# **DICE Embeddings**

Release 0.1.3.2

# **Caglar Demir**

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# **Contents:**

1	Dicee Manual	2
2	Installation       2.1 Installation from Source	<b>3</b> 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	<b>Answering Complex Queries</b>	6
8	Predicting Missing Links	8
9	<b>Downloading Pretrained Models</b>	8
10	How to Deploy	8
11	Docker	8
12	Coverage Report	8
13	How to cite	10
	dicee  14.1 Submodules  14.2 Attributes  14.3 Classes  14.4 Functions  14.5 Package Contents	12 12 165 165 166 168
Py	thon Module Index	212

Index 213

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

# 1 Dicee Manual

Version: dicee 0.1.3.2

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

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

Contact: caglar.demir@upb.de

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

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

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

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

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

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

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

- <sup>1</sup> https://github.com/dice-group/dice-embeddings
- <sup>2</sup> https://github.com/Demirrr
- 3 https://pandas.pydata.org/
- 4 https://pytorch.org/
- <sup>5</sup> https://huggingface.co/
- 6 https://pandas.pydata.org/
- <sup>7</sup> https://pytorch.org/
- 8 https://pytorch.org/
- 9 https://www.pytorchlightning.ai/
- 10 https://huggingface.co/gradio

# 2 Installation

### 2.1 Installation from Source

```
git clone https://github.com/dice-group/dice-embeddings.git conda create -n dice python=3.10.13 --no-default-packages && conda activate dice &&_ 
cd dice-embeddings && 
pip3 install -e .
```

or

```
pip install dicee
```

# 3 Download Knowledge Graphs

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

→certificate && unzip KGs.zip
```

#### To test the Installation

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

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

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

# 4 Knowledge Graph Embedding Models

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

# 5 How to Train

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

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

where the data is in the following form

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

A KGE model can also be trained from the command line

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

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

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

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

--"train_val_test"

# Train a model by only using GPU-1

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

--"train_val_test"

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

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

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

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

Similarly, models can be easily trained with torchrun

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

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

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

→9753123402351737}

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

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

→'MRR': 0.8072499937521418}

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

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

→'MRR': 0.8064032293278861}
```

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

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

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

--KGS/UMLS

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

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

--KGS/UMLS
```

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

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

where the data is in the following form

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

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

For more, please refer to examples.

# 6 Creating an Embedding Vector Database

# 6.1 Learning Embeddings

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

# 6.2 Loading Embeddings into Qdrant Vector Database

# 6.3 Launching Webservice

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

→location "localhost"
```

#### **Retrieve and Search**

Get embedding of germany

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

Get most similar things to europe

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

# 7 Answering Complex Queries

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

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

For more, please refer to examples/multi\_hop\_query\_answering.

# **8 Predicting Missing Links**

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

# 9 Downloading Pretrained Models

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

For more please look at dice-research.org/projects/DiceEmbeddings/<sup>11</sup>

# 10 How to Deploy

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

# 11 Docker

To build the Docker image:

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

To test the Docker image:

```
docker run --rm -v ~/.local/share/dicee/KGs:/dicee/KGs dice-embeddings ./main.py --
→model AConEx --embedding_dim 16
```

# 12 Coverage Report

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

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

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

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

```
→123, 146-147, 152, 165, 197, 240-254, 257-260, 263-266, 301, 314-317, 320-324, 364-
\Rightarrow375, 390-398, 413, 424-428, 555-575, 581-585, 589-591
dicee/callbacks.py
                                                           245
                                                                  102
\hookrightarrow67-73, 76, 88-93, 98-103, 106-109, 116-133, 138-142, 146-147, 276-280, 286-287, 305-
→311, 314, 319-320, 332-338, 344-353, 358-360, 405, 416-429, 433-468, 480-486
dicee/config.py
                                                            93
                                                                    2
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                                                                                141-142
dicee/dataset_classes.py
                                                           299
                                                                   74
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                                                                                41, 54, ...
→87, 93, 99-106, 109, 112, 115-139, 195-201, 204, 207-209, 314, 325-328, 344, 410-

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

dicee/eval_static_funcs.py
                                                           227
                                                                   95
                                                                         58%
                                                                                101, 106,
→ 111, 258-353, 360-411
dicee/evaluator.py
                                                           262
                                                                   51
                                                                         81%
                                                                                46, 51,_
→56, 84, 89-90, 93, 109, 126, 137, 141, 146, 177-188, 195-206, 314, 344-367, 455, □
→465, 482-487
dicee/executer.py
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                                                           113
⇒259, 291
dicee/knowledge_graph.py
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                                                                                79, 110, _
⇔114
dicee/knowledge_graph_embeddings.py
                                                           636
                                                                  443
                                                                         30%
                                                                                27, 30-
→31, 39-52, 57-90, 93-127, 131-139, 170-184, 215-228, 254-274, 324-327, 330-333, 346,
→ 381-426, 484-486, 502-503, 509-517, 522-525, 528-533, 538, 547, 592-598, 630, 688-
→1053, 1084-1145, 1149-1177, 1200, 1227-1265
dicee/models/__init__.py
                                                             9
                                                                        100%
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                                                                   31
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dicee/models/base_model.py
                                                                                54, 56, ...
→82, 88-103, 157, 190, 230, 236, 245, 248, 252, 259, 263, 265, 280, 288-289, 296-297,
→ 351, 354, 427, 439
dicee/models/clifford.py
                                                                  357
→68-117, 122-133, 156-168, 190-220, 235, 237, 241, 248-249, 276-280, 303-311, 325-
→327, 332-333, 364-384, 406, 413, 417-478, 495-499, 511, 514, 519, 524, 571-607, 625-
→631, 644, 647, 652, 657, 686-692, 705, 708, 713, 718, 728-737, 753-754, 774-845, □
→856-859, 884-909, 933-966, 1002-1006, 1019, 1029, 1032, 1037, 1042, 1047, 1051, □
→1055, 1064-1065, 1095, 1102, 1107, 1135-1139, 1167-1176, 1186-1194, 1212-1214, 1232-
→1234, 1250-1252
dicee/models/complex.py
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dicee/models/dualE.py
                                                            59
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→142-156
                                                           262
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dicee/models/function_space.py
                                                                         16%
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\Rightarrow28-37, 40-49, 53-70, 77-86, 89-98, 101-110, 114-126, 134-156, 159-165, 168-185, 188-
→194, 197-205, 208, 213-234, 243-246, 250-254, 258-267, 271-292, 301-307, 311-328, □
→332-335, 344-352, 355, 366-372, 392-406, 424-438, 443-453, 461-465, 474-478
                                                           227
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                                                                         63%
dicee/models/octonion.py
                                                                                21-44,_
\Rightarrow320-329, 334-345, 348-370, 374-416, 426-474
dicee/models/pykeen_models.py
                                                            50
                                                                    5
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dicee/models/quaternion.py
                                                                                7-21, 30-
                                                           192
                                                                   69
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→55, 68-72, 107, 185, 328-342, 345-364, 368-389, 399-426
dicee/models/real.py
                                                            61
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\leftrightarrow 66-69, 87, 103-106
dicee/models/static_funcs.py
                                                            10
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dicee/models/transformers.py
                                                           236
                                                                  189
→46, 60-75, 84-102, 105-116, 123-125, 128, 134-151, 155-180, 186-190, 193-197, 203-
→207, 210-212, 229-256, 265-268, 271-276, 279-304, 310-315, 319-372, 376-398, 404-414
```

```
dicee/query_generator.py
                                                              374
                                                                      346
                                                                               7%
                                                                                    18-52,_
\hookrightarrow56, 62-65, 69-70, 78-92, 100-147, 155-188, 192-206, 212-269, 274-303, 307-443, 453-
\hookrightarrow472, 480-501, 508-512, 517, 522-528
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dicee/read_preprocess_save_load_kg/__init__.py
dicee/read_preprocess_save_load_kg/preprocess.py
                                                              256
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\hookrightarrow78, 102-127, 133, 138-151, 184, 214, 388-389, 444
dicee/read_preprocess_save_load_kg/read_from_disk.py
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\hookrightarrow40, 47, 55, 58-72
dicee/read_preprocess_save_load_kg/save_load_disk.py
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dicee/read_preprocess_save_load_kg/util.py
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                                                                      126
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→72-73, 91-97, 100-102, 107-109, 121, 134, 140-143, 148-156, 161-167, 172-177, 182-
→187, 199-220, 226-282, 286-290, 294-295, 299, 303-304, 334, 351, 356, 363-364
                                                                       23
                                                                             57%
dicee/sanity_checkers.py
                                                               54
                                                                                    8-12, 21-
\rightarrow31, 46, 51, 58, 64-79, 85, 89, 96
dicee/static_funcs.py
                                                                      163
                                                                             61%
                                                                                    40, 50, ...
                                                              418
→56-61, 83, 105-106, 115, 138, 152, 157-159, 163-165, 167, 194-198, 246, 254, 263-
→268, 290-304, 316-336, 340-357, 362, 386-387, 392-393, 410-411, 413-414, 416-417, □
→419-420, 428, 446-450, 467-470, 474-479, 483-487, 491-492, 498-500, 526-527, 539-
\hookrightarrow 542, 547-550, 559-610, 615-627, 644-658, 661-669
dicee/static_funcs_training.py
                                                              123
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⇔223-224
dicee/static_preprocess_funcs.py
                                                              100
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\hookrightarrow 52, 56, 64, 67, 78, 91-115, 120-123, 128-131, 136-139
dicee/trainer/__init__.py
                                                                        0
                                                                            100%
                                                                1
dicee/trainer/dice_trainer.py
                                                              126
                                                                       13
                                                                             90%
                                                                                    27-32, _
\hookrightarrow 91, 98, 103-108, 147
dicee/trainer/torch_trainer.py
                                                               79
                                                                              95%
                                                                                    31, 196, _
→207-208
dicee/trainer/torch_trainer_ddp.py
                                                              152
                                                                      128
                                                                             16%
                                                                                    13-14,_
→43, 47-72, 83-112, 131-137, 140-149, 164-194, 204-217, 226-246, 251-260, 263-272, □
⇒275-299, 302-309
TOTAL
                                                             6181
                                                                     2828
                                                                             54%
```

# 13 How to cite

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

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

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

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

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

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

# 14 dicee

## 14.1 Submodules

dicee.\_\_main\_\_

dicee.abstracts

### **Classes**

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

# **Module Contents**

class dicee.abstracts.AbstractTrainer(args, callbacks)

Abstract class for Trainer class for knowledge graph embedding models

### **Parameter**

```
args
    [str]?

callbacks: list
    ?

attributes

callbacks

is_global_zero = True
global_rank = 0

local_rank = 0

strategy = None
```

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

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

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

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

Call at the end of the training.

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

# dicee.analyse\_experiments

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

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

### **Classes**

```
Experiment
```

## **Functions**

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

## **Module Contents**

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

```
val_h10 = []

test_mrr = []

test_h1 = []

test_h3 = []

test_h10 = []

runtime = []

normalization = []

scoring_technique = []

save_experiment(x)

to_df()

dicee.analyse_experiments.analyse(args)
```

## dicee.callbacks

# **Classes**

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

### **Functions**

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

# **Module Contents**

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

Abstract class for Callback class for knowledge graph embedding models

```
Parameter
```

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

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

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

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

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

Abstract class for Callback class for knowledge graph embedding models

#### **Parameter**

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

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

Parameter Perturbation:

```
Output Perturbation:

level = 'input'

ratio = 0.0

method = None

scaler = None

frequency = None

on_train_batch_start (trainer, model, batch, batch_idx)

Called when the train batch begins.
```

# dicee.config

# **Classes**

Namespace

Simple object for storing attributes.

### **Module Contents**

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

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

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

dicee.dataset\_classes

#### **Classes**

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

#### **Functions**

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

#### **Module Contents**

Reload the files from disk to construct the Pytorch dataset

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

→ torch.utils.data.Dataset

Bases: torch.utils.data.Dataset

An abstract class representing a Dataset.

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



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

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

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

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

## **1** Note

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

```
• entity_idxs - mapping.
```

- relation\_idxs mapping.
- form ?
- num\_workers int for https://pytorch.org/docs/stable/data.html#torch.utils.data.

  DataLoader

#### Return type

torch.utils.data.Dataset

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

class dicee.dataset\_classes.OnevsAllDataset(train\_set\_idx: numpy.ndarray, entity\_idxs)

Bases: torch.utils.data.Dataset

Dataset for the 1vsALL training strategy

#### **Parameters**

- train\_set\_idx Indexed triples for the training.
- entity\_idxs mapping.
- relation\_idxs mapping.
- form ?
- num\_workers int for https://pytorch.org/docs/stable/data.html#torch.utils.data.
   DataLoader

## Return type

torch.utils.data.Dataset

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

Bases: torch.utils.data.Dataset

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

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



**TODO** 

### train\_set\_idx

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

### entity\_idxs

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

#### relation idxs

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

self: torch.utils.data.Dataset

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

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

class dicee.dataset\_classes.AllvsAll(train\_set\_idx: numpy.ndarray, entity\_idxs, relation\_idxs, label smoothing rate=0.0)

Bases: torch.utils.data.Dataset

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

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

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



1 Note

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

only with 0s.

# train\_set\_idx

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

# entity idxs

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

#### relation idxs

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

self: torch.utils.data.Dataset

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

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

class dicee.dataset\_classes.OnevsSample ( $train\_set$ : numpy.ndarray,  $num\_entities$ ,  $num\_relations$ , neg sample ratio: int = None, label smoothing rate: <math>float = 0.0)

Bases: torch.utils.data.Dataset

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

#### **Parameters**

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

# train\_data

The input data converted into a PyTorch tensor.

```
Type torch. Tensor
```

#### num entities

Number of entities in the dataset.

```
Type int
```

### num\_relations

Number of relations in the dataset.

```
Type int
```

```
neg_sample_ratio
```

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

```
Type int
```

### label\_smoothing\_rate

The smoothing factor applied to the labels.

### **Type**

torch.Tensor

# collate\_fn

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

### **Type**

function, optional

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

Returns the number of samples in the dataset.

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

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

#### **Parameters**

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

# Returns

# A tuple consisting of:

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

# Return type

tuple

 $\begin{tabular}{ll} {\tt classe} & \tt dicee.dataset\_classes. {\tt KvsSampleDataset} ({\it train\_set\_idx: numpy.ndarray, entity\_idxs, relation\_idxs, form, store=None, neg\_ratio=None, label\_smoothing\_rate: float = 0.0) \end{tabular}$ 

Bases: torch.utils.data.Dataset

# **KvsSample a Dataset:**

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

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

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

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



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

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

- num\_relations relation to index mapping.
- batch\_size int
- form ?
- num\_workers int for https://pytorch.org/docs/stable/data.html#torch.utils.data.
   DataLoader

# Return type

?

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

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

An iterable or collection of iterables specifying training samples.

For more information about multiple dataloaders, see this section.

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

For data processing use the following pattern:

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

However, the above are only necessary for distributed processing.

# **A** Warning

do not assign state in prepare\_data

• fit()

- prepare\_data()
- setup()

# 1 Note

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

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

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

#### **Parameters**

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

Example:

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

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

# don't do this
        self.something = else

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

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

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

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

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

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

# **1** Note

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

#### **Parameters**

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

#### Returns

A reference to the data on the new device.

# Example:

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

# See also

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

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

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

# **▲** Warning

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

#### Example:

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

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

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

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

# Example:

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

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

This is called before requesting the dataloaders:

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

# dicee.eval\_static\_funcs

# **Functions**

```
evaluate_link_prediction_performance(→
Dict)
evaluate_link_prediction_performance_with_.

evaluate_link_prediction_performance_with_i

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

## **Module Contents**

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

# **Parameters**

• model

- triples
- er\_vocab
- re\_vocab

#### **Parameters**

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

## dicee.evaluator

# Classes

Evaluator Evaluator Class to evaluate KGE models in various downstream tasks

# **Module Contents**

class dicee.evaluator.Evaluator(args, is\_continual\_training=None)

Evaluator class to evaluate KGE models in various downstream tasks

Arguments

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

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

## dicee.executer

# **Classes**

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

# **Module Contents**

class dicee.executer.Execute(args, continuous\_training=False)

A class for Training, Retraining and Evaluation a model.

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

```
args
```

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

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

Save a knowledge graph embedding model

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

#### **Parameter**

# rtype

None

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

End training

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

## **Parameter**

#### rtype

A dict containing information about the training and/or evaluation

# $write\_report() \rightarrow None$

Report training related information in a report.json file

 $start() \rightarrow dict$ 

Start training

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

#### **Parameter**

#### rtype

A dict containing information about the training and/or evaluation

class dicee.executer.ContinuousExecute(args)

Bases: Execute

A subclass of Execute Class for retraining

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

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

 ${\tt continual\_start}\,()\,\to dict$ 

Start Continual Training

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

# **Parameter**

### rtype

A dict containing information about the training and/or evaluation

# dicee.knowledge\_graph

# **Classes**

KG Knowledge Graph

# **Module Contents**

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

```
target_dim = None

train_target_indices = None

ordered_bpe_entities = None

separator = None

description_of_input = None

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**

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

# **Parameter**

relation: Union[List[str], str]

String representation of selected relations.

tail\_entity: Union[List[str], str]

String representation of selected entities.

k: int

Highest ranked k entities.

# **Returns: Tuple**

Highest K scores and entities

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

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

#### **Parameter**

head\_entity: List[str]

String representation of selected entities.

tail\_entity: List[str]

String representation of selected entities.

k: int

Highest ranked k entities.

# **Returns: Tuple**

Highest K scores and entities

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

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

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

## **Parameter**

head\_entity: List[str]

String representation of selected entities.

tail\_entity: List[str]

String representation of selected entities.

# **Returns: Tuple**

```
scores
```

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

#### **Parameters**

- logits
- h
- r
- t
- within

Predict missing item in a given triple.

# **Parameter**

head\_entity: Union[str, List[str]]

String representation of selected entities.

relation: Union[str, List[str]]

String representation of selected relations.

tail\_entity: Union[str, List[str]]

String representation of selected entities.

k: int

Highest ranked k item.

# **Returns: Tuple**

Highest K scores and items

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

Predict triple score

#### **Parameter**

head\_entity: List[str]

String representation of selected entities.

relation: List[str]

String representation of selected relations.

tail\_entity: List[str]

String representation of selected entities.

logits: bool

If logits is True, unnormalized score returned

# **Returns: Tuple**

```
pytorch tensor of triple score
```

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

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

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

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

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

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

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

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

→ List[Tuple[str, torch.Tensor]]
```

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

Find an answer set for EPFO queries including negation and disjunction

# **Parameter**

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

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

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

tnorm: str The t-norm operator.

neg\_norm: str The negation norm.

lambda\_: float lambda parameter for sugeno and yager negation norms

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

#### returns

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

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

Find missing triples

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

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

Return (e,r,x)

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

```
confidence: float
          A threshold for an output of a sigmoid function given a triple.
          topk: int
          Highest ranked k item to select triples with f(e,r,x) > \text{confidence}.
          at most: int
          Stop after finding at most missing triples
           \{(e,r,x) \mid f(e,r,x) > \text{confidence land } (e,r,x)\}
      otin G
deploy(share: bool = False, top\_k: int = 10)
train_triples (h: List[str], r: List[str], t: List[str], labels: List[float], iteration=2, optimizer=None)
train_k_vs_all(h, r, iteration=1, lr=0.001)
      Train k vs all :param head_entity: :param relation: :param iteration: :param lr: :return:
train(kg, kr=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,
              eval\_litreal\_preds: bool = True, eval\_file\_path: str = None,
```

random\_seed=1)
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.
- eval\_litreal\_preds (bool) If True, evaluate the model after training.

lit normalization type: str = 'z-norm', batch size: int = 1024, sampling ratio: float = None,

- eval\_file\_path (str) Path to evaluation data file.
- 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.

```
\label{eq:predict_literals} \begin{array}{l} \textit{Predict_literals} \; (\textit{entity: List[str]} \; | \; \textit{str} = \textit{None}, \; \textit{attribute: List[str]} \; | \; \textit{str} = \textit{None}, \\ & \textit{denormalize\_preds: bool} = \textit{True}) \; \rightarrow \; \textit{torch.FloatTensor} \end{array}
```

Predicts literal values for given entities and attributes.

# **Parameters**

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

# Returns

Predictions for the given entities and attributes.

# Return type

torch.FloatTensor

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.

#### Returns

None

# dicee.literal\_classes

## **Classes**

GatedLinearUnit	Applies a gated linear unit (GLU) operation:
LiteralEmbeddings	A model for learning and predicting numerical literals using pre-trained KGE.
LiteralDataset	Dataset for loading and processing literal data for training Literal Embedding model.

# **Module Contents**

```
class dicee.literal_classes.GatedLinearUnit (input_dim, gated_residual=True)
```

Bases: torch.nn.Module

Applies a gated linear unit (GLU) operation: Splits the input in half along the last dimension, applies a sigmoid gate to one half and multiplies it with the other.

```
proj
```

```
gate_residual = True
```

forward (x1, x2)

class dicee.literal\_classes.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.
             torch.tensor
dropout
     Dropout rate for regularization.
         Type
             float
gate_residual
     Whether to use gated residual connections.
             bool
freeze_entity_embeddings
     Whether to freeze the entity embeddings during training.
             bool
embedding_dim
num_of_data_properties
hidden_dim
entity_embeddings
data_property_embeddings
fc
fc_out
dropout
residual
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

```
class dicee.literal_classes.LiteralDataset (file_path: str, ent_idx: dict = None,
            normalization_type: str = 'z-norm', sampling_ratio: float = None)
     Bases: torch.utils.data.Dataset
     Dataset for loading and processing literal data for training Literal Embedding model. This dataset handles the
     loading, normalization, and preparation of triples for training a literal embedding model.
     Extends torch.utils.data.Dataset for supporting PyTorch dataloaders.
     train_file_path
           Path to the training data file.
               Type
                   str
     normalization
           Type of normalization to apply ('z-norm', 'min-max', or None).
                   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
     train_file_path
     normalization_type = 'z-norm'
```

```
normalization_params
sampling_ratio = None
entity_to_idx = None
num_entities
__getitem__(index)
__len__()
```

 $static load_and_validate_literal_data(file_path: str = None) \rightarrow pandas.DataFrame$ 

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

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

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.models

**Submodules** 

dicee.models.adopt

#### **Classes**

ADOPT

Base class for all optimizers.

# **Functions**

#### **Module Contents**

```
class dicee.models.adopt.ADOPT (params: torch.optim.optimizer.ParamsT,

lr: float | torch.Tensor = 0.001, betas: Tuple[float, float] = (0.9, 0.9999), eps: float = 1e-06,

clip_lambda: Callable[[int], float] | None = lambda step: ..., weight_decay: float = 0.0,

decouple: bool = False, *, foreach: bool | None = None, maximize: bool = False,

capturable: bool = False, differentiable: bool = False, fused: bool | None = None)
```

Bases: torch.optim.optimizer.Optimizer

Base class for all optimizers.



## Warning

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

#### **Parameters**

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

```
clip_lambda
```

```
__setstate__(state)
```

step(closure=None)

Perform a single optimization step.

#### **Parameters**

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

```
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)

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

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



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

#### Variables

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

```
\label{eq:training_step_outputs} \begin{tabular}{ll} training_step_outputs = [] \\ \\ mem_of_model() \rightarrow Dict \\ \end{tabular}
```

Size of model in MB and number of params

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

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

#### **Parameters**

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

#### **Returns**

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

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

Example:

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

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

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

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

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

# **1** Note

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

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

## **Parameters**

- yhat\_batch
- y\_batch

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

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

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

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

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

def on_train_epoch_end(self):
```

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

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

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

An iterable or collection of iterables specifying test samples.

For more information about multiple dataloaders, see this section.

For data processing use the following pattern:

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

However, the above are only necessary for distributed processing.

# Warning

do not assign state in prepare\_data

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

## 1 Note

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

# 1 Note

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

# $val\_dataloader() \rightarrow None$

An iterable or collection of iterables specifying validation samples.

For more information about multiple dataloaders, see this section.

dataloader will be reloaded unless you :paramref: "~lightning.pytorch.trainer.trainer.Trainer.reload\_dataloaders\_every\_n\_epochs" to a positive integer.

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

- fit()
- validate()

- prepare\_data()
- setup()

# **1** Note

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

# 1 Note

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

### $predict_dataloader() \rightarrow None$

An iterable or collection of iterables specifying prediction samples.

For more information about multiple dataloaders, see this section.

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

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

# 1 Note

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

## Returns

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

# $\texttt{train\_dataloader}() \rightarrow None$

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

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

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

Base class for all neural network modules.

Your models should also subclass this class.

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

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

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

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

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

# **1** Note

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

## Variables

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

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

## dicee.models.clifford

## **Classes**

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

## **Module Contents**

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

Base class for all neural network modules.

Your models should also subclass this class.

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

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

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

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

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

# 1 Note

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

### **Variables**

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

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

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

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

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

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

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

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

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

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

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

```
results = [] for j in range(q - 1):
                             for k in range(j + 1, q):
                                  results.append(hq[:, :, j] * rq[:, :, k] - hq[:, :, k] * rq[:, :, j])
                    sigma_q = torch.stack(results, dim=2) assert sigma_qq.shape == (b, r, int((q * (q - 1)) / 2))
           Yet, this computation would be quite inefficient. Instead, we compute interactions along all p, e.g., e1e1,
           e1e2, e1e3,
                    e2e1, e2e2, e2e3, e3e1, e3e2, e3e3
           Then select the triangular matrix without diagonals: e1e2, e1e3, e2e3.
compute_sigma_pq(*, hp, hq, rp, rq)
           sum_{i=1}^{p} sum_{j=p+1}^{p+q} (h_i r_j - h_j r_i) e_i e_j
           results = [] sigma_pq = torch.zeros(b, r, p, q) for i in range(p):
                    for i in range(q):
                             sigma_pq[:, :, i, j] = hp[:, :, i] * rq[:, :, j] - hq[:, :, j] * rp[:, :, i]
           print(sigma_pq.shape)
apply_coefficients(hp, hq, rp, rq)
           Multiplying a base vector with its scalar coefficient
clifford_multiplication (h0, hp, hq, r0, rp, rq)
           Compute our CL multiplication
                    h = h_0 + sum_{i=1}^p h_i e_i + sum_{j=p+1}^p h_j e_j r = r_0 + sum_{i=1}^p r_i e_i + sum_{i=1}^p r_i e_i + sum_{i=1}^n p_i e_j r = r_0 + sum_{i=1}^n p_i e_i + sum_{i=1}^n p_i e_j r = r_0 + sum_{i=1}^n p_i r = r_0 + sum_{i=1}^n p_i e_j r = r_0 
                    sum_{j=p+1}^{p+q} r_j e_j
                    ei ^2 = +1 for i = < i = < p ej ^2 = -1 for p < j = < p+q ei ej = -eje1 for i
           eq j
                    h r = sigma_0 + sigma_p + sigma_q + sigma_{pp} + sigma_{q} + sigma_{pq}  where
                    (1) sigma_0 = h_0 r_0 + sum_{i=1}^p (h_0 r_i) e_i - sum_{j=p+1}^{p+q} (h_j r_j) e_j
                    (2) sigma p = sum \{i=1\}^p (h \ 0 \ r \ i + h \ i \ r \ 0) e \ i
                    (3) sigma_q = sum_{j=p+1}^{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.FloatTensor
           Compute residual score of two complex-valued embeddings. :param C_1: a tuple of two pytorch tensors
           that corresponds complex-valued embeddings :param C_2: a tuple of two pytorch tensors that corresponds
           complex-valued embeddings :return:
     forward_k_vs_all(x: torch.Tensor) \rightarrow torch.FloatTensor
     forward\_triples(x: torch.Tensor) \rightarrow torch.FloatTensor
               Parameters
     forward_k_vs_sample (x: torch.Tensor, target_entity_idx: torch.Tensor)
class dicee.models.complex.AConEx(args)
     Bases: dicee.models.base_model.BaseKGE
     Additive Convolutional ComplEx Knowledge Graph Embeddings
     name = 'AConEx'
     conv2d
     fc_num_input
     fc1
     norm_fc1
     bn_conv2d
     feature_map_dropout
     residual convolution (C 1: Tuple[torch.Tensor, torch.Tensor],
                  C 2: Tuple[torch.Tensor, torch.Tensor]) \rightarrow torch.FloatTensor
           Compute residual score of two complex-valued embeddings. :param C_1: a tuple of two pytorch tensors
           that corresponds complex-valued embeddings :param C_2: a tuple of two pytorch tensors that corresponds
           complex-valued embeddings :return:
     forward_k_vs_all(x: torch.Tensor) \rightarrow torch.FloatTensor
     forward\_triples(x: torch.Tensor) \rightarrow torch.FloatTensor
               Parameters
     forward_k_vs_sample (x: torch.Tensor, target_entity_idx: torch.Tensor)
```

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

Base class for all neural network modules.

Your models should also subclass this class.

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

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

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

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

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

# 1 Note

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

#### **Variables**

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

# **Parameters**

- emb\_h
- emb\_r
- emb E

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

forward\_k\_vs\_sample (x: torch.LongTensor, target\_entity\_idx: torch.LongTensor)

# dicee.models.dualE

### **Classes**

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

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

# Output

```
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.octonion

### **Classes**

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

### **Functions**

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

# **Module Contents**

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

Base class for all neural network modules.

Your models should also subclass this class.

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

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

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

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

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

# 1 Note

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

### Variables

**training**  $(b \circ \circ 1)$  – 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__()
```

(continued from previous page)

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

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



conv2d

# 1 Note

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

#### Variables

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

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

```
fc_num_input

fc1

bn_conv2d

norm_fc1

feature_map_dropout

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

residual_convolution(O_1, O_2)

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

Parameters

x

forward_k_vs_all(x: torch.Tensor)
```

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

# dicee.models.pykeen\_models

### **Classes**

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

# **Module Contents**

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

Notes: Pykeen\_DistMult: C Pykeen\_ComplEx: Pykeen\_QuatE: Pykeen\_MuRE: Pykeen\_CP: Pykeen\_HolE: Pykeen\_HolE: Pykeen\_TransD: Pykeen\_TransE: Pykeen\_TransF: Pykeen\_TransH: Pykeen\_TransR:

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

### forward\_k\_vs\_all (x: torch.LongTensor)

- # => Explicit version by this we can apply bn and dropout
- # (1) Retrieve embeddings of heads and relations + apply Dropout & Normalization if given. h,  $r = self.get_head_relation_representation(x) # (2) Reshape (1). if <math>self.last_dim > 0$ :
  - $\label{eq:hamma} h = h.reshape(len(x), self.embedding\_dim, self.last\_dim) \\ r = r.reshape(len(x), self.embedding\_dim, s$
- # (3) Reshape all entities. if self.last dim > 0:
  - t = self.entity\_embeddings.weight.reshape(self.num\_entities, self.embedding\_dim, self.last\_dim)

#### else:

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

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

- # => Explicit version by this we can apply bn and dropout
- # (1) Retrieve embeddings of heads, relations and tails and apply Dropout & Normalization if given. h, r, t = self.get\_triple\_representation(x) # (2) Reshape (1). if self.last\_dim > 0:
  - $h = h.reshape(len(x), self.embedding\_dim, self.last\_dim) r = r.reshape(len(x), self.embedding\_dim, self.last\_dim) t = t.reshape(len(x), self.embedding\_dim, self.last\_dim)$
- # (3) Compute the triple score return self.interaction.score(h=h, r=r, t=t, slice size=None, slice dim=0)
- abstract forward\_k\_vs\_sample (x: torch.LongTensor, target\_entity\_idx)

# dicee.models.quaternion

## **Classes**

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

# **Functions**

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

# **Module Contents**

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

class dicee.models.quaternion.QMult(args)

Bases: dicee.models.base\_model.BaseKGE

Base class for all neural network modules.

Your models should also subclass this class.

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

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

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

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

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



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

# Variables

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

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

# **Parameters**

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

### **Returns**

Triple scores.

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

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

Absolute value of a quaternion

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

L2 norm of quaternion vector:

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

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

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

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

# dicee.models.real

Entities()

## **Classes**

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

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

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

# dicee.models.static\_funcs

# **Functions**

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

# **Module Contents**

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

### dicee.models.transformers

Full definition of a GPT Language Model, all of it in this single file. References: 1) the official GPT-2 TensorFlow implementation released by OpenAI: https://github.com/openai/gpt-2/blob/master/src/model.py 2) hugging-face/transformers PyTorch implementation: https://github.com/huggingface/transformers/blob/main/src/transformers/models/gpt2/modeling\_gpt2.py

# **Classes**

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

# **Module Contents**

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

Base class for all neural network modules.

Your models should also subclass this class.

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

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

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

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

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



### 1 Note

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

### Variables

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

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

# **Parameters**

- yhat\_batch
- y\_batch

forward (x: torch.LongTensor)

### **Parameters**

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

generate (idx, max\_new\_tokens, temperature=1.0, top\_k=None)

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

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

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

# **Parameters**

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

### Returns

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

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

Example:

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

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

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

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

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

### 1 Note

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

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

Bases: torch.nn.Module

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

weight

bias

forward(input)

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

Bases: torch.nn.Module

Base class for all neural network modules.

Your models should also subclass this class.

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

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

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

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

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

# 1 Note

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

#### **Variables**

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

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

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

Base class for all neural network modules.

Your models should also subclass this class.

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

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

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

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

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

# 1 Note

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

### **Variables**

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

```
c_fc
gelu
c_proj
dropout
forward(x)

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

Base class for all neural network modules.

Your models should also subclass this class.

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

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

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

(continued from previous page)

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

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

# 1 Note

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

# Variables

**training**  $(b \circ \circ 1)$  – 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):
```

(continued from previous page)

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

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

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

# 1 Note

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

# Variables

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

config

transformer

lm\_head

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

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

# Classes

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

Table 1 - continued from previous page

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

# **Functions**

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

# **Package Contents**

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

Base class for all optimizers.

# Warning

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

#### **Parameters**

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

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

Perform a single optimization step.

### **Parameters**

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

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

Bases: lightning.LightningModule

Base class for all neural network modules.

Your models should also subclass this class.

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

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

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



### 1 Note

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

#### Variables

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

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

Size of model in MB and number of params

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

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

### **Parameters**

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

### **Returns**

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

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

# Example:

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

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

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

(continued from previous page)

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

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

# 1 Note

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

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

#### **Parameters**

- yhat\_batch
- y\_batch

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

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

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

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

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

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

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

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

An iterable or collection of iterables specifying test samples.

For more information about multiple dataloaders, see this section.

For data processing use the following pattern:

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

However, the above are only necessary for distributed processing.

# Warning

do not assign state in prepare\_data

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

# **1** Note

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

# 1 Note

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

# $val\_dataloader() \rightarrow None$

An iterable or collection of iterables specifying validation samples.

For more information about multiple dataloaders, see this section.

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

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

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

# 1 Note

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

# **1** Note

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

### $predict_dataloader() \rightarrow None$

An iterable or collection of iterables specifying prediction samples.

For more information about multiple dataloaders, see this section.

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

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

# 1 Note

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

### Returns

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

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

An iterable or collection of iterables specifying training samples.

For more information about multiple dataloaders, see this section.

dataloader return will not be reloaded unless you set :paramref: "~lightning.pytorch.trainer.trainer.Trainer.reload\_dataloaders\_every\_n\_epochs" to a positive integer.

For data processing use the following pattern:

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

However, the above are only necessary for distributed processing.

# Warning

do not assign state in prepare\_data

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

# **1** Note

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

### configure\_optimizers (parameters=None)

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

#### Returns

Any of these 6 options.

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

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

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

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

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



# 1 Note

Some things to know:

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

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

Bases: BaseKGELightning

Base class for all neural network modules.

Your models should also subclass this class.

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

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

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

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

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

# 1 Note

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

# Variables

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

#### args

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

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

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

init\_params\_with\_sanity\_checking()

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

(continued from previous page)

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

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

# **1** Note

As per the example above, an <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 = None
__call__(x)
static forward(x)

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

Base class for all neural network modules.

Your models should also subclass this class.

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

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

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

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

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

# **1** Note

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

# Variables

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

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

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

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

forward\_triples (x: torch.LongTensor)

#### **Parameters**

x

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

Bases: BaseKGELightning

Base class for all neural network modules.

Your models should also subclass this class.

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

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

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

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

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

#### 1 Note

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

## Variables

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

## args

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

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

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

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

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

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

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

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



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

#### Variables

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

• emb\_E

forward\_k\_vs\_sample (x: torch.LongTensor, target\_entity\_idx: torch.LongTensor)

```
dicee.models.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:

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

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

Bases: BaseKGELightning

Base class for all neural network modules.

Your models should also subclass this class.

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

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

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

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

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



## 1 Note

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

#### **Variables**

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

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

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

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

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

Bases: torch.nn.Module

Base class for all neural network modules.

Your models should also subclass this class.

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

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

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

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

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

# 1 Note

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

#### Variables

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

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

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

class dicee.models.QMult(args)

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

Base class for all neural network modules.

Your models should also subclass this class.

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

(continued from previous page)

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

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

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



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

## Variables

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

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

# **Parameters**

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

## Returns

Triple scores.

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

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

Absolute value of a quaternion

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

L2 norm of quaternion vector:

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

#### **Parameters**

 $\mathbf{x}$  – The vector.

# Returns

The normalized vector.

```
score (head_ent_emb: torch.FloatTensor, rel_ent_emb: torch.FloatTensor,
                   tail ent emb: torch.FloatTensor)
      k\_vs\_all\_score (bpe_head_ent_emb, bpe_rel_ent_emb, E)
                Parameters
                    • bpe_head_ent_emb
                    • bpe_rel_ent_emb
      forward_k_vs_all(x)
                Parameters
                    x
      forward_k_vs_sample (x, target_entity_idx)
           Completed. Given a head entity and a relation (h,r), we compute scores for all possible triples, i.e.,
           [score(h,r,x)|x \text{ in Entities}] => [0.0,0.1,...,0.8], shape=> (1, |Entities|) Given a batch of head entities and
           relations => shape (size of batch,| Entities|)
class dicee.models.ConvQ(args)
      Bases: dicee.models.base_model.BaseKGE
      Convolutional Quaternion Knowledge Graph Embeddings
      name = 'ConvQ'
      entity_embeddings
      relation_embeddings
      conv2d
      fc_num_input
      fc1
      bn conv1
      bn_conv2
      feature_map_dropout
      {\tt residual\_convolution}\,(Q\_1,\,Q\_2)
      \textbf{forward\_triples} \ (\textit{indexed\_triple: torch.Tensor}) \ \rightarrow \textbf{torch.Tensor}) \ \rightarrow \textbf{torch.Tensor}
                Parameters
      forward_k_vs_all (x: torch.Tensor)
           Given a head entity and a relation (h,r), we compute scores for all entities. [score(h,r,x)|x in Entities] =>
           [0.0,0.1,...,0.8], shape=> (1, |Entities|) Given a batch of head entities and relations => shape (size of batch,)
           Entities()
class dicee.models.AConvQ(args)
      Bases: dicee.models.base_model.BaseKGE
      Additive Convolutional Quaternion Knowledge Graph Embeddings
```

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

Bases: BaseKGELightning

Base class for all neural network modules.

Your models should also subclass this class.

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

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

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

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

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

# 1 Note

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

#### Variables

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

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

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

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

Bases: torch.nn.Module

Base class for all neural network modules.

Your models should also subclass this class.

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

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

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

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

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

# 1 Note

As per the example above, an \_\_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:

(continued from previous page)

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

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

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



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

### Variables

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

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

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

Bases: dicee.models.base\_model.BaseKGE

Base class for all neural network modules.

Your models should also subclass this class.

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

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

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

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

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

# 1 Note

conv2d

fc\_num\_input

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

#### Variables

**training**  $(b \circ \circ 1)$  – 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.AConvO(args: dict)
     Bases: dicee.models.base_model.BaseKGE
     Additive Convolutional Octonion Knowledge Graph Embeddings
     name = 'AConvO'
```

```
fc1
```

bn\_conv2d

norm\_fc1

feature\_map\_dropout

static octonion\_normalizer(emb\_rel\_e0, emb\_rel\_e1, emb\_rel\_e2, emb\_rel\_e3, emb\_rel\_e4,
emb\_rel\_e5, emb\_rel\_e6, emb\_rel\_e7)

 ${\tt residual\_convolution}\,(O\_1,\,O\_2)$ 

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

#### **Parameters**

x

```
forward k vs all (x: torch. Tensor)
```

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

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

Bases: dicee.models.base model.BaseKGE

Base class for all neural network modules.

Your models should also subclass this class.

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

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

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

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

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

## 1 Note

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

## **Variables**

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

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

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

Compute our CL multiplication

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

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

eq j

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

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

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. 

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

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

#### **Parameter**

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

#### rtvpe

torch.FloatTensor with (n) shape

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

Without learning dimension scaling

```
name = 'CKeci'
```

requires\_grad\_for\_interactions = False

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

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

Base class for all neural network modules.

Your models should also subclass this class.

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

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

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

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

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

# **1** Note

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

#### **Variables**

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

name = 'DeCaL'

entity\_embeddings

relation\_embeddings

q

r

re

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

## **Parameter**

x: torch.LongTensor with (n, ) shape

## rtype

torch.FloatTensor with (n) shape

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

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

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

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

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

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

and return:

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

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

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

For same bases vectors interaction we have

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

For different base vector interactions, we have

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

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

Kvsall training

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

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

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

Multiplying a base vector with its scalar coefficient

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

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

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

### **Parameter**

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

## returns

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

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

Compute .. math:

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

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

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

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

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

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

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

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

Compute

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

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

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

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

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

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):

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

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
     \texttt{forward\_triples} \ (x: torch.LongTensor) \ \to torch.Tensor
              Parameters
     forward_k_vs_all(*args, **kwargs)
     forward_k_vs_sample(*args, **kwargs)
     get_triple_representation(idx_hrt)
     get_head_relation_representation(indexed_triple)
     get_sentence_representation(x: torch.LongTensor)
              Parameters
                  • (b (x shape)
                  • 3
                  • t)
     get_bpe_head_and_relation_representation(x: torch.LongTensor)
                 → Tuple[torch.FloatTensor, torch.FloatTensor]
              Parameters
                 x (B x 2 x T)
     get_embeddings() → Tuple[numpy.ndarray, numpy.ndarray]
class dicee.models.PykeenKGE(args: dict)
     Bases: dicee.models.base_model.BaseKGE
     A class for using knowledge graph embedding models implemented in Pykeen
     Notes: Pykeen_DistMult: C Pykeen_ComplEx: Pykeen_QuatE: Pykeen_MuRE: Pykeen_CP: Pykeen_HolE: Py-
     keen_HolE: Pykeen_HolE: Pykeen_TransD: Pykeen_TransE: Pykeen_TransF: Pykeen_TransH: Pykeen_TransR:
     model_kwargs
     name
     model
     loss_history = []
     args
```

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

# (3) Compute the triple score return self.interaction.score(h=h, r=r, t=t, slice\_size=None, slice\_dim=0)

abstract forward\_k\_vs\_sample (x: torch.LongTensor, target\_entity\_idx)

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

Base class for all neural network modules.

Your models should also subclass this class.

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

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

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

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

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



# **1** Note

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

#### **Variables**

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

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

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

```
\mathtt{get\_embeddings}() \rightarrow Tuple[numpy.ndarray, numpy.ndarray]
class dicee.models.FMult(args)
     Bases: dicee.models.base_model.BaseKGE
     Learning Knowledge Neural Graphs
     name = 'FMult'
     entity_embeddings
     relation_embeddings
     num_sample = 50
     gamma
     roots
     weights
     compute\_func(weights: torch.FloatTensor, x) \rightarrow torch.FloatTensor
     chain_func (weights, x: torch.FloatTensor)
     forward\_triples(idx\_triple: torch.Tensor) \rightarrow torch.Tensor
               Parameters
                   x
class dicee.models.GFMult (args)
     Bases: dicee.models.base_model.BaseKGE
     Learning Knowledge Neural Graphs
     name = 'GFMult'
     entity_embeddings
     relation_embeddings
     k
     num_sample = 250
     roots
     weights
     compute\_func(weights: torch.FloatTensor, x) \rightarrow torch.FloatTensor
     chain_func (weights, x: torch.FloatTensor)
     forward\_triples(idx\_triple: torch.Tensor) \rightarrow torch.Tensor
               Parameters
                   x
```

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

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

class dicee.models.LFMult(args)

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

```
polynomial(coeff, x, degree)
           This function takes a matrix tensor of coefficients (coeff), a tensor vector of points x and range of integer
           [0,1,\ldots d] and return a vector tensor (coeff[0][0] + coeff[0][1]x +...+ coeff[0][d]x^d,
                coeff[1][0] + coeff[1][1]x + ... + coeff[1][d]x^d
      pop (coeff, x, degree)
           This function allow us to evaluate the composition of two polynomes without for loops:) it takes a matrix
           tensor of coefficients (coeff), a matrix tensor of points x and range of integer [0,1,...d]
                and return a tensor (coeff[0][0] + coeff[0][1]x + ... + coeff[0][d]x^d,
                    coeff[1][0] + coeff[1][1]x + ... + coeff[1][d]x^d
class dicee.models.DualE(args)
      Bases: dicee.models.base_model.BaseKGE
      Dual Quaternion Knowledge Graph Embeddings (https://ojs.aaai.org/index.php/AAAI/article/download/16850/
      16657)
      name = 'DualE'
      entity_embeddings
      relation embeddings
      num ent = None
      kvsall_score (e_1_h, e_2_h, e_3_h, e_4_h, e_5_h, e_6_h, e_7_h, e_8_h, e_1_t, e_2_t, e_3_t, e_4_t,
                   e_5_t, e_6_t, e_7_t, e_8_t, r_1, r_2, r_3, r_4, r_5, r_6, r_7, r_8) \rightarrow \text{torch.tensor}
           KvsAll scoring function
           Input
           x: torch.LongTensor with (n, ) shape
           Output
           torch.FloatTensor with (n) shape
      forward\_triples(idx\_triple: torch.tensor) \rightarrow torch.tensor
           Negative Sampling forward pass:
           Input
           x: torch.LongTensor with (n, ) shape
           Output
           torch.FloatTensor with (n) shape
      forward_k_vs_all(x)
```

KvsAll forward pass

# Input

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

# **Output**

```
torch.FloatTensor with (n) shape

T (x: torch.tensor) → torch.tensor

Transpose function

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

# dicee.query\_generator

## **Classes**

QueryGenerator

# **Module Contents**

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

```
set_global_seed(seed: int)
           Set seed
      construct\_graph(paths: List[str]) \rightarrow Tuple[Dict, Dict]
           Construct graph from triples Returns dicts with incoming and outgoing edges
      fill_query(query\_structure: List[str | List], ent_in: Dict, ent_out: Dict, answer: int) \rightarrow bool
           Private method for fill_query logic.
      achieve\_answer(query: List[str \mid List], ent\_in: Dict, ent\_out: Dict) \rightarrow set
           Private method for achieve_answer logic. @TODO: Document the code
      write_links(ent_out, small_ent_out)
      ground_queries (query_structure: List[str | List], ent_in: Dict, ent_out: Dict, small_ent_in: Dict,
                   small_ent_out: Dict, gen_num: int, query_name: str)
           Generating queries and achieving answers
      unmap (query_type, queries, tp_answers, fp_answers, fn_answers)
      unmap_query (query_structure, query, id2ent, id2rel)
      generate_queries (query_struct: List, gen_num: int, query_type: str)
           Passing incoming and outgoing edges to ground queries depending on mode [train valid or text] and getting
           queries and answers in return @ TODO: create a class for each single query struct
      save_queries (query_type: str, gen_num: int, save_path: str)
      abstract load_queries(path)
      get_queries (query_type: str, gen_num: int)
      static save_queries_and_answers (path: str, data: List[Tuple[str, Tuple[collections.defaultdict]]])
                    \rightarrow None
           Save Queries into Disk
      static load_queries_and_answers (path: str) → List[Tuple[str, Tuple[collections.defaultdict]]]
           Load Queries from Disk to Memory
dicee.read_preprocess_save_load_kg
Submodules
dicee.read_preprocess_save_load_kg.preprocess
Classes
```

PreprocessKG

Preprocess the data in memory

## **Module Contents**

```
class dicee.read_preprocess_save_load_kg.preprocess.PreprocessKG (kg) Preprocess the data in memory kg start () \rightarrow N one Preprocess train, valid and test datasets stored in knowledge graph instance
```

## **Parameter**

rtype

None

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

- (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**

```
{\tt class} \  \, {\tt dicee.read\_preprocess\_save\_load\_kg.read\_from\_disk.ReadFromDisk} \, (kg) \\  \, Read\  \, {\tt the}\  \, {\tt disk}\  \, {\tt into}\  \, {\tt 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)	
$read\_with\_polars(\rightarrow polars.DataFrame)$	Load and Preprocess via Polars
read_with_pandas(data_path[, read_only_few,])	
read_from_disk(→ Tuple[polars.DataFrame, pan-das.DataFrame])	
read_from_triple_store([endpoint])	Read triples from triple store into pandas dataframe
get_er_vocab(data[, file_path])	parameter and parameter
<pre>get_re_vocab(data[, file_path])</pre>	
<pre>get_ee_vocab(data[, file_path])</pre>	
<pre>create_constraints(triples[, file_path])</pre>	
$load\_with\_pandas(\rightarrow None)$	Deserialize data
<pre>save_numpy_ndarray(*, data, file_path)</pre>	
<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**

```
dicee.read_preprocess_save_load_kg.util.polars_dataframe_indexer( df_polars.DataFrame, idx_entity: polars.DataFrame, idx_relation: polars.DataFrame) <math>\rightarrow polars.DataFrame
```

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

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

#### **Parameters:**

#### df polars

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

## idx\_entity

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

#### idx relation

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

#### **Returns:**

#### polars.DataFrame

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

# **Example Usage:**

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

# Steps:

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

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

```
dicee.read_preprocess_save_load_kg.util.timeit(func)
```

Load and Preprocess via Polars

```
dicee.read_preprocess_save_load_kg.util.read_with_pandas(data_path, read_only_few: int = None, sample_triples_ratio: float = None, separator: str = None)
```

```
dicee.read_preprocess_save_load_kg.util.read_from_disk(data_path: str, read_only_few: int = None, sample_triples_ratio: float = None, backend: str = None, separator: str = None) → Tuple[polars.DataFrame, pandas.DataFrame]
```

```
dicee.read_preprocess_save_load_kg.util.read_from_triple_store(endpoint: str = None)
```

Read triples from triple store into pandas dataframe

```
dicee.read_preprocess_save_load_kq.util.get_er_vocab(data, file_path: str = None)
```

```
dicee.read_preprocess_save_load_kg.util.get_re_vocab(data, file_path: str = None)
```

```
dicee.read_preprocess_save_load_kg.util.get_ee_vocab(data, file_path: str = None)
```

```
dicee.read_preprocess_save_load_kg.util.create_constraints(triples, file_path: str = None)
```

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

```
dicee.read_preprocess_save_load_kg.util.load_with_pandas(self) \rightarrow None
```

Deserialize data

#### **Classes**

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

# **Package Contents**

(2) Construct vocabulary

(3) Index datasets

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

Preprocess the data in memory

kg

start() → None

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

Parameter

rtype

None

preprocess_with_byte_pair_encoding()

preprocess_with_byte_pair_encoding_with_padding() → None

preprocess_with_pandas() → None

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

(1) Add recipriocal or noisy triples
```

# **Parameter**

```
rtvpe
                    None
      {\tt preprocess\_with\_polars}\, () \, \to None
      \verb"sequential_vocabulary_construction"\,(\,)\,\to None
           (1) Read input data into memory
           (2) Remove triples with a condition
           (3) Serialize vocabularies in a pandas dataframe where
                   => the index is integer and => a single column is string (e.g. URI)
class dicee.read_preprocess_save_load_kg.LoadSaveToDisk(kg)
      kg
      save()
      load()
class dicee.read_preprocess_save_load_kg.ReadFromDisk(kg)
      Read the data from disk into memory
      kg
      \mathtt{start}() \rightarrow \mathrm{None}
           Read a knowledge graph from disk into memory
           Data will be available at the train_set, test_set, valid_set attributes.
           Parameter
           None
               rtype
                   None
```

# dicee.sanity\_checkers

add\_noisy\_triples\_into\_training()

#### **Functions**

#### **Module Contents**

dicee.sanity\_checkers.is\_sparql\_endpoint\_alive(sparql\_endpoint: str = None)

```
dicee.sanity_checkers.validate_knowledge_graph (args)
     Validating the source of knowledge graph
dicee.sanity_checkers.sanity_checking_with_arguments (args)
```

# dicee.scripts

# **Submodules**

# dicee.scripts.index\_serve

\$ docker pull qdrant/qdrant && docker run -p 6333:6333 -p 6334:6334 -v \$(pwd)/qdrant\_storage:/qdrant/storage:z qdrant/qdrant \$ dicee\_vector\_db -index -serve -path CountryEmbeddings -collection "countries\_vdb"

# **Attributes**

```
app
neural_searcher
```

## **Classes**

```
NeuralSearcher

StringListRequest !!! abstract "Usage Documentation"
```

# **Functions**

```
get_default_arguments()
index(args)

root()
search_embeddings(q)

retrieve_embeddings(q)
search_embeddings_batch(request)
serve(args)

main()
```

## **Module Contents**

```
dicee.scripts.index_serve.get_default_arguments()
dicee.scripts.index_serve.index(args)
dicee.scripts.index_serve.app
dicee.scripts.index_serve.neural searcher = None
class dicee.scripts.index_serve.NeuralSearcher(args)
     collection name
     entity_to_idx = None
     qdrant_client
     topk = 5
     retrieve_embedding (entity: str = None, entities: List[str] = None) \rightarrow List
     search (entity: str)
async dicee.scripts.index_serve.root()
async dicee.scripts.index_serve.search_embeddings(q: str)
async dicee.scripts.index_serve.retrieve_embeddings(q: str)
class dicee.scripts.index_serve.StringListRequest(/, **data: Any)
     Bases: pydantic.BaseModel
     !!! abstract "Usage Documentation"
          [Models](../concepts/models.md)
     A base class for creating Pydantic models.
     __class_vars__
          The names of the class variables defined on the model.
     __private_attributes__
          Metadata about the private attributes of the model.
          The synthesized __init__ [Signature][inspect.Signature] of the model.
     __pydantic_complete__
          Whether model building is completed, or if there are still undefined fields.
     __pydantic_core_schema__
          The core schema of the model.
     __pydantic_custom_init__
          Whether the model has a custom __init__ function.
     __pydantic_decorators__
          Metadata containing the decorators defined on the model. This replaces Model._validators_ and
          Model.__root_validators__ from Pydantic V1.
```

```
__pydantic_generic_metadata__
          Metadata for generic models; contains data used for a similar purpose to __args__, __origin__, __parame-
          ters in typing-module generics. May eventually be replaced by these.
      __pydantic_parent_namespace__
          Parent namespace of the model, used for automatic rebuilding of models.
     __pydantic_post_init__
          The name of the post-init method for the model, if defined.
      __pydantic_root_model__
          Whether the model is a [RootModel][pydantic.root_model.RootModel].
     __pydantic_serializer__
          The pydantic-core SchemaSerializer used to dump instances of the model.
     __pydantic_validator__
          The pydantic-core Schema Validator used to validate instances of the model.
     __pydantic_fields__
          A dictionary of field names and their corresponding [FieldInfo][pydantic.fields.FieldInfo] objects.
     __pydantic_computed_fields__
               dictionary
                            of
                                 computed
                                             field
                                                     names
                                                              and
                                                                     their
                                                                            corresponding
                                                                                             [ComputedField-
          Info][pydantic.fields.ComputedFieldInfo] objects.
     __pydantic_extra__
          A dictionary containing extra values, if [extra][pydantic.config.ConfigDict.extra] is set to 'allow'.
      __pydantic_fields_set__
          The names of fields explicitly set during instantiation.
     __pydantic_private__
          Values of private attributes set on the model instance.
     queries: List[str]
     reducer: str | None = None
async dicee.scripts.index_serve.search_embeddings_batch (request: StringListRequest)
dicee.scripts.index_serve.serve(args)
dicee.scripts.index_serve.main()
```

# dicee.scripts.run

# **Functions**

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

## **Module Contents**

## dicee.static\_funcs

## **Functions**

```
create_recipriocal_triples(x)
                                                         Add inverse triples into dask dataframe
get_er_vocab(data[, file_path])
get_re_vocab(data[, file_path])
get_ee_vocab(data[, file_path])
timeit(func)
save_pickle(*[, data, file_path])
load_pickle([file_path])
load_term_mapping([file_path])
select_model(args[,
                         is_continual_training,
                                                 stor-
age_path])
load_mode1(→ Tuple[object, Tuple[dict, dict]])
                                                         Load weights and initialize pytorch module from names-
                                                         pace arguments
                                                         Construct Ensemble Of weights and initialize pytorch
load_model_ensemble(...)
                                                         module from namespace arguments
save_numpy_ndarray(*, data, file_path)
numpy_data_type_changer(→ numpy.ndarray)
                                                         Detect most efficient data type for a given triples
                                                         Store Pytorch model into disk
save\_checkpoint\_model(\rightarrow None)
store(\rightarrow None)
add\_noisy\_triples(\rightarrow pandas.DataFrame)
                                                         Add randomly constructed triples
read_or_load_kg(args, cls)
intialize\_model(\rightarrow Tuple[object, str])
load_json(\rightarrow dict)
save\_embeddings(\rightarrow None)
                                                         Save it as CSV if memory allows.
random_prediction(pre_trained_kge)
deploy_triple_prediction(pre_trained_kge,
str_subject, ...)
deploy_tail_entity_prediction(pre_trained_kge,
...)
```

continues on next page

Table 2 - continued from previous page

```
deploy_head_entity_prediction(pre_trained_kge,
deploy_relation_prediction(pre_trained_kge,
...)
 vocab_to_parquet(vocab_to_idx, name, ...)
create_experiment_folder([folder_name])
continual_training_setup_executor(→ None)
exponential\_function(\rightarrow torch.FloatTensor)
load_numpy(→ numpy.ndarray)
                                                    # @TODO: CD: Renamed this function
evaluate(entity_to_idx,
                           scores,
                                      easy answers,
hard answers)
 download_file(url[, destination_folder])
download\_files\_from\_url(\rightarrow None)
download_pretrained_model(\rightarrow str)
write_csv_from_model_parallel(path)
                                                     Create
 from_pretrained_model_write_embeddings_into
None)
```

#### **Module Contents**

```
dicee.static_funcs.create_recipriocal_triples(x)
     Add inverse triples into dask dataframe :param x: :return:
dicee.static_funcs.get_er_vocab(data, file_path: str = None)
dicee.static_funcs.get_re_vocab(data, file_path: str = None)
dicee.static_funcs.get_ee_vocab(data, file_path: str = None)
dicee.static_funcs.timeit(func)
dicee.static_funcs.save_pickle(*, data: object = None, file_path=str)
dicee.static_funcs.load_pickle(file_path=str)
dicee.static_funcs.load_term_mapping(file_path=str)
dicee.static_funcs.select_model(args: dict, is_continual_training: bool = None,
           storage\_path: str = None)
dicee.static_funcs.load_model(path_of_experiment_folder: str, model_name='model.pt', verbose=0)
            → Tuple[object, Tuple[dict, dict]]
     Load weights and initialize pytorch module from namespace arguments
dicee.static_funcs.load_model_ensemble(path_of_experiment_folder: str)
            → Tuple[dicee.models.base_model.BaseKGE, Tuple[pandas.DataFrame, pandas.DataFrame]]
     Construct Ensemble Of weights and initialize pytorch module from namespace arguments
```

- (1) Detect models under given path
- (2) Accumulate parameters of detected models
- (3) Normalize parameters
- (4) Insert (3) into model.

```
dicee.static_funcs.save_numpy_ndarray(*, data: numpy.ndarray, file_path: str)
```

Detect most efficient data type for a given triples :param train\_set: :param num: :return:

dicee.static\_funcs.save\_checkpoint\_model (model, path: str) ightarrow None

Store Pytorch model into disk

dicee.static\_funcs.store(trained\_model, model\_name: str = 'model', full\_storage\_path: str = None,  $save\_embeddings\_as\_csv=False$ )  $\rightarrow$  None

Add randomly constructed triples :param train\_set: :param add\_noise\_rate: :return:

```
dicee.static_funcs.read_or_load_kg(args, cls)
```

```
dicee.static_funcs.intialize_model(args: dict, verbose=0) \rightarrow Tuple[object, str]
```

dicee.static\_funcs.load\_json(p: str)  $\rightarrow$  dict

dicee.static\_funcs.save\_embeddings (embeddings: numpy.ndarray, indexes, path:  $str) \rightarrow None$ Save it as CSV if memory allows. :param embeddings: :param indexes: :param path: :return:

dicee.static\_funcs.random\_prediction(pre\_trained\_kge)

dicee.static\_funcs.deploy\_tail\_entity\_prediction( $pre\_trained\_kge$ ,  $str\_subject$ ,  $str\_predicate$ ,  $top\_k$ )

 $\label{local_discrete_discrete} \verb|disce.static_funcs.deploy_head_entity_prediction|| (pre\_trained\_kge, str\_object, str\_predicate, top\_k)|$ 

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

dicee.static\_funcs.vocab\_to\_parquet(vocab\_to\_idx, name, path\_for\_serialization, print\_into)

dicee.static\_funcs.create\_experiment\_folder(folder\_name='Experiments')

dicee.static\_funcs.continual\_training\_setup\_executor(executor)  $\rightarrow$  None

 $\label{linear_discrete_discrete} \begin{tabular}{ll} \tt discrete_static_funcs.exponential\_function (\it{x: numpy.ndarray, lam: float, ascending\_order=True)} \\ \to torch. Float Tensor \end{tabular}$ 

dicee.static\_funcs.load\_numpy(path)  $\rightarrow$  numpy.ndarray

dicee.static\_funcs.evaluate(entity\_to\_idx, scores, easy\_answers, hard\_answers)

# @TODO: CD: Renamed this function Evaluate multi hop query answering on different query types dicee.static\_funcs.download\_file(url, destination\_folder='.')

```
dicee.static_funcs.download_files_from_url(base\_url: str, destination\_folder='.') 	o None
```

#### **Parameters**

- base\_url (e.g. "https://files.dice-research.org/projects/DiceEmbeddings/ KINSHIP-Keci-dim128-epoch256-KvsAll")
- destination\_folder(e.g. "KINSHIP-Keci-dim128-epoch256-KvsA11")

```
{\tt dicee.static\_funcs.download\_pretrained\_model}~(\textit{url: str})~\rightarrow str
```

dicee.static\_funcs.write\_csv\_from\_model\_parallel(path: str)

Create

 $\texttt{dicee.static\_funcs.from\_pretrained\_model\_write\_embeddings\_into\_csv} \ (\textit{path: str}) \rightarrow None$ 

## dicee.static funcs training

#### **Functions**

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

## **Module Contents**

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

```
dicee.static_funcs_training.evaluate_lp (model=None, triple_idx=None, num_entities=None, er_vocab: Dict[Tuple, List] = None, re_vocab: Dict[Tuple, List] = None, info='Eval Starts', batch_size=128, chunk_size=1000)
```

dicee.static\_funcs\_training.efficient\_zero\_grad(model)

# dicee.static\_preprocess\_funcs

#### **Attributes**

enable\_log

## **Functions**

```
timeit(func)
preprocesses\_input\_args(args)
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)
Sanity Checking in input arguments
get\_er\_vocab(data)
```

## **Module Contents**

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

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

dicee.trainer

**Submodules** 

dicee.trainer.dice\_trainer

**Classes** 

DICE\_Trainer implement

## **Functions**

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

## **Module Contents**

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

## **Parameter**

#### returns

- model
- form\_of\_labelling (str)

## initialize\_trainer(callbacks: List)

→ lightning.Trainer | dicee.trainer.model\_parallelism.TensorParallel | dicee.trainer.torch\_trainer.TorchTrainer | dicee.trainer.TorchTrainer | dicee.trainer.torch\_trainer.TorchTrainer | dicee.trainer.torch\_trainer.TorchTrainer | dicee.trainer.torch\_trai

```
initialize_or_load_model()
```

 $\verb"init_dataloader" (dataset: torch.utils.data.Dataset") o torch.utils.data.DataLoader$ 

 $init\_dataset() \rightarrow torch.utils.data.Dataset$ 

 $\verb|start| (knowledge\_graph: dicee.knowledge\_graph.KG \mid numpy.memmap)|$ 

→ Tuple[dicee.models.base\_model.BaseKGE, str]

Start the training

- (1) Initialize Trainer
- (2) Initialize or load a pretrained KGE model

in DDP setup, we need to load the memory map of already read/index KG.

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

Perform K-fold Cross-Validation

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

# **Parameters**

- self
- dataset

#### Returns

model

# dicee.trainer.model\_parallelism

# **Classes**

TensorParallel Abstract class for Trainer class for knowledge graph embedding models

## **Functions**

```
extract_input_outputs(z[, device])

find_good_batch_size(train_loader,

tp_ensemble_model)

forward_backward_update_loss(\rightarrow float)
```

## **Module Contents**

## dicee.trainer.torch\_trainer

## Classes

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

## **Module Contents**

```
class dicee.trainer.torch_trainer.TorchTrainer(args, callbacks)

Bases: dicee.abstracts.AbstractTrainer

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

Arguments

callbacks: list of Abstract callback instances

loss_function = None
```

```
optimizer = None
      model = None
      train_dataloaders = None
      training_step = None
      process
      fit (*args, train\_dataloaders, **kwargs) \rightarrow None
                  Training starts
                  Arguments
            kwargs:Tuple
                 empty dictionary
                  Return type
                      batch loss (float)
      \textbf{forward\_backward\_update} \ (x\_\textit{batch: torch.Tensor}, \ y\_\textit{batch: torch.Tensor}) \ \to \ \text{torch.Tensor}) \ \to \ \text{torch.Tensor})
                  Compute forward, loss, backward, and parameter update
                  Arguments
                  Return type
                      batch loss (float)
      \textbf{extract\_input\_outputs\_set\_device} \ (\textit{batch: list}) \ \rightarrow \textbf{Tuple}
                  Construct inputs and outputs from a batch of inputs with outputs From a batch of inputs and put
                  Arguments
                  Return type
                      (tuple) mini-batch on select device
dicee.trainer.torch_trainer_ddp
```

#### dicee.trainer.torch\_tra

## **Classes**

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

## **Functions**

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

# **Module Contents**

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

```
extract_input_outputs (z: list)
train()
Training loop for DDP
```

## **Classes**

DICE\_Trainer

DICE\_Trainer implement

# **Package Contents**

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

## **DICE\_Trainer implement**

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

args

is\_continual\_training:bool

storage\_path:str

evaluator:

report:dict

report

args

trainer = None

is\_continual\_training

storage\_path

evaluator = None

form\_of\_labelling = None

continual\_start (knowledge\_graph)

- (1) Initialize training.
- (2) Load model
- (3) Load trainer (3) Fit model

#### **Parameter**

# returns

- model
- form\_of\_labelling (str)

## initialize\_trainer(callbacks: List)

→ lightning.Trainer | dicee.trainer.model\_parallelism.TensorParallel | dicee.trainer.torch\_trainer.TorchTrainer | dicee.trainer.TorchTrainer | dicee.trainer.torch\_trainer.TorchTrainer | dicee.trainer.torch\_trainer.TorchTrainer | dicee.trainer.torch\_trai

## initialize\_or\_load\_model()

 $init\_dataloader$  (dataset: torch.utils.data.Dataset)  $\rightarrow$  torch.utils.data.DataLoader

 $\verb"init_dataset"() \rightarrow torch.utils.data.Dataset"$ 

 $\verb|start| (knowledge\_graph: dicee.knowledge\_graph.KG \mid numpy.memmap)|$ 

→ Tuple[dicee.models.base\_model.BaseKGE, str]

Start the training

- (1) Initialize Trainer
- (2) Initialize or load a pretrained KGE model

in DDP setup, we need to load the memory map of already read/index KG.

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

Perform K-fold Cross-Validation

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

#### **Parameters**

- self
- dataset

## Returns

model

# 14.2 Attributes

\_\_version\_\_

# 14.3 Classes

Pyke	A Physical Embedding Model for Knowledge Graphs
DistMult	Embedding Entities and Relations for Learning and Infer-
	ence in Knowledge Bases
CKeci	Without learning dimension scaling
Keci	Base class for all neural network modules.
TransE	Translating Embeddings for Modeling
DeCaL	Base class for all neural network modules.

continues on next page

Table 3 - continued from previous page

DualE	Dual Quaternion Knowledge Graph Embeddings
Duale	(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
AConvO	Additive Convolutional Octonion Knowledge Graph Em-
	beddings
AConvQ	Additive Convolutional Quaternion Knowledge Graph
	Embeddings
ConvQ	Convolutional Quaternion Knowledge Graph Embed-
	dings
ConvO	Base class for all neural network modules.
ConEx	Convolutional ComplEx Knowledge Graph Embeddings
QMult	Base class for all neural network modules.
OMult	Base class for all neural network modules.
Shallom	A shallow neural model for relation prediction (https:
	//arxiv.org/abs/2101.09090)
LFMult	Embedding with polynomial functions. We represent all
	entities and relations in the polynomial space as:
PykeenKGE	A class for using knowledge graph embedding models 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
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
CVDataModule	Create a Dataset for cross validation
QueryGenerator	

# 14.4 Functions

create_recipriocal_triples(x)	Add inverse triples into dask dataframe
	continues on next page

Table 4 - continued from previous page

```
get_er_vocab(data[, file_path])
get_re_vocab(data[, file_path])
get_ee_vocab(data[, file_path])
timeit(func)
save_pickle(*[, data, file_path])
load_pickle([file_path])
load_term_mapping([file_path])
select_model(args[,
                         is_continual_training,
                                                 stor-
age path])
load_model(→ Tuple[object, Tuple[dict, dict]])
                                                        Load weights and initialize pytorch module from names-
                                                        pace arguments
                                                        Construct Ensemble Of weights and initialize pytorch
load_model_ensemble(...)
                                                        module from namespace arguments
save_numpy_ndarray(*, data, file_path)
numpy_data_type_changer(→ numpy.ndarray)
                                                        Detect most efficient data type for a given triples
save\_checkpoint\_model(\rightarrow None)
                                                        Store Pytorch model into disk
store(\rightarrow None)
add\_noisy\_triples(\rightarrow pandas.DataFrame)
                                                        Add randomly constructed triples
read_or_load_kg(args, cls)
intialize\_model(\rightarrow Tuple[object, str])
load_json(\rightarrow dict)
                                                        Save it as CSV if memory allows.
save\_embeddings(\rightarrow None)
random_prediction(pre_trained_kge)
deploy_triple_prediction(pre_trained_kge,
str subject, ...)
deploy_tail_entity_prediction(pre_trained_kge,
deploy_head_entity_prediction(pre_trained_kge,
deploy_relation_prediction(pre_trained_kge,
vocab_to_parquet(vocab_to_idx, name, ...)
create_experiment_folder([folder_name])
continual\_training\_setup\_executor(\rightarrow None)
exponential_function(\rightarrow torch.FloatTensor)
```

continues on next page

Table 4 - continued from previous page

```
load_numpy(\rightarrow numpy.ndarray)
                                                      # @TODO: CD: Renamed this function
 evaluate(entity_to_idx,
                            scores,
                                       easy_answers,
 hard answers)
 download_file(url[, destination_folder])
 download\_files\_from\_url(\rightarrow None)
 download\_pretrained\_model(\rightarrow str)
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
class dicee.DistMult(args)
     Bases: dicee.models.base_model.BaseKGE
     Embedding Entities and Relations for Learning and Inference in Knowledge Bases https://arxiv.org/abs/1412.6575
     name = 'DistMult'
     \verb+k_vs_all_score+ (emb_h: torch.FloatTensor, emb_r: torch.FloatTensor, emb_E: torch.FloatTensor)
              Parameters
                   • emb h
                   • emb_r
                   • emb_E
```

```
forward_k_vs_all(x: torch.LongTensor)
forward_k_vs_sample(x: torch.LongTensor, target_entity_idx: torch.LongTensor)
score(h, r, t)

class dicee.CKeci(args)
Bases: Keci
Without learning dimension scaling
name = 'CKeci'
requires_grad_for_interactions = False

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

Base class for all neural network modules.

Your models should also subclass this class.

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

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

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

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

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

#### 1 Note

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

#### **Variables**

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

```
name = 'Keci'
p
q
```

```
requires_grad_for_interactions = True
compute\_sigma\_pp(hp, rp)
          Compute sigma_{pp} = sum_{i=1}^{p-1} sum_{k=i+1}^p (h_i r_k - h_k r_i) e_i e_k
          sigma_{pp} captures the interactions between along p bases For instance, let p e_1, e_2, e_3, we compute
          interactions between e 1 e 2, e 1 e 3, and e 2 e 3 This can be implemented with a nested two for loops
                  results = [] for i in range(p - 1):
                          for k in range(i + 1, p):
                               results.append(hp[:, :, i] * rp[:, :, k] - hp[:, :, k] * rp[:, :, i])
                  sigma_pp = torch.stack(results, dim=2) assert sigma_pp.shape == (b, r, int((p * (p - 1)) / 2))
          Yet, this computation would be quite inefficient. Instead, we compute interactions along all p, e.g., e1e1,
          e1e2, e1e3,
                  e2e1, e2e2, e2e3, e3e1, e3e2, e3e3
          Then select the triangular matrix without diagonals: e1e2, e1e3, e2e3.
compute\_sigma\_qq(hq, rq)
          Compute sigma_{qq} = sum_{j=1}^{p+q-1} sum_{k=j+1}^{p+q} (h_j r_k - h_k r_j) e_j e_k sigma_{q}
          captures the interactions between along q bases For instance, let q e 1, e 2, e 3, we compute interactions
          between e 1 e 2, e 1 e 3, and e 2 e 3 This can be implemented with a nested two for loops
                  results = [] for j in range(q - 1):
                          for k in range(j + 1, q):
                               results.append(hq[:,:,j]*rq[:,:,k]-hq[:,:,k]*rq[:,:,j])\\
                  sigma_qq = torch.stack(results, dim=2) assert sigma_qq.shape == (b, r, int((q * (q - 1)) / 2))
          Yet, this computation would be quite inefficient. Instead, we compute interactions along all p, e.g., e1e1,
          e1e2, e1e3,
                  e2e1, e2e2, e2e3, e3e1, e3e2, e3e3
          Then select the triangular matrix without diagonals: e1e2, e1e3, e2e3.
compute_sigma_pq(*, hp, hq, rp, rq)
          sum_{i=1}^{p} sum_{j=p+1}^{p+q} (h_i r_j - h_j r_i) e_i e_j
          results = [] sigma_pq = torch.zeros(b, r, p, q) for i in range(p):
                  for j in range(q):
                          sigma_pq[:, :, i, j] = hp[:, :, i] * rq[:, :, j] - hq[:, :, j] * rp[:, :, i]
          print(sigma_pq.shape)
apply_coefficients(hp, hq, rp, rq)
          Multiplying a base vector with its scalar coefficient
clifford_multiplication (h0, hp, hq, r0, rp, rq)
          Compute our CL multiplication
                  h = h_0 + sum_{i=1}^p h_i e_i + sum_{j=p+1}^p h_j e_j r = r_0 + sum_{i=1}^p r_i e_i + sum_{j=p+1}^n h_j e_j r = r_0 + sum_{i=1}^n h_j e_j r = r_0 + sum_{i
                  sum_{j=p+1}^{p+q} r_j e_j
                  ei ^2 = +1 for i =< i =< p ej ^2 = -1 for p < j =< p+q ei ej = -eje1 for i
          eq j
                  h r = sigma \ 0 + sigma \ p + sigma \ q + sigma \ \{pp\} + sigma \ \{q\} + sigma \ \{pq\}  where
```

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

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

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

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

#### **Parameter**

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

# returns

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

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

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

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

Kvsall training

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

forward\_k\_vs\_with\_explicit and this 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  \begin{aligned} &\text{target\_entity\_idx: torch.LongTensor with (n, k) shape k denotes the selected number of examples.} \\ & &\textbf{rtype} \\ & & & & & & & & & & & & & & & \\ & & & & & & & & & & & & & \\ & & & & & & & & & & & & \\ & & & & & & & & & & & & \\ & & & & & & & & & & & \\ & & & & & & & & & & & \\ & & & & & & & & & & & \\ & & & & & & & & & & \\ & & & & & & & & & & \\ & & & & & & & & & & \\ & & & & & & & & & & \\ & & & & & & & & & & \\ & & & & & & & & & \\ & & & & & & & & & \\ & & & & & & & & & \\ & & & & & & & & & \\ & & & & & & & & \\ & & & & & & & & \\ & & & & & & & & \\ & & & & & & & & \\ & & & & & & & & \\ & & & & & & & \\ & & & & & & & \\ & & & & & & & \\ & & & & & & & \\ & & & & & & & \\ & & & & & & & \\ & & & & & & & \\ & & & & & & & \\ & & & & & & & \\ & & & & & & & \\ & & & & & & & \\ & & & & & & & \\ & & & & & & & \\ & & & & & & & \\ & & & & & & & \\ & & & & & & \\ & & & & & & \\ & & & & & & \\ & & & & & & \\ & & & & & & \\ & & & & & & \\ & & & & & \\ & & & & & & \\ & & & & & & \\ & & & & & & \\ & & & & & & \\ & & & & & & \\ & & & & & \\ & & & & & \\ & & & & & \\ & & & & & \\ & & & & & \\ & & & & & \\ & & & & & \\ & & & & \\ & & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & \\ & & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & &
```

#### **Parameter**

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

#### rtype

torch.FloatTensor with (n) shape

```
class dicee.TransE(args)
```

Bases: dicee.models.base model.BaseKGE

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

```
name = 'TransE'

margin = 4

score (head_ent_emb, rel_ent_emb, tail_ent_emb)

forward_k_vs_all (x: torch.Tensor) → torch.FloatTensor

class dicee.DeCaL (args)

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

Base class for all neural network modules.

Your models should also subclass this class.

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

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

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

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

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

# **1** Note

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

#### **Variables**

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

name = 'DeCaL'

entity\_embeddings

relation\_embeddings

р

q

r

re

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

#### **Parameter**

x: torch.LongTensor with (n, ) shape

#### rtype

torch.FloatTensor with (n) shape

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

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

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

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

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

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

and return:

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

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

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

For same bases vectors interaction we have

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

For different base vector interactions, we have

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

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

Kvsall training

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

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

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

Multiplying a base vector with its scalar coefficient

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

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

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

#### **Parameter**

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

#### returns

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

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

Compute .. math:

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

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

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

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

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

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

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

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

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

Compute

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

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

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

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

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

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

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

# for j in range(q):

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

print(sigma\_pq.shape)

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

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

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

```
for j in range(q):
                                                                    sigma_pq[:, :, i, j] = hp[:, :, i] * rq[:, :, j] - hq[:, :, j] * rp[:, :, i]
                                       print(sigma_pq.shape)
class dicee.DualE(args)
                    Bases: dicee.models.base_model.BaseKGE
                    Dual Quaternion Knowledge Graph Embeddings (https://ojs.aaai.org/index.php/AAAI/article/download/16850/
                    16657)
                    name = 'DualE'
                    entity_embeddings
                    relation_embeddings
                    num_ent = None
                    \texttt{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\_6\_h, e\_7\_h, e\_8\_h, e\_1\_t, e\_2\_t, e\_3\_t, e\_4\_t, e\_4\_t, e\_6\_h, e\_7\_h, e\_8\_h, e\_1\_t, e\_6\_t, e\_6\_h, e\_7\_h, e\_8\_h, e\_1\_t, e\_8\_t, e\_8
                                                                 e\_5\_t, e\_6\_t, e\_7\_t, e\_8\_t, r\_1, r\_2, r\_3, r\_4, r\_5, r\_6, r\_7, r\_8) \rightarrow \text{torch.tensor}
                                       KvsAll scoring function
                                       Input
                                       x: torch.LongTensor with (n, ) shape
                                       Output
                                       torch.FloatTensor with (n) shape
                    \textbf{forward\_triples} \ (\textit{idx\_triple: torch.tensor}) \ \rightarrow \textbf{torch.tensor}) \ \rightarrow \textbf{torch.tensor}
                                       Negative Sampling forward pass:
                                       Input
                                       x: torch.LongTensor with (n, ) shape
                                       Output
                                       torch.FloatTensor with (n) shape
                    forward_k_vs_all(x)
                                       KvsAll forward pass
                                       Input
                                       x: torch.LongTensor with (n, ) shape
                                       Output
                                       torch.FloatTensor with (n) shape
                    T (x: torch.tensor) \rightarrow torch.tensor
                                       Transpose function
                                       Input: Tensor with shape (nxm) Output: Tensor with shape (mxn)
```

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

Bases: dicee.models.base\_model.BaseKGE

Base class for all neural network modules.

Your models should also subclass this class.

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

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

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

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

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

# 1 Note

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

#### **Variables**

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

## **Parameters**

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

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

forward\_k\_vs\_sample(x: torch.LongTensor, target\_entity\_idx: torch.LongTensor)

```
class dicee.AConEx(args)
```

Bases: dicee.models.base\_model.BaseKGE

Additive Convolutional ComplEx Knowledge Graph Embeddings

```
name = 'AConEx'
     conv2d
     fc_num_input
     fc1
     norm_fc1
     bn_conv2d
     feature_map_dropout
     {\tt residual\_convolution}~(\textit{C\_1: Tuple[torch.Tensor, torch.Tensor]},
                  C_2: Tuple[torch.Tensor, torch.Tensor]) \rightarrow torch.FloatTensor
           Compute residual score of two complex-valued embeddings. :param C_1: a tuple of two pytorch tensors
           that corresponds complex-valued embeddings :param C_2: a tuple of two pytorch tensors that corresponds
           complex-valued embeddings :return:
     forward_k_vs_all(x: torch.Tensor) \rightarrow torch.FloatTensor
     forward\_triples(x: torch.Tensor) \rightarrow torch.FloatTensor
               Parameters
     forward_k_vs_sample (x: torch.Tensor, target_entity_idx: torch.Tensor)
class dicee.AConvO(args: dict)
     Bases: dicee.models.base_model.BaseKGE
     Additive Convolutional Octonion Knowledge Graph Embeddings
     name = 'AConvO'
     conv2d
     fc_num_input
     fc1
     bn_conv2d
     norm_fc1
     feature_map_dropout
     static octonion_normalizer(emb_rel_e0, emb_rel_e1, emb_rel_e2, emb_rel_e3, emb_rel_e4,
                  emb_rel_e5, emb_rel_e6, emb_rel_e7)
     {\tt residual\_convolution}\,(O\_1,\,O\_2)
     forward\_triples(x: torch.Tensor) \rightarrow torch.Tensor
               Parameters
                   x
```

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

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

```
feature_map_dropout
```

```
residual_convolution (Q_1, Q_2)
```

 $forward\_triples (indexed\_triple: torch.Tensor) \rightarrow torch.Tensor$ 

#### **Parameters**

x

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

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

## class dicee.ConvO(args: dict)

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

Base class for all neural network modules.

Your models should also subclass this class.

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

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

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

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

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

## **1** Note

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

#### **Variables**

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

```
name = 'ConvO'
conv2d
fc_num_input
fc1
```

```
bn_conv2d
     norm_fc1
     feature_map_dropout
     static octonion_normalizer(emb_rel_e0, emb_rel_e1, emb_rel_e2, emb_rel_e3, emb_rel_e4,
                  emb_rel_e5, emb_rel_e6, emb_rel_e7)
     residual\_convolution(O\_1, O\_2)
     forward\_triples(x: torch.Tensor) \rightarrow torch.Tensor
               Parameters
     forward k vs all (x: torch. Tensor)
           Given a head entity and a relation (h,r), we compute scores for all entities. [score(h,r,x)|x in Entities] =>
           [0.0,0.1,...,0.8], shape=> (1, |Entities|) Given a batch of head entities and relations => shape (size of batch,|
           Entities 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
     feature_map_dropout
     residual_convolution (C_1: Tuple[torch.Tensor, torch.Tensor],
                  C_2: Tuple[torch.Tensor, torch.Tensor]) \rightarrow torch.FloatTensor
           Compute residual score of two complex-valued embeddings. :param C_1: a tuple of two pytorch tensors
           that corresponds complex-valued embeddings :param C_2: a tuple of two pytorch tensors that corresponds
           complex-valued embeddings :return:
     forward_k_vs_all(x: torch.Tensor) \rightarrow torch.FloatTensor
     forward\_triples(x: torch.Tensor) \rightarrow torch.FloatTensor
               Parameters
     forward_k_vs_sample (x: torch.Tensor, target_entity_idx: torch.Tensor)
class dicee.QMult(args)
     Bases: dicee.models.base_model.BaseKGE
     Base class for all neural network modules.
     Your models should also subclass this class.
```

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

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

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

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

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



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

#### **Variables**

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

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

#### **Parameters**

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

### Returns

Triple scores.

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

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

Absolute value of a quaternion

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

L2 norm of quaternion vector:

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

### **Parameters**

 $\mathbf{x}$  – The vector.

#### Returns

The normalized vector.

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

#### **Parameters**

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

forward\_k\_vs\_all (X)

#### **Parameters**

x

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

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

```
class dicee.OMult(args)
```

Bases: dicee.models.base\_model.BaseKGE

Base class for all neural network modules.

Your models should also subclass this class.

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

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

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

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

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

#### 1 Note

As per the example above, an \_\_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 = 'OMult'
     static octonion_normalizer(emb_rel_e0, emb_rel_e1, emb_rel_e2, emb_rel_e3, emb_rel_e4,
                  emb rel e5, emb rel e6, emb rel e7)
     \verb+score+ (head\_ent\_emb: torch.FloatTensor, rel\_ent\_emb: torch.FloatTensor,
                  tail_ent_emb: torch.FloatTensor)
     k_vs_all_score (bpe_head_ent_emb, bpe_rel_ent_emb, E)
     forward_k_vs_all(X)
           Completed. Given a head entity and a relation (h,r), we compute scores for all possible triples, i.e.,
           [score(h,r,x)|x \text{ in Entities}] => [0.0,0.1,...,0.8], shape=> (1, |Entities|) Given a batch of head entities and
           relations => shape (size of batch, | Entities|)
class dicee.Shallom(args)
     Bases: dicee.models.base_model.BaseKGE
     A shallow neural model for relation prediction (https://arxiv.org/abs/2101.09090)
     name = 'Shallom'
     shallom
     get_embeddings() → Tuple[numpy.ndarray, None]
     forward_k_vs_all (x) \rightarrow \text{torch.FloatTensor}
     forward_triples (x) \rightarrow \text{torch.FloatTensor}
               Parameters
                   x
               Returns
class dicee.LFMult(args)
     Bases: dicee.models.base_model.BaseKGE
     Embedding with polynomial functions. We represent all entities and relations in the polynomial space as: f(x) =
     sum_{i=0}^{d-1} a_k x^{i\%d} and use the three differents scoring function as in the paper to evaluate the score.
     We also consider combining with Neural Networks.
     name = 'LFMult'
     entity_embeddings
     relation_embeddings
     degree
     x values
     forward_triples (idx_triple)
               Parameters
                   x
     construct_multi_coeff(x)
```

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

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

linear (x, w, b)

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

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

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

this part implement the trilinear scoring techniques:

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

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

this part implement the vector triple product scoring techniques:

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

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

## $\mathtt{comp\_func}\,(h,r,t)$

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

#### polynomial(coeff, x, degree)

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

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

pop (coeff, x, degree)

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

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

class dicee.PykeenKGE (args: dict)

Bases: dicee.models.base\_model.BaseKGE

A class for using knowledge graph embedding models implemented in Pykeen

Notes: Pykeen\_DistMult: C Pykeen\_ComplEx: Pykeen\_QuatE: Pykeen\_MuRE: Pykeen\_CP: Pykeen\_HolE: Pykeen\_HolE: Pykeen\_TransD: Pykeen\_TransE: Pykeen\_TransF: Pykeen\_TransH: Pykeen\_TransR:

model\_kwargs

```
name
model
loss_history = []
args
entity_embeddings = None
relation_embeddings = None
forward_k_vs_all (x: torch.LongTensor)
             # => Explicit version by this we can apply bn and dropout
             # (1) Retrieve embeddings of heads and relations + apply Dropout & Normalization if given. h, r =
             self.get_head_relation_representation(x) \# (2) Reshape (1). if self.last_dim > 0:
                       h = h.reshape(len(x), self.embedding\_dim, self.last\_dim) r = r.reshape(len(x), self.embedding\_dim,
                       self.last_dim)
             # (3) Reshape all entities. if self.last_dim > 0:
                       t = self.entity embeddings.weight.reshape(self.num entities, self.embedding dim, self.last dim)
             else:
                       t = self.entity_embeddings.weight
             # (4) Call the score t from interactions to generate triple scores. return self.interaction.score t(h=h, r=r,
             all_entities=t, slice_size=1)
forward\_triples(x: torch.LongTensor) \rightarrow torch.FloatTensor
             # => Explicit version by this we can apply bn and dropout
             # (1) Retrieve embeddings of heads, relations and tails and apply Dropout & Normalization if given. h, r, t =
             self.get_triple_representation(x) \# (2) Reshape (1). if self.last_dim > 0:
                       h = h.reshape(len(x), self.embedding\_dim, self.last\_dim) r = r.reshape(len(x), self.embedding\_dim, self.embeddin
                       self.last_dim) t = t.reshape(len(x), self.embedding_dim, self.last_dim)
             # (3) Compute the triple score return self.interaction.score(h=h, r=r, t=t, slice size=None, slice dim=0)
abstract forward_k_vs_sample (x: torch.LongTensor, target_entity_idx)
Bases: dicee.models.base_model.BaseKGE
```

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

Base class for all neural network modules.

Your models should also subclass this class.

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

```
import torch.nn as nn
import torch.nn.functional as F
class Model(nn.Module):
    def __init__(self) -> None:
        super().__init__()
```

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

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



## 1 Note

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

#### Variables

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

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

## **Parameters**

- yhat\_batch
- y\_batch

forward(x: torch.LongTensor)

## **Parameters**

```
\mathbf{x} (B by T tensor)
```

generate (idx, max\_new\_tokens, temperature=1.0, top\_k=None)

Take a conditioning sequence of indices idx (LongTensor of shape (b,t)) and complete the sequence max\_new\_tokens times, feeding the predictions back into the model each time. Most likely you'll want to make sure to be in model.eval() mode of operation for this.

```
training_step(batch, batch_idx=None)
```

Here you compute and return the training loss and some additional metrics for e.g. the progress bar or logger.

#### **Parameters**

- batch The output of your data iterable, normally a DataLoader.
- batch\_idx The index of this batch.

• dataloader\_idx - The index of the dataloader that produced this batch. (only if multiple dataloaders used)

#### Returns

- Tensor The loss tensor
- dict A dictionary which can include any keys, but must include the key 'loss' in the case of automatic optimization.
- None In automatic optimization, this will skip to the next batch (but is not supported for multi-GPU, TPU, or DeepSpeed). For manual optimization, this has no special meaning, as returning the loss is not required.

In this step you'd normally do the forward pass and calculate the loss for a batch. You can also do fancier things like multiple forward passes or something model specific.

### Example:

```
def training_step(self, batch, batch_idx):
    x, y, z = batch
    out = self.encoder(x)
    loss = self.loss(out, x)
    return loss
```

To use multiple optimizers, you can switch to 'manual optimization' and control their stepping:

```
def __init__(self):
    super().__init__()
    self.automatic_optimization = False

# Multiple optimizers (e.g.: GANs)
def training_step(self, batch, batch_idx):
    opt1, opt2 = self.optimizers()

# do training_step with encoder
    ...
    opt1.step()
    # do training_step with decoder
    ...
    opt2.step()
```

## 1 Note

When accumulate\_grad\_batches > 1, the loss returned here will be automatically normalized by accumulate\_grad\_batches internally.

class dicee.BaseKGE(args: dict)

Bases: BaseKGELightning

Base class for all neural network modules.

Your models should also subclass this class.

Modules can also contain other Modules, allowing them to be nested in a tree structure. You can assign the sub-modules as regular attributes:

```
import torch.nn as nn
import torch.nn.functional as F

class Model(nn.Module):
    def __init__(self) -> None:
        super().__init__()
        self.conv1 = nn.Conv2d(1, 20, 5)
        self.conv2 = nn.Conv2d(20, 20, 5)

    def forward(self, x):
        x = F.relu(self.conv1(x))
        return F.relu(self.conv2(x))
```

Submodules assigned in this way will be registered, and will also have their parameters converted when you call to(), etc.

## 1 Note

As per the example above, an \_\_init\_\_() call to the parent class must be made before assignment on the child.

### Variables

**training** (bool) – Boolean represents whether this module is in training or evaluation mode.

### args

```
embedding_dim = None
num_entities = None
num_relations = None
num_tokens = None
learning_rate = None
learning_rate = None
apply_unit_norm = None
input_dropout_rate = None
hidden_dropout_rate = None
optimizer_name = None
feature_map_dropout_rate = None
kernel_size = None
num_of_output_channels = None
weight_decay = None
loss
selected_optimizer = None
```

```
normalizer_class = None
normalize_head_entity_embeddings
normalize_relation_embeddings
normalize_tail_entity_embeddings
hidden_normalizer
param_init
input_dp_ent_real
input_dp_rel_real
hidden_dropout
loss_history = []
byte_pair_encoding
max_length_subword_tokens
block_size
forward_byte_pair_encoded_k_vs_all (x: torch.LongTensor)
        Parameters
            x (B x 2 x T)
forward_byte_pair_encoded_triple (x: Tuple[torch.LongTensor, torch.LongTensor])
    byte pair encoded neural link predictors
        Parameters
init_params_with_sanity_checking()
forward(x: torch.LongTensor | Tuple[torch.LongTensor, torch.LongTensor],
           y_idx: torch.LongTensor = None)
        Parameters
            • x
            • y_idx
            • ordered_bpe_entities
forward\_triples(x: torch.LongTensor) \rightarrow torch.Tensor
        Parameters
forward_k_vs_all(*args, **kwargs)
forward_k_vs_sample(*args, **kwargs)
get_triple_representation(idx_hrt)
{\tt get\_head\_relation\_representation}\ (indexed\_triple)
```

```
get_sentence_representation(x: torch.LongTensor)
               Parameters
                   • (b (x shape)
                   • 3
                   • t)
     get_bpe_head_and_relation_representation(x: torch.LongTensor)
                  → Tuple[torch.FloatTensor, torch.FloatTensor]
               Parameters
                   x (B x 2 x T)
     \mathtt{get\_embeddings}() \rightarrow \mathsf{Tuple}[\mathsf{numpy}.\mathsf{ndarray}, \mathsf{numpy}.\mathsf{ndarray}]
class dicee.EnsembleKGE (seed_model=None, pretrained_models: List = None)
     name
     train_mode = True
     named_children()
     property example_input_array
     parameters()
     modules()
     __iter__()
     __len__()
     eval()
     to (device)
     mem_of_model()
     __call__(x_batch)
     step()
     get_embeddings()
     __str__()
dicee.create_recipriocal_triples(x)
     Add inverse triples into dask dataframe :param x: :return:
dicee.get_er_vocab(data, file_path: str = None)
dicee.get_re_vocab(data, file_path: str = None)
dicee.get_ee_vocab (data, file_path: str = None)
dicee.timeit(func)
dicee.save_pickle(*, data: object = None, file_path=str)
```

```
dicee.load_pickle(file_path=str)
dicee.load_term_mapping(file_path=str)
dicee.select_model(args: dict, is_continual_training: bool = None, storage_path: str = None)
dicee.load_model(path_of_experiment_folder: str, model_name='model.pt', verbose=0)
             → Tuple[object, Tuple[dict, dict]]
     Load weights and initialize pytorch module from namespace arguments
dicee.load_model_ensemble(path_of_experiment_folder: str)
             → Tuple[dicee.models.base_model.BaseKGE, Tuple[pandas.DataFrame, pandas.DataFrame]]
     Construct Ensemble Of weights and initialize pytorch module from namespace arguments
       (1) Detect models under given path
       (2) Accumulate parameters of detected models
       (3) Normalize parameters
       (4) Insert (3) into model.
dicee.save_numpy_ndarray(*, data: numpy.ndarray, file_path: str)
dicee.numpy_data_type_changer(train\_set: numpy.ndarray, num: int) \rightarrow numpy.ndarray
     Detect most efficient data type for a given triples :param train_set: :param num: :return:
dicee.save_checkpoint_model(model, path: str) \rightarrow None
     Store Pytorch model into disk
dicee.store(trained_model, model_name: str = 'model', full_storage_path: str = None,
            save\_embeddings\_as\_csv=False) \rightarrow None
dicee.add_noisy_triples(train\_set: pandas.DataFrame, add\_noise\_rate: float) \rightarrow pandas.DataFrame
     Add randomly constructed triples :param train_set: :param add_noise_rate: :return:
dicee.read_or_load_kg(args, cls)
dicee.intialize_model(args: dict, verbose=0) \rightarrow Tuple[object, str]
dicee.load_json(p: str) \rightarrow dict
dicee.save_embeddings(embeddings: numpy.ndarray, indexes, path: str) \rightarrow None
     Save it as CSV if memory allows. :param embeddings: :param indexes: :param path: :return:
dicee.random_prediction(pre_trained_kge)
dicee.deploy_triple_prediction(pre_trained_kge, str_subject, str_predicate, str_object)
dicee.deploy_tail_entity_prediction(pre_trained_kge, str_subject, str_predicate, top_k)
dicee.deploy_head_entity_prediction(pre_trained_kge, str_object, str_predicate, top_k)
dicee.deploy_relation_prediction(pre_trained_kge, str_subject, str_object, top_k)
dicee.vocab_to_parquet(vocab_to_idx, name, path_for_serialization, print_into)
dicee.create_experiment_folder(folder_name='Experiments')
dicee.continual_training_setup_executor(executor) \rightarrow None
```

```
dicee.exponential_function (x: numpy.ndarray, lam: float, ascending_order=True) \rightarrow torch.FloatTensor
dicee.load_numpy(path) \rightarrow numpy.ndarray
dicee.evaluate(entity_to_idx, scores, easy_answers, hard_answers)
     # @TODO: CD: Renamed this function Evaluate multi hop query answering on different query types
dicee.download_file (url, destination_folder='.')
dicee.download_files_from_url(base\_url: str, destination\_folder='.') \rightarrow None
           Parameters
                 base_url
                                                   "https://files.dice-research.org/projects/DiceEmbeddings/
                   KINSHIP-Keci-dim128-epoch256-KvsAll")
                 • destination_folder(e.g. "KINSHIP-Keci-dim128-epoch256-KvsAll")
dicee.download_pretrained_model(url: str) \rightarrow str
dicee.write_csv_from_model_parallel(path: str)
     Create
\texttt{dicee.from\_pretrained\_model\_write\_embeddings\_into\_csv}(\textit{path: str}) \rightarrow \texttt{None}
class dicee.DICE_Trainer(args, is_continual_training: bool, storage_path, evaluator=None)
     DICE Trainer implement
           1- Pytorch Lightning trainer (https://pytorch-lightning.readthedocs.io/en/stable/common/trainer.html)
           2- Multi-GPU Trainer(https://pytorch.org/docs/stable/generated/torch.nn.parallel.DistributedDataParallel.
           html) 3- CPU Trainer
           args
           is_continual_training:bool
           storage_path:str
           evaluator:
           report:dict
     report
     args
     trainer = None
     is_continual_training
     storage_path
     evaluator = None
     form_of_labelling = None
     continual_start (knowledge_graph)
           (1) Initialize training.
           (2) Load model
           (3) Load trainer (3) Fit model
```

#### **Parameter**

#### returns

- model
- form\_of\_labelling (str)

initialize\_trainer(callbacks: List)

→ lightning.Trainer | dicee.trainer.model\_parallelism.TensorParallel | dicee.trainer.torch\_trainer.TorchTrainer | dicee.trainer.TorchTrainer | dicee.trainer.torch\_trainer.TorchTrainer | dicee.trainer.torch\_trainer.TorchTrainer | dicee.trainer.torch\_trai

```
initialize_or_load_model()
```

 $init\_dataloader(dataset: torch.utils.data.Dataset) \rightarrow torch.utils.data.DataLoader$ 

init\_dataset() → torch.utils.data.Dataset

 $\begin{tabular}{ll} \textbf{start} & (knowledge\_graph: dicee.knowledge\_graph.KG \mid numpy.memmap) \\ & \rightarrow \textbf{Tuple}[dicee.models.base\_model.BaseKGE, str] \\ \end{tabular}$ 

Start the training

- (1) Initialize Trainer
- (2) Initialize or load a pretrained KGE model

in DDP setup, we need to load the memory map of already read/index KG.

 $\textbf{k\_fold\_cross\_validation} (\textit{dataset}) \rightarrow \text{Tuple}[\textit{dicee.models.base\_model.BaseKGE}, \text{str}]$ 

Perform K-fold Cross-Validation

- 1. Obtain K train and test splits.
- 2. For each split,
  - 2.1 initialize trainer and model 2.2. Train model with configuration provided in args. 2.3. Compute the mean reciprocal rank (MRR) score of the model on the test respective split.
- 3. Report the mean and average MRR.

## **Parameters**

- self
- dataset

#### Returns

model

class dicee. KGE (path=None, url=None, construct\_ensemble=False, model\_name=None)

 $Bases: \ \textit{dicee.abstracts.BaseInteractiveKGE}$ 

Knowledge Graph Embedding Class for interactive usage of pre-trained models

```
__str__()
```

to (device: str)  $\rightarrow$  None

 $\begin{tabular}{ll} \tt get\_transductive\_entity\_embeddings (\it indices: torch.LongTensor \mid List[str], as\_pytorch=False, \\ as\_numpy=False, as\_list=True) \rightarrow {\tt torch.FloatTensor \mid numpy.ndarray \mid List[float]} \\ \end{tabular}$ 

 $create\_vector\_database$  (collection\_name: str, distance: str, location: str = 'localhost', port: int = 6333)

```
generate (h=", r=")
eval_lp_performance (dataset=List[Tuple[str, str, str]], filtered=True)
predict_missing_head_entity (relation: List[str] | str, tail_entity: List[str] | str, within=None)
               \rightarrow Tuple
     Given a relation and a tail entity, return top k ranked head entity.
     argmax_{e} in E  f(e,r,t), where r in R, t in E.
     Parameter
     relation: Union[List[str], str]
     String representation of selected relations.
     tail_entity: Union[List[str], str]
     String representation of selected entities.
     k: int
     Highest ranked k entities.
     Returns: Tuple
     Highest K scores and entities
predict_missing_relations (head_entity: List[str] | str, tail_entity: List[str] | str, within=None)
     Given a head entity and a tail entity, return top k ranked relations.
     argmax_{r in R} f(h,r,t), where h, t in E.
     Parameter
     head_entity: List[str]
     String representation of selected entities.
     tail_entity: List[str]
     String representation of selected entities.
     k: int
     Highest ranked k entities.
     Returns: Tuple
     Highest K scores and entities
predict_missing_tail_entity (head_entity: List[str] | str, relation: List[str] | str,
              within: List[str] = None \rightarrow torch.FloatTensor
     Given a head entity and a relation, return top k ranked entities
     argmax_{e} = in E f(h,r,e), where h in E and r in R.
```

```
Parameter
```

```
head_entity: List[str]
```

String representation of selected entities.

```
tail_entity: List[str]
```

String representation of selected entities.

## **Returns: Tuple**

scores

 $predict(*, h: List[str] | str = None, r: List[str] | str = None, t: List[str] | str = None, within=None, logits=True) <math>\rightarrow$  torch. Float Tensor

## **Parameters**

- logits
- h
- r
- t
- within

Predict missing item in a given triple.

### **Parameter**

head\_entity: Union[str, List[str]]

String representation of selected entities.

relation: Union[str, List[str]]

String representation of selected relations.

tail\_entity: Union[str, List[str]]

String representation of selected entities.

k: int

Highest ranked k item.

## **Returns: Tuple**

Highest K scores and items

Predict triple score

```
Parameter
```

```
head entity: List[str]
     String representation of selected entities.
     relation: List[str]
     String representation of selected relations.
     tail_entity: List[str]
     String representation of selected entities.
     logits: bool
     If logits is True, unnormalized score returned
     Returns: Tuple
     pytorch tensor of triple score
t_norm(tens_1: torch.Tensor, tens_2: torch.Tensor, tnorm: str = 'min') \rightarrow torch.Tensor
tensor_t_norm (subquery_scores: torch.FloatTensor, tnorm: str = 'min') \rightarrow torch.FloatTensor
     Compute T-norm over [0,1] ^{n imes d} where n denotes the number of hops and d denotes number of
     entities
t\_conorm (tens_1: torch.Tensor, tens_2: torch.Tensor, tconorm: str = 'min') \rightarrow torch.Tensor
negnorm(tens\_1: torch.Tensor, lambda\_: float, neg\_norm: str = 'standard') \rightarrow torch.Tensor
return_multi_hop_query_results (aggregated_query_for_all_entities, k: int, only_scores)
single_hop_query_answering (query: tuple, only_scores: bool = True, k: int = None)
answer multi hop query (query type: str = None, query: Tuple[str | Tuple[str, str], Ellipsis] = None,
             queries: List[Tuple[str | Tuple[str, str], Ellipsis]] = None, tnorm: str = 'prod',
             neg_norm: str = 'standard', lambda_: float = 0.0, k: int = 10, only_scores=False)
              → List[Tuple[str, torch.Tensor]]
     # @TODO: Refactoring is needed # @TODO: Score computation for each query type should be done in a
     static function
     Find an answer set for EPFO queries including negation and disjunction
     Parameter
     query_type: str The type of the query, e.g., "2p".
     query: Union[str, Tuple[str, Tuple[str, str]]] The query itself, either a string or a nested tuple.
     queries: List of Tuple[Union[str, Tuple[str, str]], ...]
     tnorm: str The t-norm operator.
     neg_norm: str The negation norm.
     lambda_: float lambda parameter for sugeno and yager negation norms
     k: int The top-k substitutions for intermediate variables.
```

## returns

• List[Tuple[str, torch.Tensor]]

```
• Entities and corresponding scores sorted in the descening order of scores
find_missing_triples (confidence: float, entities: List[str] = None, relations: List[str] = None,
              topk: int = 10, at_most: int = sys.maxsize) \rightarrow Set
          Find missing triples
          Iterative over a set of entities E and a set of relation R:
     orall e in E and orall r in R f(e,r,x)
          Return (e,r,x)
     otin G and f(e,r,x) > confidence
          confidence: float
          A threshold for an output of a sigmoid function given a triple.
          topk: int
          Highest ranked k item to select triples with f(e,r,x) > confidence.
          at_most: int
          Stop after finding at_most missing triples
          \{(e,r,x) \mid f(e,r,x) > \text{confidence land } (e,r,x)\}
     otin G
deploy(share: bool = False, top\_k: int = 10)
train_triples (h: List[str], r: List[str], t: List[str], labels: List[float], iteration=2, optimizer=None)
train_k_vs_all(h, r, iteration=1, lr=0.001)
     Train k vs all :param head entity: :param relation: :param iteration: :param lr: :return:
train(kg, lr=0.1, epoch=10, batch\_size=32, neg\_sample\_ratio=10, num\_workers=1) \rightarrow None
     Retrained a pretrain model on an input KG via negative sampling.
train_literals (train_file_path: str = None, num_epochs: int = 100, lit_lr: float = 0.001,
              eval\_litreal\_preds: bool = True, eval\_file\_path: str = None,
             lit_normalization_type: str = 'z-norm', batch_size: int = 1024, sampling_ratio: float = None,
              random\_seed=1)
     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.
               • eval_litreal_preds (bool) - If True, evaluate the model after training.
               • eval_file_path (str) – Path to evaluation data file.
```

• 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.

```
predict_literals (entity: List[str] | str = None, attribute: List[str] | str = None, denormalize preds: bool = True) \rightarrow torch.FloatTensor
```

Predicts literal values for given entities and attributes.

#### **Parameters**

- entity (Union[List[str], str]) Entity or list of entities to predict literals for.
- attribute (Union[List[str], str]) Attribute or list of attributes to predict literals for.
- denormalize\_preds (bool) If True, denormalizes the predictions.

#### Returns

Predictions for the given entities and attributes.

### Return type

torch.FloatTensor

```
evaluate\_literal\_prediction (eval\_file\_path: str = None, store\_lit\_preds: bool = True, eval\_literals: bool = True)
```

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.

#### Returns

None

Bases: torch.utils.data.Dataset

An abstract class representing a Dataset.

All datasets that represent a map from keys to data samples should subclass it. All subclasses should overwrite \_\_getitem\_\_(), supporting fetching a data sample for a given key. Subclasses could also optionally overwrite \_\_len\_\_(), which is expected to return the size of the dataset by many Sampler implementations and the default options of DataLoader. Subclasses could also optionally implement \_\_getitems\_\_(), for speedup batched samples loading. This method accepts list of indices of samples of batch and returns list of samples.

## **1** Note

DataLoader by default constructs an index sampler that yields integral indices. To make it work with a mapstyle dataset with non-integral indices/keys, a custom sampler must be provided.

```
train_set
  ordered_bpe_entities
num_bpe_entities
neg_ratio
num_datapoints
  __len__()
  __getitem__(idx)
collate_fn(batch_shaped_bpe_triples: List[Tuple[torch.Tensor, torch.Tensor]])
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.

## Note

DataLoader by default constructs an index sampler that yields integral indices. To make it work with a mapstyle dataset with non-integral indices/keys, a custom sampler must be provided.

```
train_set

train_indices_target

target_dim

num_datapoints

torch_ordered_shaped_bpe_entities

collate_fn = None

__len__()
__getitem__(idx)
```

```
class dicee.MultiClassClassificationDataset (subword_units: numpy.ndarray, block_size: int = 8)
     Bases: torch.utils.data.Dataset
     Dataset for the 1vsALL training strategy
          Parameters
                • train_set_idx - Indexed triples for the training.
                • entity_idxs - mapping.
                • relation_idxs - mapping.
                • form - ?
                • num_workers - int
                                           for
                                                 https://pytorch.org/docs/stable/data.html#torch.utils.data.
                  DataLoader
          Return type
              torch.utils.data.Dataset
     train_data
     block_size = 8
     num_of_data_points
     collate_fn = None
     __len__()
     \__{\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 - ?
                                          for https://pytorch.org/docs/stable/data.html#torch.utils.data.
                • num_workers - int
                  DataLoader
          Return type
              torch.utils.data.Dataset
     train_data
     target_dim
     collate_fn = None
     __len__()
```

 $\__getitem__(idx)$ 

class dicee. KvsAll (train\_set\_idx: numpy.ndarray, entity\_idxs, relation\_idxs, form, store=None, label\_smoothing\_rate: float = 0.0)

Bases: torch.utils.data.Dataset

#### Creates a dataset for KvsAll training by inheriting from torch.utils.data.Dataset.

Let D denote a dataset for KvsAll training and be defined as D:=  $\{(x,y)_i\}_i ^N$ , where x: (h,r) is an unique tuple of an entity h in E and a relation r in R that has been seed in the input graph. y: denotes a multi-label vector in  $[0,1]^{\{E\}}$  is a binary label.

orall  $y_i = 1$  s.t. (h r  $E_i$ ) in KG



### train\_set\_idx

[numpy.ndarray] n by 3 array representing n triples

#### entity idxs

[dictonary] string representation of an entity to its integer id

## relation\_idxs

[dictonary] string representation of a relation to its integer id

self: torch.utils.data.Dataset

```
>>> a = KvsAll()
>>> a
? array([0, 1, 2, 3, 4, 5, 6, 7, 8, 9])
```

```
train_data = None
train_target = None
label_smoothing_rate
collate_fn = None
__len__()
__getitem__(idx)
```

class dicee. AllvsAll (train\_set\_idx: numpy.ndarray, entity\_idxs, relation\_idxs, label\_smoothing\_rate=0.0)

Bases: torch.utils.data.Dataset

## Creates a dataset for 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
```

AllysAll extends KysAll via none existing (h,r). Hence, it adds data points that are labelled without 1s,

only with 0s.

#### train\_set\_idx

[numpy.ndarray] n by 3 array representing n triples

#### entity\_idxs

[dictonary] string representation of an entity to its integer id

#### relation\_idxs

[dictonary] string representation of a relation to its integer id

self: torch.utils.data.Dataset

```
>>> a = AllvsAll()
>>> a
? array([0, 1, 2, 3, 4, 5, 6, 7, 8, 9])
```

```
train_data = None
train_target = None
label_smoothing_rate
collate_fn = None
target_dim
__len__()
__getitem__(idx)
```

class dicee.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.

```
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__()
     \__{\texttt{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
```

**Return type** 

An abstract class representing a Dataset.

All datasets that represent a map from keys to data samples should subclass it. All subclasses should overwrite \_\_getitem\_\_(), supporting fetching a data sample for a given key. Subclasses could also optionally overwrite \_\_len\_\_(), which is expected to return the size of the dataset by many Sampler implementations and the default options of DataLoader. Subclasses could also optionally implement \_\_getitems\_\_(), for speedup batched samples loading. This method accepts list of indices of samples of batch and returns list of samples.



DataLoader by default constructs an index sampler that yields integral indices. To make it work with a map-style dataset with non-integral indices/keys, a custom sampler must be provided.

```
neg_sample_ratio
      train_set
      length
      num_entities
      num relations
      __len__()
      getitem (idx)
class dicee. TriplePredictionDataset (train_set: numpy.ndarray, num_entities: int, num_relations: int,
             neg sample ratio: int = 1, label smoothing rate: float = 0.0)
      Bases: torch.utils.data.Dataset
           Triple Dataset
                D := \{(x)_i\}_i \ ^N, \text{ where }
                    . x:(h,r, t) in KG is a unique h in E and a relation r in R and . collact_fn => Generates
                    negative triples
                collect_fn:
      orall (h,r,t) in G obtain, create negative triples \{(h,r,x),(r,t),(h,m,t)\}
                y:labels are represented in torch.float16
           train_set_idx
                Indexed triples for the training.
           entity idxs
                mapping.
           relation_idxs
                mapping.
           form
           store
           label_smoothing_rate
           collate_fn: batch:List[torch.IntTensor] Returns ——- torch.utils.data.Dataset
```

```
label_smoothing_rate
     neg_sample_ratio
     train_set
     length
     num_entities
     num_relations
     __len__()
     \__getitem__(idx)
     collate_fn (batch: List[torch.Tensor])
class dicee. CVDataModule (train_set_idx: numpy.ndarray, num_entities, num_relations, neg_sample_ratio,
            batch size, num workers)
     Bases: \verb"pytorch_lightning.LightningDataModule" \\
     Create a Dataset for cross validation
          Parameters
                 • train_set_idx - Indexed triples for the training.
                 • num_entities - entity to index mapping.
                 • num_relations - relation to index mapping.
                 • batch_size - int
                 • form - ?
                                                  https://pytorch.org/docs/stable/data.html#torch.utils.data.
                 • num_workers -
                                        int
                                             for
                   DataLoader
           Return type
     train_set_idx
     num_entities
     num_relations
     neg_sample_ratio
     batch_size
     num_workers
     train\_dataloader() \rightarrow torch.utils.data.DataLoader
           An iterable or collection of iterables specifying training samples.
           For more information about multiple dataloaders, see this section.
                  dataloader
                               you
                                      return
                                               will
                                                      not
                                                             be
                                                                   reloaded
                                                                              unless
                                                                                        you
                                                                                                     :param-
           ref: ~pytorch_lightning.trainer.trainer.Trainer.reload_dataloaders_every_n_epochs to a positive
          integer.
           For data processing use the following pattern:
```

- download in prepare\_data()
- process and split in setup ()

However, the above are only necessary for distributed processing.

## **▲** Warning

do not assign state in prepare\_data

- fit()
- prepare\_data()
- setup()

## **1** Note

Lightning tries to add the correct sampler for distributed and arbitrary hardware. There is no need to set it yourself.

```
setup(*args, **kwargs)
```

Called at the beginning of fit (train + validate), validate, test, or predict. This is a good hook when you need to build models dynamically or adjust something about them. This hook is called on every process when using DDP.

#### **Parameters**

```
stage - either 'fit', 'validate', 'test', or 'predict'
```

Example:

```
class LitModel(...):
    def __init__(self):
        self.11 = None

def prepare_data(self):
        download_data()
        tokenize()

# don't do this
        self.something = else

def setup(self, stage):
        data = load_data(...)
        self.11 = nn.Linear(28, data.num_classes)
```

## transfer\_batch\_to\_device(\*args, \*\*kwargs)

Override this hook if your DataLoader returns tensors wrapped in a custom data structure.

The data types listed below (and any arbitrary nesting of them) are supported out of the box:

- torch. Tensor or anything that implements .to(...)
- list
- dict

• tuple

For anything else, you need to define how the data is moved to the target device (CPU, GPU, TPU, ...).



### **1** Note

This hook should only transfer the data and not modify it, nor should it move the data to any other device than the one passed in as argument (unless you know what you are doing). To check the current state of execution of this hook you can use self.trainer.training/testing/validating/predicting so that you can add different logic as per your requirement.

#### **Parameters**

- batch A batch of data that needs to be transferred to a new device.
- device The target device as defined in PyTorch.
- dataloader idx The index of the dataloader to which the batch belongs.

#### Returns

A reference to the data on the new device.

### Example:

```
def transfer_batch_to_device(self, batch, device, dataloader_idx):
   if isinstance(batch, CustomBatch):
        # move all tensors in your custom data structure to the device
       batch.samples = batch.samples.to(device)
        batch.targets = batch.targets.to(device)
   elif dataloader_idx == 0:
        # skip device transfer for the first dataloader or anything you wish
   else:
        batch = super().transfer_batch_to_device(batch, device, dataloader_
\rightarrowidx)
    return batch
```

## See also

- move\_data\_to\_device()
- apply\_to\_collection()

#### prepare\_data(\*args, \*\*kwargs)

Use this to download and prepare data. Downloading and saving data with multiple processes (distributed settings) will result in corrupted data. Lightning ensures this method is called only within a single process, so you can safely add your downloading logic within.



## Warning

DO NOT set state to the model (use setup instead) since this is NOT called on every device

## Example:

```
def prepare_data(self):
    # good
    download_data()
    tokenize()
    etc()

# bad
self.split = data_split
self.some_state = some_other_state()
```

In a distributed environment, prepare\_data can be called in two ways (using prepare\_data\_per\_node)

- 1. Once per node. This is the default and is only called on LOCAL\_RANK=0.
- 2. Once in total. Only called on GLOBAL\_RANK=0.

## Example:

```
# DEFAULT
# called once per node on LOCAL_RANK=0 of that node
class LitDataModule(LightningDataModule):
    def __init__(self):
        super().__init__()
        self.prepare_data_per_node = True

# call on GLOBAL_RANK=0 (great for shared file systems)
class LitDataModule(LightningDataModule):
    def __init__(self):
        super().__init__()
        self.prepare_data_per_node = False
```

This is called before requesting the dataloaders:

```
model.prepare_data()
initialize_distributed()
model.setup(stage)
model.train_dataloader()
model.val_dataloader()
model.test_dataloader()
model.predict_dataloader()
```

```
train_path
val_path
test_path
gen_valid = False
gen_test = True
seed = 1
```

```
max_ans_num = 1000000.0
      mode
      ent2id = None
      rel2id: Dict = None
      ent_in: Dict
      ent_out: Dict
      query_name_to_struct
      list2tuple(list_data)
      tuple2list(x: List | Tuple) \rightarrow List | Tuple
           Convert a nested tuple to a nested list.
      set_global_seed(seed: int)
           Set seed
      construct\_graph(paths: List[str]) \rightarrow Tuple[Dict, Dict]
           Construct graph from triples Returns dicts with incoming and outgoing edges
      fill_query (query_structure: List[str | List], ent_in: Dict, ent_out: Dict, answer: int) \rightarrow bool
           Private method for fill_query logic.
      achieve_answer (query: List[str | List], ent_in: Dict, ent_out: Dict) → set
           Private method for achieve_answer logic. @TODO: Document the code
      write_links(ent_out, small_ent_out)
      ground_queries (query_structure: List[str | List], ent_in: Dict, ent_out: Dict, small_ent_in: Dict,
                   small_ent_out: Dict, gen_num: int, query_name: str)
           Generating queries and achieving answers
      unmap (query_type, queries, tp_answers, fp_answers, fn_answers)
      unmap_query (query_structure, query, id2ent, id2rel)
      generate_queries (query_struct: List, gen_num: int, query_type: str)
           Passing incoming and outgoing edges to ground queries depending on mode [train valid or text] and getting
           queries and answers in return @ TODO: create a class for each single query struct
      save_queries (query_type: str, gen_num: int, save_path: str)
      abstract load_queries(path)
      get_queries (query_type: str, gen_num: int)
      static save_queries_and_answers (path: str, data: List[Tuple[str, Tuple[collections.defaultdict]]])
                    \rightarrow None
           Save Queries into Disk
      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, 17
dicee.callbacks, 19
dicee.config, 25
dicee.dataset_classes, 28
dicee.eval_static_funcs, 40
dicee.evaluator, 41
dicee.executer, 43
dicee.knowledge_graph, 44
dicee.knowledge_graph_embeddings,46
dicee.literal_classes, 51
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.octonion, 79
dicee.models.pykeen_models, 82
dicee.models.quaternion, 83
dicee.models.real, 86
dicee.models.static_funcs, 88
dicee.models.transformers, 88
dicee.query_generator, 142
dicee.read_preprocess_save_load_kg, 143
dicee.read_preprocess_save_load_kg.preprocess,
dicee.read_preprocess_save_load_kg.read_from_disk,
        144
dicee.read_preprocess_save_load_kg.save_load_disk,
dicee.read_preprocess_save_load_kg.util,
       145
dicee.sanity_checkers, 150
dicee.scripts, 151
dicee.scripts.index_serve, 151
dicee.scripts.run, 153
dicee.static_funcs, 154
dicee.static_funcs_training, 157
dicee.static_preprocess_funcs, 157
dicee.trainer, 158
dicee.trainer.dice_trainer, 158
dicee.trainer.model_parallelism, 160
dicee.trainer.torch_trainer, 161
dicee.trainer.torch_trainer_ddp, 162
```

## Index

# Non-alphabetical

```
__call__() (dicee.EnsembleKGE method), 191
 _call__() (dicee.models.base_model.IdentityClass method), 64
__call__() (dicee.models.ensemble.EnsembleKGE method), 75
__call__() (dicee.models.IdentityClass method), 105, 116, 122
__class_vars__ (dicee.scripts.index_serve.StringListRequest attribute), 152
__getitem__() (dicee.AllvsAll method), 203
__getitem__() (dicee.BPE_NegativeSamplingDataset method), 200
__getitem__() (dicee.dataset_classes.AllvsAll method), 33
__getitem__() (dicee.dataset_classes.BPE_NegativeSamplingDataset method), 30
__getitem__() (dicee.dataset_classes.KvsAll method), 32
__getitem__() (dicee.dataset_classes.KvsSampleDataset method), 35
__getitem__() (dicee.dataset_classes.MultiClassClassificationDataset method), 31
__getitem__() (dicee.dataset_classes.MultiLabelDataset method), 30
__getitem__() (dicee.dataset_classes.NegSampleDataset method), 36
__getitem__() (dicee.dataset_classes.OnevsAllDataset method), 31
__getitem__() (dicee.dataset_classes.OnevsSample method), 34
__getitem__() (dicee.dataset_classes.TriplePredictionDataset method), 36
__getitem__() (dicee.KvsAll method), 202
__getitem__() (dicee.KvsSampleDataset method), 205
__getitem__() (dicee.literal_classes.LiteralDataset method), 54
__getitem__() (dicee.MultiClassClassificationDataset method), 201
__getitem__() (dicee.MultiLabelDataset method), 200
__getitem__() (dicee.NegSampleDataset method), 206
__getitem__() (dicee.OnevsAllDataset method), 201
__getitem__() (dicee.OnevsSample method), 204
__getitem__() (dicee.TriplePredictionDataset method), 207
__iter__() (dicee.config.Namespace method), 28
__iter__() (dicee.EnsembleKGE method), 191
__iter__() (dicee.knowledge_graph.KG method), 46
__iter__() (dicee.models.ensemble.EnsembleKGE method), 75
__len__() (dicee.AllvsAll method), 203
__len__() (dicee.BPE_NegativeSamplingDataset method), 200
__len__() (dicee.dataset_classes.AllvsAll method), 33
__len__() (dicee.dataset_classes.BPE_NegativeSamplingDataset method), 30
__len__() (dicee.dataset_classes.KvsAll method), 32
__len__() (dicee.dataset_classes.KvsSampleDataset method), 35
__len__() (dicee.dataset_classes.MultiClassClassificationDataset method), 31
__len__() (dicee.dataset_classes.MultiLabelDataset method), 30
__len__() (dicee.dataset_classes.NegSampleDataset method), 36
__len__() (dicee.dataset_classes.OnevsAllDataset method), 31
__len__() (dicee.dataset_classes.OnevsSample method), 34
__len__() (dicee.dataset_classes.TriplePredictionDataset method), 36
__len__() (dicee.EnsembleKGE method), 191
__len__() (dicee.knowledge_graph.KG method), 46
  _len__() (dicee.KvsAll method), 202
__len__() (dicee.KvsSampleDataset method), 205
__len__() (dicee.literal_classes.LiteralDataset method), 54
__len__() (dicee.models.ensemble.EnsembleKGE method), 75
__len__() (dicee.MultiClassClassificationDataset method), 201
__len__() (dicee.MultiLabelDataset method), 200
__len__() (dicee.NegSampleDataset method), 206
__len__() (dicee.OnevsAllDataset method), 201
__len__() (dicee.OnevsSample method), 204
__len__() (dicee.TriplePredictionDataset method), 207
__private_attributes__(dicee.scripts.index_serve.StringListRequest attribute). 152
__pydantic_complete__ (dicee.scripts.index_serve.StringListRequest attribute), 152
__pydantic_computed_fields__ (dicee.scripts.index_serve.StringListRequest attribute), 153
__pydantic_core_schema__ (dicee.scripts.index_serve.StringListRequest attribute), 152
__pydantic_custom_init__ (dicee.scripts.index_serve.StringListRequest attribute), 152
__pydantic_decorators__ (dicee.scripts.index_serve.StringListRequest attribute), 152
__pydantic_extra__ (dicee.scripts.index_serve.StringListRequest attribute), 153
__pydantic_fields__ (dicee.scripts.index_serve.StringListRequest attribute), 153
__pydantic_fields_set__ (dicee.scripts.index_serve.StringListRequest attribute), 153
__pydantic_generic_metadata__ (dicee.scripts.index_serve.StringListRequest attribute), 152
```

```
__pydantic_parent_namespace__(dicee.scripts.index_serve.StringListRequest attribute), 153
__pydantic_post_init__ (dicee.scripts.index_serve.StringListRequest attribute), 153
__pydantic_private__ (dicee.scripts.index_serve.StringListRequest attribute), 153
__pydantic_root_model__ (dicee.scripts.index_serve.StringListRequest attribute), 153
__pydantic_serializer__(dicee.scripts.index_serve.StringListRequest attribute), 153
__pydantic_validator__ (dicee.scripts.index_serve.StringListRequest attribute), 153
__setstate__() (dicee.models.ADOPT method), 96
__setstate__() (dicee.models.adopt.ADOPT method), 55
__signature__ (dicee.scripts.index_serve.StringListRequest attribute), 152
__str__() (dicee.EnsembleKGE method), 191
__str__() (dicee.KGE method), 194
__str__() (dicee.knowledge_graph_embeddings.KGE method), 46
__str__() (dicee.models.ensemble.EnsembleKGE method), 75
__version__ (in module dicee), 211
Α
AbstractCallback (class in dicee.abstracts), 15
AbstractPPECallback (class in dicee.abstracts), 17
AbstractTrainer (class in dicee.abstracts), 12
AccumulateEpochLossCallback (class in dicee.callbacks), 19
achieve_answer() (dicee.query_generator.QueryGenerator method), 143
achieve_answer() (dicee.QueryGenerator method), 211
AConEx (class in dicee), 177
AConEx (class in dicee.models), 112
AConEx (class in dicee.models.complex), 72
AConvo (class in dicee), 178
AConvo (class in dicee.models), 124
AConvo (class in dicee.models.octonion), 81
AConvQ (class in dicee), 179
AConvQ (class in dicee.models), 118
AConvQ (class in dicee.models.quaternion), 85
adaptive_swa (dicee.config.Namespace attribute), 28
\verb|add_new_entity_embeddings()| \textit{(dicee.abstracts.BaseInteractiveKGE method)}, 15
add_noise_rate (dicee.config.Namespace attribute), 26
add_noise_rate (dicee.knowledge_graph.KG attribute), 45
add_noisy_triples() (in module dicee), 192
add_noisy_triples() (in module dicee.static_funcs), 156
add_noisy_triples_into_training() (dicee.read_preprocess_save_load_kg.read_from_disk.ReadFromDisk_method), 145
add_noisy_triples_into_training() (dicee.read_preprocess_save_load_kg.ReadFromDisk method), 150
add_reciprocal (dicee.knowledge_graph.KG attribute), 45
ADOPT (class in dicee.models), 96
ADOPT (class in dicee.models.adopt), 54
adopt () (in module dicee.models.adopt), 55
AllvsAll (class in dicee), 202
AllvsAll (class in dicee.dataset_classes), 32
alphas (dicee.abstracts.AbstractPPECallback attribute), 17
alphas (dicee.callbacks.ASWA attribute), 23
analyse () (in module dicee.analyse experiments), 19
\verb"answer_multi_hop_query()" (\textit{dicee.KGE method}), 197
\verb"answer_multi_hop_query" () \textit{ (dicee.knowledge\_graph\_embeddings.KGE method)}, 49
app (in module dicee.scripts.index_serve), 152
apply_coefficients() (dicee.DeCaL method), 174
apply_coefficients() (dicee.Keci method), 170
apply_coefficients() (dicee.models.clifford.DeCaL method), 69
apply_coefficients() (dicee.models.clifford.Keci method), 66
apply_coefficients() (dicee.models.DeCaL method), 130
apply_coefficients() (dicee.models.Keci method), 126
apply_reciprical_or_noise() (in module dicee.read_preprocess_save_load_kg.util), 148
apply_semantic_constraint (dicee.abstracts.BaseInteractiveKGE attribute), 14
apply_unit_norm (dicee.BaseKGE attribute), 189
apply_unit_norm (dicee.models.base_model.BaseKGE attribute), 62
apply_unit_norm (dicee.models.BaseKGE attribute), 103, 106, 109, 114, 120, 133, 136
args (dicee.BaseKGE attribute), 189
args (dicee.DICE_Trainer attribute), 193
args (dicee.evaluator.Evaluator attribute), 42
args (dicee.executer.Execute attribute), 43
args (dicee.models.base_model.BaseKGE attribute), 62
```

```
args (dicee.models.base model.IdentityClass attribute), 64
args (dicee.models.BaseKGE attribute), 102, 106, 109, 114, 120, 132, 136
args (dicee.models.IdentityClass attribute), 105, 116, 122
args (dicee.models.pykeen_models.PykeenKGE attribute), 82
args (dicee.models.PykeenKGE attribute), 134
args (dicee.PykeenKGE attribute), 186
args (dicee.trainer.DICE_Trainer attribute), 164
args (dicee.trainer.dice_trainer.DICE_Trainer attribute), 159
ASWA (class in dicee.callbacks), 22
aswa (dicee.analyse_experiments.Experiment attribute), 18
attn (dicee.models.transformers.Block attribute), 93
attn_dropout (dicee.models.transformers.CausalSelfAttention attribute), 91
attributes (dicee.abstracts.AbstractTrainer attribute), 12
auto_batch_finding (dicee.config.Namespace attribute), 28
В
backend (dicee.config.Namespace attribute), 26
backend (dicee.knowledge_graph.KG attribute), 45
BaseInteractiveKGE (class in dicee.abstracts), 13
BaseKGE (class in dicee), 188
BaseKGE (class in dicee.models), 102, 105, 109, 113, 119, 132, 135
BaseKGE (class in dicee.models.base_model), 61
BaseKGELightning (class in dicee.models), 96
BaseKGELightning (class in dicee.models.base_model), 55
batch_kronecker_product() (dicee.callbacks.KronE static method), 25
batch_size (dicee.analyse_experiments.Experiment attribute), 18
batch_size (dicee.callbacks.PseudoLabellingCallback attribute), 22
batch_size (dicee.config.Namespace attribute), 26
batch_size (dicee.CVDataModule attribute), 207
batch_size (dicee.dataset_classes.CVDataModule attribute), 37
bias (dicee.models.transformers.GPTConfig attribute), 93
bias (dicee.models.transformers.LayerNorm attribute), 90
Block (class in dicee.models.transformers), 92
block_size (dicee.BaseKGE attribute), 190
block_size (dicee.config.Namespace attribute), 28
block_size (dicee.dataset_classes.MultiClassClassificationDataset attribute), 31
block_size (dicee.models.base_model.BaseKGE attribute), 62
block_size (dicee.models.BaseKGE attribute), 103, 106, 110, 115, 121, 133, 137
block_size (dicee.models.transformers.GPTConfig attribute), 93
block_size (dicee.MultiClassClassificationDataset attribute), 201
bn conv1 (dicee.AConvO attribute), 179
bn_conv1 (dicee.ConvQ attribute), 179
bn_conv1 (dicee.models.AConvQ attribute), 119
bn_conv1 (dicee.models.ConvQ attribute), 118
bn_conv1 (dicee.models.quaternion.AConvQ attribute), 86
bn_conv1 (dicee.models.quaternion.ConvQ attribute), 85
bn_conv2 (dicee.AConvQ attribute), 179
bn_conv2 (dicee.ConvQ attribute), 179
bn_conv2 (dicee.models.AConvQ attribute), 119
bn_conv2 (dicee.models.ConvQ attribute), 118
bn_conv2 (dicee.models.quaternion.AConvQ attribute), 86
bn\_conv2 (dicee.models.quaternion.ConvQ attribute), 85
bn_conv2d (dicee.AConEx attribute), 178
bn_conv2d (dicee.AConvO attribute), 178
bn_conv2d (dicee.ConEx attribute), 181
bn_conv2d (dicee.ConvO attribute), 180
bn_conv2d (dicee.models.AConEx attribute), 112
bn_conv2d (dicee.models.AConvO attribute), 125
bn_conv2d (dicee.models.complex.AConEx attribute), 72
bn_conv2d (dicee.models.complex.ConEx attribute), 72
bn_conv2d (dicee.models.ConEx attribute), 111
bn_conv2d (dicee.models.ConvO attribute), 124
bn_conv2d (dicee.models.octonion.AConvO attribute), 82
bn_conv2d (dicee.models.octonion.ConvO attribute), 81
BPE_NegativeSamplingDataset (class in dicee), 199
BPE_NegativeSamplingDataset (class in dicee.dataset_classes), 29
build_chain_funcs() (dicee.models.FMult2 method), 139
```

```
build chain funcs () (dicee.models.function space.FMult2 method), 77
build_func() (dicee.models.FMult2 method), 139
build_func() (dicee.models.function_space.FMult2 method), 77
BytE (class in dicee), 186
BytE (class in dicee.models.transformers), 88
byte_pair_encoding (dicee.analyse_experiments.Experiment attribute), 18
byte_pair_encoding (dicee.BaseKGE attribute), 190
byte_pair_encoding (dicee.config.Namespace attribute), 28
byte_pair_encoding (dicee.knowledge_graph.KG attribute), 45
byte_pair_encoding (dicee.models.base_model.BaseKGE attribute), 62
byte_pair_encoding (dicee.models.BaseKGE attribute), 103, 106, 110, 115, 121, 133, 137
С
c_attn (dicee.models.transformers.CausalSelfAttention attribute), 91
c_fc (dicee.models.transformers.MLP attribute), 92
c_proj (dicee.models.transformers.CausalSelfAttention attribute), 91
c_proj (dicee.models.transformers.MLP attribute), 92
callbacks (dicee.abstracts.AbstractTrainer attribute), 12
callbacks (dicee.analyse_experiments.Experiment attribute), 18
callbacks (dicee.config.Namespace attribute), 26
callbacks (dicee.trainer.torch_trainer_ddp.NodeTrainer attribute), 163
CausalSelfAttention (class in dicee.models.transformers), 90
chain_func() (dicee.models.FMult method), 138
chain_func() (dicee.models.function_space.FMult method), 76
chain_func() (dicee.models.function_space.GFMult method), 77
chain_func() (dicee.models.GFMult method), 138
CKeci (class in dicee), 169
CKeci (class in dicee.models), 128
CKeci (class in dicee.models.clifford), 67
cl_pqr() (dicee.DeCaL method), 173
cl_pgr() (dicee.models.clifford.DeCaL method), 69
cl_pqr() (dicee.models.DeCaL method), 129
clifford_multiplication() (dicee.Keci method), 170
clifford_multiplication() (dicee.models.clifford.Keci method), 66
clifford_multiplication() (dicee.models.Keci method), 126
clip_lambda (dicee.models.ADOPT attribute), 96
clip_lambda (dicee.models.adopt.ADOPT attribute), 55
collate fn (dicee. Allvs All attribute), 203
collate_fn (dicee.dataset_classes.AllvsAll attribute), 33
collate_fn (dicee.dataset_classes.KvsAll attribute), 32
collate fn (dicee.dataset classes.KvsSampleDataset attribute), 35
collate_fn (dicee.dataset_classes.MultiClassClassificationDataset attribute), 31
collate_fn (dicee.dataset_classes.MultiLabelDataset attribute), 30
collate_fn (dicee.dataset_classes.OnevsAllDataset attribute), 31
collate_fn (dicee.dataset_classes.OnevsSample attribute), 34
collate_fn (dicee.KvsAll attribute), 202
\verb"collate_fn" (\textit{dicee.KvsSampleDataset attribute}), 205
collate fn (dicee.MultiClassClassificationDataset attribute), 201
collate_fn (dicee.MultiLabelDataset attribute), 200
collate_fn (dicee.OnevsAllDataset attribute), 201
collate_fn (dicee.OnevsSample attribute), 204
collate_fn() (dicee.BPE_NegativeSamplingDataset method), 200
collate_fn() (dicee.dataset_classes.BPE_NegativeSamplingDataset method), 30
collate_fn() (dicee.dataset_classes.TriplePredictionDataset method), 37
collate_fn() (dicee.TriplePredictionDataset method), 207
collection_name (dicee.scripts.index_serve.NeuralSearcher attribute), 152
comp\_func() (dicee.LFMult method), 185
comp_func() (dicee.models.function_space.LFMult method), 79
comp_func() (dicee.models.LFMult method), 140
Complex (class in dicee), 176
Complex (class in dicee.models), 112
Complex (class in dicee.models.complex), 72
compute_convergence() (in module dicee.callbacks), 22
compute_func() (dicee.models.FMult method), 138
compute_func() (dicee.models.FMult2 method), 139
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), 138
compute_mrr() (dicee.callbacks.ASWA static method), 23
compute_sigma_pp() (dicee.DeCaL method), 174
compute_sigma_pp() (dicee.Keci method), 170
compute_sigma_pp() (dicee.models.clifford.DeCaL method), 70
compute_sigma_pp() (dicee.models.clifford.Keci method), 65
compute_sigma_pp() (dicee.models.DeCaL method), 130
compute_sigma_pp() (dicee.models.Keci method), 126
compute_sigma_pq() (dicee.DeCaL method), 175
compute_sigma_pq() (dicee.Keci method), 170
\verb|compute_sigma_pq()| \textit{(dicee.models.clifford.DeCaL method)}, 71
compute_sigma_pq() (dicee.models.clifford.Keci method), 66
compute_sigma_pq() (dicee.models.DeCaL method), 131
compute_sigma_pq() (dicee.models.Keci method), 126
compute_sigma_pr() (dicee.DeCaL method), 175
compute_sigma_pr() (dicee.models.clifford.DeCaL method), 71
compute_sigma_pr() (dicee.models.DeCaL method), 131
compute_sigma_qq() (dicee.DeCaL method), 174
compute_sigma_qq() (dicee.Keci method), 170
\verb|compute_sigma_qq()| \textit{(dicee.models.clifford.DeCaL method)}, 70
compute_sigma_qq() (dicee.models.clifford.Keci method), 65
compute_sigma_gq() (dicee.models.DeCaL method), 131
compute_sigma_qq() (dicee.models.Keci method), 126
compute_sigma_gr() (dicee.DeCaL method), 175
compute_sigma_gr() (dicee.models.clifford.DeCaL method), 71
compute_sigma_qr() (dicee.models.DeCaL method), 132
compute_sigma_rr() (dicee.DeCaL method), 175
\verb|compute_sigma_rr()| \textit{ (dicee.models.clifford.DeCaL method)}, 70
compute_sigma_rr() (dicee.models.DeCaL method), 131
compute_sigmas_multivect() (dicee.DeCaL method), 173
compute_sigmas_multivect() (dicee.models.clifford.DeCaL method), 69
compute_sigmas_multivect() (dicee.models.DeCaL method), 130
compute_sigmas_single() (dicee.DeCaL method), 173
compute_sigmas_single() (dicee.models.clifford.DeCaL method), 69
compute_sigmas_single() (dicee.models.DeCaL method), 129
ConEx (class in dicee), 181
ConEx (class in dicee.models), 111
ConEx (class in dicee.models.complex), 71
config (dicee.BytE attribute), 187
config (dicee.models.transformers.BytE attribute), 89
config (dicee.models.transformers.GPT attribute), 94
configs (dicee.abstracts.BaseInteractiveKGE attribute), 14
configure_optimizers() (dicee.models.base_model.BaseKGELightning method), 60
configure_optimizers() (dicee.models.BaseKGELightning method), 100
configure_optimizers() (dicee.models.transformers.GPT method), 94
construct_batch_selected_cl_multivector() (dicee.Keci method), 171
construct_batch_selected_cl_multivector() (dicee.models.clifford.Keci method), 67
construct_batch_selected_cl_multivector() (dicee.models.Keci method), 127
construct_cl_multivector() (dicee.DeCaL method), 174
construct_cl_multivector() (dicee.Keci method), 171
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), 130
construct_cl_multivector() (dicee.models.Keci method), 127
construct_dataset() (in module dicee), 199
construct_dataset() (in module dicee.dataset_classes), 29
construct_ensemble (dicee.abstracts.BaseInteractiveKGE attribute), 14
construct_graph() (dicee.query_generator.QueryGenerator method), 143
construct_graph() (dicee.QueryGenerator method), 211
construct input and output () (dicee.abstracts.BaseInteractiveKGE method), 15
construct_multi_coeff() (dicee.LFMult method), 184
construct_multi_coeff() (dicee.models.function_space.LFMult method), 78
construct_multi_coeff() (dicee.models.LFMult method), 140
continual_learning (dicee.config.Namespace attribute), 28
continual_start() (dicee.DICE_Trainer method), 193
continual_start() (dicee.executer.ContinuousExecute method), 44
continual_start() (dicee.trainer.DICE_Trainer method), 164
```

```
continual start() (dicee.trainer.dice trainer.DICE Trainer method), 159
continual_training_setup_executor() (in module dicee), 192
continual_training_setup_executor() (in module dicee.static_funcs), 156
Continuous Execute (class in dicee.executer), 44
conv2d (dicee.AConEx attribute), 178
conv2d (dicee.AConvO attribute), 178
conv2d (dicee.AConvQ attribute), 179
conv2d (dicee.ConEx attribute), 181
conv2d (dicee.ConvO attribute), 180
conv2d (dicee.ConvQ attribute), 179
conv2d (dicee.models.AConEx attribute), 112
conv2d (dicee.models.AConvO attribute), 124
conv2d (dicee.models.AConvQ attribute), 119
conv2d (dicee.models.complex.AConEx attribute), 72
conv2d (dicee.models.complex.ConEx attribute), 71
conv2d (dicee.models.ConEx attribute), 111
conv2d (dicee.models.ConvO attribute), 124
conv2d (dicee.models.ConvQ attribute), 118
conv2d (dicee.models.octonion.AConvO attribute), 81
conv2d (dicee.models.octonion.ConvO attribute), 81
conv2d (dicee.models.quaternion.AConvQ attribute), 86
conv2d (dicee.models.quaternion.ConvQ attribute), 85
ConvO (class in dicee), 180
ConvO (class in dicee.models), 123
ConvO (class in dicee.models.octonion), 80
ConvQ (class in dicee), 179
ConvQ (class in dicee.models), 118
ConvQ (class in dicee.models.quaternion), 85
create_constraints() (in module dicee.read_preprocess_save_load_kg.util), 148
create_constraints() (in module dicee.static_preprocess_funcs), 158
create_experiment_folder() (in module dicee), 192
create_experiment_folder() (in module dicee.static_funcs), 156
create_random_data() (dicee.callbacks.PseudoLabellingCallback method), 22
create_recipriocal_triples() (in module dicee), 191
create_recipriocal_triples() (in module dicee.read_preprocess_save_load_kg.util), 149
create_recipriocal_triples() (in module dicee.static_funcs), 155
create_vector_database() (dicee.KGE method), 194
create_vector_database() (dicee.knowledge_graph_embeddings.KGE method), 46
crop_block_size() (dicee.models.transformers.GPT method), 94
ctx (dicee.trainer.torch_trainer_ddp.NodeTrainer attribute), 163
CVDataModule (class in dicee), 207
CVDataModule (class in dicee.dataset_classes), 37
D
data_module (dicee.callbacks.PseudoLabellingCallback attribute), 22
data_property_embeddings (dicee.literal_classes.LiteralEmbeddings attribute), 52
data_property_to_idx (dicee.literal_classes.LiteralDataset attribute), 53
dataset_dir (dicee.config.Namespace attribute), 26
dataset_dir (dicee.knowledge_graph.KG attribute), 45
dataset_sanity_checking() (in module dicee.read_preprocess_save_load_kg.util), 149
DeCaL (class in dicee), 172
DeCaL (class in dicee.models), 128
DeCal (class in dicee.models.clifford), 68
decide() (dicee.callbacks.ASWA method), 23
degree (dicee.LFMult attribute), 184
degree (dicee.models.function_space.LFMult attribute), 78
degree (dicee.models.LFMult attribute), 140
denormalize() (dicee.literal_classes.LiteralDataset static method), 54
deploy() (dicee.KGE method), 198
deploy() (dicee.knowledge_graph_embeddings.KGE method), 50
deploy_head_entity_prediction() (in module dicee), 192
deploy_head_entity_prediction() (in module dicee.static_funcs), 156
deploy_relation_prediction() (in module dicee), 192
deploy_relation_prediction() (in module dicee.static_funcs), 156
deploy_tail_entity_prediction() (in module dicee), 192
deploy_tail_entity_prediction() (in module dicee.static_funcs), 156
deploy_triple_prediction() (in module dicee), 192
```

```
deploy_triple_prediction() (in module dicee.static_funcs), 156
describe() (dicee.knowledge_graph.KG method), 46
description_of_input (dicee.knowledge_graph.KG attribute), 46
DICE_Trainer (class in dicee), 193
DICE_Trainer (class in dicee.trainer), 164
DICE_Trainer (class in dicee.trainer.dice_trainer), 159
dicee
    module, 12
dicee.___main__
    module, 12
dicee.abstracts
    module, 12
dicee.analyse_experiments
    module, 17
dicee.callbacks
    module, 19
dicee.config
    module, 25
dicee.dataset_classes
    module, 28
dicee.eval_static_funcs
    module, 40
dicee.evaluator
    module, 41
dicee.executer
    module, 43
{\tt dicee.knowledge\_graph}
    module, 44
\verb|dicee.knowledge_graph_embeddings|
    module, 46
dicee.literal_classes
    module, 51
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.octonion
    module, 79
dicee.models.pykeen_models
    module, 82
dicee.models.quaternion
    module, 83
dicee.models.real
    module, 86
dicee.models.static_funcs
    module, 88
dicee.models.transformers
    module, 88
dicee.query_generator
    module, 142
dicee.read_preprocess_save_load_kg
    module, 143
dicee.read_preprocess_save_load_kg.preprocess
    module, 143
dicee.read_preprocess_save_load_kg.read_from_disk
    module, 144
```

```
dicee.read_preprocess_save_load_kg.save_load_disk
     module, 145
dicee.read_preprocess_save_load_kg.util
     module, 145
dicee.sanity_checkers
     module, 150
dicee.scripts
    module, 151
dicee.scripts.index_serve
     module, 151
dicee.scripts.run
     module, 153
dicee.static_funcs
     module, 154
dicee.static_funcs_training
     module, 157
dicee.static_preprocess_funcs
    module, 157
dicee.trainer
     module, 158
dicee.trainer.dice_trainer
     module, 158
dicee.trainer.model_parallelism
     module, 160
dicee.trainer.torch_trainer
     module, 161
dicee.trainer.torch_trainer_ddp
     module, 162
discrete_points (dicee.models.FMult2 attribute), 139
discrete_points (dicee.models.function_space.FMult2 attribute), 77
dist_func (dicee.models.Pyke attribute), 108
dist func (dicee.models.real.Pyke attribute), 87
dist_func (dicee.Pyke attribute), 168
DistMult (class in dicee), 168
DistMult (class in dicee.models), 107
DistMult (class in dicee.models.real), 86
download file() (in module dicee), 193
download_file() (in module dicee.static_funcs), 156
download_files_from_url() (in module dicee), 193
download_files_from_url() (in module dicee.static_funcs), 156
download_pretrained_model() (in module dicee), 193
download_pretrained_model() (in module dicee.static_funcs), 157
dropout (dicee.literal_classes.LiteralEmbeddings attribute), 52
dropout (dicee.models.transformers.CausalSelfAttention attribute), 91
dropout (dicee.models.transformers.GPTConfig attribute), 93
dropout (dicee.models.transformers.MLP attribute), 92
DualE (class in dicee), 176
DualE (class in dicee.models), 141
DualE (class in dicee.models.dualE), 74
dummy_eval() (dicee.evaluator.Evaluator method), 42
\verb|dummy_id| (\textit{dicee.knowledge\_graph.KG attribute}), 45
during_training (dicee.evaluator.Evaluator attribute), 42
Ε
ee vocab (dicee.evaluator.Evaluator attribute), 41
efficient_zero_grad() (in module dicee.static_funcs_training), 157
\verb|embedding_dim| (\textit{dicee}. \textit{analyse\_experiments}. \textit{Experiment attribute}), 18
embedding_dim (dicee.BaseKGE attribute), 189
embedding_dim (dicee.config.Namespace attribute), 26
embedding_dim (dicee.literal_classes.LiteralEmbeddings attribute), 52
embedding_dim (dicee.models.base_model.BaseKGE attribute), 62
embedding_dim (dicee.models.BaseKGE attribute), 102, 106, 109, 114, 120, 132, 136
embedding_dims (dicee.literal_classes.LiteralEmbeddings attribute), 51
enable_log (in module dicee.static_preprocess_funcs), 158
enc (dicee.knowledge_graph.KG attribute), 45
end() (dicee.executer.Execute method), 43
EnsembleKGE (class in dicee), 191
```

```
EnsembleKGE (class in dicee.models.ensemble), 75
ent2id (dicee.query_generator.QueryGenerator attribute), 142
ent2id (dicee.QueryGenerator attribute), 211
ent_in (dicee.query_generator.QueryGenerator attribute), 142
ent_in (dicee.QueryGenerator attribute), 211
ent_out (dicee.query_generator.QueryGenerator attribute), 142
ent_out (dicee.QueryGenerator attribute), 211
entities_str (dicee.knowledge_graph.KG property), 46
entity_embeddings (dicee.AConvQ attribute), 179
entity_embeddings (dicee.ConvQ attribute), 179
entity_embeddings (dicee.DeCaL attribute), 173
entity_embeddings (dicee.DualE attribute), 176
entity_embeddings (dicee.LFMult attribute), 184
entity_embeddings (dicee.literal_classes.LiteralEmbeddings attribute), 52
entity_embeddings (dicee.models.AConvQ attribute), 119
entity_embeddings (dicee.models.clifford.DeCaL attribute), 68
entity_embeddings (dicee.models.ConvQ attribute), 118
entity_embeddings (dicee.models.DeCaL attribute), 129
entity_embeddings (dicee.models.DualE attribute), 141
entity_embeddings (dicee.models.dualE.DualE attribute), 74
entity_embeddings (dicee.models.FMult attribute), 138
entity_embeddings (dicee.models.FMult2 attribute), 139
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), 138
entity_embeddings (dicee.models.LFMult attribute), 140
entity_embeddings (dicee.models.LFMult1 attribute), 139
entity_embeddings (dicee.models.pykeen_models.PykeenKGE attribute), 82
entity embeddings (dicee.models.PykeenKGE attribute), 134
entity_embeddings (dicee.models.quaternion.AConvQ attribute), 86
entity_embeddings (dicee.models.quaternion.ConvQ attribute), 85
entity_embeddings (dicee.PykeenKGE attribute), 186
\verb"entity_to_idx" (\textit{dicee.knowledge\_graph.KG"} attribute), 45
entity to idx (dicee.literal classes.LiteralDataset attribute), 53, 54
entity_to_idx (dicee.scripts.index_serve.NeuralSearcher attribute), 152
epoch_count (dicee.abstracts.AbstractPPECallback attribute), 17
epoch_count (dicee.callbacks.ASWA attribute), 22
epoch_counter (dicee.callbacks.Eval attribute), 23
epoch_counter (dicee.callbacks.KGESaveCallback attribute), 21
epoch_ratio (dicee.callbacks.Eval attribute), 23
er_vocab (dicee.evaluator.Evaluator attribute), 41
estimate_mfu() (dicee.models.transformers.GPT method), 94
estimate_q() (in module dicee.callbacks), 22
Eval (class in dicee.callbacks), 23
eval() (dicee.EnsembleKGE method), 191
eval () (dicee.evaluator.Evaluator method), 42
eval() (dicee.models.ensemble.EnsembleKGE method), 75
eval_lp_performance() (dicee.KGE method), 195
eval_lp_performance() (dicee.knowledge_graph_embeddings.KGE method), 46
eval_model (dicee.config.Namespace attribute), 27
eval_model (dicee.knowledge_graph.KG attribute), 45
eval_rank_of_head_and_tail_byte_pair_encoded_entity() (dicee.evaluator.Evaluator method), 42
eval_rank_of_head_and_tail_entity() (dicee.evaluator.Evaluator method), 42
eval_with_bpe_vs_all() (dicee.evaluator.Evaluator method), 42
\verb| eval_with_byte()| \textit{ (dicee. evaluator. Evaluator method)}, 42
eval_with_data() (dicee.evaluator.Evaluator method), 42
eval_with_vs_all() (dicee.evaluator.Evaluator method), 42
evaluate () (in module dicee), 193
evaluate() (in module dicee.static_funcs), 156
evaluate_bpe_lp() (in module dicee.static_funcs_training), 157
evaluate_link_prediction_performance() (in module dicee.eval_static_funcs), 40
evaluate_link_prediction_performance_with_bpe() (in module dicee.eval_static_funcs), 41
evaluate\_link\_prediction\_performance\_with\_bpe\_reciprocals () \textit{ (in module dicee.eval\_static\_funcs)}, 41
evaluate_link_prediction_performance_with_reciprocals() (in module dicee.eval_static_funcs), 41
evaluate_literal_prediction() (dicee.KGE method), 199
```

```
evaluate_literal_prediction() (dicee.knowledge_graph_embeddings.KGE method), 51
evaluate_lp() (dicee.evaluator.Evaluator method), 42
evaluate_lp() (in module dicee.static_funcs_training), 157
evaluate_lp_bpe_k_vs_all() (dicee.evaluator.Evaluator method), 42
evaluate_lp_bpe_k_vs_all() (in module dicee.eval_static_funcs), 41
evaluate_lp_k_vs_all() (dicee.evaluator.Evaluator method), 42
evaluate_lp_with_byte() (dicee.evaluator.Evaluator method), 42
Evaluator (class in dicee.evaluator), 41
evaluator (dicee.DICE_Trainer attribute), 193
evaluator (dicee.executer.Execute attribute), 43
evaluator (dicee.trainer.DICE_Trainer attribute), 164
\verb|evaluator| (\textit{dicee.trainer.dice\_trainer.DICE\_Trainer attribute}), 159
every_x_epoch (dicee.callbacks.KGESaveCallback attribute), 21
example_input_array (dicee.EnsembleKGE property), 191
\verb|example_input_array| (\textit{dicee.models.ensemble.EnsembleKGE property}), 75
Execute (class in dicee.executer), 43
\verb|exists()| (\textit{dicee.knowledge\_graph.KG method}), 46
Experiment (class in dicee.analyse_experiments), 18
explicit (dicee.models.QMult attribute), 117
explicit (dicee.models.quaternion.QMult attribute), 84
explicit (dicee.QMult attribute), 182
exponential_function() (in module dicee), 192
exponential_function() (in module dicee.static_funcs), 156
\verb|extract_input_outputs()| \textit{(dicee.trainer.torch\_trainer\_ddp.NodeTrainer method)}, 163
extract_input_outputs() (in module dicee.trainer.model_parallelism), 161
extract_input_outputs_set_device() (dicee.trainer.torch_trainer.TorchTrainer method), 162
F
f (dicee.callbacks.KronE attribute), 25
fc (dicee.literal_classes.LiteralEmbeddings attribute), 52
fc1 (dicee.AConEx attribute), 178
fc1 (dicee.AConvO attribute), 178
fc1 (dicee.AConvQ attribute), 179
fc1 (dicee.ConEx attribute), 181
fc1 (dicee.ConvO attribute), 180
fc1 (dicee.ConvQ attribute), 179
fc1 (dicee.models.AConEx attribute), 112
fc1 (dicee.models.AConvO attribute), 124
fc1 (dicee.models.AConvQ attribute), 119
fc1 (dicee.models.complex.AConEx attribute), 72
fc1 (dicee.models.complex.ConEx attribute), 72
fc1 (dicee.models.ConEx attribute), 111
fc1 (dicee.models.ConvO attribute), 124
fc1 (dicee.models.ConvQ attribute), 118
fc1 (dicee.models.octonion.AConvO attribute), 82
fc1 (dicee.models.octonion.ConvO attribute), 81
fc1 (dicee.models.quaternion.AConvQ attribute), 86
fc1 (dicee.models.quaternion.ConvO attribute), 85
fc_num_input (dicee.AConEx attribute), 178
fc_num_input (dicee.AConvO attribute), 178
fc_num_input (dicee.AConvQ attribute), 179
fc_num_input (dicee.ConEx attribute), 181
fc_num_input (dicee.ConvO attribute), 180
fc_num_input (dicee.ConvQ attribute), 179
fc_num_input (dicee.models.AConEx attribute), 112
fc_num_input (dicee.models.AConvO attribute), 124
fc_num_input (dicee.models.AConvQ attribute), 119
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), 111
fc_num_input (dicee.models.ConvO attribute), 124
fc_num_input (dicee.models.ConvQ attribute), 118
fc_num_input (dicee.models.octonion.AConvO attribute), 81
fc_num_input (dicee.models.octonion.ConvO attribute), 81
fc_num_input (dicee.models.quaternion.AConvQ attribute), 86
fc_num_input (dicee.models.quaternion.ConvQ attribute), 85
fc_out (dicee.literal_classes.LiteralEmbeddings attribute), 52
```

```
feature_map_dropout (dicee.AConEx attribute), 178
feature_map_dropout (dicee.AConvO attribute), 178
{\tt feature\_map\_dropout}~(\textit{dicee.AConvQ attribute}),~179
feature_map_dropout (dicee.ConEx attribute), 181
feature_map_dropout (dicee.ConvO attribute), 181
feature_map_dropout (dicee.ConvQ attribute), 179
feature_map_dropout (dicee.models.AConEx attribute), 112
feature_map_dropout (dicee.models.AConvO attribute), 125
feature_map_dropout (dicee.models.AConvQ attribute), 119
{\tt feature\_map\_dropout}~(\textit{dicee.models.complex.AConEx~attribute}), 72
feature_map_dropout (dicee.models.complex.ConEx attribute), 72
{\tt feature\_map\_dropout}~(\textit{dicee.models.ConEx attribute}),~111
feature_map_dropout (dicee.models.ConvO attribute), 124
feature_map_dropout (dicee.models.ConvQ attribute), 118
feature_map_dropout (dicee.models.octonion.AConvO attribute), 82
feature_map_dropout (dicee.models.octonion.ConvO attribute), 81
feature_map_dropout (dicee.models.quaternion.AConvQ attribute), 86
feature_map_dropout (dicee.models.quaternion.ConvQ attribute), 85
feature_map_dropout_rate (dicee.BaseKGE attribute), 189
feature_map_dropout_rate (dicee.config.Namespace attribute), 28
feature_map_dropout_rate (dicee.models.base_model.BaseKGE attribute), 62
feature_map_dropout_rate (dicee.models.BaseKGE attribute), 103, 106, 110, 114, 120, 133, 136
fill_query() (dicee.query_generator.QueryGenerator method), 143
fill_query() (dicee.QueryGenerator method), 211
find_good_batch_size() (in module dicee.trainer.model_parallelism), 161
find_missing_triples() (dicee.KGE method), 198
\verb|find_missing_triples()| (\textit{dicee.knowledge\_graph\_embeddings.KGE method}), 49
fit () (dicee.trainer.model_parallelism.TensorParallel method), 161
fit () (dicee.trainer.torch_trainer_ddp.TorchDDPTrainer method), 163
fit () (dicee.trainer.torch_trainer.TorchTrainer method), 162
flash (dicee.models.transformers.CausalSelfAttention attribute), 91
FMult (class in dicee.models), 138
FMult (class in dicee.models.function_space), 76
FMult2 (class in dicee.models), 138
FMult2 (class in dicee.models.function_space), 77
form_of_labelling (dicee.DICE_Trainer attribute), 193
form of labelling (dicee.trainer.DICE Trainer attribute), 164
form_of_labelling (dicee.trainer.dice_trainer.DICE_Trainer attribute), 159
forward() (dicee.BaseKGE method), 190
forward() (dicee.BytE method), 187
forward() (dicee.literal_classes.GatedLinearUnit method), 51
forward() (dicee.literal_classes.LiteralEmbeddings method), 52
forward() (dicee.models.base_model.BaseKGE method), 63
forward() (dicee.models.base_model.IdentityClass static method), 64
forward() (dicee.models.BaseKGE method), 104, 107, 110, 115, 121, 134, 137
forward() (dicee.models.IdentityClass static method), 105, 116, 122
forward() (dicee.models.transformers.Block method), 93
forward() (dicee.models.transformers.BytE method), 89
forward() (dicee.models.transformers.CausalSelfAttention method), 91
forward() (dicee.models.transformers.GPT method), 94
forward () (dicee.models.transformers.LayerNorm method), 90
forward() (dicee.models.transformers.MLP method), 92
\verb|forward_backward_update()| \textit{(dicee.trainer.torch\_trainer.TorchTrainer method)}, 162
forward_backward_update_loss() (in module dicee.trainer.model_parallelism), 161
forward_byte_pair_encoded_k_vs_all() (dicee.BaseKGE method), 190
\verb|forward_byte_pair_encoded_k_vs_all()| \textit{(dicee.models.base\_model.BaseKGE method)}, 62
forward_byte_pair_encoded_k_vs_all() (dicee.models.BaseKGE method), 103, 106, 110, 115, 121, 133, 137
{\tt forward\_byte\_pair\_encoded\_triple()} \ (\textit{dicee.BaseKGE method}), 190
forward_byte_pair_encoded_triple() (dicee.models.base_model.BaseKGE method), 63
forward_byte_pair_encoded_triple() (dicee.models.BaseKGE method), 103, 107, 110, 115, 121, 133, 137
forward_k_vs_all() (dicee.AConEx method), 178
forward_k_vs_all() (dicee.AConvO method), 178
forward_k_vs_all() (dicee.AConvQ method), 179
forward_k_vs_all() (dicee.BaseKGE method), 190
forward_k_vs_all() (dicee.ComplEx method), 177
forward_k_vs_all() (dicee.ConEx method), 181
forward_k_vs_all() (dicee.ConvO method), 181
forward_k\_vs\_all() (dicee.ConvQ method), 180
```

```
forward_k_vs_all() (dicee.DeCaL method), 174
forward_k_vs_all() (dicee.DistMult method), 169
forward_k_vs_all() (dicee.DualE method), 176
forward_k_vs_all() (dicee.Keci method), 171
forward_k_vs_all() (dicee.models.AConEx method), 112
forward_k_vs_all() (dicee.models.AConvO method), 125
forward_k_vs_all() (dicee.models.AConvQ method), 119
forward k vs all() (dicee.models.base model.BaseKGE method), 63
forward_k_vs_all() (dicee.models.BaseKGE method), 104, 107, 111, 115, 121, 134, 137
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), 113
forward_k_vs_all() (dicee.models.complex.AConEx method), 72
forward_k_vs_all() (dicee.models.complex.ComplEx method), 73
forward_k_vs_all() (dicee.models.complex.ConEx method), 72
forward_k_vs_all() (dicee.models.ConEx method), 111
forward_k_vs_all() (dicee.models.ConvO method), 124
forward_k_vs_all() (dicee.models.ConvQ method), 118
forward_k_vs_all() (dicee.models.DeCaL method), 130
forward_k_vs_all() (dicee.models.DistMult method), 108
forward_k_vs_all() (dicee.models.DualE method), 141
forward_k_vs_all() (dicee.models.dualE.DualE method), 74
forward_k_vs_all() (dicee.models.Keci method), 127
forward_k_vs_all() (dicee.models.octonion.AConvO method), 82
forward_k_vs_all() (dicee.models.octonion.ConvO method), 81
forward_k_vs_all() (dicee.models.octonion.OMult method), 80
{\tt forward\_k\_vs\_all()} \ \textit{(dicee.models.OMult method)}, 123
forward_k_vs_all() (dicee.models.pykeen_models.PykeenKGE method), 82
forward_k_vs_all() (dicee.models.PykeenKGE method), 135
forward_k_vs_all() (dicee.models.QMult method), 118
forward_k_vs_all() (dicee.models.quaternion.AConvQ method), 86
forward_k_vs_all() (dicee.models.quaternion.ConvQ method), 85
forward_k_vs_all() (dicee.models.quaternion.QMult method), 85
forward_k_vs_all() (dicee.models.real.DistMult method), 87
forward_k_vs_all() (dicee.models.real.Shallom method), 87
forward_k_vs_all() (dicee.models.real.TransE method), 87
forward k vs all() (dicee.models.Shallom method), 108
forward_k_vs_all() (dicee.models.TransE method), 108
forward_k_vs_all() (dicee.OMult method), 184
forward_k_vs_all() (dicee.PykeenKGE method), 186
forward_k_vs_all() (dicee.QMult method), 183
forward_k_vs_all() (dicee.Shallom method), 184
forward_k_vs_all() (dicee.TransE method), 172
forward_k_vs_sample() (dicee.AConEx method), 178
forward_k_vs_sample() (dicee.BaseKGE method), 190
forward_k_vs_sample() (dicee.ComplEx method), 177
forward_k_vs_sample() (dicee.ConEx method), 181
forward_k_vs_sample() (dicee.DistMult method), 169
forward_k_vs_sample() (dicee.Keci method), 171
forward_k_vs_sample() (dicee.models.AConEx method), 112
forward_k_vs_sample() (dicee.models.base_model.BaseKGE method), 63
forward_k_vs_sample() (dicee.models.BaseKGE method), 104, 107, 111, 115, 121, 134, 137
forward_k_vs_sample() (dicee.models.clifford.Keci method), 67
forward_k_vs_sample() (dicee.models.ComplEx method), 113
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), 111
forward_k_vs_sample() (dicee.models.DistMult method), 108
forward_k_vs_sample() (dicee.models.Keci method), 128
forward_k_vs_sample() (dicee.models.pykeen_models.PykeenKGE method), 83
forward_k_vs_sample() (dicee.models.PykeenKGE method), 135
forward_k_vs_sample() (dicee.models.QMult method), 118
forward_k_vs_sample() (dicee.models.quaternion.QMult method), 85
forward_k_vs_sample() (dicee.models.real.DistMult method), 87
forward_k_vs_sample() (dicee.PykeenKGE method), 186
forward_k_vs_sample() (dicee.QMult method), 183
forward_k_vs_with_explicit() (dicee.Keci method), 171
```

```
forward_k_vs_with_explicit() (dicee.models.clifford.Keci method), 66
forward_k_vs_with_explicit() (dicee.models.Keci method), 127
forward_triples() (dicee.AConEx method), 178
forward_triples() (dicee.AConvO method), 178
forward_triples() (dicee.AConvQ method), 179
forward_triples() (dicee.BaseKGE method), 190
forward_triples() (dicee.ConEx method), 181
forward triples() (dicee.ConvO method), 181
forward_triples() (dicee.ConvQ method), 180
forward_triples() (dicee.DeCaL method), 173
forward_triples() (dicee.DualE method), 176
forward_triples() (dicee.Keci method), 172
forward_triples() (dicee.LFMult method), 184
forward_triples() (dicee.models.AConEx method), 112
forward_triples() (dicee.models.AConvO method), 125
forward_triples() (dicee.models.AConvQ method), 119
forward_triples() (dicee.models.base_model.BaseKGE method), 63
forward_triples() (dicee.models.BaseKGE method), 104, 107, 110, 115, 121, 134, 137
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), 111
forward_triples() (dicee.models.ConvO method), 124
forward_triples() (dicee.models.ConvQ method), 118
forward_triples() (dicee.models.DeCaL method), 129
forward_triples() (dicee.models.DualE method), 141
forward_triples() (dicee.models.dualE.DualE method), 74
{\tt forward\_triples()} \ \textit{(dicee.models.FMult method)}, 138
forward_triples() (dicee.models.FMult2 method), 139
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), 138
forward triples() (dicee.models.Keci method), 128
forward_triples() (dicee.models.LFMult method), 140
forward_triples() (dicee.models.LFMult1 method), 139
forward_triples() (dicee.models.octonion.AConvO method), 82
forward_triples() (dicee.models.octonion.ConvO method), 81
forward_triples() (dicee.models.Pyke method), 108
forward_triples() (dicee.models.pykeen_models.PykeenKGE method), 83
forward_triples() (dicee.models.PykeenKGE method), 135
forward_triples() (dicee.models.quaternion.AConvQ method), 86
forward_triples() (dicee.models.quaternion.ConvQ method), 85
forward_triples() (dicee.models.real.Pyke method), 87
forward_triples() (dicee.models.real.Shallom method), 87
forward_triples() (dicee.models.Shallom method), 108
forward_triples() (dicee.Pyke method), 168
forward_triples() (dicee.PykeenKGE method), 186
forward_triples() (dicee.Shallom method), 184
{\tt freeze\_entity\_embeddings}~(\textit{dicee.literal\_classes.LiteralEmbeddings}~attribute), 52
frequency (dicee.callbacks.Perturb attribute), 25
from_pretrained() (dicee.models.transformers.GPT class method), 94
from_pretrained_model_write_embeddings_into_csv() (in module dicee), 193
from_pretrained_model_write_embeddings_into_csv() (in module dicee.static_funcs), 157
full_storage_path (dicee.analyse_experiments.Experiment attribute), 18
func_triple_to_bpe_representation (dicee.evaluator.Evaluator attribute), 41
func_triple_to_bpe_representation() (dicee.knowledge_graph.KG method), 46
function() (dicee.models.FMult2 method), 139
function() (dicee.models.function_space.FMult2 method), 77
G
gamma (dicee.models.FMult attribute), 138
gamma (dicee.models.function_space.FMult attribute), 76
gate_residual (dicee.literal_classes.GatedLinearUnit attribute), 51
```

```
gate residual (dicee.literal classes.LiteralEmbeddings attribute), 52
GatedLinearUnit (class in dicee.literal_classes), 51
gelu (dicee.models.transformers.MLP attribute), 92
gen_test (dicee.query_generator.QueryGenerator attribute), 142
gen_test (dicee.QueryGenerator attribute), 210
gen_valid (dicee.query_generator.QueryGenerator attribute), 142
gen_valid (dicee.QueryGenerator attribute), 210
generate() (dicee.BytE method), 187
generate() (dicee.KGE method), 194
generate() (dicee.knowledge_graph_embeddings.KGE method), 46
generate() (dicee.models.transformers.BytE method), 89
generate_queries() (dicee.query_generator.QueryGenerator method), 143
generate_queries() (dicee.QueryGenerator method), 211
get_aswa_state_dict() (dicee.callbacks.ASWA method), 23
{\tt get\_bpe\_head\_and\_relation\_representation()} \ (\textit{dicee.BaseKGE method}), 191
get_bpe_head_and_relation_representation() (dicee.models.base_model.BaseKGE method), 63
get_bpe_head_and_relation_representation() (dicee.models.BaseKGE method), 104, 107, 111, 115, 121, 134, 137
get_bpe_token_representation() (dicee.abstracts.BaseInteractiveKGE method), 14
get_callbacks() (in module dicee.trainer.dice_trainer), 159
get_default_arguments() (in module dicee.analyse_experiments), 18
get_default_arguments() (in module dicee.scripts.index_serve), 152
get_default_arguments() (in module dicee.scripts.run), 154
get_ee_vocab() (in module dicee), 191
get_ee_vocab() (in module dicee.read_preprocess_save_load_kg.util), 148
get_ee_vocab() (in module dicee.static_funcs), 155
get_ee_vocab() (in module dicee.static_preprocess_funcs), 158
get_embeddings() (dicee.BaseKGE method), 191
get_embeddings() (dicee.EnsembleKGE method), 191
\verb"get_embeddings" () \textit{ (dicee.models.base\_model.BaseKGE method)}, 63
get_embeddings() (dicee.models.BaseKGE method), 104, 107, 111, 115, 121, 134, 137
get_embeddings() (dicee.models.ensemble.EnsembleKGE method), 75
get embeddings() (dicee.models.real.Shallom method), 87
get_embeddings() (dicee.models.Shallom method), 108
get_embeddings() (dicee.Shallom method), 184
get_entity_embeddings() (dicee.abstracts.BaseInteractiveKGE method), 15
get_entity_index() (dicee.abstracts.BaseInteractiveKGE method), 14
get er vocab() (in module dicee), 191
get_er_vocab() (in module dicee.read_preprocess_save_load_kg.util), 148
get_er_vocab() (in module dicee.static_funcs), 155
get_er_vocab() (in module dicee.static_preprocess_funcs), 158
get_eval_report() (dicee.abstracts.BaseInteractiveKGE method), 14
get_head_relation_representation() (dicee.BaseKGE method), 190
get_head_relation_representation() (dicee.models.base_model.BaseKGE method), 63
get_head_relation_representation() (dicee.models.BaseKGE method), 104, 107, 111, 115, 121, 134, 137
get_kronecker_triple_representation() (dicee.callbacks.KronE method), 25
get_num_params() (dicee.models.transformers.GPT method), 94
qet_padded_bpe_triple_representation() (dicee.abstracts.BaseInteractiveKGE method), 14
get_queries() (dicee.query_generator.QueryGenerator method), 143
get_queries() (dicee.QueryGenerator method), 211
get_re_vocab() (in module dicee), 191
get_re_vocab() (in module dicee.read_preprocess_save_load_kg.util), 148
get_re_vocab() (in module dicee.static_funcs), 155
get_re_vocab() (in module dicee.static_preprocess_funcs), 158
get_relation_embeddings() (dicee.abstracts.BaseInteractiveKGE method), 15
get_relation_index() (dicee.abstracts.BaseInteractiveKGE method), 14
\verb"get_sentence_representation"() \textit{ (dicee.BaseKGE method)}, 190
get_sentence_representation() (dicee.models.base_model.BaseKGE method), 63
get_sentence_representation() (dicee.models.BaseKGE method), 104, 107, 111, 115, 121, 134, 137
get_transductive_entity_embeddings() (dicee.KGE method), 194
get_transductive_entity_embeddings() (dicee.knowledge_graph_embeddings.KGE method), 46
get_triple_representation() (dicee.BaseKGE method), 190
get_triple_representation() (dicee.models.base_model.BaseKGE method), 63
get_triple_representation() (dicee.models.BaseKGE method), 104, 107, 111, 115, 121, 134, 137
GFMult (class in dicee.models), 138
GFMult (class in dicee.models.function_space), 76
global_rank (dicee.abstracts.AbstractTrainer attribute), 12
global_rank (dicee.trainer.torch_trainer_ddp.NodeTrainer attribute), 163
GPT (class in dicee.models.transformers), 93
```

```
GPTConfig (class in dicee.models.transformers), 93
gpus (dicee.config.Namespace attribute), 26
gradient_accumulation_steps (dicee.config.Namespace attribute), 27
ground_queries() (dicee.query_generator.QueryGenerator method), 143
ground_queries() (dicee.QueryGenerator method), 211
Н
hidden_dim (dicee.literal_classes.LiteralEmbeddings attribute), 52
hidden_dropout (dicee.BaseKGE attribute), 190
hidden_dropout (dicee.models.base_model.BaseKGE attribute), 62
hidden_dropout (dicee.models.BaseKGE attribute), 103, 106, 110, 114, 120, 133, 136
hidden_dropout_rate (dicee.BaseKGE attribute), 189
hidden_dropout_rate (dicee.config.Namespace attribute), 28
hidden_dropout_rate (dicee.models.base_model.BaseKGE attribute), 62
hidden_dropout_rate (dicee.models.BaseKGE attribute), 103, 106, 109, 114, 120, 133, 136
hidden_normalizer (dicee.BaseKGE attribute), 190
hidden_normalizer (dicee.models.base_model.BaseKGE attribute), 62
hidden_normalizer (dicee.models.BaseKGE attribute), 103, 106, 110, 114, 120, 133, 136
IdentityClass (class in dicee.models), 104, 116, 121
IdentityClass (class in dicee.models.base_model), 63
idx_entity_to_bpe_shaped (dicee.knowledge_graph.KG attribute), 45
index() (in module dicee.scripts.index_serve), 152
index_triple() (dicee.abstracts.BaseInteractiveKGE method), 15
init_dataloader() (dicee.DICE_Trainer method), 194
init_dataloader() (dicee.trainer.DICE_Trainer method), 165
init dataloader() (dicee.trainer.dice trainer.DICE Trainer method), 160
init_dataset() (dicee.DICE_Trainer method), 194
init_dataset() (dicee.trainer.DICE_Trainer method), 165
init_dataset() (dicee.trainer.dice_trainer.DICE_Trainer method), 160
init_param (dicee.config.Namespace attribute), 27
init_params_with_sanity_checking() (dicee.BaseKGE method), 190
\verb|init_params_with_sanity_checking()| \textit{(dicee.models.base\_model.BaseKGE method)}, 63
init params with sanity checking () (dicee.models.BaseKGE method), 103, 107, 110, 115, 121, 133, 137
initial_eval_setting (dicee.callbacks.ASWA attribute), 22
initialize_or_load_model() (dicee.DICE_Trainer method), 194
initialize_or_load_model() (dicee.trainer.DICE_Trainer method), 165
\verb|initialize_or_load_model()| \textit{(dicee.trainer.dice\_trainer.DICE\_Trainer method)}, 160
initialize_trainer() (dicee.DICE_Trainer method), 194
initialize_trainer() (dicee.trainer.DICE_Trainer method), 164
initialize_trainer() (dicee.trainer.dice_trainer.DICE_Trainer method), 160
initialize_trainer() (in module dicee.trainer.dice_trainer), 159
input_dp_ent_real (dicee.BaseKGE attribute), 190
input_dp_ent_real (dicee.models.base_model.BaseKGE attribute), 62
input_dp_ent_real (dicee.models.BaseKGE attribute), 103, 106, 110, 114, 120, 133, 136
input_dp_rel_real (dicee.BaseKGE attribute), 190
input_dp_rel_real (dicee.models.base_model.BaseKGE attribute), 62
input_dp_rel_real (dicee.models.BaseKGE attribute), 103, 106, 110, 114, 120, 133, 136
input_dropout_rate (dicee.BaseKGE attribute), 189
input_dropout_rate (dicee.config.Namespace attribute), 28
input_dropout_rate (dicee.models.base_model.BaseKGE attribute), 62
input_dropout_rate (dicee.models.BaseKGE attribute), 103, 106, 109, 114, 120, 133, 136
intialize_model() (in module dicee), 192
intialize_model() (in module dicee.static_funcs), 156
is_continual_training (dicee.DICE_Trainer attribute), 193
is_continual_training (dicee.evaluator.Evaluator attribute), 41
is_continual_training (dicee.executer.Execute attribute), 43
is_continual_training (dicee.trainer.DICE_Trainer attribute), 164
is_continual_training (dicee.trainer.dice_trainer.DICE_Trainer attribute), 159
is\_global\_zero (dicee.abstracts.AbstractTrainer attribute), 12
is_seen() (dicee.abstracts.BaseInteractiveKGE method), 14
is_sparql_endpoint_alive() (in module dicee.sanity_checkers), 150
K
```

```
k (dicee.models.FMult2 attribute), 139
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), 138
k_fold_cross_validation() (dicee.DICE_Trainer method), 194
k_fold_cross_validation() (dicee.trainer.DICE_Trainer method), 165
k_fold_cross_validation() (dicee.trainer.dice_trainer.DICE_Trainer method), 160
k_vs_all_score() (dicee.ComplEx static method), 177
k_vs_all_score() (dicee.DistMult method), 168
k_vs_all_score() (dicee.Keci method), 171
k_vs_all_score() (dicee.models.clifford.Keci method), 67
k_vs_all_score() (dicee.models.ComplEx static method), 113
k_vs_all_score() (dicee.models.complex.ComplEx static method), 73
k_vs_all_score() (dicee.models.DistMult method), 107
k_vs_all_score() (dicee.models.Keci method), 127
k_vs_all_score() (dicee.models.octonion.OMult method), 80
k_vs_all_score() (dicee.models.OMult method), 123
k_vs_all_score() (dicee.models.QMult method), 118
k_vs_all_score() (dicee.models.quaternion.QMult method), 85
k_vs_all_score() (dicee.models.real.DistMult method), 86
k\_vs\_all\_score() (dicee.OMult method), 184
k_vs_all_score() (dicee.QMult method), 183
Keci (class in dicee), 169
Keci (class in dicee.models), 125
Keci (class in dicee.models.clifford), 64
kernel_size (dicee.BaseKGE attribute), 189
kernel_size (dicee.config.Namespace attribute), 27
kernel_size (dicee.models.base_model.BaseKGE attribute), 62
kernel_size (dicee.models.BaseKGE attribute), 103, 106, 110, 114, 120, 133, 136
KG (class in dicee.knowledge_graph), 44
kg (dicee.callbacks.PseudoLabellingCallback attribute), 22
kg (dicee.read_preprocess_save_load_kg.LoadSaveToDisk attribute), 150
kg (dicee.read_preprocess_save_load_kg.PreprocessKG attribute), 149
kg (dicee.read_preprocess_save_load_kg.preprocess.PreprocessKG attribute), 143
kg (dicee.read_preprocess_save_load_kg.read_from_disk.ReadFromDisk attribute), 144
kg (dicee.read preprocess save load kg.ReadFromDisk attribute), 150
kg (dicee.read_preprocess_save_load_kg.save_load_disk.LoadSaveToDisk attribute), 145
KGE (class in dicee), 194
KGE (class in dicee.knowledge_graph_embeddings), 46
KGESaveCallback (class in dicee.callbacks), 21
knowledge_graph (dicee.executer.Execute attribute), 43
KronE (class in dicee.callbacks), 24
KvsAll (class in dicee), 201
KvsAll (class in dicee.dataset_classes), 31
kvsall_score() (dicee.DualE method), 176
kvsall_score() (dicee.models.DualE method), 141
kvsall_score() (dicee.models.dualE.DualE method), 74
KvsSampleDataset (class in dicee), 205
KvsSampleDataset (class in dicee.dataset_classes), 34
label_smoothing_rate (dicee.AllvsAll attribute), 203
label_smoothing_rate (dicee.config.Namespace attribute), 27
label_smoothing_rate (dicee.dataset_classes.AllvsAll attribute), 33
label_smoothing_rate (dicee.dataset_classes.KvsAll attribute), 32
label_smoothing_rate (dicee.dataset_classes.KvsSampleDataset attribute), 35
label_smoothing_rate (dicee.dataset_classes.OnevsSample attribute), 34
label_smoothing_rate (dicee.dataset_classes.TriplePredictionDataset attribute), 36
label_smoothing_rate (dicee.KvsAll attribute), 202
label_smoothing_rate (dicee.KvsSampleDataset attribute), 205
label_smoothing_rate (dicee.OnevsSample attribute), 204
label_smoothing_rate (dicee. TriplePredictionDataset attribute), 206
layer_norm (dicee.literal_classes.LiteralEmbeddings attribute), 52
LayerNorm (class in dicee.models.transformers), 90
learning_rate (dicee.BaseKGE attribute), 189
learning_rate (dicee.models.base_model.BaseKGE attribute), 62
```

```
learning rate (dicee.models.BaseKGE attribute), 103, 106, 109, 114, 120, 133, 136
length (dicee.dataset_classes.NegSampleDataset attribute), 36
length (dicee.dataset_classes.TriplePredictionDataset attribute), 36
length (dicee.NegSampleDataset attribute), 206
length (dicee. TriplePredictionDataset attribute), 207
level (dicee.callbacks.Perturb attribute), 25
LFMult (class in dicee), 184
LFMult (class in dicee.models), 139
LFMult (class in dicee.models.function_space), 78
LFMult1 (class in dicee.models), 139
LFMult1 (class in dicee.models.function_space), 77
linear() (dicee.LFMult method), 185
linear() (dicee.models.function_space.LFMult method), 78
linear() (dicee.models.LFMult method), 140
list2tuple() (dicee.query_generator.QueryGenerator method), 142
list2tuple() (dicee.QueryGenerator method), 211
LiteralDataset (class in dicee.literal_classes), 52
LiteralEmbeddings (class in dicee.literal_classes), 51
lm_head (dicee.BytE attribute), 187
lm_head (dicee.models.transformers.BytE attribute), 89
lm_head (dicee.models.transformers.GPT attribute), 94
ln_1 (dicee.models.transformers.Block attribute), 93
ln_2 (dicee.models.transformers.Block attribute), 93
load() (dicee.read_preprocess_save_load_kg.LoadSaveToDisk method), 150
load() (dicee.read_preprocess_save_load_kg.save_load_disk.LoadSaveToDisk method), 145
load_and_validate_literal_data() (dicee.literal_classes.LiteralDataset static method), 54
load_json() (in module dicee), 192
load_json() (in module dicee.static_funcs), 156
load_model() (in module dicee), 192
load_model() (in module dicee.static_funcs), 155
load_model_ensemble() (in module dicee), 192
load_model_ensemble() (in module dicee.static_funcs), 155
load_numpy() (in module dicee), 193
load_numpy() (in module dicee.static_funcs), 156
load_numpy_ndarray() (in module dicee.read_preprocess_save_load_kg.util), 148
load_pickle() (in module dicee), 191
load_pickle() (in module dicee.read_preprocess_save_load_kg.util), 149
load_pickle() (in module dicee.static_funcs), 155
load_queries() (dicee.query_generator.QueryGenerator method), 143
load_queries() (dicee.QueryGenerator method), 211
load_queries_and_answers() (dicee.query_generator.QueryGenerator static method), 143
load_queries_and_answers() (dicee.QueryGenerator static method), 211
load_term_mapping() (in module dicee), 192, 199
load_term_mapping() (in module dicee.static_funcs), 155
load_term_mapping() (in module dicee.trainer.dice_trainer), 159
load_with_pandas() (in module dicee.read_preprocess_save_load_kg.util), 148
LoadSaveToDisk (class in dicee.read_preprocess_save_load_kg), 150
LoadSaveToDisk (class in dicee.read_preprocess_save_load_kg.save_load_disk), 145
local_rank (dicee.abstracts.AbstractTrainer attribute), 12
local_rank (dicee.trainer.torch_trainer_ddp.NodeTrainer attribute), 163
loss (dicee.BaseKGE attribute), 189
loss (dicee.models.base_model.BaseKGE attribute), 62
loss (dicee.models.BaseKGE attribute), 103, 106, 110, 114, 120, 133, 136
loss_func (dicee.trainer.torch_trainer_ddp.NodeTrainer attribute), 163
loss_function (dicee.trainer.torch_trainer.TorchTrainer attribute), 161
loss_function() (dicee.BytE method), 187
loss_function() (dicee.models.base_model.BaseKGELightning method), 57
loss_function() (dicee.models.BaseKGELightning method), 98
loss_function() (dicee.models.transformers.BytE method), 89
loss_history (dicee.BaseKGE attribute), 190
loss_history (dicee.models.base_model.BaseKGE attribute), 62
loss_history (dicee.models.BaseKGE attribute), 103, 106, 110, 115, 120, 133, 137
loss_history (dicee.models.pykeen_models.PykeenKGE attribute), 82
loss_history (dicee.models.PykeenKGE attribute), 134
loss_history (dicee.PykeenKGE attribute), 186
loss_history (dicee.trainer.torch_trainer_ddp.NodeTrainer attribute), 163
1r (dicee.analyse_experiments.Experiment attribute), 18
1r (dicee.config.Namespace attribute), 26
```

## M

```
m (dicee.LFMult attribute), 184
m (dicee.models.function_space.LFMult attribute), 78
m (dicee.models.LFMult attribute), 140
main() (in module dicee.scripts.index_serve), 153
main() (in module dicee.scripts.run), 154
make_iterable_verbose() (in module dicee.static_funcs_training), 157
make_iterable_verbose() (in module dicee.trainer.torch_trainer_ddp), 163
mapping_from_first_two_cols_to_third() (in module dicee), 199
mapping_from_first_two_cols_to_third() (in module dicee.static_preprocess_funcs), 158
margin (dicee.models.Pyke attribute), 108
margin (dicee.models.real.Pyke attribute), 87
margin (dicee.models.real.TransE attribute), 87
margin (dicee.models.TransE attribute), 108
margin (dicee. Pyke attribute), 168
margin (dicee. TransE attribute), 172
max_ans_num (dicee.query_generator.QueryGenerator attribute), 142
max_ans_num (dicee.QueryGenerator attribute), 210
max_epochs (dicee.callbacks.KGESaveCallback attribute), 21
max_length_subword_tokens (dicee.BaseKGE attribute), 190
max_length_subword_tokens (dicee.knowledge_graph.KG attribute), 45
max_length_subword_tokens (dicee.models.base_model.BaseKGE attribute), 62
max_length_subword_tokens (dicee.models.BaseKGE attribute), 103, 106, 110, 115, 121, 133, 137
max_num_of_classes (dicee.dataset_classes.KvsSampleDataset attribute), 35
max_num_of_classes (dicee.KvsSampleDataset attribute), 205
mem_of_model() (dicee.EnsembleKGE method), 191
mem_of_model() (dicee.models.base_model.BaseKGELightning method), 56
mem of model() (dicee.models.BaseKGELightning method), 97
mem_of_model() (dicee.models.ensemble.EnsembleKGE method), 75
method (dicee.callbacks.Perturb attribute), 25
MLP (class in dicee.models.transformers), 91
{\tt mlp} (dicee.models.transformers.Block attribute), 93
mode (dicee.query_generator.QueryGenerator attribute), 142
mode (dicee. Query Generator attribute), 211
model (dicee.config.Namespace attribute), 26
model (dicee.models.pykeen_models.PykeenKGE attribute), 82
model (dicee.models.PykeenKGE attribute), 134
model (dicee. Pykeen KGE attribute), 186
model (dicee.trainer.torch_trainer_ddp.NodeTrainer attribute), 163
model (dicee.trainer.torch_trainer.TorchTrainer attribute), 162
model_kwargs (dicee.models.pykeen_models.PykeenKGE attribute), 82
model_kwargs (dicee.models.PykeenKGE attribute), 134
model_kwargs (dicee.PykeenKGE attribute), 185
\verb|model_name| (\textit{dicee.analyse\_experiments.Experiment attribute}), 18
module
     dicee, 12
     dicee.__main__, 12
     dicee.abstracts, 12
     dicee.analyse_experiments, 17
     dicee.callbacks, 19
     dicee.config, 25
     dicee.dataset_classes, 28
     dicee.eval_static_funcs, 40
     dicee.evaluator, 41
     dicee.executer, 43
     dicee.knowledge_graph,44
     dicee.knowledge_graph_embeddings,46
     dicee.literal_classes, 51
     {\tt dicee.models}, {\tt 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.octonion, 79
     dicee.models.pykeen_models, 82
```

```
dicee.models.quaternion, 83
     dicee.models.real, 86
     dicee.models.static funcs.88
     dicee.models.transformers, 88
     dicee.query_generator, 142
     dicee.read_preprocess_save_load_kg, 143
     dicee.read_preprocess_save_load_kg.preprocess, 143
     dicee.read_preprocess_save_load_kg.read_from_disk, 144
     dicee.read_preprocess_save_load_kg.save_load_disk, 145
     dicee.read_preprocess_save_load_kg.util, 145
     dicee.sanity_checkers, 150
     dicee.scripts, 151
     dicee.scripts.index_serve, 151
     dicee.scripts.run, 153
     dicee.static_funcs, 154
     dicee.static_funcs_training, 157
     dicee.static_preprocess_funcs, 157
     dicee.trainer, 158
     dicee.trainer.dice_trainer, 158
     dicee.trainer.model_parallelism, 160
     dicee.trainer.torch_trainer, 161
     dicee.trainer.torch_trainer_ddp, 162
modules () (dicee. Ensemble KGE method), 191
\verb|modules()| (\textit{dicee.models.ensemble.EnsembleKGE method}), 75
MultiClassClassificationDataset (class in dicee), 200
MultiClassClassificationDataset (class in dicee.dataset_classes), 30
MultiLabelDataset (class in dicee), 200
MultiLabelDataset (class in dicee.dataset_classes), 30
Ν
n (dicee.models.FMult2 attribute), 139
n (dicee.models.function_space.FMult2 attribute), 77
n_embd (dicee.models.transformers.CausalSelfAttention attribute), 91
n_embd (dicee.models.transformers.GPTConfig attribute), 93
n_head (dicee.models.transformers.CausalSelfAttention attribute), 91
n_head (dicee.models.transformers.GPTConfig attribute), 93
n_layer (dicee.models.transformers.GPTConfig attribute), 93
n_layers (dicee.models.FMult2 attribute), 139
n_layers (dicee.models.function_space.FMult2 attribute), 77
name (dicee.abstracts.BaseInteractiveKGE property), 14
name (dicee.AConEx attribute), 177
name (dicee.AConvO attribute), 178
name (dicee.AConvO attribute), 179
name (dicee.BytE attribute), 187
name (dicee. CKeci attribute), 169
name (dicee.ComplEx attribute), 177
name (dicee.ConEx attribute), 181
name (dicee.ConvO attribute), 180
name (dicee.ConvQ attribute), 179
name (dicee.DeCaL attribute), 173
name (dicee.DistMult attribute), 168
name (dicee.DualE attribute), 176
name (dicee.EnsembleKGE attribute), 191
name (dicee. Keci attribute), 169
name (dicee.LFMult attribute), 184
name (dicee.models.AConEx attribute), 112
name (dicee.models.AConvO attribute), 124
name (dicee.models.AConvQ attribute), 118
name (dicee.models.CKeci attribute), 128
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), 113
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), 111
```

```
name (dicee.models.ConvO attribute), 124
name (dicee.models.ConvQ attribute), 118
name (dicee.models.DeCaL attribute), 129
name (dicee.models.DistMult attribute), 107
name (dicee.models.DualE attribute), 141
name (dicee.models.dualE.DualE attribute), 74
name (dicee.models.ensemble.EnsembleKGE attribute), 75
name (dicee.models.FMult attribute), 138
name (dicee.models.FMult2 attribute), 139
name (dicee.models.function_space.FMult attribute), 76
name (dicee.models.function_space.FMult2 attribute), 77
\verb"name" (\textit{dicee.models.function\_space.GFMult attribute}), 76
name (dicee.models.function_space.LFMult attribute), 78
name (dicee.models.function_space.LFMult1 attribute), 77
name (dicee.models.GFMult attribute), 138
name (dicee.models.Keci attribute), 125
name (dicee.models.LFMult attribute), 140
name (dicee.models.LFMult1 attribute), 139
name (dicee.models.octonion.AConvO attribute), 81
name (dicee.models.octonion.ConvO attribute), 81
name (dicee.models.octonion.OMult attribute), 80
name (dicee.models.OMult attribute). 123
name (dicee.models.Pyke attribute), 108
name (dicee.models.pykeen_models.PykeenKGE attribute), 82
name (dicee.models.PykeenKGE attribute), 134
name (dicee.models.QMult attribute), 117
name (dicee.models.quaternion.AConvQ attribute), 86
name (dicee.models.quaternion.ConvQ attribute), 85
name (dicee.models.quaternion.QMult attribute), 84
name (dicee.models.real.DistMult attribute), 86
name (dicee.models.real.Pyke attribute), 87
name (dicee.models.real.Shallom attribute), 87
name (dicee.models.real.TransE attribute), 87
name (dicee.models.Shallom attribute), 108
name (dicee.models.TransE attribute), 108
name (dicee.models.transformers.BytE attribute), 89
name (dicee.OMult attribute), 184
name (dicee.Pyke attribute), 168
name (dicee.PykeenKGE attribute), 185
name (dicee.QMult attribute), 182
name (dicee.Shallom attribute), 184
name (dicee. TransE attribute), 172
named_children() (dicee.EnsembleKGE method), 191
named_children() (dicee.models.ensemble.EnsembleKGE method).75
Namespace (class in dicee.config), 26
\verb"neg_ratio" (\textit{dicee.BPE\_NegativeSamplingDataset attribute}), 200
neg_ratio (dicee.config.Namespace attribute), 27
neg_ratio (dicee.dataset_classes.BPE_NegativeSamplingDataset attribute), 30
neg_ratio (dicee.dataset_classes.KvsSampleDataset attribute), 35
neg_ratio (dicee.KvsSampleDataset attribute), 205
neg_sample_ratio (dicee.CVDataModule attribute), 207
neg_sample_ratio (dicee.dataset_classes.CVDataModule attribute), 37
neg_sample_ratio (dicee.dataset_classes.NegSampleDataset attribute), 35
neg_sample_ratio (dicee.dataset_classes.OnevsSample attribute), 33, 34
neg_sample_ratio (dicee.dataset_classes.TriplePredictionDataset attribute), 36
neg_sample_ratio (dicee.NegSampleDataset attribute), 206
neg_sample_ratio (dicee.OnevsSample attribute), 204
neg_sample_ratio (dicee.TriplePredictionDataset attribute), 207
negnorm() (dicee.KGE method), 197
negnorm() (dicee.knowledge_graph_embeddings.KGE method), 49
NegSampleDataset (class in dicee), 205
NegSampleDataset (class in dicee.dataset_classes), 35
neural_searcher (in module dicee.scripts.index_serve), 152
NeuralSearcher (class in dicee.scripts.index_serve), 152
NodeTrainer (class in dicee.trainer.torch_trainer_ddp), 163
norm_fc1 (dicee.AConEx attribute), 178
norm_fc1 (dicee.AConvO attribute), 178
norm_fc1 (dicee.ConEx attribute), 181
```

```
norm fc1 (dicee.ConvO attribute), 181
norm_fc1 (dicee.models.AConEx attribute), 112
norm fc1 (dicee.models.AConvO attribute), 125
norm_fc1 (dicee.models.complex.AConEx attribute), 72
norm_fc1 (dicee.models.complex.ConEx attribute), 72
norm_fc1 (dicee.models.ConEx attribute), 111
norm_fc1 (dicee.models.ConvO attribute), 124
norm fc1 (dicee.models.octonion.AConvO attribute), 82
norm_fc1 (dicee.models.octonion.ConvO attribute), 81
normalization (dicee.analyse_experiments.Experiment attribute), 19
normalization (dicee.config.Namespace attribute), 27
normalization (dicee.literal_classes.LiteralDataset attribute), 53
normalization_params (dicee.literal_classes.LiteralDataset attribute), 53
normalization_type (dicee.literal_classes.LiteralDataset attribute), 53
{\tt normalize\_head\_entity\_embeddings}~(\textit{dicee.BaseKGE attribute}),~190
normalize_head_entity_embeddings (dicee.models.base_model.BaseKGE attribute), 62
normalize_head_entity_embeddings (dicee.models.BaseKGE attribute), 103, 106, 110, 114, 120, 133, 136
normalize_relation_embeddings (dicee.BaseKGE attribute), 190
normalize_relation_embeddings (dicee.models.base_model.BaseKGE attribute), 62
normalize_relation_embeddings (dicee.models.BaseKGE attribute), 103, 106, 110, 114, 120, 133, 136
normalize_tail_entity_embeddings (dicee.BaseKGE attribute), 190
normalize_tail_entity_embeddings (dicee.models.base_model.BaseKGE attribute), 62
normalize_tail_entity_embeddings (dicee.models.BaseKGE attribute), 103, 106, 110, 114, 120, 133, 136
normalizer_class (dicee.BaseKGE attribute), 189
normalizer_class (dicee.models.base_model.BaseKGE attribute), 62
normalizer_class (dicee.models.BaseKGE attribute), 103, 106, 110, 114, 120, 133, 136
num_bpe_entities (dicee.BPE_NegativeSamplingDataset attribute), 200
num_bpe_entities (dicee.dataset_classes.BPE_NegativeSamplingDataset attribute), 30
num_bpe_entities (dicee.knowledge_graph.KG attribute), 45
num_core (dicee.config.Namespace attribute), 27
num_data_properties (dicee.literal_classes.LiteralDataset attribute), 53
num datapoints (dicee.BPE NegativeSamplingDataset attribute), 200
num_datapoints (dicee.dataset_classes.BPE_NegativeSamplingDataset attribute), 30
num_datapoints (dicee.dataset_classes.MultiLabelDataset attribute), 30
num_datapoints (dicee.MultiLabelDataset attribute), 200
num_ent (dicee.DualE attribute), 176
num ent (dicee.models.DualE attribute), 141
num_ent (dicee.models.dualE.DualE attribute), 74
num_entities (dicee.BaseKGE attribute), 189
num_entities (dicee.CVDataModule attribute), 207
num_entities (dicee.dataset_classes.CVDataModule attribute), 37
num_entities (dicee.dataset_classes.KvsSampleDataset attribute), 35
num_entities (dicee.dataset_classes.NegSampleDataset attribute), 36
num_entities (dicee.dataset_classes.OnevsSample attribute), 33, 34
num_entities (dicee.dataset_classes.TriplePredictionDataset attribute), 36
num_entities (dicee.evaluator.Evaluator attribute), 41
num_entities (dicee.knowledge_graph.KG attribute), 45
num_entities (dicee.KvsSampleDataset attribute), 205
num_entities (dicee.literal_classes.LiteralDataset attribute), 53, 54
num_entities (dicee.models.base_model.BaseKGE attribute), 62
num entities (dicee.models.BaseKGE attribute), 102, 106, 109, 114, 120, 132, 136
num_entities (dicee.NegSampleDataset attribute), 206
num_entities (dicee.OnevsSample attribute), 203, 204
num_entities (dicee. TriplePredictionDataset attribute), 207
num_epochs (dicee.abstracts.AbstractPPECallback attribute), 17
num_epochs (dicee.analyse_experiments.Experiment attribute), 18
num_epochs (dicee.callbacks.ASWA attribute), 22
num_epochs (dicee.config.Namespace attribute), 26
num_epochs (dicee.trainer.torch_trainer_ddp.NodeTrainer attribute), 163
num_folds_for_cv (dicee.config.Namespace attribute), 27
num of data points (dicee.dataset classes.MultiClassClassificationDataset attribute), 31
num_of_data_points (dicee.MultiClassClassificationDataset attribute), 201
num_of_data_properties (dicee.literal_classes.LiteralEmbeddings attribute), 51, 52
num_of_epochs (dicee.callbacks.PseudoLabellingCallback attribute), 22
num_of_output_channels (dicee.BaseKGE attribute), 189
num_of_output_channels (dicee.config.Namespace attribute), 27
num_of_output_channels (dicee.models.base_model.BaseKGE attribute), 62
num_of_output_channels (dicee.models.BaseKGE attribute), 103, 106, 110, 114, 120, 133, 136
```

```
num params (dicee.analyse experiments.Experiment attribute), 18
num_relations (dicee.BaseKGE attribute), 189
num relations (dicee.CVDataModule attribute), 207
num_relations (dicee.dataset_classes.CVDataModule attribute), 37
num_relations (dicee.dataset_classes.NegSampleDataset attribute), 36
num_relations (dicee.dataset_classes.OnevsSample attribute), 33, 34
num_relations (dicee.dataset_classes.TriplePredictionDataset attribute), 36
num relations (dicee.evaluator.Evaluator attribute), 41
num_relations (dicee.knowledge_graph.KG attribute), 45
num_relations (dicee.models.base_model.BaseKGE attribute), 62
num_relations (dicee.models.BaseKGE attribute), 102, 106, 109, 114, 120, 132, 136
\verb|num_relations| (\textit{dicee.NegSampleDataset attribute}), 206
num_relations (dicee.OnevsSample attribute), 204
num_relations (dicee. TriplePredictionDataset attribute), 207
num_sample (dicee.models.FMult attribute), 138
num_sample (dicee.models.function_space.FMult attribute), 76
num_sample (dicee.models.function_space.GFMult attribute), 76
num_sample (dicee.models.GFMult attribute), 138
num_tokens (dicee.BaseKGE attribute), 189
num_tokens (dicee.knowledge_graph.KG attribute), 45
num_tokens (dicee.models.base_model.BaseKGE attribute), 62
num_tokens (dicee.models.BaseKGE attribute), 102, 106, 109, 114, 120, 133, 136
num_workers (dicee.CVDataModule attribute), 207
num_workers (dicee.dataset_classes.CVDataModule attribute), 37
numpy_data_type_changer() (in module dicee), 192
numpy_data_type_changer() (in module dicee.static_funcs), 156
octonion_mul() (in module dicee.models), 122
octonion_mul() (in module dicee.models.octonion), 79
octonion_mul_norm() (in module dicee.models), 122
octonion_mul_norm() (in module dicee.models.octonion), 79
octonion_normalizer() (dicee.AConvO static method), 178
octonion_normalizer() (dicee.ConvO static method), 181
octonion_normalizer() (dicee.models.AConvO static method), 125
octonion_normalizer() (dicee.models.ConvO static method), 124
octonion_normalizer() (dicee.models.octonion.AConvO static method), 82
octonion_normalizer() (dicee.models.octonion.ConvO static method), 81
octonion_normalizer() (dicee.models.octonion.OMult static method), 80
octonion_normalizer() (dicee.models.OMult static method), 123
octonion_normalizer() (dicee.OMult static method), 184
OMult (class in dicee), 183
OMult (class in dicee.models), 122
OMult (class in dicee.models.octonion), 79
on_epoch_end() (dicee.callbacks.KGESaveCallback method), 22
on_epoch_end() (dicee.callbacks.PseudoLabellingCallback method), 22
on_fit_end() (dicee.abstracts.AbstractCallback method), 16
on_fit_end() (dicee.abstracts.AbstractPPECallback method), 17
on_fit_end() (dicee.abstracts.AbstractTrainer method), 13
on_fit_end() (dicee.callbacks.AccumulateEpochLossCallback method), 20
on_fit_end() (dicee.callbacks.ASWA method), 23
on_fit_end() (dicee.callbacks.Eval method), 24
on_fit_end() (dicee.callbacks.KGESaveCallback method), 22
on_fit_end() (dicee.callbacks.PrintCallback method), 20
on_fit_start() (dicee.abstracts.AbstractCallback method), 16
on_fit_start() (dicee.abstracts.AbstractPPECallback method), 17
on_fit_start() (dicee.abstracts.AbstractTrainer method), 12
on_fit_start() (dicee.callbacks.Eval method), 24
on_fit_start() (dicee.callbacks.KGESaveCallback method), 21
on_fit_start() (dicee.callbacks.KronE method), 25
on_fit_start() (dicee.callbacks.PrintCallback method), 20
on_init_end() (dicee.abstracts.AbstractCallback method), 16
on_init_start() (dicee.abstracts.AbstractCallback method), 15
on_train_batch_end() (dicee.abstracts.AbstractCallback method), 16
on_train_batch_end() (dicee.abstracts.AbstractTrainer method), 13
on_train_batch_end() (dicee.callbacks.Eval method), 24
on_train_batch_end() (dicee.callbacks.KGESaveCallback method), 21
```

```
on train batch end() (dicee.callbacks.PrintCallback method), 20
on_train_batch_start() (dicee.callbacks.Perturb method), 25
on_train_epoch_end() (dicee.abstracts.AbstractCallback method), 16
on_train_epoch_end() (dicee.abstracts.AbstractTrainer method), 13
on_train_epoch_end() (dicee.callbacks.ASWA method), 23
on_train_epoch_end() (dicee.callbacks.Eval method), 24
on_train_epoch_end() (dicee.callbacks.KGESaveCallback method), 21
on train epoch end() (dicee.callbacks.PrintCallback method), 21
on_train_epoch_end() (dicee.models.base_model.BaseKGELightning method), 57
on_train_epoch_end() (dicee.models.BaseKGELightning method), 98
OnevsAllDataset (class in dicee), 201
OnevsAllDataset (class in dicee.dataset_classes), 31
OnevsSample (class in dicee), 203
OnevsSample (class in dicee.dataset_classes), 33
optim (dicee.config.Namespace attribute), 26
optimizer (dicee.trainer.torch_trainer_ddp.NodeTrainer attribute), 163
optimizer (dicee.trainer.torch_trainer.TorchTrainer attribute), 161
optimizer_name (dicee.BaseKGE attribute), 189
optimizer_name (dicee.models.base_model.BaseKGE attribute), 62
optimizer_name (dicee.models.BaseKGE attribute), 103, 106, 109, 114, 120, 133, 136
ordered_bpe_entities (dicee.BPE_NegativeSamplingDataset attribute), 200
ordered_bpe_entities (dicee.dataset_classes.BPE_NegativeSamplingDataset attribute), 30
ordered_bpe_entities (dicee.knowledge_graph.KG attribute), 46
ordered_shaped_bpe_tokens (dicee.knowledge_graph.KG attribute), 45
p (dicee.config.Namespace attribute), 28
p (dicee.DeCaL attribute), 173
p (dicee.Keci attribute), 169
p (dicee.models.clifford.DeCaL attribute), 68
p (dicee.models.clifford.Keci attribute), 65
p (dicee.models.DeCaL attribute), 129
p (dicee.models.Keci attribute), 126
padding (dicee.knowledge_graph.KG attribute), 45
pandas_dataframe_indexer() (in module dicee.read_preprocess_save_load_kg.util), 147
param_init (dicee.BaseKGE attribute), 190
param_init (dicee.models.base_model.BaseKGE attribute), 62
param init (dicee.models.BaseKGE attribute), 103, 106, 110, 114, 120, 133, 136
parameters () (dicee.abstracts.BaseInteractiveKGE method), 15
parameters () (dicee. Ensemble KGE method), 191
parameters () (dicee.models.ensemble.EnsembleKGE method), 75
path (dicee.abstracts.AbstractPPECallback attribute), 17
path (dicee.callbacks.AccumulateEpochLossCallback attribute), 20
path (dicee.callbacks.ASWA attribute), 22
path (dicee.callbacks.Eval attribute), 23
path (dicee.callbacks.KGESaveCallback attribute), 21
path_dataset_folder (dicee.analyse_experiments.Experiment attribute), 18
path_for_deserialization (dicee.knowledge_graph.KG attribute), 45
path_for_serialization (dicee.knowledge_graph.KG attribute), 45
path_single_kg (dicee.config.Namespace attribute), 26
path_single_kg (dicee.knowledge_graph.KG attribute), 45
path_to_store_single_run (dicee.config.Namespace attribute), 26
Perturb (class in dicee.callbacks), 25
polars_dataframe_indexer() (in module dicee.read_preprocess_save_load_kg.util), 146
poly_NN() (dicee.LFMult method), 184
poly_NN() (dicee.models.function_space.LFMult method), 78
poly_NN() (dicee.models.LFMult method), 140
polynomial() (dicee.LFMult method), 185
polynomial() (dicee.models.function_space.LFMult method), 79
polynomial() (dicee.models.LFMult method), 140
pop () (dicee.LFMult method), 185
pop() (dicee.models.function_space.LFMult method), 79
pop () (dicee.models.LFMult method), 141
\verb"pq" (dicee. analyse\_experiments. Experiment \ attribute), \ 18
predict() (dicee.KGE method), 196
predict() (dicee.knowledge_graph_embeddings.KGE method), 48
predict_dataloader() (dicee.models.base_model.BaseKGELightning method), 59
```

```
predict dataloader() (dicee.models.BaseKGELightning method), 100
predict_literals() (dicee.KGE method), 198
predict_literals() (dicee.knowledge_graph_embeddings.KGE method), 50
predict_missing_head_entity() (dicee.KGE method), 195
predict_missing_head_entity() (dicee.knowledge_graph_embeddings.KGE method), 46
predict_missing_relations() (dicee.KGE method), 195
predict_missing_relations() (dicee.knowledge_graph_embeddings.KGE method), 47
predict_missing_tail_entity() (dicee.KGE method), 195
predict_missing_tail_entity() (dicee.knowledge_graph_embeddings.KGE method), 47
predict_topk() (dicee.KGE method), 196
predict_topk() (dicee.knowledge_graph_embeddings.KGE method), 48
prepare_data() (dicee.CVDataModule method), 209
prepare_data() (dicee.dataset_classes.CVDataModule method), 39
preprocess_with_byte_pair_encoding() (dicee.read_preprocess_save_load_kg.PreprocessKG method), 149
preprocess_with_byte_pair_encoding() (dicee.read_preprocess_save_load_kg.preprocess.Preprocess.Preprocess.Preprocess.Preprocess.Preprocess.Preprocess.Preprocess.Preprocess.Preprocess.Preprocess.Preprocess.Preprocess.Preprocess.Preprocess.Preprocess.Preprocess.Preprocess.Preprocess.Preprocess.Preprocess.Preprocess.Preprocess.Preprocess.Preprocess.Preprocess.Preprocess.Preprocess.Preprocess.Preprocess.Preprocess.Preprocess.Preprocess.Preprocess.Preprocess.Preprocess.Preprocess.Preprocess.Preprocess.Preprocess.Preprocess.Preprocess.Preprocess.Preprocess.Preprocess.Preprocess.Preprocess.Preprocess.Preprocess.Preprocess.Preprocess.Preprocess.Preprocess.Preprocess.Preprocess.Preprocess.Preprocess.Preprocess.Preprocess.Preprocess.Preprocess.Preprocess.Preprocess.Preprocess.Preprocess.Preprocess.Preprocess.Preprocess.Preprocess.Preprocess.Preprocess.Preprocess.Preprocess.Preprocess.Preprocess.Preprocess.Preprocess.Preprocess.Preprocess.Preprocess.Preprocess.Preprocess.Preprocess.Preprocess.Preprocess.Preprocess.Preprocess.Preprocess.Preprocess.Preprocess.Preprocess.Preprocess.Preprocess.Preprocess.Preprocess.Preprocess.Preprocess.Preprocess.Preprocess.Preprocess.Preprocess.Preprocess.Preprocess.Preprocess.Preprocess.Preprocess.Preprocess.Preprocess.Preprocess.Preprocess.Preprocess.Preprocess.Preprocess.Preprocess.Preprocess.Preprocess.Preprocess.Preprocess.Preprocess.Preprocess.Preprocess.Preprocess.Preprocess.Preprocess.Preprocess.Preprocess.Preprocess.Preprocess.Preprocess.Preprocess.Preprocess.Preprocess.Preprocess.Preprocess.Preprocess.Preprocess.Preprocess.Preprocess.Preprocess.Preprocess.Preprocess.Preprocess.Preprocess.Preprocess.Preprocess.Preprocess.Preprocess.Preprocess.Preprocess.Preprocess.Preprocess.Preprocess.Preprocess.Preprocess.Preprocess.Preprocess.Preprocess.Preprocess.Preprocess.Preprocess.Preprocess.Preprocess.Preprocess.Preprocess.Preprocess.Preprocess.Preprocess.Preprocess.Preprocess.Preprocess.Preprocess.Preprocess.Preprocess.Preprocess.Preprocess.Preprocess.Preprocess.Preprocess.Preprocess.Prep
preprocess_with_byte_pair_encoding_with_padding() (dicee.read_preprocess_save_load_kg.PreprocessKG method), 149
preprocess_with_byte_pair_encoding_with_padding() (dicee.read_preprocess_save_load_kg.preprocess.PreprocessKG method), 144
preprocess_with_pandas() (dicee.read_preprocess_save_load_kg.PreprocessKG method), 149
preprocess_with_pandas() (dicee.read_preprocess_save_load_kg.preprocess.PreprocessKG method), 144
preprocess_with_polars() (dicee.read_preprocess_save_load_kg.PreprocessKG method), 150
preprocess_with_polars() (dicee.read_preprocess_save_load_kg.preprocess.PreprocessKG method), 144
preprocesses_input_args() (in module dicee.static_preprocess_funcs), 158
PreprocessKG (class in dicee.read_preprocess_save_load_kg), 149
PreprocessKG (class in dicee.read_preprocess_save_load_kg.preprocess), 143
PrintCallback (class in dicee.callbacks), 20
process (dicee.trainer.torch_trainer.TorchTrainer attribute), 162
proj (dicee.literal_classes.GatedLinearUnit attribute), 51
PseudoLabellingCallback (class in dicee.callbacks), 22
Pyke (class in dicee), 168
Pyke (class in dicee.models), 108
Pyke (class in dicee.models.real), 87
pykeen_model_kwargs (dicee.config.Namespace attribute), 27
PykeenKGE (class in dicee), 185
PykeenKGE (class in dicee.models), 134
PykeenKGE (class in dicee.models.pykeen_models), 82
q (dicee.config.Namespace attribute), 28
q (dicee.DeCaL attribute), 173
q (dicee.Keci attribute), 169
q (dicee.models.clifford.DeCaL attribute), 68
q (dicee.models.clifford.Keci attribute), 65
q (dicee.models.DeCaL attribute), 129
q (dicee.models.Keci attribute), 126
qdrant_client (dicee.scripts.index_serve.NeuralSearcher attribute), 152
QMult (class in dicee), 181
QMult (class in dicee.models), 116
OMult (class in dicee.models.quaternion), 83
quaternion_mul() (in module dicee.models), 113
quaternion_mul() (in module dicee.models.static_funcs), 88
quaternion_mul_with_unit_norm() (in module dicee.models), 116
quaternion_mul_with_unit_norm() (in module dicee.models.quaternion), 83
quaternion_multiplication_followed_by_inner_product() (dicee.models.QMult method), 117
quaternion_multiplication_followed_by_inner_product() (dicee.models.quaternion.QMult method), 84
quaternion_multiplication_followed_by_inner_product() (dicee.QMult method), 182
quaternion_normalizer() (dicee.models.QMult static method), 117
quaternion_normalizer() (dicee.models.quaternion.QMult static method), 84
quaternion_normalizer() (dicee.QMult static method), 182
queries (dicee.scripts.index_serve.StringListRequest attribute), 153
query_name_to_struct (dicee.query_generator.QueryGenerator attribute), 142
query_name_to_struct (dicee.QueryGenerator attribute), 211
OuervGenerator (class in dicee), 210
QueryGenerator (class in dicee.query_generator), 142
r (dicee.DeCaL attribute), 173
r (dicee. Keci attribute), 169
```

```
r (dicee.models.clifford.DeCaL attribute), 68
r (dicee.models.clifford.Keci attribute), 65
r (dicee.models.DeCaL attribute), 129
r (dicee.models.Keci attribute), 126
random_prediction() (in module dicee), 192
random_prediction() (in module dicee.static_funcs), 156
random_seed (dicee.config.Namespace attribute), 27
ratio (dicee.callbacks.Perturb attribute), 25
re (dicee.DeCaL attribute), 173
re (dicee.models.clifford.DeCaL attribute), 68
re (dicee.models.DeCaL attribute), 129
re_vocab (dicee.evaluator.Evaluator attribute), 41
read_from_disk() (in module dicee.read_preprocess_save_load_kg.util), 148
read_from_triple_store() (in module dicee.read_preprocess_save_load_kg.util), 148
read_only_few (dicee.config.Namespace attribute), 27
read_only_few (dicee.knowledge_graph.KG attribute), 45
read_or_load_kg() (in module dicee), 192
read_or_load_kg() (in module dicee.static_funcs), 156
read_with_pandas() (in module dicee.read_preprocess_save_load_kg.util), 148
read_with_polars() (in module dicee.read_preprocess_save_load_kg.util), 148
ReadFromDisk (class in dicee.read_preprocess_save_load_kg), 150
ReadFromDisk (class in dicee.read_preprocess_save_load_kg.read_from_disk), 144
reducer (dicee.scripts.index_serve.StringListRequest attribute), 153
rel2id (dicee.query_generator.QueryGenerator attribute), 142
rel2id (dicee.QueryGenerator attribute), 211
relation_embeddings (dicee.AConvQ attribute), 179
relation_embeddings (dicee.ConvQ attribute), 179
relation_embeddings (dicee.DeCaL attribute), 173
relation_embeddings (dicee.DualE attribute), 176
relation_embeddings (dicee.LFMult attribute), 184
relation_embeddings (dicee.models.AConvQ attribute), 119
relation embeddings (dicee.models.clifford.DeCaL attribute), 68
relation_embeddings (dicee.models.ConvQ attribute), 118
relation_embeddings (dicee.models.DeCaL attribute), 129
relation_embeddings (dicee.models.DualE attribute), 141
relation_embeddings (dicee.models.dualE.DualE attribute), 74
relation embeddings (dicee.models.FMult attribute), 138
relation_embeddings (dicee.models.FMult2 attribute), 139
{\tt relation\_embeddings}~(\textit{dicee.models.function\_space.FMult~attribute}), 76
relation_embeddings (dicee.models.function_space.FMult2 attribute), 77
{\tt relation\_embeddings}~({\it 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), 138
relation_embeddings (dicee.models.LFMult attribute), 140
relation_embeddings (dicee.models.LFMult1 attribute), 139
relation_embeddings (dicee.models.pykeen_models.PykeenKGE attribute), 82
relation_embeddings (dicee.models.PykeenKGE attribute), 135
relation_embeddings (dicee.models.quaternion.AConvQ attribute), 86
relation_embeddings (dicee.models.quaternion.ConvQ attribute), 85
relation_embeddings (dicee.PykeenKGE attribute), 186
relation_to_idx (dicee.knowledge_graph.KG attribute), 45
relations_str (dicee.knowledge_graph.KG property), 46
reload_dataset() (in module dicee), 199
reload_dataset() (in module dicee.dataset_classes), 29
report (dicee.DICE_Trainer attribute), 193
report (dicee.evaluator.Evaluator attribute), 42
report (dicee.executer.Execute attribute), 43
report (dicee.trainer.DICE_Trainer attribute), 164
report (dicee.trainer.dice_trainer.DICE_Trainer attribute), 159
reports (dicee.callbacks.Eval attribute), 23
requires_grad_for_interactions (dicee. CKeci attribute), 169
\verb|requires_grad_for_interactions| (\textit{dicee.Keci attribute}), 169
requires_grad_for_interactions (dicee.models.CKeci attribute), 128
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), 126
resid_dropout (dicee.models.transformers.CausalSelfAttention attribute), 91
```

```
residual (dicee.literal classes.LiteralEmbeddings attribute), 52
residual_convolution() (dicee.AConEx method), 178
residual_convolution() (dicee.AConvO method), 178
residual_convolution() (dicee.AConvQ method), 179
residual_convolution() (dicee.ConEx method), 181
residual_convolution() (dicee.ConvO method), 181
residual_convolution() (dicee.ConvQ method), 180
residual convolution() (dicee.models.AConEx method), 112
residual_convolution() (dicee.models.AConvO method), 125
residual_convolution() (dicee.models.AConvQ method), 119
residual_convolution() (dicee.models.complex.AConEx method), 72
residual_convolution() (dicee.models.complex.ConEx method), 72
residual_convolution() (dicee.models.ConEx method), 111
residual_convolution() (dicee.models.ConvO method), 124
residual_convolution() (dicee.models.ConvQ method), 118
residual_convolution() (dicee.models.octonion.AConvO method), 82
residual_convolution() (dicee.models.octonion.ConvO method), 81
residual_convolution() (dicee.models.quaternion.AConvQ method), 86
residual_convolution() (dicee.models.quaternion.ConvQ method), 85
retrieve_embedding() (dicee.scripts.index_serve.NeuralSearcher method), 152
retrieve_embeddings() (in module dicee.scripts.index_serve), 152
return_multi_hop_query_results() (dicee.KGE method), 197
return_multi_hop_query_results() (dicee.knowledge_graph_embeddings.KGE method), 49
root() (in module dicee.scripts.index_serve), 152
roots (dicee.models.FMult attribute), 138
roots (dicee.models.function_space.FMult attribute), 76
{\tt roots}~(\textit{dicee.models.function\_space.GFMult~attribute}), 76
roots (dicee.models.GFMult attribute), 138
\verb"runtime" (\textit{dicee.analyse\_experiments.Experiment attribute}), 19
S
sample_counter (dicee.abstracts.AbstractPPECallback attribute), 17
sample_entity() (dicee.abstracts.BaseInteractiveKGE method), 14
sample_relation() (dicee.abstracts.BaseInteractiveKGE method), 14
sample_triples_ratio (dicee.config.Namespace attribute), 27
sample_triples_ratio (dicee.knowledge_graph.KG attribute), 45
sampling_ratio (dicee.literal_classes.LiteralDataset attribute), 53, 54
sanity_checking_with_arguments() (in module dicee.sanity_checkers), 151
save() (dicee.abstracts.BaseInteractiveKGE method), 14
save() (dicee.read_preprocess_save_load_kg.LoadSaveToDisk method), 150
save() (dicee.read_preprocess_save_load_kg.save_load_disk.LoadSaveToDisk method), 145
save_checkpoint() (dicee.abstracts.AbstractTrainer static method), 13
save_checkpoint_model() (in module dicee), 192
save_checkpoint_model() (in module dicee.static_funcs), 156
save_embeddings() (in module dicee), 192
save_embeddings() (in module dicee.static_funcs), 156
save_embeddings_as_csv (dicee.config.Namespace attribute), 26
save_experiment() (dicee.analyse_experiments.Experiment method), 19
save_model_at_every_epoch (dicee.config.Namespace attribute), 27
save_numpy_ndarray() (in module dicee), 192
save_numpy_ndarray() (in module dicee.read_preprocess_save_load_kg.util), 148
save_numpy_ndarray() (in module dicee.static_funcs), 156
save pickle() (in module dicee), 191
save_pickle() (in module dicee.read_preprocess_save_load_kg.util), 149
save_pickle() (in module dicee.static_funcs), 155
save_queries() (dicee.query_generator.QueryGenerator method), 143
save_queries() (dicee.QueryGenerator method), 211
save_queries_and_answers() (dicee.query_generator.QueryGenerator static method), 143
save_queries_and_answers() (dicee.QueryGenerator static method), 211
save_trained_model() (dicee.executer.Execute method), 43
scalar_batch_NN() (dicee.LFMult method), 185
\verb|scalar_batch_NN()| \textit{ (dicee.models.function\_space.LFMult method)}, 78
scalar_batch_NN() (dicee.models.LFMult method), 140
scaler (dicee.callbacks.Perturb attribute), 25
scaler (dicee.trainer.torch_trainer_ddp.NodeTrainer attribute), 163
score () (dicee.ComplEx static method), 177
score () (dicee.DistMult method), 169
```

```
score () (dicee. Keci method), 172
score () (dicee.models.clifford.Keci method), 67
score () (dicee.models.ComplEx static method), 113
score() (dicee.models.complex.ComplEx static method), 73
score() (dicee.models.DistMult method), 108
score() (dicee.models.Keci method), 128
score() (dicee.models.octonion.OMult method), 80
score () (dicee.models.OMult method), 123
score () (dicee.models.QMult method), 117
score () (dicee.models.quaternion.QMult method), 85
score() (dicee.models.real.DistMult method), 87
score () (dicee.models.real.TransE method), 87
score () (dicee.models.TransE method), 108
score () (dicee.OMult method), 184
score () (dicee.QMult method), 183
score () (dicee. TransE method), 172
score_func (dicee.models.FMult2 attribute), 139
score_func (dicee.models.function_space.FMult2 attribute), 77
scoring_technique (dicee.analyse_experiments.Experiment attribute), 19
scoring_technique (dicee.config.Namespace attribute), 27
search() (dicee.scripts.index_serve.NeuralSearcher method), 152
search_embeddings() (in module dicee.scripts.index_serve), 152
search_embeddings_batch() (in module dicee.scripts.index_serve), 153
seed (dicee.query_generator.QueryGenerator attribute), 142
seed (dicee.QueryGenerator attribute), 210
select_model() (in module dicee), 192
select_model() (in module dicee.static_funcs), 155
selected_optimizer (dicee.BaseKGE attribute), 189
selected_optimizer (dicee.models.base_model.BaseKGE attribute), 62
selected_optimizer (dicee.models.BaseKGE attribute), 103, 106, 110, 114, 120, 133, 136
separator (dicee.config.Namespace attribute), 27
separator (dicee.knowledge_graph.KG attribute), 46
sequential_vocabulary_construction() (dicee.read_preprocess_save_load_kg.PreprocessKG method), 150
sequential_vocabulary_construction() (dicee.read_preprocess_save_load_kg.preprocess.PreprocessKG method), 144
serve() (in module dicee.scripts.index_serve), 153
set_global_seed() (dicee.query_generator.QueryGenerator method), 142
set global seed() (dicee. Ouery Generator method), 211
set_model_eval_mode() (dicee.abstracts.BaseInteractiveKGE method), 14
set_model_train_mode() (dicee.abstracts.BaseInteractiveKGE method), 14
setup() (dicee.CVDataModule method), 208
\verb"setup"()" (\textit{dicee.dataset\_classes.CVDataModule method}), 38
setup_executor() (dicee.executer.Execute method), 43
Shallom (class in dicee), 184
Shallom (class in dicee, models), 108
Shallom (class in dicee.models.real), 87
shallom (dicee.models.real.Shallom attribute), 87
shallom (dicee.models.Shallom attribute), 108
shallom (dicee.Shallom attribute), 184
single_hop_query_answering() (dicee.KGE method), 197
single_hop_query_answering() (dicee.knowledge_graph_embeddings.KGE method), 49
spargl_endpoint (dicee.config.Namespace attribute), 26
sparql_endpoint (dicee.knowledge_graph.KG attribute), 45
start() (dicee.DICE_Trainer method), 194
start () (dicee.executer.Execute method), 44
start() (dicee.read_preprocess_save_load_kg.PreprocessKG method), 149
start() (dicee.read_preprocess_save_load_kg.preprocess.PreprocessKG method), 143
start() (dicee.read_preprocess_save_load_kg.read_from_disk.ReadFromDisk method), 144
\verb|start()| (dicee.read\_preprocess\_save\_load\_kg.ReadFromDisk method), 150|
start() (dicee.trainer.DICE_Trainer method), 165
start () (dicee.trainer.dice_trainer.DICE_Trainer method), 160
start time (dicee.callbacks.PrintCallback attribute), 20
start_time (dicee.executer.Execute attribute), 43
step() (dicee.EnsembleKGE method), 191
step() (dicee.models.ADOPT method), 96
step() (dicee.models.adopt.ADOPT method), 55
step() (dicee.models.ensemble.EnsembleKGE method), 75
storage_path (dicee.config.Namespace attribute), 26
storage_path (dicee.DICE_Trainer attribute), 193
```

```
storage path (dicee.trainer.DICE Trainer attribute), 164
storage_path (dicee.trainer.dice_trainer.DICE_Trainer attribute), 159
store() (in module dicee), 192
store() (in module dicee.static_funcs), 156
store_ensemble() (dicee.abstracts.AbstractPPECallback method), 17
strategy (dicee.abstracts.AbstractTrainer attribute), 12
StringListRequest (class in dicee.scripts.index_serve), 152
swa (dicee.config.Namespace attribute), 28
Т
T() (dicee.DualE method), 176
T() (dicee.models.DualE method), 142
T() (dicee.models.dualE.DualE method), 75
t_conorm() (dicee.KGE method), 197
t_conorm() (dicee.knowledge_graph_embeddings.KGE method), 49
t_norm() (dicee.KGE method), 197
t_norm() (dicee.knowledge_graph_embeddings.KGE method), 49
target_dim (dicee.AllvsAll attribute), 203
{\tt target\_dim}~(\textit{dicee.dataset\_classes.AllvsAll~attribute}),\,33
target_dim (dicee.dataset_classes.MultiLabelDataset attribute), 30
target_dim (dicee.dataset_classes.OnevsAllDataset attribute), 31
target_dim (dicee.knowledge_graph.KG attribute), 45
target_dim (dicee.MultiLabelDataset attribute), 200
target_dim (dicee.OnevsAllDataset attribute), 201
temperature (dicee.BytE attribute), 187
temperature (dicee.models.transformers.BytE attribute), 89
tensor_t_norm() (dicee.KGE method), 197
tensor_t_norm() (dicee.knowledge_graph_embeddings.KGE method), 49
TensorParallel (class in dicee.trainer.model_parallelism), 161
test_dataloader() (dicee.models.base_model.BaseKGELightning method), 58
test_dataloader() (dicee.models.BaseKGELightning method), 98
test_epoch_end() (dicee.models.base_model.BaseKGELightning method), 58
test_epoch_end() (dicee.models.BaseKGELightning method), 98
test_h1 (dicee.analyse_experiments.Experiment attribute), 19
test_h3 (dicee.analyse_experiments.Experiment attribute), 19
test_h10 (dicee.analyse_experiments.Experiment attribute), 19
test_mrr (dicee.analyse_experiments.Experiment attribute), 19
test_path (dicee.query_generator.QueryGenerator attribute), 142
test_path (dicee.QueryGenerator attribute), 210
\verb|timeit()| \textit{(in module dicee}), 191, 199
timeit() (in module dicee.read_preprocess_save_load_kg.util), 148
timeit() (in module dicee.static_funcs), 155
timeit() (in module dicee.static_preprocess_funcs), 158
to() (dicee.EnsembleKGE method), 191
to () (dicee.KGE method), 194
to() (dicee.knowledge_graph_embeddings.KGE method), 46
to() (dicee.models.ensemble.EnsembleKGE method), 75
to_df() (dicee.analyse_experiments.Experiment method), 19
topk (dicee.BytE attribute), 187
{\tt topk}~({\it dicee.models.transformers.BytE~attribute}),\,89
topk (dicee.scripts.index_serve.NeuralSearcher attribute), 152
torch\_ordered\_shaped\_bpe\_entities~\textit{(dicee.dataset\_classes.MultiLabelDataset~attribute)}, 30
torch_ordered_shaped_bpe_entities (dicee.MultiLabelDataset attribute), 200
TorchDDPTrainer (class in dicee.trainer.torch_trainer_ddp), 163
TorchTrainer (class in dicee.trainer.torch_trainer), 161
train() (dicee.KGE method), 198
train() (dicee.knowledge_graph_embeddings.KGE method), 50
train() (dicee.trainer.torch_trainer_ddp.NodeTrainer method), 164
train_data (dicee.AllvsAll attribute), 203
train_data (dicee.dataset_classes.AllvsAll attribute), 33
train_data (dicee.dataset_classes.KvsAll attribute), 32
train_data (dicee.dataset_classes.KvsSampleDataset attribute), 35
train_data (dicee.dataset_classes.MultiClassClassificationDataset attribute), 31
train_data (dicee.dataset_classes.OnevsAllDataset attribute), 31
train_data (dicee.dataset_classes.OnevsSample attribute), 33, 34
train_data (dicee.KvsAll attribute), 202
train_data (dicee.KvsSampleDataset attribute), 205
```

```
train data (dicee. MultiClass Classification Dataset attribute), 201
train_data (dicee.OnevsAllDataset attribute), 201
train data (dicee. Onevs Sample attribute), 203, 204
train_dataloader() (dicee.CVDataModule method), 207
train_dataloader() (dicee.dataset_classes.CVDataModule method), 37
train_dataloader() (dicee.models.base_model.BaseKGELightning method), 59
train_dataloader() (dicee.models.BaseKGELightning method), 100
train dataloaders (dicee.trainer.torch trainer.TorchTrainer attribute), 162
train_dataset_loader (dicee.trainer.torch_trainer_ddp.NodeTrainer attribute), 163
\verb|train_file_path| \textit{(dicee.literal\_classes.LiteralDataset attribute)}, 53
train_h1 (dicee.analyse_experiments.Experiment attribute), 18
train_h3 (dicee.analyse_experiments.Experiment attribute), 18
train_h10 (dicee.analyse_experiments.Experiment attribute), 18
train_indices_target (dicee.dataset_classes.MultiLabelDataset attribute), 30
train_indices_target (dicee.MultiLabelDataset attribute), 200
train_k_vs_all() (dicee.KGE method), 198
\verb|train_k_vs_all()| \textit{(dicee.knowledge\_graph\_embeddings.KGE method)}, 50
train_literals() (dicee.KGE method), 198
train_literals() (dicee.knowledge_graph_embeddings.KGE method), 50
train_mode (dicee.EnsembleKGE attribute), 191
train_mode (dicee.models.ensemble.EnsembleKGE attribute), 75
train_mrr (dicee.analyse_experiments.Experiment attribute), 18
train_path (dicee.query_generator.QueryGenerator attribute), 142
train_path (dicee.QueryGenerator attribute), 210
train_set (dicee.BPE_NegativeSamplingDataset attribute), 200
train_set (dicee.dataset_classes.BPE_NegativeSamplingDataset attribute), 29
train_set (dicee.dataset_classes.MultiLabelDataset attribute), 30
train_set (dicee.dataset_classes.NegSampleDataset attribute), 36
train_set (dicee.dataset_classes.TriplePredictionDataset attribute), 36
train_set (dicee.MultiLabelDataset attribute), 200
train_set (dicee.NegSampleDataset attribute), 206
train set (dicee. TriplePredictionDataset attribute), 207
train_set_idx (dicee.CVDataModule attribute), 207
\verb|train_set_idx| \textit{(dicee.dataset\_classes.CVDataModule attribute)}, 37
train_set_target (dicee.knowledge_graph.KG attribute), 45
train_target (dicee.AllvsAll attribute), 203
train target (dicee.dataset classes.AllvsAll attribute), 33
train_target (dicee.dataset_classes.KvsAll attribute), 32
train_target (dicee.dataset_classes.KvsSampleDataset attribute), 35
train_target (dicee.KvsAll attribute), 202
train_target (dicee.KvsSampleDataset attribute), 205
train_target_indices (dicee.knowledge_graph.KG attribute), 46
train_triples() (dicee.KGE method), 198
train_triples() (dicee.knowledge_graph_embeddings.KGE method), 50
trained_model (dicee.executer.Execute attribute), 43
trainer (dicee.config.Namespace attribute), 27
trainer (dicee.DICE_Trainer attribute), 193
trainer (dicee.executer.Execute attribute), 43
trainer (dicee.trainer.DICE_Trainer attribute), 164
trainer (dicee.trainer.dice_trainer.DICE_Trainer attribute), 159
\verb|trainer| (\textit{dicee.trainer.torch\_trainer\_ddp.NodeTrainer attribute}), 163
training_step (dicee.trainer.torch_trainer.TorchTrainer attribute), 162
training_step() (dicee.BytE method), 187
training_step() (dicee.models.base_model.BaseKGELightning method), 56
training_step() (dicee.models.BaseKGELightning method), 97
training_step() (dicee.models.transformers.BytE method), 89
training_step_outputs (dicee.models.base_model.BaseKGELightning attribute), 56
training_step_outputs (dicee.models.BaseKGELightning attribute), 97
training_technique (dicee.knowledge_graph.KG attribute), 45
TransE (class in dicee), 172
TransE (class in dicee.models), 108
TransE (class in dicee.models.real), 87
{\tt transfer\_batch\_to\_device()} \ \textit{(dicee.CVDataModule method)}, 208
transfer_batch_to_device() (dicee.dataset_classes.CVDataModule method), 38
transformer (dicee.BytE attribute), 187
transformer (dicee.models.transformers.BytE attribute), 89
transformer (dicee.models.transformers.GPT attribute), 94
trapezoid() (dicee.models.FMult2 method), 139
```

```
trapezoid() (dicee.models.function_space.FMult2 method), 77
tri_score() (dicee.LFMult method), 185
tri_score() (dicee.models.function_space.LFMult method), 78
tri_score() (dicee.models.function_space.LFMult1 method), 78
tri_score() (dicee.models.LFMult method), 140
tri_score() (dicee.models.LFMult1 method), 139
triple_score() (dicee.KGE method), 196
triple_score() (dicee.knowledge_graph_embeddings.KGE method), 48
TriplePredictionDataset (class in dicee), 206
TriplePredictionDataset (class in dicee.dataset_classes), 36
tuple2list() (dicee.query_generator.QueryGenerator method), 142
tuple2list() (dicee.QueryGenerator method), 211
U
unlabelled_size (dicee.callbacks.PseudoLabellingCallback attribute), 22
unmap() (dicee.query_generator.QueryGenerator method), 143
unmap () (dicee. Query Generator method), 211
unmap_query() (dicee.query_generator.QueryGenerator method), 143
unmap_query() (dicee.QueryGenerator method), 211
V
val_aswa (dicee.callbacks.ASWA attribute), 23
val_dataloader() (dicee.models.base_model.BaseKGELightning method), 58
val_dataloader() (dicee.models.BaseKGELightning method), 99
val_h1 (dicee.analyse_experiments.Experiment attribute), 18
val_h3 (dicee.analyse_experiments.Experiment attribute), 18
val_h10 (dicee.analyse_experiments.Experiment attribute), 18
val_mrr (dicee.analyse_experiments.Experiment attribute), 18
val_path (dicee.query_generator.QueryGenerator attribute), 142
val_path (dicee.QueryGenerator attribute), 210
validate_knowledge_graph() (in module dicee.sanity_checkers), 150
vocab_preparation() (dicee.evaluator.Evaluator method), 42
vocab_size (dicee.models.transformers.GPTConfig attribute), 93
vocab_to_parquet() (in module dicee), 192
vocab_to_parquet() (in module dicee.static_funcs), 156
vtp_score() (dicee.LFMult method), 185
vtp_score() (dicee.models.function_space.LFMult method), 78
vtp_score() (dicee.models.function_space.LFMult1 method), 78
vtp_score() (dicee.models.LFMult method), 140
vtp_score() (dicee.models.LFMult1 method), 139
W
weight (dicee.models.transformers.LayerNorm attribute), 90
weight_decay (dicee.BaseKGE attribute), 189
weight_decay (dicee.config.Namespace attribute), 27
weight_decay (dicee.models.base_model.BaseKGE attribute), 62
weight_decay (dicee.models.BaseKGE attribute), 103, 106, 110, 114, 120, 133, 136
weights (dicee.models.FMult attribute), 138
weights (dicee.models.function_space.FMult attribute), 76
weights (dicee.models.function_space.GFMult attribute), 77
weights (dicee.models.GFMult attribute), 138
write_csv_from_model_parallel() (in module dicee), 193
write_csv_from_model_parallel() (in module dicee.static_funcs), 157
write_links() (dicee.query_generator.QueryGenerator method), 143
write_links() (dicee.QueryGenerator method), 211
write_report() (dicee.executer.Execute method), 44
X
x_values (dicee.LFMult attribute), 184
x_values (dicee.models.function_space.LFMult attribute), 78
x_values (dicee.models.LFMult attribute), 140
```