerator attribute), 144
ent2id (dicee.QueryGenerator attribute), 214
ent_in (dicee.query_generator.QueryGenerator attribute), 144
ent_in (dicee.QueryGenerator attribute), 214
ent_out (dicee.query_generator.QueryGenerator attribute), 144
ent_out (dicee.QueryGenerator attribute), 214
entities_str (dicee.knowledge_graph.KG property), 50
entity_embeddings (dicee.AConvQ attribute), 180
entity_embeddings (dicee.ConvQ attribute), 181
entity_embeddings (dicee.DeCaL attribute), 174
entity_embeddings (dicee.DualE attribute), 177
entity_embeddings (dicee.LFMult attribute), 186
entity_embeddings (dicee.models.AConvQ attribute), 120
entity_embeddings (dicee.models.clifford.DeCaL attribute), 68
entity_embeddings (dicee.models.ConvQ attribute), 120
entity_embeddings (dicee.models.DeCaL attribute), 131
entity_embeddings (dicee.models.DualE attribute), 143
entity_embeddings (dicee.models.dualE.DualE attribute), 74
entity_embeddings (dicee.models.FMult attribute), 139
entity_embeddings (dicee.models.FMult2 attribute), 140
entity_embeddings (dicee.models.function_space.FMult attribute), 76
entity embeddings (dicee.models.function space.FMult2 attribute), 77
entity_embeddings (dicee.models.function_space.GFMult attribute), 76
entity_embeddings (dicee.models.function_space.LFMult attribute), 78
entity_embeddings (dicee.models.function_space.LFMult1 attribute), 77
entity_embeddings (dicee.models.GFMult attribute), 140
entity embeddings (dicee.models.LFMult attribute), 141
entity_embeddings (dicee.models.LFMult1 attribute), 141
entity_embeddings (dicee.models.literal.LiteralEmbeddings attribute), 79, 80
entity_embeddings (dicee.models.pykeen_models.PykeenKGE attribute), 84
entity_embeddings (dicee.models.PykeenKGE attribute), 136
entity_embeddings (dicee.models.quaternion.AConvQ attribute), 87
entity_embeddings (dicee.models.quaternion.ConvQ attribute), 87
entity_embeddings (dicee.PykeenKGE attribute), 187
entity_to_idx (dicee.dataset_classes.LiteralDataset attribute), 42, 43
entity_to_idx (dicee.knowledge_graph.KG attribute), 49
entity_to_idx (dicee.LiteralDataset attribute), 212, 213
entity_to_idx (dicee.scripts.index_serve.NeuralSearcher attribute), 153
epoch_count (dicee.abstracts.AbstractPPECallback attribute), 17
epoch_count (dicee.callbacks.ASWA attribute), 24
epoch counter (dicee.callbacks.Eval attribute), 25
epoch_counter (dicee.callbacks.KGESaveCallback attribute), 22
epoch_counter (dicee.callbacks.PeriodicEvalCallback attribute), 27
epoch_ratio (dicee.callbacks.Eval attribute), 25
er_vocab (dicee.evaluator.Evaluator attribute), 45
estimate_mfu() (dicee.models.transformers.GPT method), 96
estimate_q() (in module dicee.callbacks), 23
Eval (class in dicee.callbacks), 24
eval() (dicee.EnsembleKGE method), 193
eval () (dicee.evaluator.Evaluator method), 46
eval () (dicee.models.ensemble.EnsembleKGE method), 75
eval_at_epochs (dicee.config.Namespace attribute), 30
eval_epochs (dicee.callbacks.PeriodicEvalCallback attribute), 27
eval_every_n_epochs (dicee.config.Namespace attribute), 30
eval_lp_performance() (dicee.KGE method), 196
eval_lp_performance() (dicee.knowledge_graph_embeddings.KGE method), 51
eval_model (dicee.config.Namespace attribute), 29
eval_model (dicee.knowledge_graph.KG attribute), 49
```

```
eval_rank_of_head_and_tail_byte_pair_encoded_entity() (dicee.evaluator.Evaluator method), 46
eval_rank_of_head_and_tail_entity() (dicee.evaluator.Evaluator method), 46
\verb|eval_with_bpe_vs_all()| \textit{(dicee.evaluator.Evaluator method)}, 46
eval_with_byte() (dicee.evaluator.Evaluator method), 46
eval_with_data() (dicee.evaluator.Evaluator method), 47
eval_with_vs_all() (dicee.evaluator.Evaluator method), 46
evaluate() (in module dicee), 194
evaluate() (in module dicee.static funcs), 158
evaluate_bpe_lp() (in module dicee.static_funcs_training), 159
evaluate_link_prediction_performance() (in module dicee.eval_static_funcs), 44
evaluate_link_prediction_performance_with_bpe() (in module dicee.eval_static_funcs), 44
\verb| evaluate_link_prediction_performance_with_bpe_reciprocals()| \textit{(in module dicee.eval\_static\_funcs)}, 44 \\
\verb| evaluate_link_prediction_performance_with_reciprocals()| \textit{(in module dicee.eval\_static_funcs)}, 44
evaluate_literal_prediction() (in module dicee.eval_static_funcs), 45
evaluate_lp() (dicee.evaluator.Evaluator method), 46
evaluate_lp() (in module dicee.static_funcs_training), 158
evaluate_lp_bpe_k_vs_all() (dicee.evaluator.Evaluator method), 46
evaluate_lp_bpe_k_vs_all() (in module dicee.eval_static_funcs), 45
\verb|evaluate_lp_k_vs_all()| \textit{(dicee.evaluator.Evaluator method)}, 46
evaluate_lp_with_byte() (dicee.evaluator.Evaluator method), 46
Evaluator (class in dicee.evaluator), 45
evaluator (dicee.DICE_Trainer attribute), 195
evaluator (dicee. Execute attribute), 200
evaluator (dicee.executer.Execute attribute), 47
evaluator (dicee.trainer.DICE_Trainer attribute), 165
evaluator (dicee.trainer.dice_trainer.DICE_Trainer attribute), 161
every_x_epoch (dicee.callbacks.KGESaveCallback attribute), 22
example_input_array (dicee.EnsembleKGE property), 192
\verb|example_input_array| (\textit{dicee.models.ensemble.EnsembleKGE property}), 75
Execute (class in dicee), 199
Execute (class in dicee.executer), 47
\verb|exists()| (\textit{dicee.knowledge\_graph.KG method}), 50
Experiment (class in dicee.analyse_experiments), 19
experiment_dir (dicee.callbacks.PeriodicEvalCallback attribute), 27
explicit (dicee.models.QMult attribute), 119
explicit (dicee.models.quaternion.QMult attribute), 86
explicit (dicee.QMult attribute), 183
exponential_function() (in module dicee), 194
exponential_function() (in module dicee.static_funcs), 158
extract_input_outputs() (dicee.trainer.torch_trainer_ddp.NodeTrainer method), 165
extract_input_outputs() (in module dicee.trainer.model_parallelism), 162
extract_input_outputs_set_device() (dicee.trainer.torch_trainer.TorchTrainer method), 163
F
f (dicee.callbacks.KronE attribute), 26
fc (dicee.models.literal.LiteralEmbeddings attribute), 80
fc1 (dicee.AConEx attribute), 179
fc1 (dicee.AConvO attribute), 180
fc1 (dicee.AConvQ attribute), 180
fc1 (dicee.ConEx attribute), 182
fc1 (dicee.ConvO attribute), 182
fc1 (dicee.ConvQ attribute), 181
fc1 (dicee.models.AConEx attribute), 113
fc1 (dicee.models.AConvO attribute), 126
fc1 (dicee.models.AConvO attribute), 120
fc1 (dicee.models.complex.AConEx attribute), 72
fc1 (dicee.models.complex.ConEx attribute), 72
fc1 (dicee.models.ConEx attribute), 113
fc1 (dicee.models.ConvO attribute), 126
fc1 (dicee.models.ConvQ attribute), 120
fc1 (dicee.models.octonion.AConvO attribute), 83
fc1 (dicee.models.octonion.ConvO attribute), 83
fc1 (dicee.models.quaternion.AConvQ attribute), 87
fc1 (dicee.models.quaternion.ConvQ attribute), 87
fc_num_input (dicee.AConEx attribute), 179
fc_num_input (dicee.AConvO attribute), 179
fc_num_input (dicee.AConvQ attribute), 180
```

```
fc num input (dicee.ConEx attribute), 182
fc_num_input (dicee.ConvO attribute), 182
fc_num_input (dicee.ConvQ attribute), 181
fc_num_input (dicee.models.AConEx attribute), 113
fc_num_input (dicee.models.AConvO attribute), 126
fc_num_input (dicee.models.AConvQ attribute), 120
fc_num_input (dicee.models.complex.AConEx attribute), 72
fc num input (dicee.models.complex.ConEx attribute), 72
fc_num_input (dicee.models.ConEx attribute), 113
fc_num_input (dicee.models.ConvO attribute), 126
fc_num_input (dicee.models.ConvQ attribute), 120
fc_num_input (dicee.models.octonion.AConvO attribute), 83
fc_num_input (dicee.models.octonion.ConvO attribute), 82
fc_num_input (dicee.models.quaternion.AConvQ attribute), 87
fc_num_input (dicee.models.quaternion.ConvQ attribute). 87
fc_out (dicee.models.literal.LiteralEmbeddings attribute), 80
feature_map_dropout (dicee.AConEx attribute), 179
feature_map_dropout (dicee.AConvO attribute), 180
feature_map_dropout (dicee.AConvQ attribute), 180
feature_map_dropout (dicee.ConEx attribute), 182
feature_map_dropout (dicee.ConvO attribute), 182
feature_map_dropout (dicee.ConvQ attribute), 181
feature_map_dropout (dicee.models.AConEx attribute), 114
feature_map_dropout (dicee.models.AConvO attribute), 126
feature_map_dropout (dicee.models.AConvQ attribute), 121
feature_map_dropout (dicee.models.complex.AConEx attribute), 72
feature_map_dropout (dicee.models.complex.ConEx attribute), 72
feature_map_dropout (dicee.models.ConEx attribute), 113
feature_map_dropout (dicee.models.ConvO attribute), 126
feature_map_dropout (dicee.models.ConvQ attribute), 120
feature_map_dropout (dicee.models.octonion.AConvO attribute), 83
feature_map_dropout (dicee.models.octonion.ConvO attribute), 83
feature_map_dropout (dicee.models.quaternion.AConvQ attribute), 87
feature_map_dropout (dicee.models.quaternion.ConvQ attribute), 87
feature_map_dropout_rate (dicee.BaseKGE attribute), 191
feature_map_dropout_rate (dicee.config.Namespace attribute), 29
feature map dropout rate (dicee.models.base model.BaseKGE attribute), 62
feature_map_dropout_rate (dicee.models.BaseKGE attribute), 104, 108, 111, 116, 122, 134, 138
fill_query() (dicee.query_generator.QueryGenerator method), 144
fill_query() (dicee.QueryGenerator method), 214
find_good_batch_size() (in module dicee.trainer.model_parallelism), 162
find_missing_triples() (dicee.KGE method), 199
find_missing_triples() (dicee.knowledge_graph_embeddings.KGE method), 53
fit () (dicee.trainer.model_parallelism.TensorParallel method), 162
fit () (dicee.trainer.torch_trainer_ddp.TorchDDPTrainer method), 164
fit () (dicee.trainer.torch_trainer.TorchTrainer method), 163
flash (dicee.models.transformers.CausalSelfAttention attribute), 93
FMult (class in dicee.models), 139
FMult (class in dicee.models.function_space), 76
FMult2 (class in dicee.models), 140
FMult2 (class in dicee.models.function space), 77
form_of_labelling (dicee.DICE_Trainer attribute), 195
form_of_labelling (dicee.trainer.DICE_Trainer attribute), 165
form_of_labelling (dicee.trainer.dice_trainer.DICE_Trainer attribute), 161
forward() (dicee.BaseKGE method), 192
forward() (dicee.BytE method), 189
forward() (dicee.models.base_model.BaseKGE method), 63
forward() (dicee.models.base_model.IdentityClass static method), 64
forward() (dicee.models.BaseKGE method), 105, 109, 112, 117, 123, 135, 139
forward() (dicee.models.IdentityClass static method), 107, 118, 124
forward() (dicee.models.literal.LiteralEmbeddings method), 80
forward() (dicee.models.transformers.Block method), 95
forward() (dicee.models.transformers.BytE method), 91
forward() (dicee.models.transformers.CausalSelfAttention method), 93
forward() (dicee.models.transformers.GPT method), 96
forward() (dicee.models.transformers.LayerNorm method), 92
forward() (dicee.models.transformers.MLP method), 94
forward_backward_update() (dicee.trainer.torch_trainer.TorchTrainer method), 163
```

```
forward backward update loss() (in module dicee.trainer.model parallelism), 162
forward_byte_pair_encoded_k_vs_all() (dicee.BaseKGE method), 191
forward_byte_pair_encoded_k_vs_all() (dicee.models.base_model.BaseKGE method), 62
forward_byte_pair_encoded_k_vs_all() (dicee.models.BaseKGE method), 105, 108, 112, 116, 122, 135, 138
forward_byte_pair_encoded_triple() (dicee.BaseKGE method), 191
forward_byte_pair_encoded_triple() (dicee.models.base_model.BaseKGE method), 62
forward_byte_pair_encoded_triple() (dicee.models.BaseKGE method), 105, 108, 112, 116, 122, 135, 138
forward k vs all() (dicee.AConEx method), 179
forward_k_vs_all() (dicee.AConvO method), 180
{\tt forward\_k\_vs\_all()} \ (\textit{dicee.AConvQ method}), 180
forward_k_vs_all() (dicee.BaseKGE method), 192
forward_k_vs_all() (dicee.ComplEx method), 179
forward_k_vs_all() (dicee.ConEx method), 183
forward_k_vs_all() (dicee.ConvO method), 182
forward_k_vs_all() (dicee.ConvQ method), 181
forward_k_vs_all() (dicee.DeCaL method), 175
forward_k_vs_all() (dicee.DistMult method), 170
forward_k_vs_all() (dicee.DualE method), 178
forward_k_vs_all() (dicee.Keci method), 172
forward_k_vs_all() (dicee.models.AConEx method), 114
forward_k_vs_all() (dicee.models.AConvO method), 127
{\tt forward\_k\_vs\_all()} \ (\textit{dicee.models.AConvQ method}), \ 121
forward_k_vs_all() (dicee.models.base_model.BaseKGE method), 63
forward_k_vs_all() (dicee.models.BaseKGE method), 106, 109, 112, 117, 123, 136, 139
forward_k_vs_all() (dicee.models.clifford.DeCaL method), 69
forward_k_vs_all() (dicee.models.clifford.Keci method), 67
forward_k_vs_all() (dicee.models.ComplEx method), 115
forward_k_vs_all() (dicee.models.complex.AConEx method), 72
{\tt forward\_k\_vs\_all()} \ (\textit{dicee.models.complex.ComplEx method}), 73
forward_k_vs_all() (dicee.models.complex.ConEx method), 72
forward_k_vs_all() (dicee.models.ConEx method), 113
forward_k_vs_all() (dicee.models.ConvO method), 126
forward_k_vs_all() (dicee.models.ConvQ method), 120
forward_k_vs_all() (dicee.models.DeCaL method), 131
forward_k_vs_all() (dicee.models.DistMult method), 109
forward_k_vs_all() (dicee.models.DualE method), 143
forward k vs all() (dicee.models.dualE.DualE method), 74
forward_k_vs_all() (dicee.models.Keci method), 129
forward_k_vs_all() (dicee.models.octonion.AConvO method), 83
forward_k_vs_all() (dicee.models.octonion.ConvO method), 83
{\tt forward\_k\_vs\_all()} \ (\textit{dicee.models.octonion.OMult method}), \, 82
forward_k_vs_all() (dicee.models.OMult method), 125
forward_k_vs_all() (dicee.models.pykeen_models.PykeenKGE method), 84
forward_k_vs_all() (dicee.models.PykeenKGE method), 136
forward_k_vs_all() (dicee.models.QMult method), 119
forward_k_vs_all() (dicee.models.quaternion.AConvQ method), 88
forward_k_vs_all() (dicee.models.quaternion.ConvQ method), 87
forward_k_vs_all() (dicee.models.quaternion.QMult method), 86
forward_k_vs_all() (dicee.models.real.DistMult method), 88
forward_k_vs_all() (dicee.models.real.Shallom method), 89
forward_k_vs_all() (dicee.models.real.TransE method). 89
forward_k_vs_all() (dicee.models.Shallom method), 110
forward_k_vs_all() (dicee.models.TransE method), 110
forward_k_vs_all() (dicee.OMult method), 185
forward_k_vs_all() (dicee.PykeenKGE method), 187
forward_k_vs_all() (dicee.QMult method), 184
forward_k_vs_all() (dicee.Shallom method), 185
{\tt forward\_k\_vs\_all()} \ (\textit{dicee.TransE method}), 173
forward_k_vs_sample() (dicee.AConEx method), 179
forward_k_vs_sample() (dicee.BaseKGE method), 192
forward_k_vs_sample() (dicee.ComplEx method), 179
forward_k_vs_sample() (dicee.ConEx method), 183
forward_k_vs_sample() (dicee.DistMult method), 170
forward_k_vs_sample() (dicee.Keci method), 173
forward_k_vs_sample() (dicee.models.AConEx method), 114
forward_k_vs_sample() (dicee.models.base_model.BaseKGE method), 63
forward_k_vs_sample() (dicee.models.BaseKGE method), 106, 109, 112, 117, 123, 136, 139
forward_k_vs_sample() (dicee.models.clifford.Keci method), 67
```

```
forward k vs sample() (dicee.models.ComplEx method), 115
forward_k_vs_sample() (dicee.models.complex.AConEx method), 72
forward_k_vs_sample() (dicee.models.complex.ComplEx method), 73
forward_k_vs_sample() (dicee.models.complex.ConEx method), 72
forward_k_vs_sample() (dicee.models.ConEx method), 113
forward_k_vs_sample() (dicee.models.DistMult method), 109
forward_k_vs_sample() (dicee.models.Keci method), 129
forward k vs sample() (dicee.models.pykeen models.PykeenKGE method), 85
forward_k_vs_sample() (dicee.models.PykeenKGE method), 137
forward_k_vs_sample() (dicee.models.QMult method), 120
forward_k_vs_sample() (dicee.models.quaternion.QMult method), 86
forward_k_vs_sample() (dicee.models.real.DistMult method), 88
forward_k_vs_sample() (dicee.PykeenKGE method), 188
forward_k_vs_sample() (dicee.QMult method), 184
forward_k_vs_with_explicit() (dicee.Keci method), 172
forward_k_vs_with_explicit() (dicee.models.clifford.Keci method), 66
forward_k_vs_with_explicit() (dicee.models.Keci method), 129
forward_triples() (dicee.AConEx method), 179
forward_triples() (dicee.AConvO method), 180
forward_triples() (dicee.AConvQ method), 180
forward_triples() (dicee.BaseKGE method), 192
forward_triples() (dicee.ConEx method). 183
forward_triples() (dicee.ConvO method), 182
forward_triples() (dicee.ConvQ method), 181
forward_triples() (dicee.DeCaL method), 174
forward_triples() (dicee.DualE method), 177
forward_triples() (dicee.Keci method), 173
forward_triples() (dicee.LFMult method), 186
forward_triples() (dicee.models.AConEx method), 114
forward_triples() (dicee.models.AConvO method), 127
forward_triples() (dicee.models.AConvQ method), 121
forward triples() (dicee.models.base model.BaseKGE method), 63
forward_triples() (dicee.models.BaseKGE method), 105, 109, 112, 117, 123, 135, 139
forward_triples() (dicee.models.clifford.DeCaL method), 68
forward_triples() (dicee.models.clifford.Keci method), 67
forward_triples() (dicee.models.complex.AConEx method), 72
forward triples() (dicee.models.complex.ConEx method), 72
forward_triples() (dicee.models.ConEx method), 113
forward_triples() (dicee.models.ConvO method), 126
forward_triples() (dicee.models.ConvQ method), 120
forward_triples() (dicee.models.DeCaL method), 131
forward_triples() (dicee.models.DualE method), 143
forward_triples() (dicee.models.dualE.DualE method), 74
forward_triples() (dicee.models.FMult method), 140
forward_triples() (dicee.models.FMult2 method), 141
forward_triples() (dicee.models.function_space.FMult method), 76
forward_triples() (dicee.models.function_space.FMult2 method), 77
forward_triples() (dicee.models.function_space.GFMult method), 77
forward_triples() (dicee.models.function_space.LFMult method), 78
forward_triples() (dicee.models.function_space.LFMult1 method), 77
forward triples() (dicee.models.GFMult method), 140
forward_triples() (dicee.models.Keci method), 130
forward_triples() (dicee.models.LFMult method), 141
forward_triples() (dicee.models.LFMult1 method), 141
forward_triples() (dicee.models.octonion.AConvO method), 83
forward_triples() (dicee.models.octonion.ConvO method), 83
forward_triples() (dicee.models.Pyke method), 110
forward_triples() (dicee.models.pykeen_models.PykeenKGE method), 84
forward_triples() (dicee.models.PykeenKGE method), 137
forward_triples() (dicee.models.quaternion.AConvQ method), 88
forward triples() (dicee.models.quaternion.ConvO method), 87
forward_triples() (dicee.models.real.Pyke method), 89
forward_triples() (dicee.models.real.Shallom method), 89
forward_triples() (dicee.models.Shallom method), 110
forward_triples() (dicee.Pyke method), 169
forward_triples() (dicee.PykeenKGE method), 187
forward_triples() (dicee.Shallom method), 185
{\tt freeze\_entity\_embeddings}~(\textit{dicee.models.literal.LiteralEmbeddings attribute}),~80
```

```
frequency (dicee.callbacks.Perturb attribute), 26
from_pretrained() (dicee.models.transformers.GPT class method), 96
from_pretrained_model_write_embeddings_into_csv() (in module dicee), 194
from_pretrained_model_write_embeddings_into_csv() (in module dicee.static_funcs), 158
full_storage_path (dicee.analyse_experiments.Experiment attribute), 19
func_triple_to_bpe_representation (dicee.evaluator.Evaluator attribute), 46
func_triple_to_bpe_representation() (dicee.knowledge_graph.KG method), 50
function() (dicee.models.FMult2 method), 141
function() (dicee.models.function_space.FMult2 method), 77
G
gamma (dicee.models.FMult attribute), 140
gamma (dicee.models.function_space.FMult attribute), 76
gate_residual (dicee.models.literal.LiteralEmbeddings attribute), 80
gated_residual_proj (dicee.models.literal.LiteralEmbeddings attribute), 80
gelu (dicee.models.transformers.MLP attribute), 94
gen_test (dicee.query_generator.QueryGenerator attribute), 144
gen_test (dicee.QueryGenerator attribute), 214
gen_valid (dicee.query_generator.QueryGenerator attribute), 144
gen_valid (dicee.QueryGenerator attribute), 214
generate() (dicee.BytE method), 189
generate() (dicee.KGE method), 196
generate() (dicee.knowledge_graph_embeddings.KGE method), 51
generate() (dicee.models.transformers.BytE method), 91
generate_queries() (dicee.query_generator.QueryGenerator method), 144
generate_queries() (dicee.QueryGenerator method), 214
get_aswa_state_dict() (dicee.callbacks.ASWA method), 24
get_bpe_head_and_relation_representation() (dicee.BaseKGE method), 192
get_bpe_head_and_relation_representation() (dicee.models.base_model.BaseKGE method), 63
get_bpe_head_and_relation_representation() (dicee.models.BaseKGE method), 106, 109, 113, 117, 123, 136, 139
get_bpe_token_representation() (dicee.abstracts.BaseInteractiveKGE method), 14
get_callbacks() (in module dicee.trainer.dice_trainer), 160
get_default_arguments() (in module dicee.analyse_experiments), 19
get_default_arguments() (in module dicee.scripts.index_serve), 153
get_default_arguments() (in module dicee.scripts.run), 155
get_ee_vocab() (in module dicee), 193
get_ee_vocab() (in module dicee.read_preprocess_save_load_kg.util), 149
get_ee_vocab() (in module dicee.static_funcs), 156
get_ee_vocab() (in module dicee.static_preprocess_funcs), 159
get_embeddings() (dicee.BaseKGE method), 192
get_embeddings() (dicee.EnsembleKGE method), 193
get_embeddings() (dicee.models.base_model.BaseKGE method), 63
get_embeddings() (dicee.models.BaseKGE method), 106, 109, 113, 117, 123, 136, 139
get_embeddings() (dicee.models.ensemble.EnsembleKGE method), 75
get_embeddings() (dicee.models.real.Shallom method), 89
get_embeddings() (dicee.models.Shallom method), 110
get_embeddings() (dicee.Shallom method), 185
get_entity_embeddings() (dicee.abstracts.BaseInteractiveKGE method), 15
get_entity_index() (dicee.abstracts.BaseInteractiveKGE method), 15
get_er_vocab() (in module dicee), 193
get_er_vocab() (in module dicee.read_preprocess_save_load_kg.util), 149
get_er_vocab() (in module dicee.static_funcs), 156
get_er_vocab() (in module dicee.static_preprocess_funcs), 159
get_eval_report() (dicee.abstracts.BaseInteractiveKGE method), 14
get_head_relation_representation() (dicee.BaseKGE method), 192
get_head_relation_representation() (dicee.models.base_model.BaseKGE method), 63
get_head_relation_representation() (dicee.models.BaseKGE method), 106, 109, 112, 117, 123, 136, 139
get_kronecker_triple_representation() (dicee.callbacks.KronE method), 26
get_num_params() (dicee.models.transformers.GPT method), 96
get_padded_bpe_triple_representation() (dicee.abstracts.BaseInteractiveKGE method), 14
get_queries() (dicee.query_generator.QueryGenerator method), 145
get_queries() (dicee.QueryGenerator method), 215
get_re_vocab() (in module dicee), 193
get_re_vocab() (in module dicee.read_preprocess_save_load_kg.util), 149
{\tt get\_re\_vocab} \; \textit{(in module dicee.static\_funcs)}, \, 156
get_re_vocab() (in module dicee.static_preprocess_funcs), 159
\verb|get_relation_embeddings()| \textit{(dicee.abstracts.BaseInteractiveKGE method)}, 15
```

```
get relation index() (dicee.abstracts.BaseInteractiveKGE method), 15
get_sentence_representation() (dicee.BaseKGE method), 192
get_sentence_representation() (dicee.models.base_model.BaseKGE method), 63
get_sentence_representation() (dicee.models.BaseKGE method), 106, 109, 112, 117, 123, 136, 139
\verb"get_transductive_entity_embeddings()" (\textit{dicee.KGE method}), 196
get_transductive_entity_embeddings() (dicee.knowledge_graph_embeddings.KGE method), 50
get_triple_representation() (dicee.BaseKGE method), 192
get_triple_representation() (dicee.models.base_model.BaseKGE method), 63
get_triple_representation() (dicee.models.BaseKGE method), 106, 109, 112, 117, 123, 136, 139
GFMult (class in dicee.models), 140
GFMult (class in dicee.models.function_space), 76
global_rank (dicee.abstracts.AbstractTrainer attribute), 13
global_rank (dicee.trainer.torch_trainer_ddp.NodeTrainer attribute), 164
GPT (class in dicee.models.transformers), 95
GPTConfig (class in dicee.models.transformers), 95
gpus (dicee.config.Namespace attribute), 28
gradient_accumulation_steps (dicee.config.Namespace attribute), 29
ground_queries() (dicee.query_generator.QueryGenerator method), 144
ground_queries() (dicee.QueryGenerator method), 214
hidden_dim (dicee.models.literal.LiteralEmbeddings attribute), 80
hidden_dropout (dicee.BaseKGE attribute), 191
hidden_dropout (dicee.models.base_model.BaseKGE attribute), 62
hidden_dropout (dicee.models.BaseKGE attribute), 105, 108, 112, 116, 122, 135, 138
hidden_dropout_rate (dicee.BaseKGE attribute), 191
hidden_dropout_rate (dicee.config.Namespace attribute), 29
\verb|hidden_dropout_rate| (\textit{dicee.models.base\_model.BaseKGE attribute}), 62
hidden_dropout_rate (dicee.models.BaseKGE attribute), 104, 108, 111, 116, 122, 134, 138
hidden_normalizer (dicee.BaseKGE attribute), 191
hidden_normalizer (dicee.models.base_model.BaseKGE attribute), 62
hidden_normalizer (dicee.models.BaseKGE attribute), 105, 108, 112, 116, 122, 135, 138
IdentityClass (class in dicee.models), 106, 117, 123
IdentityClass (class in dicee.models.base_model), 63
idx_entity_to_bpe_shaped (dicee.knowledge_graph.KG attribute), 49
index() (in module dicee.scripts.index_serve), 153
index_triple() (dicee.abstracts.BaseInteractiveKGE method), 15
init_dataloader() (dicee.DICE_Trainer method), 195
init\_dataloader() (dicee.trainer.DICE_Trainer method), 166
init dataloader() (dicee.trainer.dice trainer.DICE Trainer method), 161
init_dataset() (dicee.DICE_Trainer method), 195
init_dataset() (dicee.trainer.DICE_Trainer method), 166
init_dataset() (dicee.trainer.dice_trainer.DICE_Trainer method), 161
init_param (dicee.config.Namespace attribute), 29
init_params_with_sanity_checking() (dicee.BaseKGE method), 192
init_params_with_sanity_checking() (dicee.models.base_model.BaseKGE method), 63
init_params_with_sanity_checking() (dicee.models.BaseKGE method), 105, 108, 112, 117, 123, 135, 139
initial_eval_setting (dicee.callbacks.ASWA attribute), 24
initialize_or_load_model() (dicee.DICE_Trainer method), 195
initialize_or_load_model() (dicee.trainer.DICE_Trainer method), 166
initialize_or_load_model() (dicee.trainer.dice_trainer.DICE_Trainer method), 161
initialize_trainer() (dicee.DICE_Trainer method), 195
initialize_trainer() (dicee.trainer.DICE_Trainer method), 166
initialize_trainer() (dicee.trainer.dice_trainer.DICE_Trainer method), 161
initialize_trainer() (in module dicee.trainer.dice_trainer), 160
input_dp_ent_real (dicee.BaseKGE attribute), 191
input_dp_ent_real (dicee.models.base_model.BaseKGE attribute), 62
input_dp_ent_real (dicee.models.BaseKGE attribute), 105, 108, 112, 116, 122, 135, 138
input_dp_rel_real (dicee.BaseKGE attribute), 191
input_dp_rel_real (dicee.models.base_model.BaseKGE attribute), 62
input_dp_rel_real (dicee.models.BaseKGE attribute), 105, 108, 112, 116, 122, 135, 138
input_dropout_rate (dicee.BaseKGE attribute), 191
input_dropout_rate (dicee.config.Namespace attribute), 29
input_dropout_rate (dicee.models.base_model.BaseKGE attribute), 62
input_dropout_rate (dicee.models.BaseKGE attribute), 104, 108, 111, 116, 122, 134, 138
```

```
InteractiveQueryDecomposition (class in dicee.abstracts), 16
intialize_model() (in module dicee), 194
intialize_model() (in module dicee.static_funcs), 157
is_continual_training (dicee.DICE_Trainer attribute), 195
{\tt is\_continual\_training}~(\textit{dicee.evaluator.Evaluator~attribute}), 46
is_continual_training (dicee.Execute attribute), 199
is_continual_training (dicee.executer.Execute attribute), 47
is continual training (dicee.trainer.DICE Trainer attribute), 165
is_continual_training (dicee.trainer.dice_trainer.DICE_Trainer attribute), 160
is_global_zero (dicee.abstracts.AbstractTrainer attribute), 13
is_seen() (dicee.abstracts.BaseInteractiveKGE method), 15
is_sparql_endpoint_alive() (in module dicee.sanity_checkers), 152
K
k (dicee.models.FMult attribute), 139
k (dicee.models.FMult2 attribute), 140
k (dicee.models.function_space.FMult attribute), 76
k (dicee.models.function_space.FMult2 attribute), 77
k (dicee.models.function_space.GFMult attribute), 76
k (dicee.models.GFMult attribute), 140
\verb|k_fold_cross_validation()| \textit{(dicee.DICE\_Trainer method)}, 196
k_fold_cross_validation() (dicee.trainer.DICE_Trainer method), 166
\verb|k_fold_cross_validation()| \textit{(dicee.trainer.dice\_trainer.DICE\_Trainer method)}, 161
k_vs_all_score() (dicee.ComplEx static method), 179
k_vs_all_score() (dicee.DistMult method), 170
k_vs_all_score() (dicee.Keci method), 172
k_vs_all_score() (dicee.models.clifford.Keci method), 67
k_vs_all_score() (dicee.models.ComplEx static method), 115
k_vs_all_score() (dicee.models.complex.ComplEx static method), 73
k_vs_all_score() (dicee.models.DistMult method), 109
k_vs_all_score() (dicee.models.Keci method), 129
k_vs_all_score() (dicee.models.octonion.OMult method), 82
\verb|k_vs_all_score|()| \textit{(dicee.models.OMult method)}, 125
k_vs_all_score() (dicee.models.QMult method), 119
k_vs_all_score() (dicee.models.quaternion.QMult method), 86
k_vs_all_score() (dicee.models.real.DistMult method), 88
k_vs_all_score() (dicee.OMult method), 185
k_vs_all_score() (dicee.QMult method), 184
Keci (class in dicee), 170
Keci (class in dicee.models), 127
Keci (class in dicee.models.clifford), 64
kernel_size (dicee.BaseKGE attribute), 191
kernel_size (dicee.config.Namespace attribute), 29
kernel_size (dicee.models.base_model.BaseKGE attribute), 62
kernel_size (dicee.models.BaseKGE attribute), 104, 108, 111, 116, 122, 134, 138
KG (class in dicee.knowledge_graph), 49
kg (dicee.callbacks.PseudoLabellingCallback attribute), 23
kg (dicee.read_preprocess_save_load_kg.LoadSaveToDisk attribute), 151
kg (dicee.read_preprocess_save_load_kg.PreprocessKG attribute), 150
\verb|kg|| (dicee.read\_preprocess\_save\_load\_kg.preprocess.PreprocessKG| attribute), 145
kg (dicee.read_preprocess_save_load_kg.read_from_disk.ReadFromDisk attribute), 146
kg (dicee.read_preprocess_save_load_kg.ReadFromDisk attribute), 151
kg (dicee.read_preprocess_save_load_kg.save_load_disk.LoadSaveToDisk attribute), 147
KGE (class in dicee), 196
{\tt KGE}~(class~in~dicee.knowledge\_graph\_embeddings),~50
KGESaveCallback (class in dicee.callbacks), 22
knowledge_graph (dicee.Execute attribute), 200
knowledge_graph (dicee.executer.Execute attribute), 47
KronE (class in dicee.callbacks), 25
KvsAll (class in dicee), 203
KvsAll (class in dicee.dataset_classes), 33
kvsall_score() (dicee.DualE method), 177
kvsall_score() (dicee.models.DualE method), 143
kvsall_score() (dicee.models.dualE.DualE method), 74
KvsSampleDataset (class in dicee), 206
KvsSampleDataset (class in dicee.dataset_classes), 36
```

```
L
label_smoothing_rate (dicee.AllvsAll attribute), 204
label_smoothing_rate (dicee.config.Namespace attribute), 29
label_smoothing_rate (dicee.dataset_classes.AllvsAll attribute), 34
label_smoothing_rate (dicee.dataset_classes.KvsAll attribute), 34
label_smoothing_rate (dicee.dataset_classes.KvsSampleDataset attribute), 37
label_smoothing_rate (dicee.dataset_classes.OnevsSample attribute), 35, 36
{\tt label\_smoothing\_rate}~(\textit{dicee.dataset\_classes.TriplePredictionDataset~attribute}), 38
label_smoothing_rate (dicee.KvsAll attribute), 204
label_smoothing_rate (dicee.KvsSampleDataset attribute), 207
label_smoothing_rate (dicee. OnevsSample attribute), 205, 206
label_smoothing_rate (dicee. TriplePredictionDataset attribute), 208
layer_norm (dicee.models.literal.LiteralEmbeddings attribute), 80
LayerNorm (class in dicee.models.transformers), 92
learning_rate (dicee.BaseKGE attribute), 191
learning_rate (dicee.models.base_model.BaseKGE attribute), 62
learning_rate (dicee.models.BaseKGE attribute), 104, 108, 111, 116, 122, 134, 138
length (dicee.dataset classes.NegSampleDataset attribute), 37
length (dicee.dataset_classes.TriplePredictionDataset attribute), 38
length (dicee.NegSampleDataset attribute), 207
length (dicee. TriplePredictionDataset attribute), 208
level (dicee.callbacks.Perturb attribute), 26
LFMult (class in dicee), 186
LFMult (class in dicee.models), 141
LFMult (class in dicee.models.function_space), 78
LFMult1 (class in dicee.models), 141
LFMult1 (class in dicee.models.function_space), 77
linear() (dicee.LFMult method), 186
linear() (dicee.models.function_space.LFMult method), 78
linear() (dicee.models.LFMult method), 142
list2tuple() (dicee.query_generator.QueryGenerator method), 144
list2tuple() (dicee.QueryGenerator method), 214
LiteralDataset (class in dicee), 212
LiteralDataset (class in dicee.dataset_classes), 42
LiteralEmbeddings (class in dicee.models.literal), 79
lm_head (dicee.BytE attribute), 188
lm_head (dicee.models.transformers.BytE attribute), 91
lm_head (dicee.models.transformers.GPT attribute), 96
ln_1 (dicee.models.transformers.Block attribute), 95
ln_2 (dicee.models.transformers.Block attribute), 95
load() (dicee.read_preprocess_save_load_kg.LoadSaveToDisk method), 151
load() (dicee.read_preprocess_save_load_kg.save_load_disk.LoadSaveToDisk method), 147
load_and_validate_literal_data() (dicee.dataset_classes.LiteralDataset static method), 43
load_and_validate_literal_data() (dicee.LiteralDataset static method), 213
load_json() (in module dicee), 194
load_json() (in module dicee.static_funcs), 157
load_model() (in module dicee), 193
load_model() (in module dicee.static_funcs), 157
load_model_ensemble() (in module dicee), 193
load_model_ensemble() (in module dicee.static_funcs), 157
load_numpy() (in module dicee), 194
load_numpy() (in module dicee.static_funcs), 158
load_numpy_ndarray() (in module dicee.read_preprocess_save_load_kg.util), 150
load_pickle() (in module dicee), 193
load_pickle() (in module dicee.read_preprocess_save_load_kg.util), 150
load_pickle() (in module dicee.static_funcs), 157
load gueries () (dicee.query generator.QueryGenerator method), 145
load_queries() (dicee.QueryGenerator method), 215
load_queries_and_answers() (dicee.query_generator.QueryGenerator static method), 145
load_queries_and_answers() (dicee.QueryGenerator static method), 215
load_term_mapping() (in module dicee), 193, 201
load_term_mapping() (in module dicee.static_funcs), 157
load_term_mapping() (in module dicee.trainer.dice_trainer), 160
load_with_pandas() (in module dicee.read_preprocess_save_load_kg.util), 150
loader_backend (dicee.dataset_classes.LiteralDataset attribute), 43
loader_backend (dicee.LiteralDataset attribute), 213
LoadSaveToDisk (class in dicee.read_preprocess_save_load_kg), 151
LoadSaveToDisk (class in dicee.read_preprocess_save_load_kg.save_load_disk), 147
```

```
local rank (dicee.abstracts.AbstractTrainer attribute), 13
local_rank (dicee.trainer.torch_trainer_ddp.NodeTrainer attribute), 164
loss (dicee.BaseKGE attribute), 191
loss (dicee.models.base_model.BaseKGE attribute), 62
loss (dicee.models.BaseKGE attribute), 105, 108, 111, 116, 122, 135, 138
loss_func (dicee.trainer.torch_trainer_ddp.NodeTrainer attribute), 165
loss_function (dicee.trainer.torch_trainer.TorchTrainer attribute), 163
loss function() (dicee.BytE method), 189
loss_function() (dicee.models.base_model.BaseKGELightning method), 57
loss_function() (dicee.models.BaseKGELightning method), 100
loss_function() (dicee.models.transformers.BytE method), 91
loss_history (dicee.BaseKGE attribute), 191
loss_history (dicee.models.base_model.BaseKGE attribute), 62
loss_history (dicee.models.BaseKGE attribute), 105, 108, 112, 116, 122, 135, 138
loss_history (dicee.models.pykeen_models.PykeenKGE attribute), 84
loss_history (dicee.models.PykeenKGE attribute), 136
loss_history (dicee.PykeenKGE attribute), 187
loss_history (dicee.trainer.torch_trainer_ddp.NodeTrainer attribute), 165
1r (dicee.analyse_experiments.Experiment attribute), 19
1r (dicee.config.Namespace attribute), 28
M
m (dicee.LFMult attribute), 186
m (dicee.models.function_space.LFMult attribute), 78
m (dicee.models.LFMult attribute), 141
main() (in module dicee.scripts.index_serve), 155
main() (in module dicee.scripts.run), 155
make_iterable_verbose() (in module dicee.static_funcs_training), 158
make_iterable_verbose() (in module dicee.trainer.torch_trainer_ddp), 164
mapping_from_first_two_cols_to_third() (in module dicee), 200
mapping_from_first_two_cols_to_third() (in module dicee.static_preprocess_funcs), 160
margin (dicee.models.Pyke attribute), 110
margin (dicee.models.real.Pyke attribute), 89
margin (dicee.models.real.TransE attribute), 89
margin (dicee.models.TransE attribute), 110
margin (dicee.Pyke attribute), 169
margin (dicee. TransE attribute), 173
max_ans_num (dicee.query_generator.QueryGenerator attribute), 144
max_ans_num (dicee.QueryGenerator attribute), 214
max_epochs (dicee.callbacks.KGESaveCallback attribute), 22
max epochs (dicee.callbacks.PeriodicEvalCallback attribute), 27
max_length_subword_tokens (dicee.BaseKGE attribute), 191
\verb|max_length_subword_tokens| (\textit{dicee.knowledge\_graph.KG attribute}), 50
max_length_subword_tokens (dicee.models.base_model.BaseKGE attribute), 62
max_length_subword_tokens (dicee.models.BaseKGE attribute), 105, 108, 112, 116, 122, 135, 138
max_num_of_classes (dicee.dataset_classes.KvsSampleDataset attribute), 37
max_num_of_classes (dicee.KvsSampleDataset attribute), 207
mem_of_model() (dicee.EnsembleKGE method), 193
mem_of_model() (dicee.models.base_model.BaseKGELightning method), 56
mem_of_model() (dicee.models.BaseKGELightning method), 99
mem_of_model() (dicee.models.ensemble.EnsembleKGE method), 75
method (dicee.callbacks.Perturb attribute), 26
MLP (class in dicee.models.transformers), 93
mlp (dicee.models.transformers.Block attribute), 95
mode (dicee.query_generator.QueryGenerator attribute), 144
mode (dicee. Query Generator attribute), 214
model (dicee.config.Namespace attribute), 28
model (dicee.models.pykeen_models.PykeenKGE attribute), 84
model (dicee.models.PykeenKGE attribute), 136
model (dicee.PykeenKGE attribute), 187
model (dicee.trainer.torch_trainer_ddp.NodeTrainer attribute), 165
\verb|model| (\textit{dicee.trainer.torch\_trainer.TorchTrainer attribute}), 163
model_kwargs (dicee.models.pykeen_models.PykeenKGE attribute), 84
model_kwargs (dicee.models.PykeenKGE attribute), 136
model_kwargs (dicee.PykeenKGE attribute), 187
model_name (dicee.analyse_experiments.Experiment attribute), 19
module
```

```
dicee, 12
     dicee.__main__, 12
     dicee.abstracts, 12
     dicee.analyse_experiments, 19
     dicee.callbacks, 20
     dicee.config, 27
     dicee.dataset_classes, 30
     dicee.eval static funcs, 44
     dicee.evaluator, 45
     dicee.executer.47
     dicee.knowledge_graph, 49
     dicee.knowledge_graph_embeddings, 50
     dicee.models, 54
     dicee.models.adopt, 54
     dicee.models.base_model, 55
     dicee.models.clifford, 64
     dicee.models.complex, 71
     dicee.models.dualE, 74
     dicee.models.ensemble, 75
     dicee.models.function_space, 76
     dicee.models.literal, 79
     {\tt dicee.models.octonion, 81}
     dicee.models.pykeen_models, 84
     dicee.models.quaternion, 85
     dicee.models.real, 88
     dicee.models.static_funcs, 89
     dicee.models.transformers, 90
     dicee.query_generator, 143
     dicee.read_preprocess_save_load_kg, 145
     dicee.read_preprocess_save_load_kg.preprocess, 145
     {\tt dicee.read\_preprocess\_save\_load\_kg.read\_from\_disk, 146}
     dicee.read_preprocess_save_load_kg.save_load_disk, 146
     dicee.read_preprocess_save_load_kg.util, 147
     dicee.sanity_checkers, 151
     dicee.scripts, 152
     dicee.scripts.index_serve, 152
     dicee.scripts.run, 155
     dicee.static_funcs, 155
     dicee.static_funcs_training, 158
     dicee.static_preprocess_funcs, 159
     dicee.trainer, 160
     dicee.trainer.dice_trainer, 160
     dicee.trainer.model_parallelism, 162
     dicee.trainer.torch_trainer, 162
     dicee.trainer.torch_trainer_ddp, 164
modules() (dicee.EnsembleKGE method), 192
modules () (dicee.models.ensemble.EnsembleKGE method), 75
MultiClassClassificationDataset (class in dicee), 202
MultiClassClassificationDataset (class in dicee.dataset_classes), 32
MultiLabelDataset (class in dicee), 201
MultiLabelDataset (class in dicee.dataset_classes), 31
Ν
n (dicee.models.FMult2 attribute), 140
n (dicee.models.function_space.FMult2 attribute), 77
n_embd (dicee.models.transformers.CausalSelfAttention attribute), 93
n_embd (dicee.models.transformers.GPTConfig attribute), 95
n_epochs_eval_model (dicee.callbacks.PeriodicEvalCallback attribute), 27
n_epochs_eval_model (dicee.config.Namespace attribute), 30
n_head (dicee.models.transformers.CausalSelfAttention attribute), 93
n_head (dicee.models.transformers.GPTConfig attribute), 95
n_layer (dicee.models.transformers.GPTConfig attribute), 95
n_layers (dicee.models.FMult2 attribute), 140
n_layers (dicee.models.function_space.FMult2 attribute), 77
name (dicee.abstracts.BaseInteractiveKGE property), 15
name (dicee.AConEx attribute), 179
name (dicee. AConvO attribute), 179
```

```
name (dicee.AConvO attribute), 180
name (dicee.BytE attribute), 188
name (dicee.CKeci attribute), 170
name (dicee.ComplEx attribute), 179
name (dicee.ConEx attribute), 182
name (dicee.ConvO attribute), 182
name (dicee.ConvQ attribute), 181
name (dicee.DeCaL attribute), 174
name (dicee.DistMult attribute), 170
name (dicee.DualE attribute), 177
name (dicee.EnsembleKGE attribute), 192
name (dicee. Keci attribute), 171
name (dicee.LFMult attribute), 186
name (dicee.models.AConEx attribute), 113
name (dicee.models.AConvO attribute), 126
name (dicee.models.AConvQ attribute), 120
name (dicee.models.CKeci attribute), 130
name (dicee.models.clifford.CKeci attribute), 67
name (dicee.models.clifford.DeCaL attribute), 68
name (dicee.models.clifford.Keci attribute), 65
name (dicee.models.ComplEx attribute), 114
name (dicee.models.complex.AConEx attribute), 72
name (dicee.models.complex.ComplEx attribute), 73
name (dicee.models.complex.ConEx attribute), 71
name (dicee.models.ConEx attribute), 113
name (dicee.models.ConvO attribute), 126
name (dicee.models.ConvQ attribute), 120
name (dicee.models.DeCaL attribute), 131
name (dicee.models.DistMult attribute), 109
name (dicee.models.DualE attribute), 142
name (dicee.models.dualE.DualE attribute), 74
name (dicee.models.ensemble.EnsembleKGE attribute), 75
name (dicee.models.FMult attribute), 139
name (dicee.models.FMult2 attribute), 140
name (dicee.models.function_space.FMult attribute), 76
name (dicee.models.function_space.FMult2 attribute), 77
name (dicee.models.function space.GFMult attribute), 76
{\tt name}~(\textit{dicee.models.function\_space.LFMult~attribute}), 78
name (dicee.models.function_space.LFMult1 attribute), 77
name (dicee.models.GFMult attribute), 140
name (dicee.models.Keci attribute), 127
name (dicee.models.LFMult attribute), 141
name (dicee.models.LFMult1 attribute), 141
name (dicee.models.octonion.AConvO attribute), 83
name (dicee.models.octonion.ConvO attribute), 82
name (dicee.models.octonion.OMult attribute), 82
name (dicee.models.OMult attribute), 125
name (dicee.models.Pyke attribute), 110
name (dicee.models.pykeen_models.PykeenKGE attribute), 84
name (dicee.models.PykeenKGE attribute), 136
name (dicee.models.QMult attribute), 119
name (dicee.models.quaternion.AConvQ attribute), 87
name (dicee.models.quaternion.ConvQ attribute), 87
name (dicee.models.quaternion.QMult attribute), 86
name (dicee.models.real.DistMult attribute), 88
name (dicee.models.real.Pyke attribute), 89
name (dicee.models.real.Shallom attribute), 89
name (dicee.models.real.TransE attribute), 88
name (dicee.models.Shallom attribute), 110
name (dicee.models.TransE attribute), 110
name (dicee.models.transformers.BytE attribute), 91
name (dicee.OMult attribute), 185
name (dicee.Pyke attribute), 169
name (dicee.PykeenKGE attribute), 187
name (dicee.QMult attribute), 183
name (dicee.Shallom attribute), 185
name (dicee. TransE attribute), 173
named_children() (dicee.EnsembleKGE method), 192
```

```
named children() (dicee.models.ensemble.EnsembleKGE method), 75
Namespace (class in dicee.config), 27
neg_ratio (dicee.BPE_NegativeSamplingDataset attribute), 201
neg_ratio (dicee.config.Namespace attribute), 28
neg_ratio (dicee.dataset_classes.BPE_NegativeSamplingDataset attribute), 31
neg_ratio (dicee.dataset_classes.KvsSampleDataset attribute), 37
neg_ratio (dicee.KvsSampleDataset attribute), 207
neg sample ratio (dicee.CVDataModule attribute), 209
neg_sample_ratio (dicee.dataset_classes.CVDataModule attribute), 39
neg_sample_ratio (dicee.dataset_classes.NegSampleDataset attribute), 37
neg_sample_ratio (dicee.dataset_classes.OnevsSample attribute), 35, 36
neg_sample_ratio (dicee.dataset_classes.TriplePredictionDataset attribute), 38
neg_sample_ratio (dicee.NegSampleDataset attribute), 207
neg_sample_ratio (dicee.OnevsSample attribute), 205, 206
neg_sample_ratio (dicee.TriplePredictionDataset attribute), 208
negnorm() (dicee.abstracts.InteractiveQueryDecomposition method), 16
NegSampleDataset (class in dicee), 207
NegSampleDataset (class in dicee.dataset_classes), 37
neural_searcher (in module dicee.scripts.index_serve), 153
NeuralSearcher (class in dicee.scripts.index_serve), 153
NodeTrainer (class in dicee.trainer.torch_trainer_ddp), 164
norm_fc1 (dicee.AConEx attribute), 179
norm_fc1 (dicee.AConvO attribute), 180
norm_fc1 (dicee.ConEx attribute), 182
norm_fc1 (dicee.ConvO attribute), 182
norm_fc1 (dicee.models.AConEx attribute), 114
norm_fc1 (dicee.models.AConvO attribute), 126
norm_fc1 (dicee.models.complex.AConEx attribute), 72
norm_fc1 (dicee.models.complex.ConEx attribute), 72
norm_fc1 (dicee.models.ConEx attribute), 113
norm_fc1 (dicee.models.ConvO attribute), 126
norm fc1 (dicee.models.octonion.AConvO attribute), 83
norm_fc1 (dicee.models.octonion.ConvO attribute), 83
normalization (dicee.analyse_experiments.Experiment attribute), 20
normalization (dicee.config.Namespace attribute), 28
normalization (dicee.dataset_classes.LiteralDataset attribute), 42
normalization (dicee.LiteralDataset attribute), 212
normalization_params (dicee.dataset_classes.LiteralDataset attribute), 42, 43
normalization_params (dicee.LiteralDataset attribute), 212, 213
normalization_type (dicee.dataset_classes.LiteralDataset attribute), 43
normalization_type (dicee.LiteralDataset attribute), 213
normalize_head_entity_embeddings (dicee.BaseKGE attribute), 191
normalize_head_entity_embeddings (dicee.models.base_model.BaseKGE attribute), 62
normalize_head_entity_embeddings (dicee.models.BaseKGE attribute), 105, 108, 112, 116, 122, 135, 138
normalize_relation_embeddings (dicee.BaseKGE attribute), 191
\verb|normalize_relation_embeddings| \textit{(dicee.models.base\_model.BaseKGE attribute)}, 62
normalize_relation_embeddings (dicee.models.BaseKGE attribute), 105, 108, 112, 116, 122, 135, 138
normalize_tail_entity_embeddings (dicee.BaseKGE attribute), 191
normalize_tail_entity_embeddings (dicee.models.base_model.BaseKGE attribute), 62
normalize_tail_entity_embeddings (dicee.models.BaseKGE attribute), 105, 108, 112, 116, 122, 135, 138
normalizer_class (dicee.BaseKGE attribute), 191
normalizer_class (dicee.models.base_model.BaseKGE attribute), 62
normalizer_class (dicee.models.BaseKGE attribute), 105, 108, 111, 116, 122, 135, 138
num_bpe_entities (dicee.BPE_NegativeSamplingDataset attribute), 201
num_bpe_entities (dicee.dataset_classes.BPE_NegativeSamplingDataset attribute), 31
num_bpe_entities (dicee.knowledge_graph.KG attribute), 49
num_core (dicee.config.Namespace attribute), 29
num_data_properties (dicee.dataset_classes.LiteralDataset attribute), 43
num_data_properties (dicee.LiteralDataset attribute), 213
num_datapoints (dicee.BPE_NegativeSamplingDataset attribute), 201
num datapoints (dicee.dataset classes.BPE NegativeSamplingDataset attribute), 31
num_datapoints (dicee.dataset_classes.MultiLabelDataset attribute), 32
num_datapoints (dicee.MultiLabelDataset attribute), 202
num_ent (dicee.DualE attribute), 177
num_ent (dicee.models.DualE attribute), 143
num_ent (dicee.models.dualE.DualE attribute), 74
num_entities (dicee.BaseKGE attribute), 191
num_entities (dicee.CVDataModule attribute), 209
```

```
num entities (dicee.dataset classes.CVDataModule attribute), 39
num_entities (dicee.dataset_classes.KvsSampleDataset attribute), 37
num_entities (dicee.dataset_classes.LiteralDataset attribute), 43
num_entities (dicee.dataset_classes.NegSampleDataset attribute), 37
num_entities (dicee.dataset_classes.OnevsSample attribute), 35, 36
num_entities (dicee.dataset_classes.TriplePredictionDataset attribute), 38
num_entities (dicee.evaluator.Evaluator attribute), 46
num entities (dicee.knowledge graph.KG attribute), 49
num_entities (dicee.KvsSampleDataset attribute), 207
num_entities (dicee.LiteralDataset attribute), 212, 213
num_entities (dicee.models.base_model.BaseKGE attribute), 62
num_entities (dicee.models.BaseKGE attribute), 104, 107, 111, 116, 121, 134, 138
num_entities (dicee.NegSampleDataset attribute), 207
num_entities (dicee. Onevs Sample attribute), 205
num_entities (dicee. TriplePredictionDataset attribute), 208
num_epochs (dicee.abstracts.AbstractPPECallback attribute), 17
num_epochs (dicee.analyse_experiments.Experiment attribute), 19
num_epochs (dicee.callbacks.ASWA attribute), 23
num_epochs (dicee.config.Namespace attribute), 28
num_epochs (dicee.trainer.torch_trainer_ddp.NodeTrainer attribute), 165
num_folds_for_cv (dicee.config.Namespace attribute), 29
num_of_data_points (dicee.dataset_classes.MultiClassClassificationDataset attribute), 32
num_of_data_points (dicee.MultiClassClassificationDataset attribute), 202
num_of_data_properties (dicee.models.literal.LiteralEmbeddings attribute), 79, 80
num_of_epochs (dicee.callbacks.PseudoLabellingCallback attribute), 23
num_of_output_channels (dicee.BaseKGE attribute), 191
num_of_output_channels (dicee.config.Namespace attribute), 29
\verb|num_of_output_channels| (\textit{dicee.models.base\_model.BaseKGE attribute}), 62
num_of_output_channels (dicee.models.BaseKGE attribute), 105, 108, 111, 116, 122, 135, 138
num_params (dicee.analyse_experiments.Experiment attribute), 19
num_relations (dicee.BaseKGE attribute), 191
num relations (dicee, CVD ata Module attribute), 209
num_relations (dicee.dataset_classes.CVDataModule attribute), 39
\verb|num_relations| (\textit{dicee.dataset\_classes.NegSampleDataset attribute}), 37
num_relations (dicee.dataset_classes.OnevsSample attribute), 35, 36
num_relations (dicee.dataset_classes.TriplePredictionDataset attribute), 38
num relations (dicee.evaluator.Evaluator attribute), 46
num_relations (dicee.knowledge_graph.KG attribute), 49
num_relations (dicee.models.base_model.BaseKGE attribute), 62
num_relations (dicee.models.BaseKGE attribute), 104, 107, 111, 116, 122, 134, 138
num_relations (dicee.NegSampleDataset attribute), 207
num_relations (dicee. Onevs Sample attribute), 205
num_relations (dicee. TriplePredictionDataset attribute), 208
num_sample (dicee.models.FMult attribute), 139
{\tt num\_sample}~(\textit{dicee.models.function\_space.FMult~attribute}), 76
num_sample (dicee.models.function_space.GFMult attribute), 76
num_sample (dicee.models.GFMult attribute), 140
num_tokens (dicee.BaseKGE attribute), 191
num_tokens (dicee.knowledge_graph.KG attribute), 49
num_tokens (dicee.models.base_model.BaseKGE attribute), 62
num_tokens (dicee.models.BaseKGE attribute), 104, 108, 111, 116, 122, 134, 138
num_workers (dicee.CVDataModule attribute), 209
num_workers (dicee.dataset_classes.CVDataModule attribute), 39
numpy_data_type_changer() (in module dicee), 193
numpy_data_type_changer() (in module dicee.static_funcs), 157
O
octonion_mul() (in module dicee.models), 124
octonion_mul() (in module dicee.models.octonion), 81
octonion_mul_norm() (in module dicee.models), 124
octonion_mul_norm() (in module dicee.models.octonion), 81
octonion_normalizer() (dicee.AConvO static method), 180
octonion_normalizer() (dicee.ConvO static method), 182
octonion_normalizer() (dicee.models.AConvO static method), 126
octonion_normalizer() (dicee.models.ConvO static method), 126
octonion_normalizer() (dicee.models.octonion.AConvO static method), 83
octonion_normalizer() (dicee.models.octonion.ConvO static method), 83
```

```
octonion normalizer() (dicee.models.octonion.OMult static method), 82
octonion_normalizer() (dicee.models.OMult static method), 125
octonion_normalizer() (dicee.OMult static method), 185
OMult (class in dicee), 184
OMult (class in dicee.models), 124
OMult (class in dicee.models.octonion), 81
on_epoch_end() (dicee.callbacks.KGESaveCallback method), 23
on epoch end() (dicee.callbacks.PseudoLabellingCallback method), 23
on_fit_end() (dicee.abstracts.AbstractCallback method), 17
on_fit_end() (dicee.abstracts.AbstractPPECallback method), 18
on_fit_end() (dicee.abstracts.AbstractTrainer method), 13
on_fit_end() (dicee.callbacks.AccumulateEpochLossCallback method), 21
on_fit_end() (dicee.callbacks.ASWA method), 24
on_fit_end() (dicee.callbacks.Eval method), 25
on_fit_end() (dicee.callbacks.KGESaveCallback method), 23
on_fit_end() (dicee.callbacks.PeriodicEvalCallback method), 27
on_fit_end() (dicee.callbacks.PrintCallback method), 21
on_fit_start() (dicee.abstracts.AbstractCallback method), 16
on_fit_start() (dicee.abstracts.AbstractPPECallback method), 17
on_fit_start() (dicee.abstracts.AbstractTrainer method), 13
on_fit_start() (dicee.callbacks.Eval method), 25
on_fit_start() (dicee.callbacks.KGESaveCallback method), 22
on_fit_start() (dicee.callbacks.KronE method), 26
on_fit_start() (dicee.callbacks.PrintCallback method), 21
on_init_end() (dicee.abstracts.AbstractCallback method), 16
on_init_start() (dicee.abstracts.AbstractCallback method), 16
on_train_batch_end() (dicee.abstracts.AbstractCallback method), 17
on_train_batch_end() (dicee.abstracts.AbstractTrainer method), 13
on_train_batch_end() (dicee.callbacks.Eval method), 25
on_train_batch_end() (dicee.callbacks.KGESaveCallback method), 22
on_train_batch_end() (dicee.callbacks.PrintCallback method), 21
on_train_batch_start() (dicee.callbacks.Perturb method), 26
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), 24
on_train_epoch_end() (dicee.callbacks.Eval method), 25
on train epoch end() (dicee.callbacks.KGESaveCallback method), 22
on_train_epoch_end() (dicee.callbacks.PeriodicEvalCallback method), 27
on_train_epoch_end() (dicee.callbacks.PrintCallback method), 22
on_train_epoch_end() (dicee.models.base_model.BaseKGELightning method), 57
on_train_epoch_end() (dicee.models.BaseKGELightning method), 100
OnevsAllDataset (class in dicee), 202
OnevsAllDataset (class in dicee.dataset_classes), 33
OnevsSample (class in dicee), 204
OnevsSample (class in dicee.dataset_classes), 35
optim (dicee.config.Namespace attribute), 28
optimizer (dicee.trainer.torch_trainer_ddp.NodeTrainer attribute), 164
optimizer (dicee.trainer.torch_trainer.TorchTrainer attribute), 163
optimizer_name (dicee.BaseKGE attribute), 191
optimizer_name (dicee.models.base_model.BaseKGE attribute), 62
optimizer_name (dicee.models.BaseKGE attribute), 104, 108, 111, 116, 122, 134, 138
ordered_bpe_entities (dicee.BPE_NegativeSamplingDataset attribute), 201
ordered_bpe_entities (dicee.dataset_classes.BPE_NegativeSamplingDataset attribute), 31
ordered_bpe_entities (dicee.knowledge_graph.KG attribute), 50
ordered_shaped_bpe_tokens (dicee.knowledge_graph.KG attribute), 49
P
p (dicee.config.Namespace attribute), 29
p (dicee.DeCaL attribute), 174
p (dicee.Keci attribute), 171
p (dicee.models.clifford.DeCaL attribute), 68
p (dicee.models.clifford.Keci attribute), 65
p (dicee.models.DeCaL attribute), 131
p (dicee.models.Keci attribute), 127
padding (dicee.knowledge_graph.KG attribute), 50
pandas_dataframe_indexer() (in module dicee.read_preprocess_save_load_kg.util), 149
param_init (dicee.BaseKGE attribute), 191
```

```
param init (dicee.models.base model.BaseKGE attribute), 62
param_init (dicee.models.BaseKGE attribute), 105, 108, 112, 116, 122, 135, 138
parameters () (dicee.abstracts.BaseInteractiveKGE method), 15
parameters () (dicee.EnsembleKGE method), 192
parameters () (dicee.models.ensemble.EnsembleKGE method), 75
path (dicee.abstracts.AbstractPPECallback attribute), 17
path (dicee.callbacks.AccumulateEpochLossCallback attribute), 21
path (dicee.callbacks.ASWA attribute), 23
path (dicee.callbacks.Eval attribute), 25
path (dicee.callbacks.KGESaveCallback attribute), 22
path_dataset_folder (dicee.analyse_experiments.Experiment attribute), 19
path_for_deserialization (dicee.knowledge_graph.KG attribute), 49
path_for_serialization (dicee.knowledge_graph.KG attribute), 49
path_single_kg (dicee.config.Namespace attribute), 28
path_single_kg (dicee.knowledge_graph.KG attribute), 49
path_to_store_single_run (dicee.config.Namespace attribute), 27
PeriodicEvalCallback (class in dicee.callbacks), 26
Perturb (class in dicee.callbacks), 26
polars_dataframe_indexer() (in module dicee.read_preprocess_save_load_kg.util), 148
poly_NN() (dicee.LFMult method), 186
poly_NN() (dicee.models.function_space.LFMult method), 78
poly_NN() (dicee.models.LFMult method), 142
polynomial() (dicee.LFMult method), 187
polynomial() (dicee.models.function_space.LFMult method), 79
polynomial() (dicee.models.LFMult method), 142
pop () (dicee.LFMult method), 187
pop() (dicee.models.function_space.LFMult method), 79
pop () (dicee.models.LFMult method), 142
pq (dicee.analyse_experiments.Experiment attribute), 19
predict () (dicee.KGE method), 197
predict() (dicee.knowledge_graph_embeddings.KGE method), 52
predict dataloader() (dicee.models.base model.BaseKGELightning method), 59
predict_dataloader() (dicee.models.BaseKGELightning method), 101
predict_literals() (dicee.KGE method), 199
predict_literals() (dicee.knowledge_graph_embeddings.KGE method), 54
predict_missing_head_entity() (dicee.KGE method), 196
predict_missing_head_entity() (dicee.knowledge_graph_embeddings.KGE method), 51
predict_missing_relations() (dicee.KGE method), 197
\verb|predict_missing_relations()| \textit{(dicee.knowledge\_graph\_embeddings.KGE method)}, 51|
predict_missing_tail_entity() (dicee.KGE method), 197
\verb|predict_missing_tail_entity()| \textit{(dicee.knowledge\_graph\_embeddings.KGE method)}, 51
predict_topk() (dicee.KGE method), 197
predict_topk() (dicee.knowledge_graph_embeddings.KGE method), 52
prepare_data() (dicee.CVDataModule method), 211
prepare_data() (dicee.dataset_classes.CVDataModule method), 41
preprocess_with_byte_pair_encoding() (dicee.read_preprocess_save_load_kg.PreprocessKG method), 150
preprocess_with_byte_pair_encoding() (dicee.read_preprocess_save_load_kg.preprocess.PreprocessKG method), 145
preprocess_with_byte_pair_encoding_with_padding() (dicee.read_preprocess_save_load_kg.PreprocessKG method), 150
preprocess_with_byte_pair_encoding_with_padding() (dicee.read_preprocess_save_load_kg.preprocess.PreprocessKG method), 145
preprocess_with_pandas() (dicee.read_preprocess_save_load_kg.PreprocessKG method), 150
preprocess_with_pandas() (dicee.read_preprocess_save_load_kg.preprocess.PreprocessKG method), 145
preprocess_with_polars() (dicee.read_preprocess_save_load_kg.PreprocessKG method), 151
\verb|preprocess_save_load_kg.preprocess.Preprocess.Preprocess.Preprocess.Preprocess.Preprocess.Preprocess.Preprocess.Preprocess.Preprocess.Preprocess.Preprocess.Preprocess.Preprocess.Preprocess.Preprocess.Preprocess.Preprocess.Preprocess.Preprocess.Preprocess.Preprocess.Preprocess.Preprocess.Preprocess.Preprocess.Preprocess.Preprocess.Preprocess.Preprocess.Preprocess.Preprocess.Preprocess.Preprocess.Preprocess.Preprocess.Preprocess.Preprocess.Preprocess.Preprocess.Preprocess.Preprocess.Preprocess.Preprocess.Preprocess.Preprocess.Preprocess.Preprocess.Preprocess.Preprocess.Preprocess.Preprocess.Preprocess.Preprocess.Preprocess.Preprocess.Preprocess.Preprocess.Preprocess.Preprocess.Preprocess.Preprocess.Preprocess.Preprocess.Preprocess.Preprocess.Preprocess.Preprocess.Preprocess.Preprocess.Preprocess.Preprocess.Preprocess.Preprocess.Preprocess.Preprocess.Preprocess.Preprocess.Preprocess.Preprocess.Preprocess.Preprocess.Preprocess.Preprocess.Preprocess.Preprocess.Preprocess.Preprocess.Preprocess.Preprocess.Preprocess.Preprocess.Preprocess.Preprocess.Preprocess.Preprocess.Preprocess.Preprocess.Preprocess.Preprocess.Preprocess.Preprocess.Preprocess.Preprocess.Preprocess.Preprocess.Preprocess.Preprocess.Preprocess.Preprocess.Preprocess.Preprocess.Preprocess.Preprocess.Preprocess.Preprocess.Preprocess.Preprocess.Preprocess.Preprocess.Preprocess.Preprocess.Preprocess.Preprocess.Preprocess.Preprocess.Preprocess.Preprocess.Preprocess.Preprocess.Preprocess.Preprocess.Preprocess.Preprocess.Preprocess.Preprocess.Preprocess.Preprocess.Preprocess.Preprocess.Preprocess.Preprocess.Preprocess.Preprocess.Preprocess.Preprocess.Preprocess.Preprocess.Preprocess.Preprocess.Preprocess.Preprocess.Preprocess.Preprocess.Preprocess.Preprocess.Preprocess.Preprocess.Preprocess.Preprocess.Preprocess.Preprocess.Preprocess.Preprocess.Preprocess.Preprocess.Preprocess.Preprocess.Preprocess.Preprocess.Preprocess.Preprocess.Preprocess.Preprocess.Preprocess.Preprocess.Preprocess.Preprocess.Preprocess.Preprocess.Preprocess.Preprocess.Preprocess.Prepr
preprocesses_input_args() (in module dicee.static_preprocess_funcs), 159
PreprocessKG (class in dicee.read_preprocess_save_load_kg), 150
PreprocessKG (class in dicee.read_preprocess_save_load_kg.preprocess), 145
PrintCallback (class in dicee.callbacks), 21
process (dicee.trainer.torch_trainer.TorchTrainer attribute), 163
PseudoLabellingCallback (class in dicee.callbacks), 23
Pyke (class in dicee), 169
Pyke (class in dicee.models), 110
Pyke (class in dicee.models.real), 89
pykeen_model_kwargs (dicee.config.Namespace attribute), 29
PykeenKGE (class in dicee), 187
PykeenKGE (class in dicee.models), 136
PykeenKGE (class in dicee.models.pykeen_models), 84
```

```
Q
```

```
q (dicee.config.Namespace attribute), 29
q (dicee.DeCaL attribute), 174
q (dicee.Keci attribute), 171
q (dicee.models.clifford.DeCaL attribute), 68
q (dicee.models.clifford.Keci attribute), 65
q (dicee.models.DeCaL attribute), 131
q (dicee.models.Keci attribute), 127
qdrant_client (dicee.scripts.index_serve.NeuralSearcher attribute), 153
QMult (class in dicee), 183
QMult (class in dicee.models), 118
QMult (class in dicee.models.quaternion), 85
quaternion_mul() (in module dicee.models), 115
quaternion_mul() (in module dicee.models.static_funcs), 89
quaternion_mul_with_unit_norm() (in module dicee.models), 118
quaternion_mul_with_unit_norm() (in module dicee.models.quaternion), 85
quaternion_multiplication_followed_by_inner_product() (dicee.models.QMult method), 119
quaternion_multiplication_followed_by_inner_product() (dicee.models.quaternion.QMult method), 86
quaternion_multiplication_followed_by_inner_product() (dicee.QMult method), 183
quaternion_normalizer() (dicee.models.QMult static method), 119
quaternion normalizer() (dicee.models.quaternion.QMult static method), 86
quaternion_normalizer() (dicee.QMult static method), 184
queries (dicee.scripts.index_serve.StringListRequest attribute), 154
query_name_to_struct (dicee.query_generator.QueryGenerator attribute), 144
query_name_to_struct (dicee.QueryGenerator attribute), 214
QueryGenerator (class in dicee), 213
QueryGenerator (class in dicee.query_generator), 144
r (dicee.DeCaL attribute), 174
r (dicee, Keci attribute), 171
r (dicee.models.clifford.DeCaL attribute), 68
r (dicee.models.clifford.Keci attribute), 65
r (dicee.models.DeCaL attribute), 131
r (dicee.models.Keci attribute), 127
random_prediction() (in module dicee), 194
random_prediction() (in module dicee.static_funcs), 157
random_seed (dicee.config.Namespace attribute), 29
ratio (dicee.callbacks.Perturb attribute), 26
re (dicee.DeCaL attribute), 174
re (dicee.models.clifford.DeCaL attribute), 68
re (dicee.models.DeCaL attribute), 131
re_vocab (dicee.evaluator.Evaluator attribute), 45
read_from_disk() (in module dicee.read_preprocess_save_load_kg.util), 149
read_from_triple_store() (in module dicee.read_preprocess_save_load_kg.util), 149
read_only_few (dicee.config.Namespace attribute), 29
read_only_few (dicee.knowledge_graph.KG attribute), 49
read_or_load_kg() (in module dicee), 194
read_or_load_kg() (in module dicee.static_funcs), 157
read_with_pandas() (in module dicee.read_preprocess_save_load_kg.util), 149
read_with_polars() (in module dicee.read_preprocess_save_load_kg.util), 149
ReadFromDisk (class in dicee.read_preprocess_save_load_kg), 151
ReadFromDisk (class in dicee.read_preprocess_save_load_kg.read_from_disk), 146
reducer (dicee.scripts.index_serve.StringListRequest attribute), 154
rel2id (dicee.query_generator.QueryGenerator attribute), 144
rel2id (dicee.QueryGenerator attribute), 214
relation_embeddings (dicee.AConvQ attribute), 180
relation_embeddings (dicee.ConvQ attribute), 181
relation_embeddings (dicee.DeCaL attribute), 174
relation_embeddings (dicee.DualE attribute), 177
relation embeddings (dicee.LFMult attribute), 186
relation_embeddings (dicee.models.AConvQ attribute), 120
relation_embeddings (dicee.models.clifford.DeCaL attribute), 68
relation_embeddings (dicee.models.ConvQ attribute), 120
relation_embeddings (dicee.models.DeCaL attribute), 131
relation_embeddings (dicee.models.DualE attribute), 143
relation_embeddings (dicee.models.dualE.DualE attribute), 74
```

```
relation embeddings (dicee.models.FMult attribute), 139
relation_embeddings (dicee.models.FMult2 attribute), 141
relation_embeddings (dicee.models.function_space.FMult attribute), 76
relation_embeddings (dicee.models.function_space.FMult2 attribute), 77
relation_embeddings (dicee.models.function_space.GFMult attribute), 76
relation_embeddings (dicee.models.function_space.LFMult attribute), 78
relation_embeddings (dicee.models.function_space.LFMult1 attribute), 77
relation embeddings (dicee.models.GFMult attribute), 140
relation_embeddings (dicee.models.LFMult attribute), 141
relation_embeddings (dicee.models.LFMult1 attribute). 141
relation_embeddings (dicee.models.pykeen_models.PykeenKGE attribute), 84
{\tt relation\_embeddings}~(\textit{dicee.models.PykeenKGE attribute}),\,136
relation_embeddings (dicee.models.quaternion.AConvQ attribute), 87
relation_embeddings (dicee.models.quaternion.ConvQ attribute), 87
relation_embeddings (dicee.PykeenKGE attribute), 187
relation_to_idx (dicee.knowledge_graph.KG attribute), 49
\verb|relations_str| (\textit{dicee.knowledge\_graph.KG property}), 50
reload_dataset() (in module dicee), 201
reload_dataset() (in module dicee.dataset_classes), 31
report (dicee.DICE_Trainer attribute), 195
report (dicee.evaluator.Evaluator attribute), 46
report (dicee. Execute attribute), 200
report (dicee.executer.Execute attribute), 47
report (dicee.trainer.DICE_Trainer attribute), 165
report (dicee.trainer.dice_trainer.DICE_Trainer attribute), 160
reports (dicee.callbacks.Eval attribute), 25
reports (dicee.callbacks.PeriodicEvalCallback attribute), 27
requires_grad_for_interactions (dicee.CKeci attribute), 170
{\tt requires\_grad\_for\_interactions}~(\textit{dicee.Keci attribute}),~171
requires_grad_for_interactions (dicee.models.CKeci attribute), 130
requires_grad_for_interactions (dicee.models.clifford.CKeci attribute), 67
requires_grad_for_interactions (dicee.models.clifford.Keci attribute), 65
requires_grad_for_interactions (dicee.models.Keci attribute), 127
\verb|resid_dropout| \textit{(dicee.models.transformers.CausalSelfAttention attribute)}, 93
residual_convolution() (dicee.AConEx method), 179
residual_convolution() (dicee.AConvO method), 180
residual convolution() (dicee.AConvO method), 180
residual_convolution() (dicee.ConEx method), 182
residual_convolution() (dicee.ConvO method), 182
residual_convolution() (dicee.ConvQ method), 181
residual_convolution() (dicee.models.AConEx method), 114
residual_convolution() (dicee.models.AConvO method), 126
residual_convolution() (dicee.models.AConvQ method), 121
residual_convolution() (dicee.models.complex.AConEx method), 72
residual_convolution() (dicee.models.complex.ConEx method), 72
residual_convolution() (dicee.models.ConEx method), 113
residual_convolution() (dicee.models.ConvO method), 126
residual_convolution() (dicee.models.ConvQ method), 120
residual_convolution() (dicee.models.octonion.AConvO method), 83
residual_convolution() (dicee.models.octonion.ConvO method), 83
residual_convolution() (dicee.models.quaternion.AConvQ method), 88
residual_convolution() (dicee.models.quaternion.ConvQ method), 87
retrieve_embedding() (dicee.scripts.index_serve.NeuralSearcher method), 153
retrieve_embeddings() (in module dicee.scripts.index_serve), 153
return_multi_hop_query_results() (dicee.KGE method), 198
return_multi_hop_query_results() (dicee.knowledge_graph_embeddings.KGE method), 53
root() (in module dicee.scripts.index_serve), 153
roots (dicee.models.FMult attribute), 140
roots (dicee.models.function_space.FMult attribute), 76
roots (dicee.models.function_space.GFMult attribute), 76
roots (dicee.models.GFMult attribute), 140
runtime (dicee.analyse_experiments.Experiment attribute), 20
S
sample_counter (dicee.abstracts.AbstractPPECallback attribute), 17
sample_entity() (dicee.abstracts.BaseInteractiveKGE method), 15
sample\_relation() (dicee.abstracts.BaseInteractiveKGE method), 15
```

```
sample_triples_ratio (dicee.config.Namespace attribute), 29
sample_triples_ratio (dicee.knowledge_graph.KG attribute), 49
sampling_ratio (dicee.dataset_classes.LiteralDataset attribute), 42, 43
sampling_ratio (dicee.LiteralDataset attribute), 212, 213
sanity_checking_with_arguments() (in module dicee.sanity_checkers), 152
save() (dicee.abstracts.BaseInteractiveKGE method), 15
save() (dicee.read_preprocess_save_load_kg.LoadSaveToDisk method), 151
save() (dicee.read_preprocess_save_load_kg.save_load_disk.LoadSaveToDisk method), 147
save_checkpoint() (dicee.abstracts.AbstractTrainer static method), 13
save_checkpoint_model() (in module dicee), 193
save_checkpoint_model() (in module dicee.static_funcs), 157
save_embeddings() (in module dicee), 194
save_embeddings() (in module dicee.static_funcs), 157
save_embeddings_as_csv (dicee.config.Namespace attribute), 27
save_every_n_epochs (dicee.config.Namespace attribute), 30
save_experiment() (dicee.analyse_experiments.Experiment method), 20
save_model_at_every_epoch (dicee.config.Namespace attribute), 29
save_model_every_n_epoch (dicee.callbacks.PeriodicEvalCallback attribute), 27
save_numpy_ndarray() (in module dicee), 193
save_numpy_ndarray() (in module dicee.read_preprocess_save_load_kg.util), 150
save_numpy_ndarray() (in module dicee.static_funcs), 157
save_pickle() (in module dicee), 193
save_pickle() (in module dicee.read_preprocess_save_load_kg.util), 150
save_pickle() (in module dicee.static_funcs), 157
save_queries() (dicee.query_generator.QueryGenerator method), 145
save_queries() (dicee.QueryGenerator method), 214
{\tt save\_queries\_and\_answers()} \ (\textit{dicee.query\_generator.QueryGenerator static method}), 145
save_queries_and_answers() (dicee.QueryGenerator static method), 215
save_trained_model() (dicee.Execute method), 200
save_trained_model() (dicee.executer.Execute method), 47
scalar_batch_NN() (dicee.LFMult method), 186
scalar_batch_NN() (dicee.models.function_space.LFMult method), 78
scalar_batch_NN() (dicee.models.LFMult method), 142
scaler (dicee.callbacks.Perturb attribute), 26
scaler (dicee.trainer.torch_trainer_ddp.NodeTrainer attribute), 165
score () (dicee.ComplEx static method), 179
score () (dicee.DistMult method), 170
score () (dicee. Keci method), 173
score () (dicee.models.clifford.Keci method), 67
score () (dicee.models.ComplEx static method), 115
score() (dicee.models.complex.ComplEx static method), 73
score () (dicee.models.DistMult method), 110
score() (dicee.models.Keci method), 130
score () (dicee.models.octonion.OMult method), 82
score () (dicee.models.OMult method), 125
score() (dicee.models.QMult method), 119
score () (dicee.models.quaternion.QMult method), 86
score() (dicee.models.real.DistMult method), 88
score() (dicee.models.real.TransE method), 89
score () (dicee.models.TransE method), 110
score() (dicee.OMult method), 185
score() (dicee.QMult method), 184
score() (dicee. TransE method), 173
score_func (dicee.models.FMult2 attribute), 140
score_func (dicee.models.function_space.FMult2 attribute), 77
scoring_technique (dicee.analyse_experiments.Experiment attribute), 20
scoring_technique (dicee.config.Namespace attribute), 28
search() (dicee.scripts.index_serve.NeuralSearcher method), 153
search_embeddings() (in module dicee.scripts.index_serve), 153
search_embeddings_batch() (in module dicee.scripts.index_serve), 155
seed (dicee.query generator.QueryGenerator attribute), 144
seed (dicee.QueryGenerator attribute), 214
select_model() (in module dicee), 193
select_model() (in module dicee.static_funcs), 157
selected_optimizer (dicee.BaseKGE attribute), 191
selected_optimizer (dicee.models.base_model.BaseKGE attribute), 62
selected_optimizer (dicee.models.BaseKGE attribute), 105, 108, 111, 116, 122, 135, 138
separator (dicee.config.Namespace attribute), 28
```

```
separator (dicee.knowledge_graph.KG attribute), 50
sequential_vocabulary_construction() (dicee.read_preprocess_save_load_kg.PreprocessKG method), 151
sequential\_vocabulary\_construction () \ \textit{(dicee.read\_preprocess\_save\_load\_kg.preprocess.PreprocessKG method)}, 146
serve() (in module dicee.scripts.index_serve), 155
set_global_seed() (dicee.query_generator.QueryGenerator method), 144
set_global_seed() (dicee.QueryGenerator method), 214
set_model_eval_mode() (dicee.abstracts.BaseInteractiveKGE method), 14
set model train mode() (dicee.abstracts.BaseInteractiveKGE method), 14
setup() (dicee.CVDataModule method), 209
setup() (dicee.dataset_classes.CVDataModule method), 40
setup_executor() (dicee.Execute method), 200
setup_executor() (dicee.executer.Execute method), 47
Shallom (class in dicee), 185
Shallom (class in dicee.models), 110
Shallom (class in dicee.models.real), 89
shallom (dicee.models.real.Shallom attribute), 89
shallom (dicee.models.Shallom attribute), 110
shallom (dicee.Shallom attribute), 185
single_hop_query_answering() (dicee.KGE method), 198
\verb|single_hop_query_answering()| \textit{(dicee.knowledge\_graph\_embeddings.KGE method)}, 53
sparql_endpoint (dicee.config.Namespace attribute), 28
sparql_endpoint (dicee.knowledge_graph.KG attribute), 49
start() (dicee.DICE_Trainer method), 195
start () (dicee.Execute method), 200
start () (dicee.executer.Execute method), 48
start() (dicee.read_preprocess_save_load_kg.PreprocessKG method), 150
\verb|start()| (dicee.read\_preprocess\_save\_load\_kg.preprocess.PreprocessKG method), 145
start() (dicee.read_preprocess_save_load_kg.read_from_disk.ReadFromDisk method), 146
start() (dicee.read_preprocess_save_load_kg.ReadFromDisk method), 151
start () (dicee.trainer.DICE_Trainer method), 166
start () (dicee.trainer.dice_trainer.DICE_Trainer method), 161
start time (dicee.callbacks.PrintCallback attribute), 21
start_time (dicee.Execute attribute), 200
start_time (dicee.executer.Execute attribute), 47
step() (dicee.EnsembleKGE method), 193
step() (dicee.models.ADOPT method), 98
step() (dicee.models.adopt.ADOPT method), 55
step() (dicee.models.ensemble.EnsembleKGE method), 75
storage_path (dicee.config.Namespace attribute), 27
storage_path (dicee.DICE_Trainer attribute), 195
storage_path (dicee.trainer.DICE_Trainer attribute), 165
storage_path (dicee.trainer.dice_trainer.DICE_Trainer attribute), 161
store() (in module dicee), 193
store() (in module dicee.static_funcs), 157
store_ensemble() (dicee.abstracts.AbstractPPECallback method), 18
strategy (dicee.abstracts.AbstractTrainer attribute), 13
StringListRequest (class in dicee.scripts.index_serve), 153
swa (dicee.config.Namespace attribute), 30
T() (dicee.DualE method), 178
T() (dicee.models.DualE method), 143
T() (dicee.models.dualE.DualE method), 75
t\_conorm() (dicee.abstracts.InteractiveQueryDecomposition method), 16
t_norm() (dicee.abstracts.InteractiveQueryDecomposition method), 16
target_dim (dicee.AllvsAll attribute), 204
target\_dim(dicee.dataset\_classes.AllvsAll\ attribute), 35
target_dim(dicee.dataset_classes.MultiLabelDataset attribute), 32
target_dim (dicee.dataset_classes.OnevsAllDataset attribute), 33
target_dim (dicee.knowledge_graph.KG attribute), 50
target_dim (dicee.MultiLabelDataset attribute), 202
target_dim (dicee.OnevsAllDataset attribute), 203
temperature (dicee.BytE attribute), 188
temperature (dicee.models.transformers.BytE attribute), 91
tensor_t_norm() (dicee.abstracts.InteractiveQueryDecomposition method), 16
TensorParallel (class in dicee.trainer.model_parallelism), 162
\verb|test_dataloader()| \textit{ (dicee.models.base\_model.BaseKGELightning method)}, 57
```

```
test dataloader() (dicee.models.BaseKGELightning method), 100
test_epoch_end() (dicee.models.base_model.BaseKGELightning method), 57
test_epoch_end() (dicee.models.BaseKGELightning method), 100
test_h1 (dicee.analyse_experiments.Experiment attribute), 20
\verb|test_h3| (\textit{dicee.analyse\_experiments.Experiment attribute}), 20
test_h10 (dicee.analyse_experiments.Experiment attribute), 20
test_mrr (dicee.analyse_experiments.Experiment attribute), 20
test path (dicee.query generator.QueryGenerator attribute), 144
test_path (dicee.QueryGenerator attribute), 214
timeit() (in module dicee), 193, 201
timeit() (in module dicee.read_preprocess_save_load_kg.util), 149
timeit() (in module dicee.static_funcs), 157
timeit() (in module dicee.static_preprocess_funcs), 159
to() (dicee.EnsembleKGE method), 193
to() (dicee.KGE method), 196
to() (dicee.knowledge_graph_embeddings.KGE method), 50
to () (dicee.models.ensemble.EnsembleKGE method), 75
to_df() (dicee.analyse_experiments.Experiment method), 20
topk (dicee.BytE attribute), 188
topk (dicee.models.transformers.BytE attribute), 91
topk (dicee.scripts.index_serve.NeuralSearcher attribute), 153
{\tt torch\_ordered\_shaped\_bpe\_entities}~(\textit{dicee.dataset\_classes.MultiLabelDataset~attribute}), 32
torch_ordered_shaped_bpe_entities (dicee.MultiLabelDataset attribute), 202
TorchDDPTrainer (class in dicee.trainer.torch_trainer_ddp), 164
TorchTrainer (class in dicee.trainer.torch_trainer), 163
train() (dicee.abstracts.BaseInteractiveTrainKGE method), 18
train() (dicee.trainer.torch_trainer_ddp.NodeTrainer method), 165
train_data (dicee.AllvsAll attribute), 204
train_data (dicee.dataset_classes.AllvsAll attribute), 34
train_data (dicee.dataset_classes.KvsAll attribute), 34
train_data (dicee.dataset_classes.KvsSampleDataset attribute), 37
train data (dicee.dataset classes.MultiClassClassificationDataset attribute), 32
train_data (dicee.dataset_classes.OnevsAllDataset attribute), 33
train_data (dicee.dataset_classes.OnevsSample attribute), 35, 36
train_data (dicee.KvsAll attribute), 203
train_data (dicee.KvsSampleDataset attribute), 207
train data (dicee.MultiClassClassificationDataset attribute), 202
train_data (dicee.OnevsAllDataset attribute), 203
train_data (dicee.OnevsSample attribute), 205
train_dataloader() (dicee.CVDataModule method), 209
train_dataloader() (dicee.dataset_classes.CVDataModule method), 39
train_dataloader() (dicee.models.base_model.BaseKGELightning method), 59
train_dataloader() (dicee.models.BaseKGELightning method), 102
train_dataloaders (dicee.trainer.torch_trainer.TorchTrainer attribute), 163
train_dataset_loader (dicee.trainer.torch_trainer_ddp.NodeTrainer attribute), 165
train_file_path (dicee.dataset_classes.LiteralDataset attribute), 42, 43
train_file_path (dicee.LiteralDataset attribute), 212, 213
train_h1 (dicee.analyse_experiments.Experiment attribute), 19
train_h3 (dicee.analyse_experiments.Experiment attribute), 19
train_h10 (dicee.analyse_experiments.Experiment attribute), 19
train_indices_target (dicee.dataset_classes.MultiLabelDataset attribute), 32
train_indices_target (dicee.MultiLabelDataset attribute), 202
train_k_vs_all() (dicee.abstracts.BaseInteractiveTrainKGE method), 18
train_literals() (dicee.abstracts.BaseInteractiveTrainKGE method), 18
train_mode (dicee.EnsembleKGE attribute), 192
train_mode (dicee.models.ensemble.EnsembleKGE attribute), 75
train_mrr (dicee.analyse_experiments.Experiment attribute), 19
train_path (dicee.query_generator.QueryGenerator attribute), 144
train_path (dicee.QueryGenerator attribute), 214
train_set (dicee.BPE_NegativeSamplingDataset attribute), 201
train set (dicee.dataset classes.BPE NegativeSamplingDataset attribute), 31
train_set (dicee.dataset_classes.MultiLabelDataset attribute), 32
train_set (dicee.dataset_classes.NegSampleDataset attribute), 37
train_set (dicee.dataset_classes.TriplePredictionDataset attribute), 38
train_set (dicee.MultiLabelDataset attribute), 202
train_set (dicee.NegSampleDataset attribute), 207
train_set (dicee. TriplePredictionDataset attribute), 208
train_set_idx (dicee.CVDataModule attribute), 209
```

```
train set idx (dicee.dataset classes.CVDataModule attribute), 39
train_set_target (dicee.knowledge_graph.KG attribute), 50
train target (dicee. Allvs All attribute), 204
train_target (dicee.dataset_classes.AllvsAll attribute), 34
train_target (dicee.dataset_classes.KvsAll attribute), 34
train_target (dicee.dataset_classes.KvsSampleDataset attribute), 37
train_target (dicee.KvsAll attribute), 204
train target (dicee.KvsSampleDataset attribute), 207
train_target_indices (dicee.knowledge_graph.KG attribute), 50
train_triples() (dicee.abstracts.BaseInteractiveTrainKGE method), 18
trained_model (dicee.Execute attribute), 200
trained_model (dicee.executer.Execute attribute), 47
trainer (dicee.config.Namespace attribute), 28
trainer (dicee.DICE_Trainer attribute), 195
trainer (dicee. Execute attribute), 200
trainer (dicee.executer.Execute attribute), 47
trainer (dicee.trainer.DICE_Trainer attribute), 165
trainer (dicee.trainer.dice_trainer.DICE_Trainer attribute), 160
trainer (dicee.trainer.torch_trainer_ddp.NodeTrainer attribute), 164
training_step (dicee.trainer.torch_trainer.TorchTrainer attribute), 163
training_step() (dicee.BytE method), 189
training_step() (dicee.models.base_model.BaseKGELightning method), 56
training_step() (dicee.models.BaseKGELightning method), 99
training_step() (dicee.models.transformers.BytE method), 91
training_step_outputs (dicee.models.base_model.BaseKGELightning attribute), 56
training_step_outputs (dicee.models.BaseKGELightning attribute), 99
training_technique (dicee.knowledge_graph.KG attribute), 49
TransE (class in dicee), 173
TransE (class in dicee.models), 110
TransE (class in dicee.models.real), 88
transfer_batch_to_device() (dicee.CVDataModule method), 210
transfer_batch_to_device() (dicee.dataset_classes.CVDataModule method), 40
transformer (dicee. BytE attribute), 188
{\tt transformer} \ (\textit{dicee.models.transformers.BytE attribute}), 91
transformer (dicee.models.transformers.GPT attribute), 96
trapezoid() (dicee.models.FMult2 method), 141
trapezoid() (dicee.models.function space.FMult2 method), 77
tri_score() (dicee.LFMult method), 186
\verb|tri_score()| (\textit{dicee.models.function\_space.LFMult method}), 78
tri_score() (dicee.models.function_space.LFMult1 method), 78
tri_score() (dicee.models.LFMult method), 142
tri_score() (dicee.models.LFMult1 method), 141
triple_score() (dicee.KGE method), 198
\verb|triple_score|()| (\textit{dicee.knowledge\_graph\_embeddings.KGE method}), 52
TriplePredictionDataset (class in dicee), 207
TriplePredictionDataset (class in dicee.dataset_classes), 38
tuple2list() (dicee.query_generator.QueryGenerator method), 144
tuple2list() (dicee.QueryGenerator method), 214
U
unlabelled_size (dicee.callbacks.PseudoLabellingCallback attribute), 23
unmap() (dicee.query_generator.QueryGenerator method), 144
unmap () (dicee. Query Generator method), 214
unmap_query() (dicee.query_generator.QueryGenerator method), 144
unmap_query() (dicee.QueryGenerator method), 214
V
val_aswa (dicee.callbacks.ASWA attribute), 24
val_dataloader() (dicee.models.base_model.BaseKGELightning method), 58
val_dataloader() (dicee.models.BaseKGELightning method), 101
val_h1 (dicee.analyse_experiments.Experiment attribute), 20
val_h3 (dicee.analyse_experiments.Experiment attribute), 20
val_h10 (dicee.analyse_experiments.Experiment attribute), 20
val_mrr (dicee.analyse_experiments.Experiment attribute), 19
val_path (dicee.query_generator.QueryGenerator attribute), 144
val_path (dicee.QueryGenerator attribute), 214
validate_knowledge_graph() (in module dicee.sanity_checkers), 152
```

```
vocab_preparation() (dicee.evaluator.Evaluator method), 46
vocab_size (dicee.models.transformers.GPTConfig attribute), 95
vocab_to_parquet() (in module dicee), 194
vocab_to_parquet() (in module dicee.static_funcs), 158
vtp_score() (dicee.LFMult method), 186
vtp_score() (dicee.models.function_space.LFMult method), 78
vtp_score() (dicee.models.function_space.LFMult1 method), 78
vtp_score() (dicee.models.LFMult method), 142
vtp_score() (dicee.models.LFMult1 method), 141
W
weight (dicee.models.transformers.LayerNorm attribute), 92
weight_decay (dicee.BaseKGE attribute), 191
weight_decay (dicee.config.Namespace attribute), 28
weight_decay (dicee.models.base_model.BaseKGE attribute), 62
weight_decay (dicee.models.BaseKGE attribute), 105, 108, 111, 116, 122, 135, 138
weights (dicee.models.FMult attribute), 140
weights (dicee.models.function_space.FMult attribute), 76
weights (dicee.models.function_space.GFMult attribute), 77
weights (dicee.models.GFMult attribute), 140
write_csv_from_model_parallel() (in module dicee), 194
write_csv_from_model_parallel() (in module dicee.static_funcs), 158
write_links() (dicee.query_generator.QueryGenerator method), 144
write_links() (dicee.QueryGenerator method), 214
write_report() (dicee.Execute method), 200
write_report() (dicee.executer.Execute method), 48
X
x_values (dicee.LFMult attribute), 186
x_values (dicee.models.function_space.LFMult attribute), 78
```

x_values (dicee.models.LFMult attribute), 141