# **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	Download Knowledge Graphs	3
4	Knowledge Graph Embedding Models	3
5	How to Train	3
6	Creating an Embedding Vector Database 6.1 Learning Embeddings	5 6 6
7	Answering Complex Queries	6
8	Predicting Missing Links	8
9	Downloading Pretrained Models	8
10	How to Deploy	8
11	Docker	8
12	Coverage Report	8
13	How to cite	10
14	dicee	12
	14.1 Subpackages	12
	14.2 Submodules	111
	14.3 Attributes	156
	14.4 Classes	156
	14.5 Functions	158
	14.6 Package Contents	

Index 204

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

# 1 Dicee Manual

**Version:** dicee 0.1.3.2

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

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

Contact: caglar.demir@upb.de

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

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

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

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

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

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

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

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

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

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

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

<sup>5</sup> https://huggingface.co/

<sup>6</sup> https://pandas.pydata.org/

<sup>7</sup> https://pytorch.org/

<sup>8</sup> https://pytorch.org/

<sup>9</sup> https://www.pytorchlightning.ai/

<sup>10</sup> https://huggingface.co/gradio

# 2 Installation

### 2.1 Installation from Source

```
git clone https://github.com/dice-group/dice-embeddings.git conda create -n dice python=3.10.13 --no-default-packages && conda activate dice &&_ 
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
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dicee/dataset_classes.py
                                                           299
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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
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                                                                                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
                                                                          96%
                                                                                116, 258-
                                                           113
⇒259, 291
dicee/knowledge_graph.py
                                                            65
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⇔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
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dicee/models/base_model.py
                                                                                54, 56, ...
→82, 88-103, 157, 190, 230, 236, 245, 248, 252, 259, 263, 265, 280, 288-289, 296-297,

→ 351, 354, 427, 439

dicee/models/clifford.py
                                                                  357
→68-117, 122-133, 156-168, 190-220, 235, 237, 241, 248-249, 276-280, 303-311, 325-
→327, 332-333, 364-384, 406, 413, 417-478, 495-499, 511, 514, 519, 524, 571-607, 625-
→631, 644, 647, 652, 657, 686-692, 705, 708, 713, 718, 728-737, 753-754, 774-845, □
→856-859, 884-909, 933-966, 1002-1006, 1019, 1029, 1032, 1037, 1042, 1047, 1051, □
→1055, 1064-1065, 1095, 1102, 1107, 1135-1139, 1167-1176, 1186-1194, 1212-1214, 1232-
→1234, 1250-1252
dicee/models/complex.py
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dicee/models/dualE.py
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→142-156
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                                                                  221
dicee/models/function_space.py
                                                                          16%
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\Rightarrow28-37, 40-49, 53-70, 77-86, 89-98, 101-110, 114-126, 134-156, 159-165, 168-185, 188-
→194, 197-205, 208, 213-234, 243-246, 250-254, 258-267, 271-292, 301-307, 311-328, □
→332-335, 344-352, 355, 366-372, 392-406, 424-438, 443-453, 461-465, 474-478
                                                           227
                                                                   83
                                                                          63%
dicee/models/octonion.py
                                                                                21-44,_
\Rightarrow320-329, 334-345, 348-370, 374-416, 426-474
dicee/models/pykeen_models.py
                                                            50
                                                                    5
                                                                          90%
                                                                                60-63, _
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
                                                                   12
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\leftrightarrow 66-69, 87, 103-106
dicee/models/static_funcs.py
                                                            10
                                                                    0
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dicee/models/transformers.py
                                                           236
                                                                   189
\hookrightarrow46, 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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                                                                            100%
dicee/read_preprocess_save_load_kg/__init__.py
dicee/read_preprocess_save_load_kg/preprocess.py
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                                                                                    34, 40, _
\hookrightarrow78, 102-127, 133, 138-151, 184, 214, 388-389, 444
dicee/read_preprocess_save_load_kg/read_from_disk.py
                                                               36
                                                                       11
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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
                                                              219
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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
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                                                                                    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
                                                                       63
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                                                                                    118-215, _
⇔223-224
dicee/static_preprocess_funcs.py
                                                              100
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                                                                             56%
                                                                                    17-25.
\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:)

```
@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 Subpackages

dicee.models

**Submodules** 

dicee.models.base\_model

### **Classes**

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

### **Module Contents**

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

Bases: lightning.LightningModule

Base class for all neural network modules.

Your models should also subclass this class.

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

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

class Model(nn.Module):
    def __init__ (self) -> 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 have their parameters converted too when you call to (), etc.

# 1 Note

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

#### **Variables**

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

```
\label{eq:continuous_step_outputs} \begin{tabular}{ll} \textbf{training\_step\_outputs} &= & [\ ] \\ \\ \textbf{mem\_of\_model} \ () &\to Dict \\ \\ \textbf{Size of model in MB and number of params} \\ \end{tabular}
```

Size of model in MD and number of param

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

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

#### **Parameters**

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

### **Returns**

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

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

### Example:

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

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

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

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

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

# 1 Note

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

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

### **Parameters**

- yhat\_batch
- y\_batch

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

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

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

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

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

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

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

```
\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()



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

1 Note

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

# ${\tt val\_dataloader}\,()\,\to None$

An iterable or collection of iterables specifying validation samples.

For more information about multiple dataloaders, see this section.

The dataloader return will not be reloaded unless :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.

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

An iterable or collection of iterables specifying training samples.

For more information about multiple dataloaders, see this section.

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

For data processing use the following pattern:

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

However, the above are only necessary for distributed processing.

# Warning

do not assign state in prepare\_data

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

# **1** Note

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

### configure\_optimizers (parameters=None)

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

#### Returns

Any of these 6 options.

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

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

```
lr_scheduler_config = {
    # REQUIRED: The scheduler instance
   "scheduler": lr_scheduler,
    # The unit of the scheduler's step size, could also be 'step'.
    # 'epoch' updates the scheduler on epoch end whereas 'step'
    # updates it after a optimizer update.
   "interval": "epoch",
   # How many epochs/steps should pass between calls to
    # `scheduler.step()`. 1 corresponds to updating the learning
    # rate after every epoch/step.
   "frequency": 1,
    # Metric to 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 to nest them in a tree structure. You can assign the submodules as regular attributes:

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

class Model(nn.Module):
    def __init__ (self) -> 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 have their parameters converted too when you call to(), etc.

# **1** Note

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

# Variables

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

# args

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

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

```
init_params_with_sanity_checking()
     forward (x: torch.LongTensor | Tuple[torch.LongTensor, torch.LongTensor],
                 y idx: torch.LongTensor = None)
              Parameters
                  • x
                  y_idx
                  • ordered_bpe_entities
     \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.base_model.IdentityClass(args=None)
     Bases: torch.nn.Module
```

Base class for all neural network modules.

Your models should also subclass this class.

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

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

class Model(nn.Module):
    def __init__(self) -> 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 have their parameters converted too when you call to(), etc.



### **1** Note

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

### Variables

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

```
args
\_\_call\_\_(x)
static forward (x)
```

### dicee.models.clifford

### Classes

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

# **Module Contents**

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

Base class for all neural network modules.

Your models should also subclass this class.

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

```
import torch.nn as nn
import torch.nn.functional as F
class Model (nn.Module):
    def __init__(self) -> 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 have their parameters converted too 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**

name = 'Keci'

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

```
r
requires_grad_for_interactions = True
compute_sigma_pp (hp, rp)
   Compute sigma_{pp} = sum_{i=1}^{p-1} sum_{k=i+1}^p (h_i r_k - h_k r_i) e_i e_k
   sigma_{pp} captures the interactions between along p bases For instance, let p e_1, e_2, e_3, we compute
   interactions between e_1 e_2, e_1 e_3, and e_2 e_3 This can be implemented with a nested two for loops
   results = [] for i in range(p - 1):
        for k in range(i + 1, p):
        results.append(hp[:, :, i] * rp[:, :, k] - hp[:, :, k] * rp[:, :, i])
```

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

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

```
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.

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

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

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

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

 ${\tt clifford\_multiplication}\,(h0,\,hp,\,hq,\,r0,\,rp,\,rq)$ 

Compute our CL multiplication

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

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

eq j

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

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

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

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

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

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

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

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

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

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

### **Parameter**

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

### returns

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

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

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

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

Kvsall training

(1) Retrieve real-valued embedding vectors for heads and relations mathbb $\{R\}^d$ .

- (2) Construct head entity and relation embeddings according to  $Cl_{p,q}(mathbb{R}^d)$ .
- (3) Perform Cl multiplication
- (4) Inner product of (3) and all entity embeddings

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

 $\begin{tabular}{ll} \begin{tabular}{ll} \beg$ 

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

 $\verb"score"\,(h,\,r,\,t)$ 

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

# **Parameter**

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

# rtype

torch.FloatTensor with (n) shape

class dicee.models.clifford.KeciBase(args)

Bases: Keci

Without learning dimension scaling

name = 'KeciBase'

requires\_grad\_for\_interactions = False

class dicee.models.clifford.DeCaL(args)

Bases: dicee.models.base\_model.BaseKGE

Base class for all neural network modules.

Your models should also subclass this class.

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

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

class Model(nn.Module):
    def __init__ (self) -> 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 have their parameters converted too when you call to(), etc.



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

### **Variables**

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

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

# **Parameter**

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

### rtype

torch.FloatTensor with (n) shape

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

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

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

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

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

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

and return:

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

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

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

For same bases vectors interaction we have

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

For different base vector interactions, we have

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

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

Kvsall training

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

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

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

Multiplying a base vector with its scalar coefficient

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

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

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

### **Parameter**

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

### returns

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

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

Compute .. math:

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

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

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

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

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

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

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

Compute

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

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

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

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

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

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

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

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

compute sigma rr(hk, rk)

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

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

Compute

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

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

## for j in range(q):

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

```
print(sigma_pq.shape)

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

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

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

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

print(sigma_pq.shape)

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

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

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

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

print(sigma_pq.shape)
```

# dicee.models.complex

### **Classes**

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

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

```
import torch.nn as nn
import torch.nn.functional as F
class Model (nn.Module):
    def __init__(self) -> 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 have their parameters converted too when you call to(), etc.

# 1 Note

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

### Variables

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

```
name = 'ComplEx'
static score (head_ent_emb: torch.FloatTensor, rel_ent_emb: torch.FloatTensor,
            tail_ent_emb: torch.FloatTensor)
static k_vs_all_score (emb_h: torch.FloatTensor, emb_r: torch.FloatTensor,
            emb_E: torch.FloatTensor)
         Parameters
```

- emb h
- emb\_r
- emb\_E

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

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

### dicee.models.dualE

# **Classes**

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

```
class dicee.models.dualE.DualE(args)
                     Bases: dicee.models.base_model.BaseKGE
                     Dual Quaternion Knowledge Graph Embeddings (https://ojs.aaai.org/index.php/AAAI/article/download/16850/
                     16657)
                     name = 'DualE'
                     entity embeddings
                     relation embeddings
                     num_ent
                     {\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
                     forward\_triples(idx\_triple: torch.tensor) \rightarrow torch.tensor
                                         Negative Sampling forward pass:
                                        Input
                                         x: torch.LongTensor with (n, ) shape
                                         Output
                                        torch.FloatTensor with (n) shape
                     forward_k_vs_all(x)
                                         KvsAll forward pass
                                         Input
                                         x: torch.LongTensor with (n, ) shape
                                         Output
                                        torch.FloatTensor with (n) shape
                     T (x: torch.tensor) \rightarrow torch.tensor
                                        Transpose function
                                         Input: Tensor with shape (nxm) Output: Tensor with shape (mxn)
```

# dicee.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
     tuned_embedding_dim = False
     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
                   x
     construct_multi_coeff(X)
     poly_NN(x, coefh, coefr, coeft)
           Constructing a 2 layers NN to represent the embeddings. h = sigma(wh^T x + bh), r = sigma(wr^T x + br),
           t = sigma(wt^T x + bt)
     linear(x, w, b)
     scalar_batch_NN(a, b, c)
           element wise multiplication between a,b and c: Inputs: a, b, c ====> torch.tensor of size batch_size x m x
           d Output: a tensor of size batch size x d
     tri_score (coeff_h, coeff_r, coeff_t)
           this part implement the trilinear scoring techniques:
           score(h,r,t) = int_{0}{1} h(x)r(x)t(x) dx = sum_{i,j,k} = 0}^{d-1} dfrac{a_i*b_j*c_k}{1+(i+j+k)%d}
            1. generate the range for i, j and k from [0 d-1]
           2. perform dfrac\{a_i*b_j*c_k\}\{1+(i+j+k)\%d\} in parallel for every batch
            3. take the sum over each batch
```

```
\mathtt{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

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

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

```
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)

### dicee.models.octonion

# **Classes**

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

# **Functions**

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

```
dicee.models.octonion.octonion_mul(*, O_1, O_2)
dicee.models.octonion.octonion mul norm(*, O_1, O_2)
```

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

Base class for all neural network modules.

Your models should also subclass this class.

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

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

class Model(nn.Module):
    def __init__ (self) -> 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 have their parameters converted too 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.

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

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

Base class for all neural network modules.

Your models should also subclass this class.

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

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

class Model(nn.Module):
    def __init__(self) -> 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 have their parameters converted too when you call to (), etc.

### 1 Note

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

#### Variables

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

```
name = 'Conv0'

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

# dicee.models.pykeen\_models

### Classes

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

### **Module Contents**

```
class dicee.models.pykeen_models.PykeenKGE (args: dict)

Bases: dicee.models.base_model.BaseKGE

A class for using knowledge graph embedding models implemented in Pykeen

Notes: Pykeen_DistMult: C Pykeen_ComplEx: Pykeen_QuatE: Pykeen_MuRE: Pykeen_CP: Pykeen_HolE: Pykeen_HolE:

model_kwargs

name

model
```

```
loss_history = []
args
entity_embeddings = None
relation_embeddings = None
forward_k_vs_all (x: torch.LongTensor)
    # => Explicit version by this we can apply bn and dropout
```

# (1) Retrieve embeddings of heads and relations + apply Dropout & Normalization if given. h, r = self.get\_head\_relation\_representation(x) # (2) Reshape (1). if 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)

# (3) Reshape all entities. if self.last\_dim > 0:

 $t = self.entity\_embeddings.weight.reshape(self.num\_entities, self.embedding\_dim, self.last\_dim)$ 

#### else:

t = self.entity\_embeddings.weight

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

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

# => Explicit version by this we can apply bn and dropout

# (1) Retrieve embeddings of heads, relations and tails and apply Dropout & Normalization if given. h, r, t = self.get\_triple\_representation(x) # (2) Reshape (1). if self.last\_dim > 0:

 $h = h.reshape(len(x), self.embedding_dim, self.last_dim) r = r.reshape(len(x), self.embedding_dim,$ self.last\_dim) t = t.reshape(len(x), self.embedding\_dim, self.last\_dim)

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

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

# dicee.models.quaternion

#### Classes

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

### **Functions**

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

### **Module Contents**

```
dicee.models.quaternion.quaternion_mul_with_unit_norm(*, Q_1, Q_2)
class dicee.models.quaternion.QMult(args)
Bases: dicee.models.base_model.BaseKGE
```

Base class for all neural network modules.

Your models should also subclass this class.

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

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

class Model(nn.Module):
    def __init__ (self) -> 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 have their parameters converted too 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.

```
\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) → torch.FloatTensor

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

Absolute value of a quaternion

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

L2 norm of quaternion vector:

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

### **Parameters**

 $\mathbf{x}$  – The vector.

#### Returns

The normalized vector.

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

#### **Parameters**

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

 $forward_k_vs_all(x)$ 

#### **Parameters**

x

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

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

class dicee.models.quaternion.ConvQ(args)

Bases: dicee.models.base\_model.BaseKGE

Convolutional Quaternion Knowledge Graph Embeddings

name = 'ConvQ'

entity\_embeddings

relation\_embeddings

conv2d

fc\_num\_input

fc1

bn conv1

bn\_conv2

```
feature_map_dropout
      {\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 l)
class dicee.models.quaternion.AConvQ(args)
      Bases: dicee.models.base_model.BaseKGE
      Additive Convolutional Quaternion Knowledge Graph Embeddings
      name = 'AConvQ'
      entity_embeddings
      relation_embeddings
      conv2d
      fc_num_input
      fc1
      bn_conv1
      bn conv2
      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,|
```

### dicee.models.real

Entities l)

### **Classes**

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

### **Module Contents**

```
class dicee.models.real.DistMult(args)
      Bases: dicee.models.base_model.BaseKGE
      Embedding Entities and Relations for Learning and Inference in Knowledge Bases https://arxiv.org/abs/1412.6575
      name = 'DistMult'
      k vs all score (emb h: torch.FloatTensor, emb r: torch.FloatTensor, emb E: torch.FloatTensor)
               Parameters
                    • emb h
                    • emb_r
                    • emb_E
      forward_k_vs_all (x: torch.LongTensor)
      forward_k_vs_sample (x: torch.LongTensor, target_entity_idx: torch.LongTensor)
      score(h, r, t)
class dicee.models.real.TransE(args)
      Bases: dicee.models.base_model.BaseKGE
      Translating Embeddings for Modeling Multi-relational Data https://proceedings.neurips.cc/paper/2013/file/
      1cecc7a77928ca8133fa24680a88d2f9-Paper.pdf
      name = 'TransE'
     margin = 4
      score (head_ent_emb, rel_ent_emb, tail_ent_emb)
      forward_k_vs_all(x: torch.Tensor) \rightarrow torch.FloatTensor
class dicee.models.real.Shallom(args)
      Bases: dicee.models.base_model.BaseKGE
      A shallow neural model for relation prediction (https://arxiv.org/abs/2101.09090)
      name = 'Shallom'
      shallom_width
      shallom
      \mathtt{get\_embeddings}() \rightarrow \mathsf{Tuple}[\mathsf{numpy}.\mathsf{ndarray}, \mathsf{None}]
      \mathbf{forward\_k\_vs\_all}\;(x)\;\to \mathrm{torch.FloatTensor}
      forward_triples (x) \rightarrow \text{torch.FloatTensor}
               Parameters
               Returns
```

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

# dicee.models.static\_funcs

#### **Functions**

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

### **Module Contents**

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

### dicee.models.transformers

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

### **Classes**

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

### **Module Contents**

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

Base class for all neural network modules.

Your models should also subclass this class.

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

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

class Model(nn.Module):
    def __init__ (self) -> 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 have their parameters converted too when you call to (), etc.

# **1** Note

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

#### Variables

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

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

#### **Parameters**

- yhat\_batch
- y\_batch

forward(x: torch.LongTensor)

#### **Parameters**

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

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

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

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

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

#### **Parameters**

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

### Returns

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

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

Example:

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

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

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

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

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

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```
opt2.step()
```

# **1** Note

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

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

Bases: torch.nn.Module

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

weight

bias

forward(input)

class dicee.models.transformers.CausalSelfAttention(config)

Bases: torch.nn.Module

Base class for all neural network modules.

Your models should also subclass this class.

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

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

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 have their parameters converted too when you call to (), etc.

### 1 Note

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

#### Variables

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

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

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

Your models should also subclass this class.

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

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

class Model(nn.Module):
    def __init__(self) -> 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 have their parameters converted too when you call to(), etc.

### 1 Note

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

#### **Variables**

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

c\_fc

gelu

```
c_proj
dropout
forward(x)

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

Your models should also subclass this class.

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

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

class Model(nn.Module):
    def __init__ (self) -> 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 have their parameters converted too when you call to (), etc.

### 1 Note

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

### Variables

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

```
ln_1
attn
ln_2
mlp
forward(x)

class dicee.models.transformers.GPTConfig
block_size: int = 1024
vocab_size: int = 50304
```

```
n_layer: int = 12

n_head: int = 12

n_embd: int = 768

dropout: float = 0.0

bias: bool = False

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

Your models should also subclass this class.

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

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

class Model(nn.Module):
    def __init__ (self) -> 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 have their parameters converted too when you call to(), etc.

# **1** Note

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

#### **Variables**

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

config

transformer

lm\_head

weight

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

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

# **Classes**

BaseKGELightning	Base class for all neural network modules.
BaseKGE	Base class for all neural network modules.
	Base class for all neural network modules.
IdentityClass	Base class for all neural network modules.
BaseKGE	
DistMult	Embedding Entities and Relations for Learning and Inference in Knowledge Bases
TransE	Translating Embeddings for Modeling
Shallom	A shallow neural model for relation prediction (https://arxiv.org/abs/2101.09090)
Pyke	A Physical Embedding Model for Knowledge Graphs
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.
OMult	Base class for all neural network modules.
ConvQ	Convolutional Quaternion Knowledge Graph Embeddings
AConvQ	Additive Convolutional Quaternion Knowledge Graph Embeddings
BaseKGE	Base class for all neural network modules.
IdentityClass	Base class for all neural network modules.
OMult	Base class for all neural network modules.
ConvO	Base class for all neural network modules.
AConv0	Additive Convolutional Octonion Knowledge Graph Embeddings
Keci	Base class for all neural network modules.
KeciBase	Without learning dimension scaling
DeCaL	Base class for all neural network modules.
BaseKGE	Base class for all neural network modules.
PykeenKGE	A class for using knowledge graph embedding models im-
*	plemented in Pykeen
BaseKGE	Base class for all neural network modules.
FMult	Learning Knowledge Neural Graphs
GFMult	Learning Knowledge Neural Graphs
FMult2	Learning Knowledge Neural Graphs
LFMult1	Embedding with trigonometric functions. We represent
111 114 L L	all entities and relations in the complex number space as:

continues on next page

Table 1 - continued from previous page

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**

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

Bases: lightning.LightningModule

Base class for all neural network modules.

Your models should also subclass this class.

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

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

class Model(nn.Module):
    def __init__(self) -> 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 have their parameters converted too when you call to (), etc.

### 1 Note

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

#### **Variables**

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

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

Size of model in MB and number of params

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

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

### **Parameters**

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

#### **Returns**

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

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

# Example:

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

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

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

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

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

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

loss function(yhat batch: torch.FloatTensor, y batch: torch.FloatTensor)

#### **Parameters**

- yhat\_batch
- y\_batch

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

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

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

```
class MyLightningModule(L.LightningModule):
   def __init__(self):
        super().__init__()
        self.training_step_outputs = []
   def training_step(self):
        loss = \dots
        self.training_step_outputs.append(loss)
        return loss
   def on_train_epoch_end(self):
        # do something with all training_step outputs, for example:
        epoch_mean = torch.stack(self.training_step_outputs).mean()
        self.log("training_epoch_mean", epoch_mean)
        # free up the memory
        self.training_step_outputs.clear()
```

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

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

An iterable or collection of iterables specifying test samples.

For more information about multiple dataloaders, see this section.

For data processing use the following pattern:

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

However, the above are only necessary for distributed processing.

### Warning

do not assign state in prepare\_data

• test()

- prepare\_data()
- setup()

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

## 1 Note

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

### ${\tt val\_dataloader}\,()\,\to None$

An iterable or collection of iterables specifying validation samples.

For more information about multiple dataloaders, see this section.

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

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

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

### 1 Note

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

# **1** Note

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

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

An iterable or collection of iterables specifying prediction samples.

For more information about multiple dataloaders, see this section.

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

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

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

#### Returns

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

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

An iterable or collection of iterables specifying training samples.

For more information about multiple dataloaders, see this section.

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

For data processing use the following pattern:

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

However, the above are only necessary for distributed processing.

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

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

class Model (nn.Module):
    def __init__ (self) -> 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 have their parameters converted too when you call to(), etc.

## 1 Note

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

#### **Variables**

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

#### args

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

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

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

Your models should also subclass this class.

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

```
import torch.nn as nn
import torch.nn.functional as F
class Model(nn.Module):
    def __init__(self) -> 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 have their parameters converted too when you call to(), etc.

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

#### **Variables**

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

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

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

Base class for all neural network modules.

Your models should also subclass this class.

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

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

class Model(nn.Module):
    def __init__ (self) -> 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 have their parameters converted too when you call to(), etc.

### **1** Note

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

#### **Variables**

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

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

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

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

```
forward_k_vs_sample (x: torch.LongTensor, target_entity_idx: torch.LongTensor)
     \mathtt{score}\,(h,r,t)
class dicee.models.TransE(args)
     Bases: dicee.models.base_model.BaseKGE
     Translating Embeddings for Modeling Multi-relational Data https://proceedings.neurips.cc/paper/2013/file/
     1cecc7a77928ca8133fa24680a88d2f9-Paper.pdf
     name = 'TransE'
     margin = 4
     score (head_ent_emb, rel_ent_emb, tail_ent_emb)
     forward_k_vs_all(x: torch.Tensor) \rightarrow torch.FloatTensor
class dicee.models.Shallom(args)
     Bases: dicee.models.base model.BaseKGE
     A shallow neural model for relation prediction (https://arxiv.org/abs/2101.09090)
     name = 'Shallom'
     shallom_width
     shallom
     \mathtt{get\_embeddings}() \rightarrow \mathsf{Tuple}[\mathsf{numpy}.\mathsf{ndarray}, \mathsf{None}]
     forward_k_vs_all(x) \rightarrow torch.FloatTensor
     forward\_triples(x) \rightarrow torch.FloatTensor
               Parameters
                   x
               Returns
class dicee.models.Pyke(args)
     Bases: dicee.models.base_model.BaseKGE
     A Physical Embedding Model for Knowledge Graphs
     name = 'Pyke'
     dist_func
     margin = 1.0
     forward_triples (x: torch.LongTensor)
               Parameters
                   x
class dicee.models.BaseKGE (args: dict)
     Bases: BaseKGELightning
     Base class for all neural network modules.
     Your models should also subclass this class.
```

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

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

class Model(nn.Module):
    def __init__ (self) -> 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 have their parameters converted too when you call to(), etc.

# 1 Note

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

#### **Variables**

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

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

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

```
get_head_relation_representation(indexed_triple)
     get_sentence_representation(x: torch.LongTensor)
              Parameters
                   • (b (x shape)
                   • 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.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
```

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:

```
\label{eq:continuous_problem} \begin{split} \textbf{forward_k\_vs\_all} & (x: torch.Tensor) \rightarrow \text{torch.FloatTensor} \\ \textbf{forward\_triples} & (x: torch.Tensor) \rightarrow \text{torch.FloatTensor} \\ \textbf{Parameters} \\ & \textbf{x} \end{split}
```

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

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

Bases: dicee.models.base\_model.BaseKGE

Base class for all neural network modules.

Your models should also subclass this class.

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

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

class Model(nn.Module):
    def __init__(self) -> 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 have their parameters converted too when you call to (), etc.

### 1 Note

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

### Variables

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

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

Your models should also subclass this class.

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

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

class Model(nn.Module):
    def __init__(self) -> 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 have their parameters converted too 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)
                  \rightarrow Tuple[torch.FloatTensor, torch.FloatTensor]
              Parameters
                  x (B x 2 x T)
     \mathtt{get\_embeddings}() \rightarrow Tuple[numpy.ndarray, numpy.ndarray]
class dicee.models.IdentityClass(args=None)
     Bases: torch.nn.Module
```

Your models should also subclass this class.

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

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

class Model(nn.Module):
    def __init__(self) -> 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 have their parameters converted too when you call to (), etc.

### 1 Note

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

### Variables

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

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

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

class dicee.models.QMult(args)

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

Base class for all neural network modules.

Your models should also subclass this class.

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

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

class Model(nn.Module):
    def __init__ (self) -> 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 have their parameters converted too when you call to(), etc.

# 1 Note

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

### **Variables**

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

name = 'OMult'

explicit = True

 $quaternion_multiplication_followed_by_inner_product(h, r, t)$ 

### **Parameters**

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

### **Returns**

Triple scores.

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

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

Absolute value of a quaternion

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

L2 norm of quaternion vector:

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

# **Parameters**

 $\mathbf{x}$  – The vector.

### Returns

The normalized vector.

score (head\_ent\_emb: torch.FloatTensor, rel\_ent\_emb: torch.FloatTensor, tail ent emb: torch.FloatTensor)

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

### **Parameters**

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

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

```
\label{lem:bn_conv1} $$ bn_conv2$ $$ feature_map_dropout $$ $$ residual_convolution ($Q_1$, $Q_2$) $$ forward_triples ($indexed_triple: torch.Tensor) $$ $$ $$ $$ $$ $$ $$ torch.Tensor $$
```

### **Parameters**

x

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

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

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

Bases: BaseKGELightning

Base class for all neural network modules.

Your models should also subclass this class.

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

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

class Model(nn.Module):
    def __init__ (self) -> 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 have their parameters converted too when you call to(), etc.

# 1 Note

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

### **Variables**

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

### args

embedding\_dim = None

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

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

Base class for all neural network modules.

Your models should also subclass this class.

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

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

class Model(nn.Module):
    def __init__(self) -> 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 have their parameters converted too when you call to (), etc.

# **1** Note

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

### Variables

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

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

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

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

class dicee.models.OMult(args)

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

Base class for all neural network modules.

Your models should also subclass this class.

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

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

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

def forward(self, x):
```

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

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

# 1 Note

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

### Variables

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

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

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

Bases: dicee.models.base\_model.BaseKGE

Base class for all neural network modules.

Your models should also subclass this class.

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

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

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 have their parameters converted too when you call to(), etc.

### 1 Note

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

### **Variables**

name = 'ConvO'

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

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

```
\begin{tabular}{ll} {\bf residual\_convolution} & (O\_1,O\_2) \\ {\bf forward\_triples} & (x:torch.Tensor) & \rightarrow {\bf torch}.{\bf Tensor} \\ & {\bf Parameters} \\ & {\bf x} \\ \end{tabular}
```

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.

forward\_k\_vs\_all (x: torch.Tensor)

Your models should also subclass this class.

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

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

class Model (nn.Module):
    def __init__ (self) -> 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 have their parameters converted too when you call to (), etc.

# **1** Note

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

# Variables

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

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

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

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

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

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

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

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

### **Parameter**

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

### returns

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

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

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

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

Kvsall training

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

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

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

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

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

### **Parameter**

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

### returns

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

 $forward_k\_vs\_sample$  (x: torch.LongTensor, target\_entity\_idx: torch.LongTensor)  $\rightarrow$  torch.FloatTensor

### **Parameter**

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

Base class for all neural network modules.

Your models should also subclass this class.

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

```
import torch.nn as nn
import torch.nn.functional as F
class Model (nn.Module):
    def __init__(self) -> 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 have their parameters converted too when you call to(), etc.

# **1** Note

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

### Variables

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

name = 'DeCaL'

entity\_embeddings

relation embeddings

p

q

r

re

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

### **Parameter**

x: torch.LongTensor with (n, ) shape

### rtype

torch.FloatTensor with (n) shape

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

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

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

 $\verb|compute_sigmas_single| (\textit{list}\_h\_\textit{emb}, \textit{list}\_r\_\textit{emb}, \textit{list}\_t\_\textit{emb})$ 

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

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

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

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

For different base vector interactions, we have

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

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

Kvsall training

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

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

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

Multiplying a base vector with its scalar coefficient

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

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

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

### **Parameter**

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

### returns

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

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

Compute .. math:

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

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

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

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

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

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

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

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

Compute

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

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

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

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

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

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

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

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

 $compute\_sigma\_rr(hk, rk)$ 

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

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

Compute

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

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

### for j in range(q):

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

print(sigma\_pq.shape)

 $\texttt{compute\_sigma\_pr} \ (*, hp, hk, rp, rk)$ 

Compute

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

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

### for j in range(q):

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

print(sigma\_pq.shape)

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

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

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

# for j in range(q):

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

print(sigma\_pq.shape)

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

Bases: BaseKGELightning

Base class for all neural network modules.

Your models should also subclass this class.

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

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

class Model(nn.Module):
    def __init__ (self) -> 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 have their parameters converted too 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
                                                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.PykeenKGE(args: dict)
              Bases: dicee.models.base_model.BaseKGE
              A class for using knowledge graph embedding models implemented in Pykeen
              Notes: Pykeen_DistMult: C Pykeen_ComplEx: Pykeen_QuatE: Pykeen_MuRE: Pykeen_CP: Pykeen_HolE: Py-
              keen HolE:
              model_kwargs
              name
              model
              loss_history = []
              args
              entity_embeddings = None
              relation_embeddings = None
              forward_k_vs_all (x: torch.LongTensor)
                           # => Explicit version by this we can apply bn and dropout
                           # (1) Retrieve embeddings of heads and relations + apply Dropout & Normalization if given. h, r =
                           self.get_head_relation_representation(x) \# (2) Reshape (1). if self.last_dim > 0:
                                     h = h.reshape(len(x), self.embedding\_dim, self.last\_dim) r = r.reshape(len(x), self.embedding\_dim, self.embeddin
                                     self.last_dim)
                           \# (3) Reshape all entities. if self.last_dim > 0:
```

t = self.entity\_embeddings.weight.reshape(self.num\_entities, self.embedding\_dim, self.last\_dim)

### else:

t = self.entity\_embeddings.weight

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

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

- # => Explicit version by this we can apply bn and dropout
- # (1) Retrieve embeddings of heads, relations and tails and apply Dropout & Normalization if given. h, r, t = self.get\_triple\_representation(x) # (2) Reshape (1). if self.last\_dim > 0:
  - $$\label{eq:hamma} \begin{split} &h = h.reshape(len(x), self.embedding\_dim, self.last\_dim) \ r = r.reshape(len(x), self.embedding\_dim, self.last\_dim) \end{split}$$
      $& self.last\_dim) \ t = t.reshape(len(x), self.embedding\_dim, self.last\_dim) \end{split}$
- # (3) Compute the triple score return self.interaction.score(h=h, r=r, t=t, slice\_size=None, slice\_dim=0)

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

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

Bases: BaseKGELightning

Base class for all neural network modules.

Your models should also subclass this class.

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

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

class Model(nn.Module):
    def __init__(self) -> 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 have their parameters converted too when you call to (), etc.

### 1 Note

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

# Variables

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

args

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

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

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

```
discrete_points
     entity_embeddings
     relation_embeddings
     build_func(Vec)
     build_chain_funcs(list_Vec)
     compute\_func(W, b, x) \rightarrow torch.FloatTensor
     function (list_W, list_b)
     trapezoid(list_W, list_b)
     forward_triples (idx\_triple: torch.Tensor) \rightarrow torch.Tensor
               Parameters
                   x
class dicee.models.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
     \texttt{tri\_score}(h, r, t)
     \mathtt{vtp\_score}(h, r, t)
class dicee.models.LFMult(args)
     Bases: dicee.models.base_model.BaseKGE
     Embedding with polynomial functions. We represent all entities and relations in the polynomial space as: f(x) =
     sum_{i=0}^{d-1} a_k x^{i\%} and use the three differents scoring function as in the paper to evaluate the score.
     We also consider combining with Neural Networks.
     name = 'LFMult'
     entity_embeddings
     relation_embeddings
     degree
     x_values
```

forward\_triples (idx\_triple)

### **Parameters**

x

construct\_multi\_coeff(X)

poly NN (x, coefh, coefr, coeft)

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

linear(x, w, b)

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

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

tri\_score (coeff\_h, coeff\_r, coeff\_t)

this part implement the trilinear scoring techniques:

```
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} \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

```
comp_func(h, r, t)
```

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

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

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

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

pop (coeff, x, degree)

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

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

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

class dicee.models.DualE(args)

Bases: dicee.models.base\_model.BaseKGE

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

```
name = 'DualE'
      entity_embeddings
      relation_embeddings
      num_ent
      kvsall_score (e_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) \rightarrow torch.tensor
           Transpose function
           Input: Tensor with shape (nxm) Output: Tensor with shape (mxn)
dicee.read_preprocess_save_load_kg
Submodules
dicee.read_preprocess_save_load_kg.preprocess
Classes
```

PreprocessKG

Preprocess the data in memory

# **Module Contents**

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

# Classes

ReadFromDisk

Read the data from disk into memory

# **Module Contents**

```
\begin{tabular}{ll} {\bf class} & {\tt dicee.read\_preprocess\_save\_load\_kg.read\_from\_disk.ReadFromDisk} \end{tabular} \label{table_load_kg}. \\ & {\tt Read} & {\tt the} & {\tt data} & {\tt from} & {\tt disk} & {\tt into} & {\tt memory} \\ & {\tt kg} & \\ \end{tabular}
```

```
start () → 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>apply_reciprical_or_noise(add_reciprical, eval_model)</pre>	
timeit(func)	
read_with_polars(→ polars.DataFrame)	Load and Preprocess via Polars
read_with_pandas(data_path[, read_only_few,])	r
<pre>read_from_disk(data_path[, read_only_few,])</pre>	
<pre>read_from_triple_store([endpoint])</pre>	Read triples from triple store into pandas dataframe
<pre>get_er_vocab(data[, file_path])</pre>	
<pre>get_re_vocab(data[, file_path])</pre>	
<pre>get_ee_vocab(data[, file_path])</pre>	
<pre>create_constraints(triples[, file_path])</pre>	
$load\_with\_pandas(\rightarrow None)$	Deserialize data
<pre>save_numpy_ndarray(*, data, file_path)</pre>	
<pre>load_numpy_ndarray(*, file_path)</pre>	
<pre>save_pickle(*, data[, file_path])</pre>	
<pre>load_pickle(*[, file_path])</pre>	
create_recipriocal_triples(x)	Add inverse triples into dask dataframe
<pre>index_triples_with_pandas(→ das.core.frame.DataFrame)</pre>	1-
$dataset\_sanity\_checking(\rightarrow None)$	

### **Module Contents**

```
\label{local_discrete_discrete} $$ discrete_read_preprocess\_save\_load_kg.util.polars\_dataframe\_indexer ($$ df\_polars: polars.DataFrame, idx\_entity: polars.DataFrame, idx\_relation: polars.DataFrame) $$ \rightarrow polars.DataFrame $$
```

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.

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

```
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)

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

Read triples from triple store into pandas dataframe

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

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

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

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

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

```
\label{eq:cond_preprocess_save_load_kg.util.load_with_pandas} (\textit{self}) \rightarrow None \\ Descrialize \ data
```

dicee.read\_preprocess\_save\_load\_kg.util.index\_triples\_with\_pandas(train\_set, entity to idx: dict, relation to idx: dict) → pandas.core.frame.DataFrame

### **Parameters**

- train set pandas dataframe
- entity\_to\_idx a mapping from str to integer index
- relation\_to\_idx a mapping from str to integer index
- num\_core number of cores to be used

### Returns

indexed triples, i.e., pandas dataframe

dicee.read\_preprocess\_save\_load\_kg.util.dataset\_sanity\_checking(  $train\_set: numpy.ndarray, num\_entities: int, num\_relations: int) \rightarrow None$ 

### **Parameters**

- train set
- num\_entities
- num\_relations

### Returns

# **Classes**

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

# **Package Contents**

kg

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

```
save()
     load()
\verb|class| dicee.read_preprocess_save_load_kg.ReadFromDisk| (kg)
     Read the data from disk into memory
     kg
     start() \rightarrow None
           Read a knowledge graph from disk into memory
           Data will be available at the train_set, test_set, valid_set attributes.
           Parameter
           None
               rtype
                   None
     add_noisy_triples_into_training()
dicee.scripts
```

**Submodules** 

dicee.scripts.index

# **Functions**

```
get_default_arguments()
main()
```

# **Module Contents**

```
dicee.scripts.index.get_default_arguments()
dicee.scripts.index.main()
```

# dicee.scripts.run

### **Functions**

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

# **Module Contents**

# dicee.scripts.serve

### **Attributes**

```
app
neural_searcher
```

### **Classes**

NeuralSearcher

### **Functions**

```
get_default_arguments()

root()

search_embeddings(q)

retrieve_embeddings(q)

main()
```

# **Module Contents**

```
model
    qdrant_client
    get (entity: str)
    search (entity: str)

dicee.scripts.serve.main()
```

dicee.trainer

**Submodules** 

dicee.trainer.dice\_trainer

**Classes** 

DICE\_Trainer

DICE\_Trainer implement

### **Functions**

```
load_term_mapping([file_path])
initialize_trainer(args, callbacks)
get_callbacks(args)
```

# **Module Contents**

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

    model

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

- self
- dataset

# Returns

model

# dicee.trainer.torch trainer

### **Classes**

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

### **Module Contents**

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

### dicee.trainer.torch\_trainer\_ddp

#### **Classes**

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

### **Functions**

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

### **Module Contents**

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

```
optimizer

train_dataset_loader

loss_func

callbacks

model

num_epochs

loss_history = []

ptdtype

ctx

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, storage\_path, evaluator=None)

### **DICE\_Trainer implement**

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

args

is\_continual\_training:bool

storage\_path:str

evaluator:

report:dict

report

args

trainer = None

is\_continual\_training

storage\_path

evaluator

form\_of\_labelling = None

### continual\_start()

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

#### **Parameter**

#### returns

- model
- form\_of\_labelling (str)

```
initialize\_trainer(callbacks: List) \rightarrow lightning.Trainer
```

Initialize Trainer from input arguments

```
initialize_or_load_model()
```

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

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

 $\begin{tabular}{ll} \textbf{start} & (knowledge\_graph: dicee.knowledge\_graph.KG \mid numpy.memmap) \\ & \rightarrow \textbf{Tuple}[dicee.models.base\_model.BaseKGE, str] \end{tabular}$ 

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

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

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

### 14.2 Submodules

dicee.\_\_main\_\_

dicee.abstracts

### Classes

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

### **Module Contents**

class dicee.abstracts.AbstractTrainer(args, callbacks)

Abstract class for Trainer class for knowledge graph embedding models

```
Parameter
```

kwargs

**rtype**None

```
args
     [str] ?
callbacks: list
attributes
callbacks
is_global_zero = True
strategy = None
on_fit_start(*args, **kwargs)
     A function to call callbacks before the training starts.
     Parameter
     args
     kwargs
         rtype
             None
on_fit_end(*args, **kwargs)
     A function to call callbacks at the ned of the training.
     Parameter
     args
```

```
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
      apply_semantic_constraint
      configs
      \texttt{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]}
          Parameters
               str_entity_or_relation(corresponds to a str or a list of strings to
              be tokenized via BPE and shaped.)
          Return type
              A list integer(s) or a list of lists containing integer(s)
\texttt{get\_padded\_bpe\_triple\_representation} (triples: List[List[str]]) \rightarrow Tuple[List, List, List]
          Parameters
              triples
\verb"set_model_train_mode"() \to None
     Setting the model into training mode
     Parameter
\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: \verb"abc.ABC", \verb"lightning.pytorch.callbacks.Callback"
     Abstract class for Callback class for knowledge graph embedding models
     Parameter
     on_init_start(*args, **kwargs)
           Parameter
           trainer:
           model:
               rtype
                   None
     on_init_end(*args, **kwargs)
           Call at the beginning of the training.
           Parameter
           trainer:
           model:
               rtype
                   None
```

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

```
path
sample_counter = 0
epoch_count = 0
alphas = None
on_fit_start(trainer, model)
     Call at the beginning of the training.
     Parameter
     trainer:
     model:
         rtype
             None
on\_fit\_end(trainer, model)
     Call at the end of the training.
     Parameter
     trainer:
     model:
         rtype
             None
\verb|store_ensemble| (param_ensemble)| \rightarrow None
```

## dicee.analyse\_experiments

This script should be moved to dicee/scripts

## Classes

Experiment

### **Functions**

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

### **Module Contents**

```
\verb|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
<pre>compute_convergence(seq, i)</pre>	

### **Module Contents**

```
Bases: dicee.abstracts.AbstractCallback

Abstract class for Callback class for knowledge graph embedding models

Parameter

path

on_fit_end(trainer, model) → None

Store epoch loss

Parameter

trainer:

model:
```

**rtype**None

class dicee.callbacks.AccumulateEpochLossCallback(path: str)

```
class dicee.callbacks.PrintCallback
      Bases: dicee.abstracts.AbstractCallback
      Abstract class for Callback class for knowledge graph embedding models
      Parameter
      start_time
      \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
      \verb"on_fit_start" (\textit{trainer}, \textit{pl}\_\textit{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
     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)
     decide (running_model_state_dict, ensemble_state_dict, val_running_model,
                 mrr_updated_ensemble_model)
          Perform Hard Update, software or rejection
              Parameters
                   • running_model_state_dict
                   • ensemble_state_dict
                  • val_running_model
                   • mrr_updated_ensemble_model
     on_train_epoch_end(trainer, model)
          Call at the end of each epoch during training.
          Parameter
          trainer:
          model:
              rtype
                  None
class dicee.callbacks.Eval (path, epoch_ratio: int = None)
     Bases: dicee.abstracts.AbstractCallback
     Abstract class for Callback class for knowledge graph embedding models
     Parameter
     path
     reports = []
     epoch_ratio
     epoch_counter = 0
     on_fit_start (trainer, model)
```

Call at the beginning of the training.

```
Parameter
           trainer:
           model:
               rtype
                   None
     on_fit_end(trainer, model)
           Call at the end of the training.
           Parameter
           trainer:
           model:
               rtype
                   None
     \verb"on_train_epoch_end" (\textit{trainer}, \textit{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:
               rtvpe
                   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
     ratio
     method
     scaler
     frequency
     on_train_batch_start (trainer, model, batch, batch_idx)
           Called when the train batch begins.
dicee.config
```

# **Classes**

Namespace

Simple object for storing attributes.

### **Module Contents**

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

Bases: argparse.Namespace

Simple object for storing attributes.

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

```
dataset_dir: str = None
     The path of a folder containing train.txt, and/or valid.txt and/or test.txt
save_embeddings_as_csv: bool = False
     Embeddings of entities and relations are stored into CSV files to facilitate easy usage.
storage_path: str = 'Experiments'
     A directory named with time of execution under -storage_path that contains related data about embeddings.
path_to_store_single_run: str = None
     A single directory created that contains related data about embeddings.
path_single_kg = None
     Path of a file corresponding to the input knowledge graph
sparql_endpoint = None
     An endpoint of a triple store.
model: str = 'Keci'
     KGE model
optim: str = 'Adam'
     Optimizer
embedding_dim: int = 64
     Size of continuous vector representation of an entity/relation
num_epochs: int = 150
     Number of pass over the training data
batch_size: int = 1024
     Mini-batch size if it is None, an automatic batch finder technique applied
lr: float = 0.1
     Learning rate
add_noise_rate: float = None
     The ratio of added random triples into training dataset
gpus = None
     Number GPUs to be used during training
callbacks
     10}}
         Type
             Callbacks, e.g., {"PPE"
             { "last_percent_to_consider"
backend: str = 'pandas'
     Backend to read, process, and index input knowledge graph. pandas, polars and rdflib available
separator: str = '\\s+'
     separator for extracting head, relation and tail from a triple
trainer: str = 'torchCPUTrainer'
     Trainer for knowledge graph embedding model
```

```
scoring_technique: str = 'KvsAll'
    Scoring technique for knowledge graph embedding models
neg_ratio: int = 0
    Negative ratio for a true triple in NegSample training_technique
weight decay: float = 0.0
    Weight decay for all trainable params
normalization: str = 'None'
    LayerNorm, BatchNorm1d, or None
init_param: str = None
    xavier_normal or None
gradient_accumulation_steps: int = 0
    Not tested e
num_folds_for_cv: int = 0
    Number of folds for CV
eval_model: str = 'train_val_test'
    ["None", "train", "train_val", "train_val_test", "test"]
        Type
            Evaluate trained model choices
save_model_at_every_epoch: int = None
    Not tested
label_smoothing_rate: float = 0.0
num_core: int = 0
    Number of CPUs to be used in the mini-batch loading process
random_seed: int = 0
    Random Seed
sample_triples_ratio: float = None
    Read some triples that are uniformly at random sampled. Ratio being between 0 and 1
read_only_few: int = None
    Read only first few triples
pykeen_model_kwargs
    Additional keyword arguments for pykeen models
kernel_size: int = 3
    Size of a square kernel in a convolution operation
num_of_output_channels: int = 32
    Number of slices in the generated feature map by convolution.
p: int = 0
    P parameter of Clifford Embeddings
q: int = 1
    Q parameter of Clifford Embeddings
```

```
input_dropout_rate: float = 0.0
    Dropout rate on embeddings of input triples
hidden_dropout_rate: float = 0.0
    Dropout rate on hidden representations of input triples
feature_map_dropout_rate: float = 0.0
    Dropout rate on a feature map generated by a convolution operation
byte_pair_encoding: bool = False
    Byte pair encoding
        Type
            WIP
adaptive_swa: bool = False
    Adaptive stochastic weight averaging
swa: bool = False
    Stochastic weight averaging
block_size: int = None
    block size of LLM
continual_learning = None
    Path of a pretrained model size of LLM
__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 <code>\_\_getitem\_\_()</code>, supporting fetching a data sample for a given key. Subclasses could also optionally overwrite <code>\_\_len\_\_()</code>, which is expected to return the size of the dataset by many <code>Sampler</code> implementations and the default options of <code>DataLoader</code>. Subclasses could also optionally implement <code>\_\_getitems\_\_()</code>, for speedup batched samples loading. This method accepts list of indices of samples of batch and returns list of samples.

### **1** Note

**Parameters** 

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

```
• train_set_idx - Indexed triples for the training.
```

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

### Return type

torch.utils.data.Dataset

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

Bases: torch.utils.data.Dataset

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

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

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



\_\_\_\_

TODO

### train\_set\_idx

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

### entity\_idxs

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

### relation\_idxs

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

self: torch.utils.data.Dataset

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

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

```
collate_fn = None
__len__()
\__getitem__(idx)
```

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

Bases: torch.utils.data.Dataset

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

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

only with 0s.

#### train set idx

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

### entity\_idxs

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

### relation\_idxs

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

self: torch.utils.data.Dataset

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

```
train_data = None
train_target = None
label_smoothing_rate
collate_fn = None
target_dim
store
__len__()
\_getitem\_(idx)
```

class dicee.dataset\_classes.OnevsSample ( $train\_set$ : numpy.ndarray,  $num\_entities$ ,  $num\_relations$ ,  $neg\_sample\_ratio$ : int = None,  $label\_smoothing\_rate$ : float = 0.0)

Bases: torch.utils.data.Dataset

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

#### **Parameters**

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

### train\_data

The input data converted into a PyTorch tensor.

#### Type

torch.Tensor

#### num entities

Number of entities in the dataset.

### **Type**

int

### num\_relations

Number of relations in the dataset.

#### **Type**

int

### neg\_sample\_ratio

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

### Type

int

#### label\_smoothing\_rate

The smoothing factor applied to the labels.

#### Туре

torch.Tensor

### collate\_fn

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

#### Туре

function, optional

### train\_data

num\_entities

```
num_relations
      neg_sample_ratio
      label_smoothing_rate
      collate_fn = None
      __len__()
           Returns the number of samples in the dataset.
      \__getitem\__(idx)
           Retrieves a single data sample from the dataset at the given index.
                    idx (int) – The index of the sample to retrieve.
                Returns
                    A tuple consisting of:
                      • x (torch.Tensor): The head and relation part of the triple.
                      • y_idx (torch.Tensor): The concatenated indices of the true object (tail entity) and the
                         indices of the negative samples.
                      • y_vec (torch.Tensor): A vector containing the labels for the positive and negative samples,
                         with label smoothing applied.
                Return type
                    tuple
class dicee.dataset_classes.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

num_entities

label_smoothing_rate

collate_fn = None

store

max_num_of_classes
__len__()
__getitem__(idx)

class dicee.dataset_classes.NegSampleDataset(train_set: numpy.ndarray, num_entities: int, num_relations: int, neg_sample_ratio: int = 1)

Bases: torch.utils.data.Dataset
```

An abstract class representing a Dataset.

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

### 1 Note

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

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

• num workers int for https://pytorch.org/docs/stable/data.html#torch.utils.data. DataLoader

### Return type

train set idx

num\_entities

num\_relations

neg\_sample\_ratio

batch\_size

num\_workers

train\_dataloader() → torch.utils.data.DataLoader

An iterable or collection of iterables specifying training samples.

For more information about multiple dataloaders, see this section.

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

For data processing use the following pattern:

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

However, the above are only necessary for distributed processing.

### 🛕 Warning

do not assign state in prepare\_data

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

#### 1 Note

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

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

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

#### **Parameters**

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

#### Example:

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

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

# don't do this
        self.something = else

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

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

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

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

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

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

### 1 Note

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

### **Parameters**

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

#### **Returns**

A reference to the data on the new device.

#### Example:

```
def transfer_batch_to_device(self, batch, device, dataloader_idx):
    if isinstance(batch, CustomBatch):
        # move all tensors in your custom data structure to the device
        batch.samples = batch.samples.to(device)
        batch.targets = batch.targets.to(device)
        (continues on next page)
```

(continued from previous page)

```
elif dataloader_idx == 0:
    # skip device transfer for the first dataloader or anything you wish
    pass
else:
    batch = super().transfer_batch_to_device(batch, device, dataloader_
→idx)
    return batch
```

```
See alsomove_data_to_device()apply_to_collection()
```

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

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

## **A** Warning

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

### Example:

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

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

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

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

### Example:

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

(continues on next page)

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```
# 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**

### **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

num_entities = None

num_relations = None

args

report

during_training = False

vocab_preparation (dataset) → None

A function to wait future objects for the attributes of executor
```

Return type

None

```
eval (dataset: dicee.knowledge_graph.KG, trained_model, form_of_labelling, during_training=False)
             \rightarrow None
eval_rank_of_head_and_tail_entity(*, train_set, valid_set=None, test_set=None, trained_model)
eval_rank_of_head_and_tail_byte_pair_encoded_entity(*, train_set=None, valid_set=None,
             test_set=None, ordered_bpe_entities, trained_model)
eval_with_byte (*, raw_train_set, raw_valid_set=None, raw_test_set=None, trained_model,
             form\_of\_labelling) \rightarrow None
     Evaluate model after reciprocal triples are added
eval_with_bpe_vs_all (*, raw_train_set, raw_valid_set=None, raw_test_set=None, trained_model,
            form\_of\_labelling) \rightarrow None
     Evaluate model after reciprocal triples are added
eval_with_vs_all (*, train_set, valid_set=None, test_set=None, trained_model, form_of_labelling)
              \rightarrow None
     Evaluate model after reciprocal triples are added
\verb|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
storage\_path = None
trainer = None
trained\_model = None
knowledge\_graph = None
report
evaluator = None
start\_time = None
continual\_training\_setup\_executor() → None
read\_preprocess\_index\_serialize\_data() → None

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

Read & Preprocess & Index & Serialize Input Data

(2) Store the statistics of the data.

#### **Parameter**

rtype

None

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

Save a knowledge graph embedding model

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

### **Parameter**

rtype

None

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

End training

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

### **Parameter**

#### rtype

A dict containing information about the training and/or evaluation

### $write\_report() \rightarrow None$

Report training related information in a report. json file

 $start() \rightarrow dict$ 

Start training

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

#### **Parameter**

#### rtype

A dict containing information about the training and/or evaluation

class dicee.executer.ContinuousExecute(args)

Bases: Execute

A subclass of Execute Class for retraining

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

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

previous\_args

args

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

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
     sparql_endpoint
     path_single_kg
     byte_pair_encoding
     ordered_shaped_bpe_tokens = None
     add_noise_rate
     num_entities = None
     num_relations = None
     path_for_deserialization
     add_reciprocal
     eval_model
     read_only_few
     sample_triples_ratio
     path_for_serialization
     entity_to_idx
     relation_to_idx
     backend
     training_technique
     idx_entity_to_bpe_shaped
     enc
     num_tokens
     num_bpe_entities = None
     padding
     dummy_id
     max_length_subword_tokens = None
```

```
train_set_target = None

target_dim = None

train_target_indices = None

ordered_bpe_entities = None

separator

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
```

within. List[sit] = None)  $\rightarrow$  to characteristic

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} \begin{split} \texttt{triple\_score} \ (h: List[str] \mid str = None, \, r: \, List[str] \mid str = None, \, t: \, List[str] \mid str = None, \, logits = False) \\ &\rightarrow \mathsf{torch.FloatTensor} \end{split}
```

Predict triple score

### **Parameter**

head\_entity: List[str]

String representation of selected entities.

relation: List[str]

String representation of selected relations.

tail\_entity: List[str]

String representation of selected entities.

logits: bool

If logits is True, unnormalized score returned

# **Returns: Tuple**

```
pytorch tensor of triple score
```

```
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) | f(e,r,x) > confidence land (e,r,x)

otin G

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

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

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

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

train (kg, lr=0.1, epoch=10, batch_size=32, neg_sample_ratio=10, num_workers=1) → None

Retrained a pretrain model on an input KG via negative sampling.
```

# dicee.query\_generator

### **Classes**

QueryGenerator

# **Module Contents**

```
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) \rightarrow List[Tuple[str, Tuple[collections.defaultdict]]]
     Load Queries from Disk to Memory
```

# dicee.sanity\_checkers

### **Functions**

# **Module Contents**

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

# dicee.static\_funcs

# **Functions**

<pre>create_recipriocal_triples(x)</pre>	Add inverse triples into dask dataframe
get_er_vocab(data[, file_path])	
(dotal flath))	
<pre>get_re_vocab(data[, file_path])</pre>	
get_ee_vocab(data[, file_path])	
-	
timeit(func)	
save_pickle(*[, data, file_path])	
parto_profite( [, amm, mo_pmm])	
load_pickle([file_path])	
([61 <sub>2</sub>	
<pre>load_term_mapping([file_path])</pre>	
select_model(args[, is_continual_training, stor-	
age_path])	
$load_model( \rightarrow Tuple[object, Tuple[dict, dict]])$	Load weights and initialize pytorch module from names-
load_model_ensemble()	pace arguments  Construct Ensemble Of weights and initialize pytorch
ioad_model_ensemble()	module from namespace arguments
save_numpy_ndarray(*, data, file_path)	ı C
numpy_data_type_changer(→ numpy.ndarray)	Detect most efficient data type for a given triples
$save\_checkpoint\_model(\rightarrow None)$ $store(\rightarrow None)$	Store Pytorch model into disk Store trained_model model and save embeddings into csv
Score( / None)	file.
$add\_noisy\_triples(\rightarrow pandas.DataFrame)$	Add randomly constructed triples
read_or_load_kg(args, cls)	
intialize_model(→ Tuple[object, str])	
THETATIZE_HOUGET(→ Tupic[Object, Sti])	
load_json(→ dict)	
save_embeddings(→ None)	Save it as CSV if memory allows.
random_prediction(pre_trained_kge)	
deploy_triple_prediction(pre_trained_kge,	
str_subject,)	
	continues on next page

continues on next page

Table 2 - continued from previous page

```
deploy_tail_entity_prediction(pre_trained_kge,
...)
deploy_head_entity_prediction(pre_trained_kge,
...)
deploy_relation_prediction(pre_trained_kge,
...)
vocab_to_parquet(vocab_to_idx, name, ...)
create_experiment_folder([folder_name])
continual\_training\_setup\_executor(\rightarrow None)
exponential\_function(\rightarrow torch.FloatTensor)
load_numpy(\rightarrow numpy.ndarray)
evaluate(entity_to_idx,
                            scores,
                                       easy_answers,
                                                       # @TODO: CD: Renamed this function
hard answers)
download_file(url[, destination_folder])
download_files_from_url(\rightarrow None)
download\_pretrained\_model(\rightarrow str)
```

### **Module Contents**

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

```
\texttt{dicee.static\_funcs.save\_checkpoint\_model} \ (\textit{model}, \textit{path: str}) \ \rightarrow None
```

Store Pytorch model into disk

```
dicee.static_funcs.store(trainer, trained_model, model_name: str = 'model', full_storage_path: str = None, save_embeddings_as_csv=False) \rightarrow None
```

Store trained\_model model and save embeddings into csv file. :param trainer: an instance of trainer class :param full\_storage\_path: path to save parameters. :param model\_name: string representation of the name of the model. :param trained\_model: an instance of BaseKGE see core.models.base\_model . :param save\_embeddings\_as\_csv: for easy access of embeddings. :return:

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)
```

```
\label{local_condition} \mbox{disce.static\_funcs.deploy\_tail\_entity\_prediction} \mbox{$(pre\_trained\_kge, str\_subject, str\_predicate, top\_k)$}
```

```
\label{local_condition} \begin{tabular}{ll} dice.static\_funcs.deploy\_head\_entity\_prediction (pre\_trained\_kge, str\_object, str\_predicate, \\ top\_k) \end{tabular}
```

```
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='.') \rightarrow None
```

### **Parameters**

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

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

# dicee.static\_funcs\_training

### **Functions**

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

efficient_zero_grad(model)
```

### **Module Contents**

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

Evaluate model in a standard link prediction task

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

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

# dicee.static\_preprocess\_funcs

# **Attributes**

enable\_log

### **Functions**

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

## **Module Contents**

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

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

# 14.3 Attributes

```
__version__
```

# 14.4 Classes

Pyke	A Physical Embedding Model for Knowledge Graphs
DistMult	Embedding Entities and Relations for Learning and Infer-
	ence in Knowledge Bases
KeciBase	Without learning dimension scaling

continues on next page

Table 3 - continued from previous page

Keci	Base class for all neural network modules.
TransE	Translating Embeddings for Modeling
DeCaL	Base class for all neural network modules.
DualE	Dual Quaternion Knowledge Graph Embeddings
	(https://ojs.aaai.org/index.php/AAAI/article/download/16850/16657)
ComplEx	Base class for all neural network modules.
AConEx	Additive Convolutional ComplEx Knowledge Graph Embeddings
AConvO	Additive Convolutional Octonion Knowledge Graph Embeddings
AConvQ	Additive Convolutional Quaternion Knowledge Graph Embeddings
ConvQ	Convolutional Quaternion Knowledge Graph Embeddings
ConvO	Base class for all neural network modules.
ConEx	Convolutional ComplEx Knowledge Graph Embeddings
QMult	Base class for all neural network modules.
OMult	Base class for all neural network modules.
Shallom	A shallow neural model for relation prediction (https://arxiv.org/abs/2101.09090)
LFMult	Embedding with polynomial functions. We represent all entities and relations in the polynomial space as:
PykeenKGE	A class for using knowledge graph embedding models implemented in Pykeen
BytE	Base class for all neural network modules.
BaseKGE	Base class for all neural network modules.
DICE_Trainer	DICE_Trainer implement
KGE	Knowledge Graph Embedding Class for interactive usage of pre-trained models
Execute	A class for Training, Retraining and Evaluation a model.
BPE_NegativeSamplingDataset	An abstract class representing a Dataset.
MultiLabelDataset	An abstract class representing a Dataset.
MultiClassClassificationDataset	Dataset for the 1vsALL training strategy
OnevsAllDataset	Dataset for the 1vsALL training strategy
KvsAll	Creates a dataset for KvsAll training by inheriting from torch.utils.data.Dataset.
AllvsAll	Creates a dataset for AllvsAll training by inheriting from torch.utils.data.Dataset.
OnevsSample	A custom PyTorch Dataset class for knowledge graph embeddings, which includes
KvsSampleDataset	KvsSample a Dataset:
NegSampleDataset	An abstract class representing a Dataset.
TriplePredictionDataset	Triple Dataset
CVDataModule	Create a Dataset for cross validation
QueryGenerator	

# 14.5 Functions

```
Add inverse triples into dask dataframe
create_recipriocal_triples(x)
get_er_vocab(data[, file_path])
get_re_vocab(data[, file_path])
get_ee_vocab(data[, file_path])
timeit(func)
save_pickle(*[, data, file_path])
load_pickle([file_path])
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
load_model_ensemble(...)
                                                        Construct Ensemble Of weights and initialize pytorch
                                                        module from namespace arguments
save_numpy_ndarray(*, data, file_path)
numpy\_data\_type\_changer(\rightarrow numpy.ndarray)
                                                        Detect most efficient data type for a given triples
save\_checkpoint\_model(\rightarrow None)
                                                        Store Pytorch model into disk
store(\rightarrow None)
                                                        Store trained model model and save embeddings into csv
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,
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])
```

continues on next page

Table 4 - continued from previous page

```
continual\_training\_setup\_executor(\rightarrow None)
exponential\_function(\rightarrow torch.FloatTensor)
load_numpy(→ numpy.ndarray)
                                                        # @TODO: CD: Renamed this function
evaluate(entity_to_idx,
                             scores,
                                        easy_answers,
hard_answers)
download_file(url[, destination_folder])
download\_files\_from\_url(\rightarrow None)
download\_pretrained\_model(\rightarrow str)
mapping_from_first_two_cols_to_third(train_se
timeit(func)
load_term_mapping([file_path])
reload_dataset(path, form of labelling, ...)
                                                        Reload the files from disk to construct the Pytorch dataset
construct_dataset(→ torch.utils.data.Dataset)
```

# 14.6 Package Contents

```
class dicee.Pyke(args)
     Bases: dicee.models.base_model.BaseKGE
     A Physical Embedding Model for Knowledge Graphs
     name = 'Pyke'
     dist_func
     margin = 1.0
     forward_triples (x: torch.LongTensor)
              Parameters
                  x
class dicee.DistMult(args)
     Bases: dicee.models.base_model.BaseKGE
     Embedding Entities and Relations for Learning and Inference in Knowledge Bases https://arxiv.org/abs/1412.6575
     name = 'DistMult'
     k_vs_all_score (emb_h: torch.FloatTensor, emb_r: torch.FloatTensor, emb_E: torch.FloatTensor)
              Parameters
                  • emb_h
                  • emb_r
```

```
forward_k_vs_all (x: torch.LongTensor)
forward_k_vs_sample (x: torch.LongTensor, target_entity_idx: torch.LongTensor)
score (h, r, t)

class dicee.KeciBase (args)
Bases: Keci
Without learning dimension scaling
name = 'KeciBase'
requires_grad_for_interactions = False

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

Base class for all neural network modules.

Your models should also subclass this class.

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

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

class Model (nn.Module):
    def __init__ (self) -> 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 have their parameters converted too when you call to(), etc.

# **1** Note

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

### **Variables**

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

```
name = 'Keci'
p
q
```

eq j

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

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

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

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

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

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

### **Parameter**

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

### returns

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

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

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

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

Kvsall training

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

 $\textbf{forward\_k\_vs\_sample} \ (x: torch.LongTensor, target\_entity\_idx: torch.LongTensor) \ \rightarrow \textbf{torch.FloatTensor}$ 

### **Parameter**

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

*rtype**
torch.FloatTensor with (n, k) shape

*score*(h, r, t)

*forward triples*(x: torch.Tensor)* \rightarrow torch.FloatTensor
```

### **Parameter**

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

### rtype

torch.FloatTensor with (n) shape

```
class dicee.TransE(args)
```

Bases: dicee.models.base model.BaseKGE

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

```
name = 'TransE'

margin = 4

score (head_ent_emb, rel_ent_emb, tail_ent_emb)

forward_k_vs_all (x: torch.Tensor) → torch.FloatTensor

class dicee.DeCaL(args)

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

Base class for all neural network modules.

Your models should also subclass this class.

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

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

class Model(nn.Module):
    def __init__(self) -> 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 have their parameters converted too when you call to(), etc.

# 1 Note

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

### **Variables**

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

name = 'DeCaL'

entity\_embeddings

relation\_embeddings

р

q

r

re

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

### **Parameter**

x: torch.LongTensor with (n, ) shape

### rtype

torch.FloatTensor with (n) shape

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

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

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

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

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

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

and return:

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

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

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

For same bases vectors interaction we have

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

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

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

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[:, :, j] \* rq[:, :, k] - hq[:, :, k] \* rq[:, :, j])

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

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

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

 $compute\_sigma\_rr(hk, rk)$ 

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

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

Compute

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

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

### for j in range(q):

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

print(sigma\_pq.shape)

compute\_sigma\_pr(\*, hp, hk, rp, rk)

Compute

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

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

# for j in range(q):

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

print(sigma\_pq.shape)

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

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

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

```
for j in range(q):
                                                                     sigma_pq[:, :, i, j] = hp[:, :, i] * rq[:, :, j] - hq[:, :, j] * rp[:, :, i]
                                       print(sigma_pq.shape)
class dicee.DualE(args)
                    Bases: dicee.models.base_model.BaseKGE
                    Dual Quaternion Knowledge Graph Embeddings (https://ojs.aaai.org/index.php/AAAI/article/download/16850/
                    16657)
                    name = 'DualE'
                    entity_embeddings
                    relation_embeddings
                    num_ent
                    \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 to nest them in a tree structure. You can assign the submodules as regular attributes:

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

class Model(nn.Module):
    def __init__ (self) -> 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 have their parameters converted too 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.

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

```
import torch.nn as nn
import torch.nn.functional as F
class Model(nn.Module):
    def __init__(self) -> 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 have their parameters converted too when you call to(), etc.

# **1** Note

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

### **Variables**

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

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

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

class Model(nn.Module):
    def __init__ (self) -> 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 have their parameters converted too when you call to (), etc.



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

### **Variables**

**training**  $(b \circ o 1)$  – 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 to nest them in a tree structure. You can assign the submodules as regular attributes:

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

class Model(nn.Module):
    def __init__(self) -> 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 have their parameters converted too when you call to (), etc.

### 1 Note

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

## Variables

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

```
name = 'OMult'
     static octonion_normalizer(emb_rel_e0, emb_rel_e1, emb_rel_e2, emb_rel_e3, emb_rel_e4,
                  emb rel e5, emb rel e6, emb rel e7)
     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_width
     shallom
     get_embeddings() → Tuple[numpy.ndarray, None]
     forward_k_vs_all (x) \rightarrow \text{torch.FloatTensor}
     forward\_triples(x) \rightarrow torch.FloatTensor
               Parameters
                   x
               Returns
class dicee.LFMult(args)
     Bases: dicee.models.base_model.BaseKGE
     Embedding with polynomial functions. We represent all entities and relations in the polynomial space as: f(x) =
     sum_{i=0}^{d-1} a_k x^{i}d and use the three differents scoring function as in the paper to evaluate the score.
     We also consider combining with Neural Networks.
     name = 'LFMult'
     entity_embeddings
     relation_embeddings
     degree
     m
     x_values
     forward_triples (idx_triple)
               Parameters
                   x
```

```
construct_multi_coeff(X)
```

 $poly_NN(x, coefh, coefr, coeft)$ 

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

linear(x, w, b)

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

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

# tri\_score (coeff\_h, coeff\_r, coeff\_t)

this part implement the trilinear scoring techniques:

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

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

### vtp score (h, r, t)

this part implement the vector triple product scoring techniques:

```
score(h,r,t) = int_{0}{1} \quad h(x)r(x)t(x) \quad dx = sum_{i,j,k} = 0^{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

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

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] + 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.PykeenKGE(args: dict)

Bases: dicee.models.base\_model.BaseKGE

A class for using knowledge graph embedding models implemented in Pykeen

Notes: Pykeen\_DistMult: C Pykeen\_ComplEx: Pykeen\_QuatE: Pykeen\_MuRE: Pykeen\_CP: Pykeen\_HolE: Pykeen\_HolE: Pykeen\_HolE:

model\_kwargs

```
name
model
loss_history = []
args
entity_embeddings = None
relation_embeddings = None
forward_k_vs_all (x: torch.LongTensor)
     # => Explicit version by this we can apply bn and dropout
     # (1) Retrieve embeddings of heads and relations + apply Dropout & Normalization if given. h, r =
     self.get_head_relation_representation(x) \# (2) Reshape (1). if self.last_dim > 0:
          h = h.reshape(len(x), self.embedding\_dim, self.last\_dim) r = r.reshape(len(x), self.embedding\_dim,
          self.last_dim)
     # (3) Reshape all entities. if self.last_dim > 0:
          t = self.entity embeddings.weight.reshape(self.num entities, self.embedding dim, self.last dim)
     else:
          t = self.entity embeddings.weight
     # (4) Call the score_t from interactions to generate triple scores. return self.interaction.score_t(h=h, r=r,
     all_entities=t, slice_size=1)
forward\_triples(x: torch.LongTensor) \rightarrow torch.FloatTensor
     # => Explicit version by this we can apply bn and dropout
     # (1) Retrieve embeddings of heads, relations and tails and apply Dropout & Normalization if given. h, r, t =
     self.get_triple_representation(x) \# (2) Reshape (1). if self.last_dim > 0:
          h = h.reshape(len(x), self.embedding\_dim, self.last\_dim) r = r.reshape(len(x), self.embedding\_dim,
          self.last_dim) t = t.reshape(len(x), self.embedding_dim, self.last_dim)
     # (3) Compute the triple score return self.interaction.score(h=h, r=r, t=t, slice size=None, slice dim=0)
abstract forward_k_vs_sample (x: torch.LongTensor, target_entity_idx)
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 to nest them in a tree structure. You can assign the submodules as regular attributes:

```
import torch.nn as nn
import torch.nn.functional as F
class Model(nn.Module):
    def __init__(self) -> None:
        super().__init__()
```

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(continued from previous page)

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

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



# 1 Note

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

### Variables

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

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

### **Parameters**

- yhat\_batch
- y\_batch

forward(x: torch.LongTensor)

## **Parameters**

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

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

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

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

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

### **Parameters**

- batch The output of your data iterable, normally a DataLoader.
- batch\_idx The index of this batch.

dataloader\_idx – The index of the dataloader that produced this batch. (only if multiple dataloaders used)

### Returns

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

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

Example:

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

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

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

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

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

# **1** Note

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

class dicee.BaseKGE(args: dict)

Bases: BaseKGELightning

Base class for all neural network modules.

Your models should also subclass this class.

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

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

class Model(nn.Module):
    def __init__(self) -> 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 have their parameters converted too when you call to(), etc.

# 1 Note

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

### Variables

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

### args

```
embedding_dim = None
num_entities = None
num_relations = None
num_tokens = None
learning_rate = None
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)
      get_embeddings() → Tuple[numpy.ndarray, numpy.ndarray]
dicee.create_recipriocal_triples(x)
      Add inverse triples into dask dataframe :param x: :return:
dicee.get_er_vocab(data, file_path: str = None)
dicee.get_re_vocab(data, file_path: str = None)
dicee.get_ee_vocab(data, file_path: str = None)
dicee.timeit(func)
dicee.save_pickle(*, data: object = None, file_path=str)
dicee.load_pickle(file_path=str)
dicee.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)
\texttt{dicee.numpy\_data\_type\_changer} (\textit{train\_set: numpy.ndarray}, \textit{num: int}) \rightarrow \texttt{numpy.ndarray}
      Detect most efficient data type for a given triples :param train_set: :param num: :return:
\texttt{dicee.save\_checkpoint\_model} \ (\textit{model}, \textit{path: str}) \ \rightarrow None
      Store Pytorch model into disk
```

```
dicee.store(trainer, trained_model, model_name: str = 'model', full_storage_path: str = None,
            save embeddings as csv=False) \rightarrow None
      Store trained_model model and save embeddings into csv file. :param trainer: an instance of trainer class :param
      full_storage_path: path to save parameters. :param model_name: string representation of the name of the model.
      :param trained_model: an instance of BaseKGE see core.models.base_model . :param save_embeddings_as_csv:
      for easy access of embeddings. :return:
dicee.add\_noisy\_triples (train_set: pandas.DataFrame, add_noise_rate: float) \rightarrow pandas.DataFrame
      Add randomly constructed triples :param train set: :param add noise rate: :return:
dicee.read_or_load_kg(args, cls)
dicee.intialize_model(args: dict, verbose=0) → Tuple[object, str]
dicee.load_json(p: str) \rightarrow dict
dicee.save_embeddings(embeddings: numpy.ndarray, indexes, path: str) \rightarrow None
      Save it as CSV if memory allows. :param embeddings: :param indexes: :param path: :return:
dicee.random_prediction(pre_trained_kge)
dicee.deploy_triple_prediction(pre_trained_kge, str_subject, str_predicate, str_object)
dicee.deploy_tail_entity_prediction(pre_trained_kge, str_subject, str_predicate, top_k)
dicee.deploy_head_entity_prediction(pre_trained_kge, str_object, str_predicate, top_k)
dicee.deploy_relation_prediction(pre_trained_kge, str_subject, str_object, top_k)
dicee.vocab_to_parquet(vocab_to_idx, name, path_for_serialization, print_into)
dicee.create_experiment_folder(folder_name='Experiments')
{\tt dicee.continual\_training\_setup\_executor}(\textit{executor}) \rightarrow None
dicee.exponential_function (x: numpy.ndarray, lam: float, ascending\_order=True) \rightarrow torch.FloatTensor
dicee.load_numpy(path) \rightarrow numpy.ndarray
dicee.evaluate(entity_to_idx, scores, easy_answers, hard_answers)
      # @TODO: CD: Renamed this function Evaluate multi hop query answering on different query types
dicee.download_file(url, destination_folder='.')
dicee.download_files_from_url(base\_url: str, destination\_folder='.') \rightarrow None
           Parameters
                                                    "https://files.dice-research.org/projects/DiceEmbeddings/
                  • base_url
```

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

 ${\tt dicee.download\_pretrained\_model}\,(\mathit{url}:\mathit{str})\,\to \mathit{str}$ 

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

# **DICE\_Trainer implement**

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

```
args
     is_continual_training:bool
     storage_path:str
     evaluator:
     report:dict
report
args
trainer = None
is_continual_training
storage_path
evaluator
form_of_labelling = None
continual_start()
     (1) Initialize training.
     (2) Load model
     (3) Load trainer (3) Fit model
     Parameter
         returns

    model

              • form_of_labelling (str)
initialize\_trainer(callbacks: List) \rightarrow lightning.Trainer
     Initialize Trainer from input arguments
initialize_or_load_model()
init_dataloader (dataset: torch.utils.data.Dataset) → torch.utils.data.DataLoader
init_dataset() → torch.utils.data.Dataset
start (knowledge_graph: dicee.knowledge_graph.KG | numpy.memmap)
             → Tuple[dicee.models.base_model.BaseKGE, str]
     in DDP setup, we need to load the memory map of already read/index KG. Ther
k\_fold\_cross\_validation(dataset) \rightarrow Tuple[dicee.models.base\_model.BaseKGE, str]
     Perform K-fold Cross-Validation
      1. Obtain K train and test splits.
      2. For each split,
             2.1 initialize trainer and model 2.2. Train model with configuration provided in args. 2.3. Compute
             the mean reciprocal rank (MRR) score of the model on the test respective split.
```

3. Report the mean and average MRR.

```
Parameters
```

- self
- dataset

#### Returns

model

```
class dicee.KGE (path=None, url=None, construct_ensemble=False, model_name=None)
      Bases: dicee.abstracts.BaseInteractiveKGE
      Knowledge Graph Embedding Class for interactive usage of pre-trained models
      __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
      predict_missing_relations (head_entity: List[str] | str, tail_entity: List[str] | str, within=None)
                     \rightarrow Tuple
            Given a head entity and a tail entity, return top k ranked relations.
            argmax_{r} in R \} f(h,r,t), where h, t in E.
```

```
Parameter
```

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

String representation of selected entities.

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

String representation of selected entities.

k: int

Highest ranked k entities.

## **Returns: Tuple**

Highest K scores and entities

```
\verb|predict_missing_tail_entity| (\textit{head\_entity: List[str]} \mid \textit{str}, \textit{relation: List[str]} \mid \textit{str},
```

*within:* List[str] = None  $\rightarrow$  torch.FloatTensor

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

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

#### **Parameter**

head\_entity: List[str]

String representation of selected entities.

tail\_entity: List[str]

String representation of selected entities.

#### **Returns: Tuple**

scores

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

# **Parameters**

- logits
- h
- r
- t
- within

Predict missing item in a given triple.

### **Parameter**

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

String representation of selected entities.

relation: Union[str, List[str]]

```
tail_entity: Union[str, List[str]]
     String representation of selected entities.
     k: int
     Highest ranked k item.
     Returns: Tuple
     Highest K scores and items
triple_score (h: List[str] | str = None, r: List[str] | str = None, t: List[str] | str = None, logits=False)
              \rightarrow torch.FloatTensor
     Predict triple score
     Parameter
     head_entity: List[str]
     String representation of selected entities.
     relation: List[str]
     String representation of selected relations.
     tail_entity: List[str]
     String representation of selected entities.
     logits: bool
     If logits is True, unnormalized score returned
     Returns: Tuple
     pytorch tensor of triple score
t_norm(tens_1: torch.Tensor, tens_2: torch.Tensor, tnorm: str = 'min') \rightarrow torch.Tensor
tensor_t_norm(subquery\_scores: torch.FloatTensor, tnorm: str = 'min') \rightarrow torch.FloatTensor
     Compute T-norm over [0,1] ^{n imes d} where n denotes the number of hops and d denotes number of
t\_conorm (tens_1: torch.Tensor, tens_2: torch.Tensor, tconorm: str = 'min') \rightarrow torch.Tensor
negnorm(tens\_1: torch.Tensor, lambda\_: float, neg\_norm: str = 'standard') \rightarrow torch.Tensor
return_multi_hop_query_results (aggregated_query_for_all_entities, k: int, only_scores)
single_hop_query_answering (query: tuple, only_scores: bool = True, k: int = None)
answer_multi_hop_query (query_type: str = None, query: Tuple[str | Tuple[str, str], Ellipsis] = None,
              queries: List[Tuple[str | Tuple[str, str], Ellipsis]] = None, tnorm: str = 'prod',
             neg_norm: str = 'standard', lambda_: float = 0.0, k: int = 10, only_scores=False)
              \rightarrow List[Tuple[str, torch.Tensor]]
     # @TODO: Refactoring is needed # @TODO: Score computation for each query type should be done in a
     static function
     Find an answer set for EPFO queries including negation and disjunction
```

String representation of selected relations.

#### **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.
                 Highest ranked k item to select triples with f(e,r,x) > \text{confidence}.
                 at most: int
                 Stop after finding at_most missing triples
                 \{(e,r,x) \mid f(e,r,x) > \text{confidence land } (e,r,x)\}
            otin G
      deploy(share: bool = False, top\_k: int = 10)
      train_triples (h: List[str], r: List[str], t: List[str], labels: List[float], iteration=2, optimizer=None)
      train_k_vs_all(h, r, iteration=1, lr=0.001)
            Train k vs all :param head_entity: :param relation: :param iteration: :param lr: :return:
      train (kg, lr=0.1, epoch=10, batch \ size=32, neg \ sample \ ratio=10, num \ workers=1) \rightarrow None
            Retrained a pretrain model on an input KG via negative sampling.
class dicee.Execute(args, continuous_training=False)
      A class for Training, Retraining and Evaluation a model.
        (1) Loading & Preprocessing & Serializing input data.
```

(2) Training & Validation & Testing

(3) Storing all necessary info args is\_continual\_training storage\_path = None trainer = None trained\_model = None knowledge\_graph = None report evaluator = None start\_time = None  $\verb"continual_training_setup_executor"\,(\,)\,\to None$  ${\tt read\_preprocess\_index\_serialize\_data}\,()\,\to None$ 

Read & Preprocess & Index & Serialize Input Data

- (1) Read or load the data from disk into memory.
- (2) Store the statistics of the data.

#### **Parameter**

rtype

None

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

Save a knowledge graph embedding model

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

#### **Parameter**

rtype

None

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

End training

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

#### **Parameter**

```
rtype
```

A dict containing information about the training and/or evaluation

```
write report () \rightarrow None
```

Report training related information in a report json file

 $start() \rightarrow dict$ 

Start training

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

#### **Parameter**

#### rtype

A dict containing information about the training and/or evaluation

```
dicee.mapping_from_first_two_cols_to_third(train_set_idx)
dicee.timeit(func)
dicee.load_term_mapping(file_path=str)
dicee.reload_dataset(path: str, form_of_labelling, scoring_technique, neg_ratio, label_smoothing_rate)
     Reload the files from disk to construct the Pytorch dataset
dicee.construct_dataset(*, train_set: numpy.ndarray | list, valid_set=None, test_set=None,
```

ordered bpe entities=None, train target indices=None, target dim: int = None, entity to idx: dict, relation\_to\_idx: dict, form\_of\_labelling: str, scoring\_technique: str, neg\_ratio: int, *label\_smoothing\_rate: float, byte\_pair\_encoding=None, block\_size: int = None)*  $\rightarrow$  torch.utils.data.Dataset

class dicee.BPE\_NegativeSamplingDataset(train\_set: torch.LongTensor, ordered\_shaped\_bpe\_entities: torch.LongTensor, neg\_ratio: int)

Bases: torch.utils.data.Dataset

An abstract class representing a Dataset.

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



### 1 Note

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

train\_set ordered\_bpe\_entities num\_bpe\_entities

```
neg_ratio
num_datapoints
__len__()
__getitem__(idx)
collate_fn(batch_shaped_bpe_triples: List[Tuple[torch.Tensor, torch.Tensor]])
```

Bases: torch.utils.data.Dataset

An abstract class representing a Dataset.

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

# 1 Note

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

```
train_set

train_indices_target

target_dim

num_datapoints

torch_ordered_shaped_bpe_entities

collate_fn = None

__len__()
__getitem__(idx)
```

class dicee.MultiClassClassificationDataset (subword\_units: numpy.ndarray, block\_size: int = 8)

Bases: torch.utils.data.Dataset

Dataset for the 1vsALL training strategy

#### **Parameters**

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

```
Return type
```

torch.utils.data.Dataset

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

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

Bases: torch.utils.data.Dataset

Dataset for the 1vsALL training strategy

#### **Parameters**

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

### Return type

torch.utils.data.Dataset

```
train_data
target_dim
collate_fn = None
__len__()
\__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  $[0,1]^{\{|\mathbf{E}|\}}$  is a binary label.

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



1 Note

**TODO** 

#### train set idx

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

#### entity idxs

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

#### relation idxs

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

self: torch.utils.data.Dataset

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

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

class dicee. 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:=  $\{(x,y) \mid i \mid i \land N, \text{ where } x : (h,r) \text{ is a possible } i \land N, \text{ is a possibl$ 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
```

```
train_data = None

train_target = None

label_smoothing_rate

collate_fn = None

target_dim

store

__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
label_smoothing_rate
collate_fn = None
__len__()
    Returns the number of samples in the dataset.
```

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

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

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

#### **Returns**

#### A tuple consisting of:

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

# Return type

tuple

class dicee.KvsSampleDataset(train\_set\_idx: numpy.ndarray, entity\_idxs, relation\_idxs, form, store=None, neg ratio=None, label smoothing rate: float = 0.0

Bases: torch.utils.data.Dataset

#### **KvsSample a Dataset:**

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

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

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

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

lnew\_yl << IEI new\_y contains all 1's if sum(y)< neg\_sample ratio new\_y contains</pre>

```
train set idx
              Indexed triples for the training.
          entity_idxs
              mapping.
          relation idxs
              mapping.
          form
          store
          label_smoothing_rate
          torch.utils.data.Dataset
     train data = None
     train_target = None
     neg_ratio
     num_entities
     label_smoothing_rate
     collate_fn = None
     store
     max_num_of_classes
     __len__()
     \__getitem__(idx)
class dicee. NegSampleDataset (train_set: numpy.ndarray, num_entities: int, num_relations: int,
           neg sample ratio: int = 1)
     Bases: torch.utils.data.Dataset
```

An abstract class representing a Dataset.

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

# 1 Note

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

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: pytorch_lightning.LightningDataModule
     Create a Dataset for cross validation
           Parameters
                 • train_set_idx - Indexed triples for the training.
```

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

#### Return type

?

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

train\_dataloader() → torch.utils.data.DataLoader

An iterable or collection of iterables specifying training samples.

For more information about multiple dataloaders, see this section.

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

For data processing use the following pattern:

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

However, the above are only necessary for distributed processing.

# Warning

do not assign state in prepare\_data

- fit()
- prepare\_data()

• setup()



#### 1 Note

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

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

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

#### **Parameters**

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

Example:

```
class LitModel(...):
   def __init__(self):
        self.11 = None
   def prepare_data(self):
        download_data()
        tokenize()
        # don't do this
        self.something = else
   def setup(self, stage):
        data = load_data(...)
        self.l1 = nn.Linear(28, data.num_classes)
```

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

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

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

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

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



#### **1** Note

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

#### **Parameters**

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

#### Returns

A reference to the data on the new device.

#### Example:

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

# See alsomove\_data\_to\_device()apply\_to\_collection()

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

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

# **A** Warning

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

#### Example:

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

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

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

1. Once per node. This is the default and is only called on LOCAL\_RANK=0.

2. Once in total. Only called on GLOBAL\_RANK=0.

Example:

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

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

This is called before requesting the dataloaders:

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

class dicee.QueryGenerator(train\_path, val\_path: str, test\_path: str, ent2id: Dict = None, rel2id: Dict = None, seed: int = 1, gen\_valid: bool = False, gen\_test: bool = True)

```
train_path

val_path

test_path

gen_valid

gen_test

seed

max_ans_num = 1000000.0

mode

ent2id

rel2id: Dict

ent_in: Dict

ent_out: Dict

query_name_to_struct

list2tuple(list_data)
```

```
tuple21ist (x: List \mid Tuple) \rightarrow List \mid Tuple
            Convert a nested tuple to a nested list.
      set_global_seed (seed: int)
            Set seed
      construct graph (paths: List[str]) → Tuple[Dict, Dict]
            Construct graph from triples Returns dicts with incoming and outgoing edges
      fill_query (query_structure: List[str | List], ent_in: Dict, ent_out: Dict, answer: int) → bool
            Private method for fill_query logic.
      achieve\_answer(query: List[str | List], ent\_in: Dict, ent\_out: Dict) \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
      \textbf{static load\_queries\_and\_answers} (\textit{path: str}) \rightarrow 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__,111
dicee.abstracts, 111
dicee.analyse_experiments, 117
dicee.callbacks, 119
dicee.config, 125
dicee.dataset_classes, 128
dicee.eval_static_funcs, 140
dicee.evaluator, 141
dicee.executer, 142
dicee.knowledge_graph, 144
dicee.knowledge_graph_embeddings, 146
dicee.models, 12
dicee.models.base_model, 12
dicee.models.clifford, 21
dicee.models.complex, 28
dicee.models.dualE, 30
dicee.models.function_space, 32
dicee.models.octonion, 35
dicee.models.pykeen_models, 38
dicee.models.quaternion, 39
dicee.models.real, 42
dicee.models.static_funcs, 44
dicee.models.transformers, 44
dicee.query_generator, 150
dicee.read_preprocess_save_load_kg, 97
dicee.read_preprocess_save_load_kg.preprocess,
dicee.read_preprocess_save_load_kg.read_from_disk,
dicee.read_preprocess_save_load_kg.save_load_disk,
dicee.read_preprocess_save_load_kg.util, 99
dicee.sanity_checkers, 151
dicee.scripts, 104
dicee.scripts.index, 104
dicee.scripts.run, 104
dicee.scripts.serve, 105
dicee.static_funcs, 152
dicee.static_funcs_training, 155
dicee.static_preprocess_funcs, 155
dicee.trainer, 106
dicee.trainer.dice_trainer, 106
dicee.trainer.torch_trainer, 108
dicee.trainer.torch_trainer_ddp, 109
```

# Index

# Non-alphabetical

```
__call__() (dicee.models.base_model.IdentityClass method), 21
 _call__() (dicee.models.IdentityClass method), 61, 72, 78
__getitem__() (dicee.AllvsAll method), 194
__getitem__() (dicee.BPE_NegativeSamplingDataset method), 191
__getitem__() (dicee.dataset_classes.AllvsAll method), 132
__getitem__() (dicee.dataset_classes.BPE_NegativeSamplingDataset method), 129
__getitem__() (dicee.dataset_classes.KvsAll method), 132
__getitem__() (dicee.dataset_classes.KvsSampleDataset method), 135
__getitem__() (dicee.dataset_classes.MultiClassClassificationDataset method), 130
__getitem__() (dicee.dataset_classes.MultiLabelDataset method), 130
__getitem__() (dicee.dataset_classes.NegSampleDataset method), 135
__getitem__() (dicee.dataset_classes.OnevsAllDataset method), 131
__getitem__() (dicee.dataset_classes.OnevsSample method), 134
__getitem__() (dicee.dataset_classes.TriplePredictionDataset method), 136
__getitem__() (dicee.KvsAll method), 193
__getitem__() (dicee.KvsSampleDataset method), 196
__getitem__() (dicee.MultiClassClassificationDataset method), 192
__getitem__() (dicee.MultiLabelDataset method), 191
__getitem__() (dicee.NegSampleDataset method), 197
__getitem__() (dicee.OnevsAllDataset method), 192
__getitem__() (dicee.OnevsSample method), 195
__getitem__() (dicee.TriplePredictionDataset method), 197
__iter__() (dicee.config.Namespace method), 128
__iter__() (dicee.knowledge_graph.KG method), 146
__len__() (dicee.AllvsAll method), 194
  _len__() (dicee.BPE_NegativeSamplingDataset method), 191
__len__() (dicee.dataset_classes.AllvsAll method), 132
__len__() (dicee.dataset_classes.BPE_NegativeSamplingDataset method), 129
__len__() (dicee.dataset_classes.KvsAll method), 132
__len__() (dicee.dataset_classes.KvsSampleDataset method), 135
  _len__() (dicee.dataset_classes.MultiClassClassificationDataset method), 130
__len__() (dicee.dataset_classes.MultiLabelDataset method), 130
__len__() (dicee.dataset_classes.NegSampleDataset method), 135
__len__() (dicee.dataset_classes.OnevsAllDataset method), 131
__len__() (dicee.dataset_classes.OnevsSample method), 134
__len__() (dicee.dataset_classes.TriplePredictionDataset method), 136
__len__() (dicee.knowledge_graph.KG method), 146
__len__() (dicee.KvsAll method), 193
__len__() (dicee.KvsSampleDataset method), 196
__len__() (dicee.MultiClassClassificationDataset method), 192
__len__() (dicee.MultiLabelDataset method), 191
__len__() (dicee.NegSampleDataset method), 197
__len__() (dicee.OnevsAllDataset method), 192
__len__() (dicee.OnevsSample method), 195
  _len__() (dicee.TriplePredictionDataset method), 197
__str__() (dicee.KGE method), 185
__str__() (dicee.knowledge_graph_embeddings.KGE method), 146
__version__ (in module dicee), 202
AbstractCallback (class in dicee.abstracts), 115
AbstractPPECallback (class in dicee.abstracts), 116
AbstractTrainer (class in dicee.abstracts), 112
AccumulateEpochLossCallback (class in dicee.callbacks), 119
achieve_answer() (dicee.query_generator.QueryGenerator method), 151
achieve_answer() (dicee.QueryGenerator method), 202
AConEx (class in dicee), 168
AConEx (class in dicee.models), 67
AConEx (class in dicee.models.complex), 29
AConvO (class in dicee), 169
AConvO (class in dicee.models), 80
AConvO (class in dicee.models.octonion), 37
AConvo (class in dicee), 170
AConvQ (class in dicee.models), 74
```

```
AConvo (class in dicee.models.quaternion), 42
adaptive_swa (dicee.config.Namespace attribute), 128
add_new_entity_embeddings() (dicee.abstracts.BaseInteractiveKGE method), 115
add_noise_rate (dicee.config.Namespace attribute), 126
add_noise_rate (dicee.knowledge_graph.KG attribute), 145
add_noisy_triples() (in module dicee), 183
add_noisy_triples() (in module dicee.static_funcs), 154
add_noisy_triples_into_training() (dicee.read_preprocess_save_load_kg.read_from_disk.ReadFromDisk method), 99
add_noisy_triples_into_training() (dicee.read_preprocess_save_load_kg.ReadFromDisk method), 104
\verb"add_reciprocal" (\textit{dicee.knowledge\_graph.KG attribute}), 145
AllvsAll (class in dicee), 193
AllvsAll (class in dicee.dataset_classes), 132
alphas (dicee.abstracts.AbstractPPECallback attribute), 117
alphas (dicee.callbacks.ASWA attribute), 122
analyse() (in module dicee.analyse_experiments), 119
answer_multi_hop_query() (dicee.KGE method), 187
answer_multi_hop_query() (dicee.knowledge_graph_embeddings.KGE method), 149
app (in module dicee.scripts.serve), 105
apply_coefficients() (dicee.DeCaL method), 165
apply_coefficients() (dicee.Keci method), 161
apply_coefficients() (dicee.models.clifford.DeCaL method), 26
apply_coefficients() (dicee.models.clifford.Keci method), 23
apply_coefficients() (dicee.models.DeCaL method), 86
apply_coefficients() (dicee.models.Keci method), 82
apply_reciprical_or_noise() (in module dicee.read_preprocess_save_load_kg.util), 101
apply_semantic_constraint (dicee.abstracts.BaseInteractiveKGE attribute), 113
apply_unit_norm (dicee.BaseKGE attribute), 180
apply_unit_norm (dicee.models.base_model.BaseKGE attribute), 19
apply_unit_norm (dicee.models.BaseKGE attribute), 58, 62, 65, 70, 76, 88, 92
args (dicee.BaseKGE attribute), 180
args (dicee.DICE_Trainer attribute), 184
args (dicee.evaluator.Evaluator attribute), 141
args (dicee.Execute attribute), 189
args (dicee.executer.ContinuousExecute attribute), 144
args (dicee.executer.Execute attribute), 143
args (dicee.models.base_model.BaseKGE attribute), 18
args (dicee.models.base model.IdentityClass attribute), 21
args (dicee.models.BaseKGE attribute), 58, 61, 65, 69, 75, 88, 91
args (dicee.models.IdentityClass attribute), 61, 72, 78
args (dicee.models.pykeen_models.PykeenKGE attribute), 39
args (dicee.models.PykeenKGE attribute), 90
args (dicee. Pykeen KGE attribute), 177
args (dicee.trainer.DICE_Trainer attribute), 110
args (dicee.trainer.dice_trainer.DICE_Trainer attribute), 106
ASWA (class in dicee.callbacks), 122
aswa (dicee.analyse_experiments.Experiment attribute), 118
attn (dicee.models.transformers.Block attribute), 49
attn_dropout (dicee.models.transformers.CausalSelfAttention attribute), 48
attributes (dicee.abstracts.AbstractTrainer attribute), 112
В
backend (dicee.config.Namespace attribute), 126
backend (dicee.knowledge_graph.KG attribute), 145
BaseInteractiveKGE (class in dicee.abstracts), 113
BaseKGE (class in dicee), 179
BaseKGE (class in dicee.models), 57, 61, 64, 69, 75, 87, 91
BaseKGE (class in dicee.models.base_model), 18
BaseKGELightning (class in dicee.models), 52
BaseKGELightning (class in dicee.models.base_model), 12
batch_kronecker_product() (dicee.callbacks.KronE static method), 124
batch_size (dicee.analyse_experiments.Experiment attribute), 118
batch_size (dicee.callbacks.PseudoLabellingCallback attribute), 122
batch_size (dicee.config.Namespace attribute), 126
batch_size (dicee.CVDataModule attribute), 198
batch_size (dicee.dataset_classes.CVDataModule attribute), 137
bias (dicee.models.transformers.GPTConfig attribute), 50
bias (dicee.models.transformers.LayerNorm attribute), 47
```

```
Block (class in dicee.models.transformers), 49
block_size (dicee.BaseKGE attribute), 181
block_size (dicee.config.Namespace attribute), 128
block_size (dicee.dataset_classes.MultiClassClassificationDataset attribute), 130
block_size (dicee.models.base_model.BaseKGE attribute), 19
block_size (dicee.models.BaseKGE attribute), 59, 62, 66, 70, 76, 89, 92
block_size (dicee.models.transformers.GPTConfig attribute), 49
block size (dicee.MultiClassClassificationDataset attribute), 192
bn_conv1 (dicee.AConvQ attribute), 170
bn_conv1 (dicee.ConvQ attribute), 170
bn_conv1 (dicee.models.AConvQ attribute), 74
bn_conv1 (dicee.models.ConvQ attribute), 74
bn_conv1 (dicee.models.quaternion.AConvQ attribute), 42
bn_conv1 (dicee.models.quaternion.ConvQ attribute), 41
bn_conv2 (dicee.AConvQ attribute), 170
bn_conv2 (dicee.ConvQ attribute), 170
bn_conv2 (dicee.models.AConvQ attribute), 75
bn_conv2 (dicee.models.ConvQ attribute), 74
bn_conv2 (dicee.models.quaternion.AConvQ attribute), 42
bn_conv2 (dicee.models.quaternion.ConvQ attribute), 41
bn_conv2d (dicee.AConEx attribute), 169
bn_conv2d (dicee.AConvO attribute), 169
bn_conv2d (dicee.ConEx attribute), 172
bn_conv2d (dicee.ConvO attribute), 171
bn_conv2d (dicee.models.AConEx attribute), 68
bn_conv2d (dicee.models.AConvO attribute), 80
bn_conv2d (dicee.models.complex.AConEx attribute), 29
bn_conv2d (dicee.models.complex.ConEx attribute), 28
bn_conv2d (dicee.models.ConEx attribute), 67
bn_conv2d (dicee.models.ConvO attribute), 80
bn_conv2d (dicee.models.octonion.AConvO attribute), 38
bn conv2d (dicee.models.octonion.ConvO attribute), 37
BPE_NegativeSamplingDataset (class in dicee), 190
BPE_NegativeSamplingDataset (class in dicee.dataset_classes), 129
build_chain_funcs() (dicee.models.FMult2 method), 95
build_chain_funcs() (dicee.models.function_space.FMult2 method), 33
build func() (dicee.models.FMult2 method), 95
build_func() (dicee.models.function_space.FMult2 method), 33
BytE (class in dicee), 177
BytE (class in dicee.models.transformers), 45
byte_pair_encoding (dicee.analyse_experiments.Experiment attribute), 118
byte_pair_encoding (dicee.BaseKGE attribute), 181
byte_pair_encoding (dicee.config.Namespace attribute), 128
byte_pair_encoding (dicee.knowledge_graph.KG attribute), 145
byte_pair_encoding (dicee.models.base_model.BaseKGE attribute), 19
byte_pair_encoding (dicee.models.BaseKGE attribute), 59, 62, 66, 70, 76, 89, 92
c_attn (dicee.models.transformers.CausalSelfAttention attribute), 47
c_fc (dicee.models.transformers.MLP attribute), 48
c_proj (dicee.models.transformers.CausalSelfAttention attribute), 48
c_proj (dicee.models.transformers.MLP attribute), 48
callbacks (dicee.abstracts.AbstractTrainer attribute), 112
callbacks (dicee.analyse_experiments.Experiment attribute), 118
callbacks (dicee.config.Namespace attribute), 126
callbacks (dicee.trainer.torch_trainer_ddp.NodeTrainer attribute), 110
CausalSelfAttention (class in dicee.models.transformers), 47
chain_func() (dicee.models.FMult method), 94
chain_func() (dicee.models.function_space.FMult method), 32
chain_func() (dicee.models.function_space.GFMult method), 33
chain_func() (dicee.models.GFMult method), 94
cl_pqr() (dicee.DeCaL method), 164
cl_pgr() (dicee.models.clifford.DeCaL method), 25
cl_pqr() (dicee.models.DeCaL method), 85
clifford_multiplication() (dicee.Keci method), 161
clifford_multiplication() (dicee.models.clifford.Keci method), 23
clifford_multiplication() (dicee.models.Keci method), 82
```

```
collate fn (dicee. Allvs All attribute), 194
collate_fn (dicee.dataset_classes.AllvsAll attribute), 132
collate fn (dicee.dataset classes.KvsAll attribute), 131
collate_fn (dicee.dataset_classes.KvsSampleDataset attribute), 135
collate_fn (dicee.dataset_classes.MultiClassClassificationDataset attribute), 130
collate_fn (dicee.dataset_classes.MultiLabelDataset attribute), 130
collate_fn (dicee.dataset_classes.OnevsAllDataset attribute), 131
collate fn (dicee.dataset classes.OnevsSample attribute), 133, 134
collate_fn (dicee.KvsAll attribute), 193
collate_fn (dicee.KvsSampleDataset attribute), 196
collate_fn (dicee.MultiClassClassificationDataset attribute), 192
collate_fn (dicee.MultiLabelDataset attribute), 191
collate_fn (dicee.OnevsAllDataset attribute), 192
collate_fn (dicee.OnevsSample attribute), 195
collate_fn() (dicee.BPE_NegativeSamplingDataset method), 191
collate_fn() (dicee.dataset_classes.BPE_NegativeSamplingDataset method), 129
collate_fn() (dicee.dataset_classes.TriplePredictionDataset method), 136
collate_fn() (dicee. TriplePredictionDataset method), 197
collection_name (dicee.scripts.serve.NeuralSearcher attribute), 105
comp_func() (dicee.LFMult method), 176
comp_func() (dicee.models.function_space.LFMult method), 35
comp_func() (dicee.models.LFMult method), 96
Complex (class in dicee), 167
Complex (class in dicee.models), 68
Complex (class in dicee.models.complex), 29
compute_convergence() (in module dicee.callbacks), 122
compute_func() (dicee.models.FMult method), 94
compute_func() (dicee.models.FMult2 method), 95
compute_func() (dicee.models.function_space.FMult method), 32
compute_func() (dicee.models.function_space.FMult2 method), 33
compute_func() (dicee.models.function_space.GFMult method), 33
compute func() (dicee.models.GFMult method), 94
compute_mrr() (dicee.callbacks.ASWA static method), 123
compute_sigma_pp() (dicee.DeCaL method), 165
compute_sigma_pp() (dicee.Keci method), 161
compute_sigma_pp() (dicee.models.clifford.DeCaL method), 26
compute_sigma_pp() (dicee.models.clifford.Keci method), 22
compute_sigma_pp() (dicee.models.DeCaL method), 86
compute_sigma_pp() (dicee.models.Keci method), 81
compute_sigma_pq() (dicee.DeCaL method), 166
compute_sigma_pq() (dicee.Keci method), 161
compute_sigma_pq() (dicee.models.clifford.DeCaL method), 27
compute_sigma_pq() (dicee.models.clifford.Keci method), 23
compute_sigma_pq() (dicee.models.DeCaL method), 87
compute_sigma_pq() (dicee.models.Keci method), 82
compute_sigma_pr() (dicee.DeCaL method), 166
compute_sigma_pr() (dicee.models.clifford.DeCaL method), 28
compute_sigma_pr() (dicee.models.DeCaL method), 87
compute_sigma_qq() (dicee.DeCaL method), 165
compute_sigma_qq() (dicee.Keci method), 161
compute_sigma_qq() (dicee.models.clifford.DeCaL method), 27
compute_sigma_qq() (dicee.models.clifford.Keci method), 22
compute_sigma_qq() (dicee.models.DeCaL method), 86
compute_sigma_qq() (dicee.models.Keci method), 82
compute_sigma_qr() (dicee.DeCaL method), 166
compute_sigma_qr() (dicee.models.clifford.DeCaL method), 28
compute_sigma_qr() (dicee.models.DeCaL method), 87
compute_sigma_rr() (dicee.DeCaL method), 166
compute_sigma_rr() (dicee.models.clifford.DeCaL method), 27
compute_sigma_rr() (dicee.models.DeCaL method), 87
compute sigmas multivect() (dicee.DeCaL method), 164
compute_sigmas_multivect() (dicee.models.clifford.DeCaL method), 26
\verb|compute_sigmas_multivect(|)| \textit{(dicee.models.DeCaL method)}, 85
compute_sigmas_single() (dicee.DeCaL method), 164
\verb|compute_sigmas_single()| \textit{(dicee.models.clifford.DeCaL method)}, 26
compute_sigmas_single() (dicee.models.DeCaL method), 85
ConEx (class in dicee), 172
ConEx (class in dicee.models), 67
```

```
ConEx (class in dicee.models.complex), 28
config (dicee.BytE attribute), 178
config (dicee.models.transformers.BytE attribute), 45
config (dicee.models.transformers.GPT attribute), 50
configs (dicee.abstracts.BaseInteractiveKGE attribute), 113
configure_optimizers() (dicee.models.base_model.BaseKGELightning method), 16
configure_optimizers() (dicee.models.BaseKGELightning method), 56
configure_optimizers() (dicee.models.transformers.GPT method), 51
construct_batch_selected_cl_multivector() (dicee.Keci method), 162
\verb|construct_batch_selected_cl_multivector()| \textit{(dicee.models.clifford.Keci method)}, 24
construct_batch_selected_cl_multivector() (dicee.models.Keci method), 83
construct_cl_multivector() (dicee.DeCaL method), 165
construct_cl_multivector() (dicee.Keci method), 162
construct_cl_multivector() (dicee.models.clifford.DeCaL method), 26
construct_cl_multivector() (dicee.models.clifford.Keci method), 23
construct_cl_multivector() (dicee.models.DeCaL method), 86
construct_cl_multivector() (dicee.models.Keci method), 83
construct_dataset() (in module dicee), 190
construct_dataset() (in module dicee.dataset_classes), 129
construct_ensemble (dicee.abstracts.BaseInteractiveKGE attribute), 113
construct_graph() (dicee.query_generator.QueryGenerator method), 151
construct_graph() (dicee.QueryGenerator method), 202
construct_input_and_output() (dicee.abstracts.BaseInteractiveKGE method), 115
construct_multi_coeff() (dicee.LFMult method), 175
construct_multi_coeff() (dicee.models.function_space.LFMult method), 34
construct_multi_coeff() (dicee.models.LFMult method), 96
continual_learning (dicee.config.Namespace attribute), 128
continual_start() (dicee.DICE_Trainer method), 184
continual_start() (dicee.executer.ContinuousExecute method), 144
continual_start() (dicee.trainer.DICE_Trainer method), 110
continual_start() (dicee.trainer.dice_trainer.DICE_Trainer method), 107
continual_training_setup_executor() (dicee.Execute method), 189
continual_training_setup_executor() (dicee.executer.Execute method), 143
continual_training_setup_executor() (in module dicee), 183
continual_training_setup_executor() (in module dicee.static_funcs), 154
Continuous Execute (class in dicee.executer), 144
conv2d (dicee.AConEx attribute), 169
conv2d (dicee.AConvO attribute), 169
conv2d (dicee.AConvQ attribute), 170
conv2d (dicee.ConEx attribute), 172
conv2d (dicee.ConvO attribute), 171
conv2d (dicee.ConvQ attribute), 170
conv2d (dicee.models.AConEx attribute), 67
conv2d (dicee.models.AConvO attribute), 80
conv2d (dicee.models.AConvQ attribute), 74
conv2d (dicee.models.complex.AConEx attribute), 29
conv2d (dicee.models.complex.ConEx attribute), 28
conv2d (dicee.models.ConEx attribute), 67
conv2d (dicee.models.ConvO attribute), 80
conv2d (dicee.models.ConvQ attribute), 74
conv2d (dicee.models.octonion.AConvO attribute), 38
conv2d (dicee.models.octonion.ConvO attribute), 37
conv2d (dicee.models.quaternion.AConvQ attribute), 42
conv2d (dicee.models.quaternion.ConvQ attribute), 41
ConvO (class in dicee), 171
ConvO (class in dicee.models), 79
ConvO (class in dicee.models.octonion), 36
ConvO (class in dicee), 170
ConvQ (class in dicee.models), 74
ConvQ (class in dicee.models.quaternion), 41
create_constraints() (in module dicee.read_preprocess_save_load_kg.util), 102
create_constraints() (in module dicee.static_preprocess_funcs), 156
create_experiment_folder() (in module dicee), 183
create_experiment_folder() (in module dicee.static_funcs), 154
create_random_data() (dicee.callbacks.PseudoLabellingCallback method), 122
create_recipriocal_triples() (in module dicee), 182
create_recipriocal_triples() (in module dicee.read_preprocess_save_load_kg.util), 102
create_recipriocal_triples() (in module dicee.static_funcs), 153
```

```
create_vector_database() (dicee.KGE method), 185
\verb|create_vector_database()| \textit{(dicee.knowledge\_graph\_embeddings.KGE method)}, 146
crop_block_size() (dicee.models.transformers.GPT method), 51
ctx (dicee.trainer.torch_trainer_ddp.NodeTrainer attribute), 110
CVDataModule (class in dicee), 198
CVDataModule (class in dicee.dataset_classes), 136
data_module (dicee.callbacks.PseudoLabellingCallback attribute), 122
dataset_dir (dicee.config.Namespace attribute), 125
dataset_dir (dicee.knowledge_graph.KG attribute), 145
dataset_sanity_checking() (in module dicee.read_preprocess_save_load_kg.util), 102
DeCal (class in dicee), 163
DeCal (class in dicee.models), 84
DeCal (class in dicee.models.clifford), 24
decide() (dicee.callbacks.ASWA method), 123
degree (dicee.LFMult attribute), 175
degree (dicee.models.function_space.LFMult attribute), 34
degree (dicee.models.LFMult attribute), 95
deploy() (dicee.KGE method), 188
{\tt deploy()} \ (\textit{dicee.knowledge\_graph\_embeddings.KGE method}), 150
deploy_head_entity_prediction() (in module dicee), 183
deploy_head_entity_prediction() (in module dicee.static_funcs), 154
deploy_relation_prediction() (in module dicee), 183
deploy_relation_prediction() (in module dicee.static_funcs), 154
deploy_tail_entity_prediction() (in module dicee), 183
deploy_tail_entity_prediction() (in module dicee.static_funcs), 154
deploy_triple_prediction() (in module dicee), 183
deploy_triple_prediction() (in module dicee.static_funcs), 154
describe() (dicee.knowledge_graph.KG method), 146
description_of_input (dicee.knowledge_graph.KG attribute), 146
DICE_Trainer (class in dicee), 183
DICE_Trainer (class in dicee.trainer), 110
DICE_Trainer (class in dicee.trainer.dice_trainer), 106
dicee
     module, 12
dicee.___main_
     module, 111
dicee.abstracts
    module, 111
dicee.analyse_experiments
    module, 117
dicee.callbacks
     module, 119
dicee.config
     module, 125
dicee.dataset_classes
     module, 128
dicee.eval_static_funcs
     module, 140
dicee.evaluator
     module, 141
dicee.executer
     module, 142
dicee.knowledge_graph
     module, 144
dicee.knowledge_graph_embeddings
     module, 146
dicee.models
     module, 12
dicee.models.base_model
    module, 12
dicee.models.clifford
     module, 21
dicee.models.complex
     module, 28
dicee.models.dualE
```

```
module, 30
dicee.models.function_space
    module, 32
dicee.models.octonion
    module, 35
dicee.models.pykeen_models
    module, 38
dicee.models.quaternion
    module, 39
dicee.models.real
    module, 42
dicee.models.static_funcs
    module, 44
dicee.models.transformers
    module, 44
dicee.query_generator
    module, 150
dicee.read_preprocess_save_load_kg
    module, 97
dicee.read_preprocess_save_load_kg.preprocess
dicee.read_preprocess_save_load_kg.read_from_disk
    module, 98
\verb|dicee.read_preprocess_save_load_kg.save_load_disk|
    module, 99
dicee.read_preprocess_save_load_kg.util
    module, 99
dicee.sanity_checkers
    module, 151
dicee.scripts
    module, 104
dicee.scripts.index
    module, 104
dicee.scripts.run
    module, 104
dicee.scripts.serve
    module, 105
dicee.static_funcs
    module, 152
dicee.static_funcs_training
    module, 155
dicee.static_preprocess_funcs
    module, 155
dicee.trainer
    module, 106
dicee.trainer.dice_trainer
    module, 106
dicee.trainer.torch_trainer
    module, 108
dicee.trainer.torch_trainer_ddp
    module, 109
discrete_points (dicee.models.FMult2 attribute), 94
discrete_points (dicee.models.function_space.FMult2 attribute), 33
dist_func (dicee.models.Pyke attribute), 64
dist_func (dicee.models.real.Pyke attribute), 44
dist_func (dicee.Pyke attribute), 159
DistMult (class in dicee), 159
DistMult (class in dicee.models), 63
DistMult (class in dicee.models.real), 43
download_file() (in module dicee), 183
download_file() (in module dicee.static_funcs), 155
download_files_from_url() (in module dicee), 183
download_files_from_url() (in module dicee.static_funcs), 155
download_pretrained_model() (in module dicee), 183
download_pretrained_model() (in module dicee.static_funcs), 155
dropout (dicee.models.transformers.CausalSelf Attention attribute), 48
dropout (dicee.models.transformers.GPTConfig attribute), 50
dropout (dicee.models.transformers.MLP attribute), 49
```

```
DualE (class in dicee), 167
DualE (class in dicee.models), 96
DualE (class in dicee.models.dualE), 31
dummy_eval() (dicee.evaluator.Evaluator method), 142
dummy_id (dicee.knowledge_graph.KG attribute), 145
during_training (dicee.evaluator.Evaluator attribute), 141
ee_vocab (dicee.evaluator.Evaluator attribute), 141
efficient_zero_grad() (in module dicee.static_funcs_training), 155
embedding_dim (dicee.analyse_experiments.Experiment attribute), 118
embedding_dim (dicee.BaseKGE attribute), 180
embedding_dim (dicee.config.Namespace attribute), 126
embedding_dim (dicee.models.base_model.BaseKGE attribute), 18
embedding_dim (dicee.models.BaseKGE attribute), 58, 61, 65, 70, 75, 88, 91
enable_log (in module dicee.static_preprocess_funcs), 156
enc (dicee.knowledge_graph.KG attribute), 145
end() (dicee.Execute method), 189
end () (dicee.executer.Execute method), 143
ent2id (dicee.query_generator.QueryGenerator attribute), 150
ent2id (dicee.QueryGenerator attribute), 201
ent_in (dicee.query_generator.QueryGenerator attribute), 150
ent_in (dicee.QueryGenerator attribute), 201
ent_out (dicee.query_generator.QueryGenerator attribute), 151
ent_out (dicee.QueryGenerator attribute), 201
entities_str (dicee.knowledge_graph.KG property), 146
entity_embeddings (dicee.AConvQ attribute), 170
entity_embeddings (dicee.ConvQ attribute), 170
entity_embeddings (dicee.DeCaL attribute), 164
entity_embeddings (dicee.DualE attribute), 167
entity_embeddings (dicee.LFMult attribute), 175
entity_embeddings (dicee.models.AConvQ attribute), 74
entity_embeddings (dicee.models.clifford.DeCaL attribute), 25
entity_embeddings (dicee.models.ConvQ attribute), 74
entity_embeddings (dicee.models.DeCaL attribute), 85
entity_embeddings (dicee.models.DualE attribute), 97
entity_embeddings (dicee.models.dualE.DualE attribute), 31
entity_embeddings (dicee.models.FMult attribute), 93
entity_embeddings (dicee.models.FMult2 attribute), 95
entity_embeddings (dicee.models.function_space.FMult attribute), 32
entity_embeddings (dicee.models.function_space.FMult2 attribute), 33
entity_embeddings (dicee.models.function_space.GFMult attribute), 32
entity_embeddings (dicee.models.function_space.LFMult attribute), 34
entity_embeddings (dicee.models.function_space.LFMult1 attribute), 33
entity_embeddings (dicee.models.GFMult attribute), 94
entity_embeddings (dicee.models.LFMult attribute), 95
entity_embeddings (dicee.models.LFMult1 attribute), 95
entity embeddings (dicee.models.pykeen models.PykeenKGE attribute), 39
entity_embeddings (dicee.models.PykeenKGE attribute), 90
entity_embeddings (dicee.models.quaternion.AConvQ attribute), 42
entity_embeddings (dicee.models.quaternion.ConvQ attribute), 41
entity_embeddings (dicee.PykeenKGE attribute), 177
entity_to_idx (dicee.knowledge_graph.KG attribute), 145
{\tt epoch\_count}~({\it dicee.abstracts.AbstractPPECallback~attribute}),~117
epoch_count (dicee.callbacks.ASWA attribute), 122
epoch_counter (dicee.callbacks.Eval attribute), 123
epoch_counter (dicee.callbacks.KGESaveCallback attribute), 121
epoch_ratio (dicee.callbacks.Eval attribute), 123
er_vocab (dicee.evaluator.Evaluator attribute), 141
estimate_mfu() (dicee.models.transformers.GPT method), 51
estimate_q() (in module dicee.callbacks), 122
Eval (class in dicee.callbacks), 123
eval () (dicee.evaluator.Evaluator method), 141
eval_lp_performance() (dicee.KGE method), 185
eval_lp_performance() (dicee.knowledge_graph_embeddings.KGE method), 146
eval_model (dicee.config.Namespace attribute), 127
eval_model (dicee.knowledge_graph.KG attribute), 145
```

```
eval_rank_of_head_and_tail_byte_pair_encoded_entity() (dicee.evaluator.Evaluator method), 142
eval_rank_of_head_and_tail_entity() (dicee.evaluator.Evaluator method), 142
eval_with_bpe_vs_all() (dicee.evaluator.Evaluator method), 142
eval_with_byte() (dicee.evaluator.Evaluator method), 142
\verb|eval_with_data()| \textit{(dicee.evaluator.Evaluator method)}, 142
eval_with_vs_all() (dicee.evaluator.Evaluator method), 142
evaluate() (in module dicee), 183
evaluate() (in module dicee.static funcs), 154
evaluate_bpe_lp() (in module dicee.static_funcs_training), 155
evaluate_link_prediction_performance() (in module dicee.eval_static_funcs), 140
evaluate_link_prediction_performance_with_bpe() (in module dicee.eval_static_funcs), 140
evaluate_link_prediction_performance_with_bpe_reciprocals() (in module dicee.eval_static_funcs), 140
evaluate_link_prediction_performance_with_reciprocals() (in module dicee.eval_static_funcs), 140
evaluate_lp() (dicee.evaluator.Evaluator method), 142
evaluate_lp() (in module dicee.static_funcs_training), 155
evaluate_lp_bpe_k_vs_all() (dicee.evaluator.Evaluator method), 142
evaluate_lp_bpe_k_vs_all() (in module dicee.eval_static_funcs), 141
evaluate_lp_k_vs_all() (dicee.evaluator.Evaluator method), 142
evaluate_lp_with_byte() (dicee.evaluator.Evaluator method), 142
Evaluator (class in dicee.evaluator), 141
evaluator (dicee.DICE_Trainer attribute), 184
evaluator (dicee. Execute attribute), 189
evaluator (dicee.executer.Execute attribute), 143
evaluator (dicee.trainer.DICE_Trainer attribute), 110
evaluator (dicee.trainer.dice_trainer.DICE_Trainer attribute), 107
every_x_epoch (dicee.callbacks.KGESaveCallback attribute), 121
Execute (class in dicee), 188
Execute (class in dicee.executer), 142
\verb|exists()| (\textit{dicee.knowledge\_graph.KG method}), 146
Experiment (class in dicee.analyse_experiments), 118
explicit (dicee.models.QMult attribute), 73
explicit (dicee.models.quaternion.QMult attribute), 40
explicit (dicee.QMult attribute), 173
exponential_function() (in module dicee), 183
exponential_function() (in module dicee.static_funcs), 154
extract_input_outputs() (dicee.trainer.torch_trainer_ddp.NodeTrainer method), 110
extract_input_outputs_set_device() (dicee.trainer.torch_trainer.TorchTrainer method), 108
f (dicee.callbacks.KronE attribute), 124
fc1 (dicee.AConEx attribute), 169
fc1 (dicee.AConvO attribute), 169
fc1 (dicee.AConvO attribute), 170
fc1 (dicee.ConEx attribute), 172
fc1 (dicee.ConvO attribute), 171
fc1 (dicee.ConvQ attribute), 170
fc1 (dicee.models.AConEx attribute), 68
fc1 (dicee.models.AConvO attribute), 80
fc1 (dicee.models.AConvQ attribute), 74
fc1 (dicee.models.complex.AConEx attribute), 29
fc1 (dicee.models.complex.ConEx attribute), 28
fc1 (dicee.models.ConEx attribute), 67
fc1 (dicee.models.ConvO attribute), 80
fc1 (dicee.models.ConvQ attribute), 74
fc1 (dicee.models.octonion.AConvO attribute), 38
fc1 (dicee.models.octonion.ConvO attribute), 37
fc1 (dicee.models.quaternion.AConvQ attribute), 42
fc1 (dicee.models.quaternion.ConvQ attribute), 41
fc_num_input (dicee.AConEx attribute), 169
fc_num_input (dicee.AConvO attribute), 169
fc_num_input (dicee.AConvQ attribute), 170
fc_num_input (dicee.ConEx attribute), 172
fc_num_input (dicee.ConvO attribute), 171
fc_num_input (dicee.ConvQ attribute), 170
fc_num_input (dicee.models.AConEx attribute), 67
fc_num_input (dicee.models.AConvO attribute), 80
fc_num_input (dicee.models.AConvQ attribute), 74
```

```
fc num input (dicee.models.complex.AConEx attribute), 29
fc_num_input (dicee.models.complex.ConEx attribute), 28
fc_num_input (dicee.models.ConEx attribute), 67
fc_num_input (dicee.models.ConvO attribute), 80
fc_num_input (dicee.models.ConvQ attribute), 74
fc_num_input (dicee.models.octonion.AConvO attribute), 38
fc_num_input (dicee.models.octonion.ConvO attribute), 37
fc num input (dicee.models.quaternion.AConvO attribute), 42
fc_num_input (dicee.models.quaternion.ConvQ attribute), 41
feature_map_dropout (dicee.AConEx attribute), 169
feature_map_dropout (dicee.AConvO attribute), 169
{\tt feature\_map\_dropout}~(\textit{dicee.AConvQ attribute}),~170
feature_map_dropout (dicee.ConEx attribute), 172
feature_map_dropout (dicee.ConvO attribute), 172
feature_map_dropout (dicee.ConvQ attribute), 170
feature_map_dropout (dicee.models.AConEx attribute), 68
feature_map_dropout (dicee.models.AConvO attribute), 80
feature_map_dropout (dicee.models.AConvQ attribute), 75
feature_map_dropout (dicee.models.complex.AConEx attribute), 29
feature_map_dropout (dicee.models.complex.ConEx attribute), 28
feature_map_dropout (dicee.models.ConEx attribute), 67
feature_map_dropout (dicee.models.ConvO attribute), 80
feature_map_dropout (dicee.models.ConvQ attribute), 74
feature_map_dropout (dicee.models.octonion.AConvO attribute), 38
feature_map_dropout (dicee.models.octonion.ConvO attribute), 37
feature_map_dropout (dicee.models.quaternion.AConvQ attribute), 42
feature_map_dropout (dicee.models.quaternion.ConvQ attribute), 41
feature_map_dropout_rate (dicee.BaseKGE attribute), 180
{\tt feature\_map\_dropout\_rate}~(\textit{dicee.config.Namespace attribute}),~128
feature_map_dropout_rate (dicee.models.base_model.BaseKGE attribute), 19
feature_map_dropout_rate (dicee.models.BaseKGE attribute), 58, 62, 65, 70, 76, 88, 92
fill query () (dicee.query generator.QueryGenerator method), 151
fill_query() (dicee.QueryGenerator method), 202
find_missing_triples() (dicee.KGE method), 188
find_missing_triples() (dicee.knowledge_graph_embeddings.KGE method), 149
\verb|fit()| (dicee.trainer.torch\_trainer\_ddp.TorchDDPTrainer\_method), 109
fit () (dicee.trainer.torch trainer.TorchTrainer method), 108
flash (dicee.models.transformers.CausalSelfAttention attribute), 48
FMult (class in dicee.models), 93
FMult (class in dicee.models.function_space), 32
FMult2 (class in dicee.models), 94
FMult2 (class in dicee.models.function_space), 33
form_of_labelling (dicee.DICE_Trainer attribute), 184
form_of_labelling (dicee.trainer.DICE_Trainer attribute), 110
form_of_labelling (dicee.trainer.dice_trainer.DICE_Trainer attribute), 107
forward() (dicee.BaseKGE method), 181
forward() (dicee.BytE method), 178
forward() (dicee.models.base_model.BaseKGE method), 20
forward() (dicee.models.base_model.IdentityClass static method), 21
forward() (dicee.models.BaseKGE method), 59, 63, 66, 71, 77, 89, 93
forward() (dicee.models.IdentityClass static method), 61, 72, 78
forward() (dicee.models.transformers.Block method), 49
forward() (dicee.models.transformers.BytE method), 45
forward() (dicee.models.transformers.CausalSelfAttention method), 48
forward() (dicee.models.transformers.GPT method), 50
forward() (dicee.models.transformers.LayerNorm method), 47
forward() (dicee.models.transformers.MLP method), 49
\verb|forward_backward_update()| \textit{(dicee.trainer.torch\_trainer.TorchTrainer method)}, 108
forward_byte_pair_encoded_k_vs_all() (dicee.BaseKGE method), 181
forward_byte_pair_encoded_k_vs_all() (dicee.models.base_model.BaseKGE method), 19
forward_byte_pair_encoded_k_vs_all() (dicee.models.BaseKGE method), 59, 62, 66, 70, 76, 89, 92
forward_byte_pair_encoded_triple() (dicee.BaseKGE method), 181
forward_byte_pair_encoded_triple() (dicee.models.base_model.BaseKGE method), 19
forward_byte_pair_encoded_triple() (dicee.models.BaseKGE method), 59, 62, 66, 70, 76, 89, 92
forward_k_vs_all() (dicee.AConEx method), 169
forward_k_vs_all() (dicee.AConvO method), 169
forward_k_vs_all() (dicee.AConvQ method), 170
forward_k_vs_all() (dicee.BaseKGE method), 181
```

```
forward_k_vs_all() (dicee.ComplEx method), 168
forward_k_vs_all() (dicee.ConEx method), 172
forward_k_vs_all() (dicee.ConvO method), 172
forward_k_vs_all() (dicee.ConvQ method), 171
forward_k_vs_all() (dicee.DeCaL method), 165
forward_k_vs_all() (dicee.DistMult method), 160
forward_k_vs_all() (dicee.DualE method), 167
forward k vs all() (dicee. Keci method), 162
forward_k_vs_all() (dicee.models.AConEx method), 68
forward_k_vs_all() (dicee.models.AConvO method), 81
forward_k_vs_all() (dicee.models.AConvQ method), 75
forward_k_vs_all() (dicee.models.base_model.BaseKGE method), 20
forward_k_vs_all() (dicee.models.BaseKGE method), 60, 63, 66, 71, 77, 90, 93
forward_k_vs_all() (dicee.models.clifford.DeCaL method), 26
forward_k_vs_all() (dicee.models.clifford.Keci method). 23
forward_k_vs_all() (dicee.models.ComplEx method), 69
forward_k_vs_all() (dicee.models.complex.AConEx method), 29
forward_k_vs_all() (dicee.models.complex.ComplEx method), 30
forward_k_vs_all() (dicee.models.complex.ConEx method), 29
forward_k_vs_all() (dicee.models.ConEx method), 67
forward_k_vs_all() (dicee.models.ConvO method), 80
{\tt forward\_k\_vs\_all()} \ (\textit{dicee.models.ConvQ method}), 74
forward_k_vs_all() (dicee.models.DeCaL method), 85
forward_k_vs_all() (dicee.models.DistMult method), 63
forward_k_vs_all() (dicee.models.DualE method), 97
forward_k_vs_all() (dicee.models.dualE.DualE method), 31
forward_k_vs_all() (dicee.models.Keci method), 83
forward_k_vs_all() (dicee.models.octonion.AConvO method), 38
{\tt forward\_k\_vs\_all()} \ (\textit{dicee.models.octonion.ConvO method}), 37
forward_k_vs_all() (dicee.models.octonion.OMult method), 36
forward_k_vs_all() (dicee.models.OMult method), 79
forward_k_vs_all() (dicee.models.pykeen_models.PykeenKGE method), 39
forward_k_vs_all() (dicee.models.PykeenKGE method), 90
forward_k_vs_all() (dicee.models.QMult method), 73
forward_k_vs_all() (dicee.models.quaternion.AConvQ method), 42
forward_k_vs_all() (dicee.models.quaternion.ConvQ method), 42
forward k vs all() (dicee.models.quaternion.OMult method), 41
forward_k_vs_all() (dicee.models.real.DistMult method), 43
forward_k_vs_all() (dicee.models.real.Shallom method), 43
forward_k_vs_all() (dicee.models.real.TransE method), 43
forward_k_vs_all() (dicee.models.Shallom method), 64
forward_k_vs_all() (dicee.models.TransE method), 64
forward_k_vs_all() (dicee.OMult method), 175
forward_k_vs_all() (dicee.PykeenKGE method), 177
forward_k_vs_all() (dicee.QMult method), 174
forward_k_vs_all() (dicee.Shallom method), 175
forward_k_vs_all() (dicee. TransE method), 163
forward_k_vs_sample() (dicee.AConEx method), 169
forward_k_vs_sample() (dicee.BaseKGE method), 181
forward_k_vs_sample() (dicee.ComplEx method), 168
forward_k_vs_sample() (dicee.ConEx method), 172
forward_k_vs_sample() (dicee.DistMult method), 160
forward_k_vs_sample() (dicee.Keci method), 162
forward_k_vs_sample() (dicee.models.AConEx method), 68
forward_k_vs_sample() (dicee.models.base_model.BaseKGE method), 20
forward_k_vs_sample() (dicee.models.BaseKGE method), 60, 63, 66, 71, 77, 90, 93
forward_k_vs_sample() (dicee.models.clifford.Keci method), 24
forward_k_vs_sample() (dicee.models.ComplEx method), 69
forward_k_vs_sample() (dicee.models.complex.AConEx method), 29
forward_k_vs_sample() (dicee.models.complex.ComplEx method), 30
forward_k_vs_sample() (dicee.models.complex.ConEx method), 29
forward_k_vs_sample() (dicee.models.ConEx method), 67
forward_k_vs_sample() (dicee.models.DistMult method), 63
forward_k_vs_sample() (dicee.models.Keci method), 83
forward_k_vs_sample() (dicee.models.pykeen_models.PykeenKGE method), 39
forward_k_vs_sample() (dicee.models.PykeenKGE method), 91
forward_k_vs_sample() (dicee.models.QMult method), 74
{\tt forward\_k\_vs\_sample()} \ (\textit{dicee.models.quaternion.QMult method}), 41
```

```
forward k vs sample() (dicee.models.real.DistMult method), 43
forward_k_vs_sample() (dicee.PykeenKGE method), 177
forward_k_vs_sample() (dicee.QMult method), 174
forward_k_vs_with_explicit() (dicee.Keci method), 162
forward_k_vs_with_explicit() (dicee.models.clifford.Keci method), 23
forward_k_vs_with_explicit() (dicee.models.Keci method), 83
forward_triples() (dicee.AConEx method), 169
forward triples() (dicee.AConvO method), 169
forward_triples() (dicee.AConvQ method), 170
forward_triples() (dicee.BaseKGE method), 181
forward_triples() (dicee.ConEx method), 172
forward_triples() (dicee.ConvO method), 172
forward_triples() (dicee.ConvQ method), 171
forward_triples() (dicee.DeCaL method), 164
forward_triples() (dicee.DualE method), 167
forward_triples() (dicee.Keci method), 163
forward_triples() (dicee.LFMult method), 175
forward_triples() (dicee.models.AConEx method), 68
forward_triples() (dicee.models.AConvO method), 81
forward_triples() (dicee.models.AConvQ method), 75
forward_triples() (dicee.models.base_model.BaseKGE method), 20
forward_triples() (dicee.models.BaseKGE method), 59, 63, 66, 71, 77, 89, 93
forward_triples() (dicee.models.clifford.DeCaL method), 25
forward_triples() (dicee.models.clifford.Keci method), 24
forward_triples() (dicee.models.complex.AConEx method), 29
forward_triples() (dicee.models.complex.ConEx method), 29
forward_triples() (dicee.models.ConEx method), 67
forward_triples() (dicee.models.ConvO method), 80
forward_triples() (dicee.models.ConvQ method), 74
forward_triples() (dicee.models.DeCaL method), 85
forward_triples() (dicee.models.DualE method), 97
forward_triples() (dicee.models.dualE.DualE method), 31
forward_triples() (dicee.models.FMult method), 94
forward_triples() (dicee.models.FMult2 method), 95
forward_triples() (dicee.models.function_space.FMult method), 32
forward_triples() (dicee.models.function_space.FMult2 method), 33
forward triples () (dicee.models.function space.GFMult method), 33
forward_triples() (dicee.models.function_space.LFMult method), 34
forward_triples() (dicee.models.function_space.LFMult1 method), 34
forward_triples() (dicee.models.GFMult method), 94
forward_triples() (dicee.models.Keci method), 84
forward_triples() (dicee.models.LFMult method), 95
forward_triples() (dicee.models.LFMult1 method), 95
forward_triples() (dicee.models.octonion.AConvO method), 38
forward_triples() (dicee.models.octonion.ConvO method), 37
{\tt forward\_triples()} \ ({\it dicee.models.Pyke method}), 64
forward_triples() (dicee.models.pykeen_models.PykeenKGE method), 39
forward_triples() (dicee.models.PykeenKGE method), 91
forward_triples() (dicee.models.quaternion.AConvQ method), 42
forward_triples() (dicee.models.quaternion.ConvQ method), 42
forward_triples() (dicee.models.real.Pyke method), 44
forward_triples() (dicee.models.real.Shallom method), 43
forward_triples() (dicee.models.Shallom method), 64
forward_triples() (dicee.Pyke method), 159
forward_triples() (dicee.PykeenKGE method), 177
forward_triples() (dicee.Shallom method), 175
frequency (dicee.callbacks.Perturb attribute), 125
{\tt from\_pretrained()} \ (\textit{dicee.models.transformers.GPT class method}), 51
full_storage_path (dicee.analyse_experiments.Experiment attribute), 118
func_triple_to_bpe_representation (dicee.evaluator.Evaluator attribute), 141
func_triple_to_bpe_representation() (dicee.knowledge_graph.KG method), 146
function() (dicee.models.FMult2 method), 95
function() (dicee.models.function_space.FMult2 method), 33
G
gamma (dicee.models.FMult attribute), 94
```

gamma (dicee.models.function\_space.FMult attribute), 32

```
gelu (dicee.models.transformers.MLP attribute), 48
gen_test (dicee.query_generator.QueryGenerator attribute), 150
gen_test (dicee.QueryGenerator attribute), 201
gen_valid (dicee.query_generator.QueryGenerator attribute), 150
gen_valid (dicee.QueryGenerator attribute), 201
generate() (dicee.BytE method), 178
generate() (dicee.KGE method), 185
generate() (dicee.knowledge_graph_embeddings.KGE method), 146
generate() (dicee.models.transformers.BytE method), 46
generate_queries() (dicee.query_generator.QueryGenerator method), 151
generate_queries() (dicee.QueryGenerator method), 202
get () (dicee.scripts.serve.NeuralSearcher method), 106
get_aswa_state_dict() (dicee.callbacks.ASWA method), 123
get_bpe_head_and_relation_representation() (dicee.BaseKGE method), 182
\verb|get_bpe_head_and_relation_representation()| \textit{(dicee.models.base\_model.BaseKGE method)}, 20
get_bpe_head_and_relation_representation() (dicee.models.BaseKGE method), 60, 63, 67, 71, 77, 90, 93
get_bpe_token_representation() (dicee.abstracts.BaseInteractiveKGE method), 113
get_callbacks() (in module dicee.trainer.dice_trainer), 106
get_default_arguments() (in module dicee.analyse_experiments), 118
get_default_arguments() (in module dicee.scripts.index), 104
get_default_arguments() (in module dicee.scripts.run), 105
get_default_arguments() (in module dicee.scripts.serve), 105
get_ee_vocab() (in module dicee), 182
get_ee_vocab() (in module dicee.read_preprocess_save_load_kg.util), 102
get_ee_vocab() (in module dicee.static_funcs), 153
get_ee_vocab() (in module dicee.static_preprocess_funcs), 156
get_embeddings() (dicee.BaseKGE method), 182
get_embeddings() (dicee.models.base_model.BaseKGE method), 20
get_embeddings() (dicee.models.BaseKGE method), 60, 63, 67, 71, 77, 90, 93
get_embeddings() (dicee.models.real.Shallom method), 43
get_embeddings() (dicee.models.Shallom method), 64
get embeddings() (dicee.Shallom method), 175
get_entity_embeddings() (dicee.abstracts.BaseInteractiveKGE method), 115
get_entity_index() (dicee.abstracts.BaseInteractiveKGE method), 114
get_er_vocab() (in module dicee), 182
get_er_vocab() (in module dicee.read_preprocess_save_load_kg.util), 102
get_er_vocab() (in module dicee.static_funcs), 153
get_er_vocab() (in module dicee.static_preprocess_funcs), 156
get_eval_report() (dicee.abstracts.BaseInteractiveKGE method), 113
get_head_relation_representation() (dicee.BaseKGE method), 181
{\tt get\_head\_relation\_representation()} \ \textit{(dicee.models.base\_model.BaseKGE method)}, 20
get_head_relation_representation() (dicee.models.BaseKGE method), 60, 63, 66, 71, 77, 90, 93
get_kronecker_triple_representation() (dicee.callbacks.KronE method), 124
get_num_params() (dicee.models.transformers.GPT method), 50
get_padded_bpe_triple_representation() (dicee.abstracts.BaseInteractiveKGE method), 114
get_queries() (dicee.query_generator.QueryGenerator method), 151
get_queries() (dicee.QueryGenerator method), 202
get_re_vocab() (in module dicee), 182
get_re_vocab() (in module dicee.read_preprocess_save_load_kg.util), 102
get_re_vocab() (in module dicee.static_funcs), 153
get_re_vocab() (in module dicee.static_preprocess_funcs), 156
get_relation_embeddings() (dicee.abstracts.BaseInteractiveKGE method), 115
get_relation_index() (dicee.abstracts.BaseInteractiveKGE method), 114
get_sentence_representation() (dicee.BaseKGE method), 181
get_sentence_representation() (dicee.models.base_model.BaseKGE method), 20
get_sentence_representation() (dicee.models.BaseKGE method), 60, 63, 67, 71, 77, 90, 93
get_transductive_entity_embeddings() (dicee.KGE method), 185
\verb|get_transductive_entity_embeddings()| \textit{(dicee.knowledge\_graph\_embeddings.KGE method)}, 146
get_triple_representation() (dicee.BaseKGE method), 181
get_triple_representation() (dicee.models.base_model.BaseKGE method), 20
get_triple_representation() (dicee.models.BaseKGE method), 60, 63, 66, 71, 77, 90, 93
GFMult (class in dicee.models), 94
GFMult (class in dicee.models.function_space), 32
global_rank (dicee.trainer.torch_trainer_ddp.NodeTrainer attribute), 109
GPT (class in dicee.models.transformers), 50
GPTConfig (class in dicee.models.transformers), 49
gpus (dicee.config.Namespace attribute), 126
gradient_accumulation_steps (dicee.config.Namespace attribute), 127
```

```
ground queries () (dicee.query generator.QueryGenerator method), 151
ground_queries() (dicee.QueryGenerator method), 202
Н
hidden_dropout (dicee.BaseKGE attribute), 181
hidden_dropout (dicee.models.base_model.BaseKGE attribute), 19
hidden_dropout (dicee.models.BaseKGE attribute), 59, 62, 66, 70, 76, 89, 92
hidden_dropout_rate (dicee.BaseKGE attribute), 180
\verb|hidden_dropout_rate| (\textit{dicee.config.Namespace attribute}), 128
hidden_dropout_rate (dicee.models.base_model.BaseKGE attribute), 19
hidden_dropout_rate (dicee.models.BaseKGE attribute), 58, 62, 65, 70, 76, 88, 92
hidden_normalizer (dicee.BaseKGE attribute), 181
hidden_normalizer (dicee.models.base_model.BaseKGE attribute), 19
hidden_normalizer (dicee.models.BaseKGE attribute), 59, 62, 66, 70, 76, 89, 92
IdentityClass (class in dicee.models), 60, 71, 77
IdentityClass (class in dicee.models.base_model), 20
idx_entity_to_bpe_shaped (dicee.knowledge_graph.KG attribute), 145
index_triple() (dicee.abstracts.BaseInteractiveKGE method), 114
index_triples_with_pandas() (in module dicee.read_preprocess_save_load_kg.util), 102
init_dataloader() (dicee.DICE_Trainer method), 184
init_dataloader() (dicee.trainer.DICE_Trainer method), 111
init_dataloader() (dicee.trainer.dice_trainer.DICE_Trainer method), 107
init_dataset() (dicee.DICE_Trainer method), 184
init_dataset() (dicee.trainer.DICE_Trainer method), 111
init_dataset() (dicee.trainer.dice_trainer.DICE_Trainer method), 107
init_param (dicee.config.Namespace attribute), 127
init_params_with_sanity_checking() (dicee.BaseKGE method), 181
\verb|init_params_with_sanity_checking()| \textit{(dicee.models.base\_model.BaseKGE method)}, 19
init_params_with_sanity_checking() (dicee.models.BaseKGE method), 59, 62, 66, 71, 77, 89, 93
initial_eval_setting (dicee.callbacks.ASWA attribute), 122
initialize_or_load_model() (dicee.DICE_Trainer method), 184
initialize_or_load_model() (dicee.trainer.DICE_Trainer method), 111
initialize or load model() (dicee.trainer.dice trainer.DICE Trainer method), 107
initialize_trainer() (dicee.DICE_Trainer method), 184
initialize_trainer() (dicee.trainer.DICE_Trainer method), 111
initialize_trainer() (dicee.trainer.dice_trainer.DICE_Trainer method), 107
initialize_trainer() (in module dicee.trainer.dice_trainer), 106
input_dp_ent_real (dicee.BaseKGE attribute), 181
input_dp_ent_real (dicee.models.base_model.BaseKGE attribute), 19
input_dp_ent_real (dicee.models.BaseKGE attribute), 59, 62, 66, 70, 76, 89, 92
input_dp_rel_real (dicee.BaseKGE attribute), 181
\verb"input_dp_rel_real" (\textit{dicee.models.base\_model.BaseKGE attribute}), 19
input_dp_rel_real (dicee.models.BaseKGE attribute), 59, 62, 66, 70, 76, 89, 92
input_dropout_rate (dicee.BaseKGE attribute), 180
input_dropout_rate (dicee.config.Namespace attribute), 127
input_dropout_rate (dicee.models.base_model.BaseKGE attribute), 19
input_dropout_rate (dicee.models.BaseKGE attribute), 58, 62, 65, 70, 76, 88, 92
intialize_model() (in module dicee), 183
intialize_model() (in module dicee.static_funcs), 154
is_continual_training (dicee.DICE_Trainer attribute), 184
is_continual_training (dicee.evaluator.Evaluator attribute), 141
is_continual_training (dicee.Execute attribute), 189
is_continual_training (dicee.executer.Execute attribute), 143
is_continual_training (dicee.trainer.DICE_Trainer attribute), 110
is_continual_training (dicee.trainer.dice_trainer.DICE_Trainer attribute), 107
is_global_zero (dicee.abstracts.AbstractTrainer attribute), 112
is seen() (dicee.abstracts.BaseInteractiveKGE method), 114
is_sparql_endpoint_alive() (in module dicee.sanity_checkers), 152
K
k (dicee.models.FMult attribute), 93
k (dicee.models.FMult2 attribute), 94
k (dicee.models.function_space.FMult attribute), 32
k (dicee.models.function_space.FMult2 attribute), 33
```

```
k (dicee.models.function space.GFMult attribute), 32
k (dicee.models.GFMult attribute), 94
k_fold_cross_validation() (dicee.DICE_Trainer method), 184
k_fold_cross_validation() (dicee.trainer.DICE_Trainer method), 111
k_fold_cross_validation() (dicee.trainer.dice_trainer.DICE_Trainer method), 107
k_vs_all_score() (dicee.ComplEx static method), 168
k_vs_all_score() (dicee.DistMult method), 159
k vs all score() (dicee.Keci method), 162
k_vs_all_score() (dicee.models.clifford.Keci method), 23
k_vs_all_score() (dicee.models.ComplEx static method), 69
k_vs_all_score() (dicee.models.complex.ComplEx static method), 30
k_vs_all_score() (dicee.models.DistMult method), 63
k_vs_all_score() (dicee.models.Keci method), 83
k\_vs\_all\_score() (dicee.models.octonion.OMult method), 36
k_vs_all_score() (dicee.models.OMult method), 79
k_vs_all_score() (dicee.models.QMult method), 73
k_vs_all_score() (dicee.models.quaternion.QMult method), 41
k_vs_all_score() (dicee.models.real.DistMult method), 43
k_vs_all_score() (dicee.OMult method), 175
k_vs_all_score() (dicee.QMult method), 174
Keci (class in dicee), 160
Keci (class in dicee.models), 81
Keci (class in dicee.models.clifford), 21
KeciBase (class in dicee), 160
KeciBase (class in dicee.models), 84
KeciBase (class in dicee.models.clifford), 24
kernel_size (dicee.BaseKGE attribute), 180
kernel_size (dicee.config.Namespace attribute), 127
kernel_size (dicee.models.base_model.BaseKGE attribute), 19
kernel_size (dicee.models.BaseKGE attribute), 58, 62, 65, 70, 76, 88, 92
KG (class in dicee.knowledge_graph), 145
kg (dicee.callbacks.PseudoLabellingCallback attribute), 122
kg (dicee.read_preprocess_save_load_kg.LoadSaveToDisk attribute), 103
kg (dicee.read_preprocess_save_load_kg.PreprocessKG attribute), 103
kg (dicee.read_preprocess_save_load_kg.preprocess.PreprocessKG attribute), 98
kg (dicee.read_preprocess_save_load_kg.read_from_disk.ReadFromDisk attribute), 98
kg (dicee.read preprocess save load kg.ReadFromDisk attribute), 104
kg (dicee.read_preprocess_save_load_kg.save_load_disk.LoadSaveToDisk attribute), 99
KGE (class in dicee), 185
KGE (class in dicee.knowledge_graph_embeddings), 146
KGESaveCallback (class in dicee.callbacks), 120
knowledge_graph (dicee.Execute attribute), 189
knowledge_graph (dicee.executer.Execute attribute), 143
KronE (class in dicee.callbacks), 124
KvsAll (class in dicee), 192
KvsAll (class in dicee.dataset_classes), 131
kvsall_score() (dicee.DualE method), 167
kvsall_score() (dicee.models.DualE method), 97
kvsall_score() (dicee.models.dualE.DualE method), 31
KvsSampleDataset (class in dicee), 195
KvsSampleDataset (class in dicee.dataset_classes), 134
label_smoothing_rate (dicee.AllvsAll attribute), 194
label_smoothing_rate (dicee.config.Namespace attribute), 127
label_smoothing_rate (dicee.dataset_classes.AllvsAll attribute), 132
label_smoothing_rate (dicee.dataset_classes.KvsAll attribute), 131
label_smoothing_rate (dicee.dataset_classes.KvsSampleDataset attribute), 135
label_smoothing_rate (dicee.dataset_classes.OnevsSample attribute), 133, 134
label_smoothing_rate (dicee.dataset_classes.TriplePredictionDataset attribute), 136
label_smoothing_rate (dicee.KvsAll attribute), 193
label_smoothing_rate (dicee.KvsSampleDataset attribute), 196
label_smoothing_rate (dicee. Onevs Sample attribute), 194, 195
label_smoothing_rate (dicee. TriplePredictionDataset attribute), 197
LayerNorm (class in dicee.models.transformers), 47
learning_rate (dicee.BaseKGE attribute), 180
learning_rate (dicee.models.base_model.BaseKGE attribute), 19
```

```
learning rate (dicee.models.BaseKGE attribute), 58, 62, 65, 70, 76, 88, 92
length (dicee.dataset_classes.NegSampleDataset attribute), 135
length (dicee.dataset_classes.TriplePredictionDataset attribute), 136
length (dicee.NegSampleDataset attribute), 197
length (dicee. TriplePredictionDataset attribute), 197
level (dicee.callbacks.Perturb attribute), 125
LFMult (class in dicee), 175
LFMult (class in dicee.models), 95
LFMult (class in dicee.models.function_space), 34
LFMult1 (class in dicee.models), 95
LFMult1 (class in dicee.models.function_space), 33
linear() (dicee.LFMult method), 176
linear() (dicee.models.function_space.LFMult method), 34
linear() (dicee.models.LFMult method), 96
list2tuple() (dicee.query_generator.QueryGenerator method), 151
list2tuple() (dicee.QueryGenerator method), 201
lm_head (dicee.BytE attribute), 178
lm_head (dicee.models.transformers.BytE attribute), 45
lm_head (dicee.models.transformers.GPT attribute), 50
ln_1 (dicee.models.transformers.Block attribute), 49
ln_2 (dicee.models.transformers.Block attribute), 49
load() (dicee.read_preprocess_save_load_kg.LoadSaveToDisk method), 104
load() (dicee.read_preprocess_save_load_kg.save_load_disk.LoadSaveToDisk method), 99
load_json() (in module dicee), 183
load_json() (in module dicee.static_funcs), 154
load_model() (in module dicee), 182
load_model() (in module dicee.static_funcs), 153
load_model_ensemble() (in module dicee), 182
load_model_ensemble() (in module dicee.static_funcs), 153
load_numpy() (in module dicee), 183
load_numpy() (in module dicee.static_funcs), 154
load_numpy_ndarray() (in module dicee.read_preprocess_save_load_kg.util), 102
load_pickle() (in module dicee), 182
load_pickle() (in module dicee.read_preprocess_save_load_kg.util), 102
load_pickle() (in module dicee.static_funcs), 153
load_queries() (dicee.query_generator.QueryGenerator method), 151
load gueries () (dicee. Ouery Generator method), 202
load_queries_and_answers() (dicee.query_generator.QueryGenerator static method), 151
load_queries_and_answers() (dicee.QueryGenerator static method), 202
load_term_mapping() (in module dicee), 182, 190
load_term_mapping() (in module dicee.static_funcs), 153
load_term_mapping() (in module dicee.trainer.dice_trainer), 106
load_with_pandas() (in module dicee.read_preprocess_save_load_kg.util), 102
LoadSaveToDisk (class in dicee.read_preprocess_save_load_kg), 103
LoadSaveToDisk (class in dicee.read_preprocess_save_load_kg.save_load_disk), 99
local_rank (dicee.trainer.torch_trainer_ddp.NodeTrainer attribute), 109
loss (dicee.BaseKGE attribute), 180
loss (dicee.models.base_model.BaseKGE attribute), 19
loss (dicee.models.BaseKGE attribute), 59, 62, 65, 70, 76, 89, 92
loss_func (dicee.trainer.torch_trainer_ddp.NodeTrainer attribute), 110
loss_function (dicee.trainer.torch_trainer.TorchTrainer attribute), 108
loss_function() (dicee.BytE method), 178
{\tt loss\_function()} \ (\textit{dicee.models.base\_model.BaseKGELightning method}), 14
loss_function() (dicee.models.BaseKGELightning method), 54
loss_function() (dicee.models.transformers.BytE method), 45
loss_history (dicee.BaseKGE attribute), 181
loss_history (dicee.models.base_model.BaseKGE attribute), 19
loss_history (dicee.models.BaseKGE attribute), 59, 62, 66, 70, 76, 89, 92
loss_history (dicee.models.pykeen_models.PykeenKGE attribute), 38
loss_history (dicee.models.PykeenKGE attribute), 90
loss_history (dicee.PykeenKGE attribute), 177
loss_history (dicee.trainer.torch_trainer_ddp.NodeTrainer attribute), 110
1r (dicee.analyse_experiments.Experiment attribute), 118
1r (dicee.config.Namespace attribute), 126
```

## M

m (dicee.LFMult attribute), 175

```
m (dicee.models.function space.LFMult attribute), 34
m (dicee.models.LFMult attribute), 95
main() (in module dicee.scripts.index), 104
main() (in module dicee.scripts.run), 105
main() (in module dicee.scripts.serve), 106
make_iterable_verbose() (in module dicee.trainer.torch_trainer_ddp), 109
mapping_from_first_two_cols_to_third() (in module dicee), 190
mapping_from_first_two_cols_to_third() (in module dicee.static_preprocess_funcs), 156
margin (dicee.models.Pyke attribute), 64
margin (dicee.models.real.Pyke attribute), 44
margin (dicee.models.real.TransE attribute), 43
margin (dicee.models.TransE attribute), 64
margin (dicee. Pyke attribute), 159
margin (dicee. TransE attribute), 163
max_ans_num (dicee.query_generator.QueryGenerator attribute), 150
max_ans_num (dicee.QueryGenerator attribute), 201
max_epochs (dicee.callbacks.KGESaveCallback attribute), 121
max_length_subword_tokens (dicee.BaseKGE attribute), 181
max_length_subword_tokens (dicee.knowledge_graph.KG attribute), 145
max_length_subword_tokens (dicee.models.base_model.BaseKGE attribute), 19
max_length_subword_tokens (dicee.models.BaseKGE attribute), 59, 62, 66, 70, 76, 89, 92
max_num_of_classes (dicee.dataset_classes.KvsSampleDataset attribute), 135
max_num_of_classes (dicee.KvsSampleDataset attribute), 196
mem_of_model() (dicee.models.base_model.BaseKGELightning method), 13
mem_of_model() (dicee.models.BaseKGELightning method), 53
method (dicee.callbacks.Perturb attribute), 125
MLP (class in dicee.models.transformers), 48
mlp (dicee.models.transformers.Block attribute), 49
\verb+mode+ (\textit{dicee.query\_generator.QueryGenerator attribute}), 150
mode (dicee.QueryGenerator attribute), 201
model (dicee.config.Namespace attribute), 126
model (dicee.models.pykeen_models.PykeenKGE attribute), 38
model (dicee.models.PykeenKGE attribute), 90
model (dicee.PykeenKGE attribute), 177
model (dicee.scripts.serve.NeuralSearcher attribute), 105
model (dicee.trainer.torch_trainer_ddp.NodeTrainer attribute), 110
model (dicee.trainer.torch trainer.TorchTrainer attribute), 108
{\tt model\_kwargs} (dicee.models.pykeen_models.PykeenKGE attribute), 38
model_kwargs (dicee.models.PykeenKGE attribute), 90
model_kwargs (dicee.PykeenKGE attribute), 176
model_name (dicee.analyse_experiments.Experiment attribute), 118
module
     dicee, 12
     dicee.___main___, 111
     dicee.abstracts, 111
     dicee.analyse_experiments, 117
     dicee.callbacks, 119
     dicee.config, 125
     dicee.dataset_classes, 128
     dicee.eval_static_funcs, 140
     dicee.evaluator, 141
     dicee.executer, 142
     dicee.knowledge_graph, 144
     dicee.knowledge_graph_embeddings, 146
     dicee.models, 12
     dicee.models.base_model, 12
     dicee.models.clifford, 21
     dicee.models.complex, 28
     dicee.models.dualE, 30
     dicee.models.function_space, 32
     dicee.models.octonion.35
     dicee.models.pykeen_models, 38
     dicee.models.quaternion, 39
     dicee.models.real, 42
     dicee.models.static_funcs, 44
     dicee.models.transformers, 44
     dicee.query_generator, 150
     dicee.read_preprocess_save_load_kg,97
```

```
dicee.read_preprocess_save_load_kg.preprocess, 97
      dicee.read_preprocess_save_load_kg.read_from_disk,98
      dicee.read_preprocess_save_load_kg.save_load_disk,99
      dicee.read_preprocess_save_load_kg.util,99
      dicee.sanity_checkers, 151
      dicee.scripts, 104
      dicee.scripts.index, 104
      dicee.scripts.run, 104
      dicee.scripts.serve, 105
      dicee.static_funcs, 152
      dicee.static_funcs_training, 155
      dicee.static_preprocess_funcs, 155
      dicee.trainer, 106
      dicee.trainer.dice_trainer, 106
      dicee.trainer.torch_trainer, 108
      dicee.trainer.torch_trainer_ddp, 109
MultiClassClassificationDataset (class in dicee), 191
MultiClassClassificationDataset (class in dicee.dataset_classes), 130
MultiLabelDataset (class in dicee), 191
MultiLabelDataset (class in dicee.dataset_classes), 129
Ν
n (dicee.models.FMult2 attribute), 94
n (dicee.models.function_space.FMult2 attribute), 33
n_embd (dicee.models.transformers.CausalSelfAttention attribute), 48
n_embd (dicee.models.transformers.GPTConfig attribute), 50
n_head (dicee.models.transformers.CausalSelfAttention attribute), 48
n_head (dicee.models.transformers.GPTConfig attribute), 50
n_layer (dicee.models.transformers.GPTConfig attribute), 49
n_layers (dicee.models.FMult2 attribute), 94
n_layers (dicee.models.function_space.FMult2 attribute), 33
name (dicee.abstracts.BaseInteractiveKGE property), 114
name (dicee.AConEx attribute), 168
name (dicee.AConvO attribute), 169
name (dicee.AConvQ attribute), 170
name (dicee.BytE attribute), 178
name (dicee.ComplEx attribute), 168
name (dicee.ConEx attribute), 172
name (dicee.ConvO attribute), 171
name (dicee.ConvQ attribute), 170
name (dicee.DeCaL attribute), 164
name (dicee.DistMult attribute), 159
name (dicee.DualE attribute), 167
name (dicee.Keci attribute), 160
name (dicee.KeciBase attribute), 160
name (dicee.LFMult attribute), 175
name (dicee.models.AConEx attribute), 67
name (dicee.models.AConvO attribute), 80
name (dicee.models.AConvQ attribute), 74
name (dicee.models.clifford.DeCaL attribute), 25
name (dicee.models.clifford.Keci attribute), 22
name (dicee.models.clifford.KeciBase attribute), 24
name (dicee.models.ComplEx attribute), 69
\verb"name" (\textit{dicee.models.complex.AConEx attribute}), 29
name (dicee.models.complex.ComplEx attribute), 30
name (dicee.models.complex.ConEx attribute), 28
name (dicee.models.ConEx attribute), 67
name (dicee.models.ConvO attribute), 80
name (dicee.models.ConvQ attribute), 74
name (dicee.models.DeCaL attribute), 85
name (dicee.models.DistMult attribute), 63
name (dicee.models.DualE attribute), 96
name (dicee.models.dualE.DualE attribute), 31
name (dicee.models.FMult attribute), 93
name (dicee.models.FMult2 attribute), 94
name (dicee.models.function_space.FMult attribute), 32
name (dicee.models.function_space.FMult2 attribute), 33
```

```
name (dicee.models.function_space.GFMult attribute), 32
name (dicee.models.function_space.LFMult attribute), 34
name (dicee.models.function_space.LFMult1 attribute), 33
name (dicee.models.GFMult attribute), 94
name (dicee.models.Keci attribute), 81
name (dicee.models.KeciBase attribute), 84
name (dicee.models.LFMult attribute), 95
name (dicee.models.LFMult1 attribute), 95
name (dicee.models.octonion.AConvO attribute), 38
name (dicee.models.octonion.ConvO attribute), 37
name (dicee.models.octonion.OMult attribute), 36
name (dicee.models.OMult attribute), 79
name (dicee.models.Pyke attribute), 64
name (dicee.models.pykeen_models.PykeenKGE attribute), 38
name (dicee.models.PykeenKGE attribute), 90
name (dicee.models.QMult attribute), 73
name (dicee.models.quaternion.AConvQ attribute), 42
name (dicee.models.quaternion.ConvQ attribute), 41
name (dicee.models.quaternion.QMult attribute), 40
name (dicee.models.real.DistMult attribute), 43
name (dicee.models.real.Pyke attribute), 44
name (dicee.models.real.Shallom attribute). 43
name (dicee.models.real.TransE attribute), 43
name (dicee.models.Shallom attribute), 64
name (dicee.models.TransE attribute), 64
name (dicee.models.transformers.BytE attribute), 45
name (dicee.OMult attribute), 175
name (dicee.Pyke attribute), 159
name (dicee.PykeenKGE attribute), 176
name (dicee.QMult attribute), 173
name (dicee.Shallom attribute), 175
name (dicee.TransE attribute), 163
Namespace (class in dicee.config), 125
neg_ratio (dicee.BPE_NegativeSamplingDataset attribute), 190
neg_ratio (dicee.config.Namespace attribute), 127
neg_ratio (dicee.dataset_classes.BPE_NegativeSamplingDataset attribute), 129
neg ratio (dicee.dataset classes.KvsSampleDataset attribute), 135
neg_ratio (dicee.KvsSampleDataset attribute), 196
neg_sample_ratio (dicee.CVDataModule attribute), 198
neg_sample_ratio (dicee.dataset_classes.CVDataModule attribute), 137
neg_sample_ratio (dicee.dataset_classes.NegSampleDataset attribute), 135
neg_sample_ratio (dicee.dataset_classes.OnevsSample attribute), 133, 134
neg_sample_ratio (dicee.dataset_classes.TriplePredictionDataset attribute), 136
neg_sample_ratio (dicee.NegSampleDataset attribute), 196
neg_sample_ratio (dicee.OnevsSample attribute), 194, 195
neg_sample_ratio (dicee. TriplePredictionDataset attribute), 197
negnorm() (dicee.KGE method), 187
negnorm() (dicee.knowledge_graph_embeddings.KGE method), 149
NegSampleDataset (class in dicee), 196
NegSampleDataset (class in dicee.dataset_classes), 135
neural searcher (in module dicee.scripts.serve), 105
Neural Searcher (class in dicee.scripts.serve), 105
NodeTrainer (class in dicee.trainer.torch_trainer_ddp), 109
norm_fc1 (dicee.AConEx attribute), 169
norm_fc1 (dicee.AConvO attribute), 169
norm_fc1 (dicee.ConEx attribute), 172
norm_fc1 (dicee.ConvO attribute), 172
norm_fc1 (dicee.models.AConEx attribute), 68
norm_fc1 (dicee.models.AConvO attribute), 80
{\tt norm\_fc1} (dicee.models.complex.AConEx attribute), 29
norm fc1 (dicee.models.complex.ConEx attribute), 28
norm_fc1 (dicee.models.ConEx attribute), 67
norm_fc1 (dicee.models.ConvO attribute), 80
norm_fc1 (dicee.models.octonion.AConvO attribute), 38
norm_fc1 (dicee.models.octonion.ConvO attribute), 37
normalization (dicee.analyse_experiments.Experiment attribute), 118
normalization (dicee.config.Namespace attribute), 127
normalize_head_entity_embeddings (dicee.BaseKGE attribute), 181
```

```
normalize_head_entity_embeddings (dicee.models.base_model.BaseKGE attribute), 19
normalize_head_entity_embeddings (dicee.models.BaseKGE attribute), 59, 62, 66, 70, 76, 89, 92
normalize_relation_embeddings (dicee.BaseKGE attribute), 181
normalize_relation_embeddings (dicee.models.base_model.BaseKGE attribute), 19
normalize_relation_embeddings (dicee.models.BaseKGE attribute), 59, 62, 66, 70, 76, 89, 92
normalize_tail_entity_embeddings (dicee.BaseKGE attribute), 181
normalize_tail_entity_embeddings (dicee.models.base_model.BaseKGE attribute), 19
normalize_tail_entity_embeddings (dicee.models.BaseKGE attribute), 59, 62, 66, 70, 76, 89, 92
normalizer_class (dicee.BaseKGE attribute), 180
normalizer_class (dicee.models.base_model.BaseKGE attribute), 19
normalizer_class (dicee.models.BaseKGE attribute), 59, 62, 66, 70, 76, 89, 92
num_bpe_entities (dicee.BPE_NegativeSamplingDataset attribute), 190
num_bpe_entities (dicee.dataset_classes.BPE_NegativeSamplingDataset attribute), 129
num_bpe_entities (dicee.knowledge_graph.KG attribute), 145
num_core (dicee.config.Namespace attribute), 127
num_datapoints (dicee.BPE_NegativeSamplingDataset attribute), 191
num_datapoints (dicee.dataset_classes.BPE_NegativeSamplingDataset attribute), 129
num_datapoints (dicee.dataset_classes.MultiLabelDataset attribute), 130
num_datapoints (dicee.MultiLabelDataset attribute), 191
num_ent (dicee.DualE attribute), 167
num_ent (dicee.models.DualE attribute), 97
num ent (dicee.models.dualE.DualE attribute), 31
num_entities (dicee.BaseKGE attribute), 180
num_entities (dicee.CVDataModule attribute), 198
num_entities (dicee.dataset_classes.CVDataModule attribute), 137
num_entities (dicee.dataset_classes.KvsSampleDataset attribute), 135
\verb|num_entities| (dicee. dataset\_classes. Neg Sample Dataset\ attribute),\ 135
num_entities (dicee.dataset_classes.OnevsSample attribute), 133
\verb|num_entities| (\textit{dicee.dataset\_classes.TriplePredictionDataset\ attribute}), 136
num_entities (dicee.evaluator.Evaluator attribute), 141
num_entities (dicee.knowledge_graph.KG attribute), 145
num entities (dicee.KvsSampleDataset attribute), 196
num_entities (dicee.models.base_model.BaseKGE attribute), 18
num_entities (dicee.models.BaseKGE attribute), 58, 61, 65, 70, 75, 88, 92
num_entities (dicee.NegSampleDataset attribute), 197
num_entities (dicee.OnevsSample attribute), 194, 195
num entities (dicee. TriplePredictionDataset attribute), 197
num_epochs (dicee.abstracts.AbstractPPECallback attribute), 116
num_epochs (dicee.analyse_experiments.Experiment attribute), 118
num_epochs (dicee.callbacks.ASWA attribute), 122
num_epochs (dicee.config.Namespace attribute), 126
num_epochs (dicee.trainer.torch_trainer_ddp.NodeTrainer attribute), 110
num_folds_for_cv (dicee.config.Namespace attribute), 127
\verb|num_of_data_points| (\textit{dicee.dataset\_classes.MultiClassClassificationDataset\ attribute}), 130
num_of_data_points (dicee.MultiClassClassificationDataset attribute), 192
num_of_epochs (dicee.callbacks.PseudoLabellingCallback attribute), 122
num_of_output_channels (dicee.BaseKGE attribute), 180
num_of_output_channels (dicee.config.Namespace attribute), 127
num_of_output_channels (dicee.models.base_model.BaseKGE attribute), 19
num_of_output_channels (dicee.models.BaseKGE attribute), 59, 62, 65, 70, 76, 89, 92
num_params (dicee.analyse_experiments.Experiment attribute), 118
num_relations (dicee.BaseKGE attribute), 180
num_relations (dicee.CVDataModule attribute), 198
num_relations (dicee.dataset_classes.CVDataModule attribute), 137
num_relations (dicee.dataset_classes.NegSampleDataset attribute), 135
num_relations (dicee.dataset_classes.OnevsSample attribute), 133
num_relations (dicee.dataset_classes.TriplePredictionDataset attribute), 136
num_relations (dicee.evaluator.Evaluator attribute), 141
num_relations (dicee.knowledge_graph.KG attribute), 145
num_relations (dicee.models.base_model.BaseKGE attribute), 18
num relations (dicee.models.BaseKGE attribute), 58, 61, 65, 70, 76, 88, 92
num_relations (dicee.NegSampleDataset attribute), 197
num_relations (dicee. Onevs Sample attribute), 194, 195
num_relations (dicee. TriplePredictionDataset attribute), 197
num_sample (dicee.models.FMult attribute), 93
num_sample (dicee.models.function_space.FMult attribute), 32
num_sample (dicee.models.function_space.GFMult attribute), 32
num_sample (dicee.models.GFMult attribute), 94
```

```
num tokens (dicee.BaseKGE attribute), 180
num_tokens (dicee.knowledge_graph.KG attribute), 145
num_tokens (dicee.models.base_model.BaseKGE attribute), 18
num_tokens (dicee.models.BaseKGE attribute), 58, 62, 65, 70, 76, 88, 92
num_workers (dicee.CVDataModule attribute), 198
num_workers (dicee.dataset_classes.CVDataModule attribute), 137
numpy_data_type_changer() (in module dicee), 182
numpy_data_type_changer() (in module dicee.static_funcs), 154
octonion_mul() (in module dicee.models), 78
octonion_mul() (in module dicee.models.octonion), 35
octonion_mul_norm() (in module dicee.models), 78
octonion_mul_norm() (in module dicee.models.octonion), 35
octonion_normalizer() (dicee.AConvO static method), 169
octonion_normalizer() (dicee.ConvO static method), 172
octonion_normalizer() (dicee.models.AConvO static method), 80
octonion_normalizer() (dicee.models.ConvO static method), 80
octonion_normalizer() (dicee.models.octonion.AConvO static method), 38
octonion_normalizer() (dicee.models.octonion.ConvO static method), 37
\verb|octonion_normalizer()| \textit{(dicee.models.octonion.OMult static method)}, 36
octonion_normalizer() (dicee.models.OMult static method), 79
octonion_normalizer() (dicee.OMult static method), 175
OMult (class in dicee), 174
OMult (class in dicee.models), 78
OMult (class in dicee.models.octonion), 35
on_epoch_end() (dicee.callbacks.KGESaveCallback method), 122
on_epoch_end() (dicee.callbacks.PseudoLabellingCallback method), 122
on_fit_end() (dicee.abstracts.AbstractCallback method), 116
on_fit_end() (dicee.abstracts.AbstractPPECallback method), 117
on_fit_end() (dicee.abstracts.AbstractTrainer method), 112
on_fit_end() (dicee.callbacks.AccumulateEpochLossCallback method), 119
on\_fit\_end() (dicee.callbacks.ASWA method), 122
on_fit_end() (dicee.callbacks.Eval method), 124
on_fit_end() (dicee.callbacks.KGESaveCallback method), 121
on_fit_end() (dicee.callbacks.PrintCallback method), 120
on_fit_start() (dicee.abstracts.AbstractCallback method), 115
on_fit_start() (dicee.abstracts.AbstractPPECallback method), 117
on_fit_start() (dicee.abstracts.AbstractTrainer method), 112
on_fit_start() (dicee.callbacks.Eval method), 123
on_fit_start() (dicee.callbacks.KGESaveCallback method), 121
on_fit_start() (dicee.callbacks.KronE method), 125
on_fit_start() (dicee.callbacks.PrintCallback method), 120
on_init_end() (dicee.abstracts.AbstractCallback method), 115
on_init_start() (dicee.abstracts.AbstractCallback method), 115
on_train_batch_end() (dicee.abstracts.AbstractCallback method), 116
on_train_batch_end() (dicee.abstracts.AbstractTrainer method), 113
on_train_batch_end() (dicee.callbacks.Eval method), 124
on_train_batch_end() (dicee.callbacks.KGESaveCallback method), 121
\verb"on_train_batch_end()" (\textit{dicee.callbacks.PrintCallback method}), 120
on_train_batch_start() (dicee.callbacks.Perturb method), 125
on_train_epoch_end() (dicee.abstracts.AbstractCallback method), 116
on_train_epoch_end() (dicee.abstracts.AbstractTrainer method), 112
on_train_epoch_end() (dicee.callbacks.ASWA method), 123
on_train_epoch_end() (dicee.callbacks.Eval method), 124
on_train_epoch_end() (dicee.callbacks.KGESaveCallback method), 121
on_train_epoch_end() (dicee.callbacks.PrintCallback method), 120
on_train_epoch_end() (dicee.models.base_model.BaseKGELightning method), 14
on_train_epoch_end() (dicee.models.BaseKGELightning method), 54
OnevsAllDataset (class in dicee), 192
OnevsAllDataset (class in dicee.dataset_classes), 130
OnevsSample (class in dicee), 194
OnevsSample (class in dicee.dataset_classes), 132
optim (dicee.config.Namespace attribute), 126
optimizer (dicee.trainer.torch_trainer_ddp.NodeTrainer attribute), 109
optimizer (dicee.trainer.torch_trainer.TorchTrainer attribute), 108
optimizer_name (dicee.BaseKGE attribute), 180
```

```
optimizer name (dicee.models.base model.BaseKGE attribute), 19
optimizer_name (dicee.models.BaseKGE attribute), 58, 62, 65, 70, 76, 88, 92
ordered_bpe_entities (dicee.BPE_NegativeSamplingDataset attribute), 190
ordered_bpe_entities (dicee.dataset_classes.BPE_NegativeSamplingDataset attribute), 129
ordered_bpe_entities (dicee.knowledge_graph.KG attribute), 146
ordered_shaped_bpe_tokens (dicee.knowledge_graph.KG attribute), 145
p (dicee.config.Namespace attribute), 127
p (dicee.DeCaL attribute), 164
p (dicee.Keci attribute), 160
p (dicee.models.clifford.DeCaL attribute), 25
p (dicee.models.clifford.Keci attribute), 22
p (dicee.models.DeCaL attribute), 85
p (dicee.models.Keci attribute), 81
padding (dicee.knowledge_graph.KG attribute), 145
param_init (dicee.BaseKGE attribute), 181
param_init (dicee.models.base_model.BaseKGE attribute), 19
param_init (dicee.models.BaseKGE attribute), 59, 62, 66, 70, 76, 89, 92
parameters () (dicee.abstracts.BaseInteractiveKGE method), 115
path (dicee.abstracts.AbstractPPECallback attribute), 116
path (dicee.callbacks.AccumulateEpochLossCallback attribute), 119
path (dicee.callbacks.ASWA attribute), 122
path (dicee.callbacks.Eval attribute), 123
path (dicee.callbacks.KGESaveCallback attribute), 121
path_dataset_folder (dicee.analyse_experiments.Experiment attribute), 118
path_for_deserialization (dicee.knowledge_graph.KG attribute), 145
path_for_serialization (dicee.knowledge_graph.KG attribute), 145
path_single_kg (dicee.config.Namespace attribute), 126
path_single_kg (dicee.knowledge_graph.KG attribute), 145
path_to_store_single_run (dicee.config.Namespace attribute), 126
Perturb (class in dicee.callbacks), 125
polars_dataframe_indexer() (in module dicee.read_preprocess_save_load_kg.util), 100
poly_NN() (dicee.LFMult method), 176
poly_NN() (dicee.models.function_space.LFMult method), 34
poly_NN() (dicee.models.LFMult method), 96
polynomial() (dicee.LFMult method), 176
polynomial() (dicee.models.function_space.LFMult method), 35
polynomial () (dicee.models.LFMult method), 96
pop() (dicee.LFMult method), 176
pop() (dicee.models.function_space.LFMult method), 35
pop () (dicee.models.LFMult method), 96
pq (dicee.analyse_experiments.Experiment attribute), 118
predict() (dicee.KGE method), 186
predict() (dicee.knowledge_graph_embeddings.KGE method), 148
predict_dataloader() (dicee.models.base_model.BaseKGELightning method), 15
predict_dataloader() (dicee.models.BaseKGELightning method), 55
predict_missing_head_entity() (dicee.KGE method), 185
predict_missing_head_entity() (dicee.knowledge_graph_embeddings.KGE method), 146
predict_missing_relations() (dicee.KGE method), 185
predict_missing_relations() (dicee.knowledge_graph_embeddings.KGE method), 147
predict_missing_tail_entity() (dicee.KGE method), 186
predict_missing_tail_entity() (dicee.knowledge_graph_embeddings.KGE method), 147
predict_topk() (dicee.KGE method), 186
\verb|predict_topk()| \textit{(dicee.knowledge\_graph\_embeddings.KGE method)}, 148
prepare_data() (dicee.CVDataModule method), 200
prepare_data() (dicee.dataset_classes.CVDataModule method), 139
preprocess_with_byte_pair_encoding() (dicee.read_preprocess_save_load_kg.PreprocessKG method), 103
preprocess_with_byte_pair_encoding() (dicee.read_preprocess_save_load_kg.preprocess.PreprocessKG method), 98
preprocess_with_byte_pair_encoding_with_padding() (dicee.read_preprocess_save_load_kg.PreprocessKG method), 103
preprocess_with_byte_pair_encoding_with_padding() (dicee.read_preprocess_save_load_kg.preprocess.PreprocessKG method), 98
preprocess_with_pandas() (dicee.read_preprocess_save_load_kg.PreprocessKG method), 103
preprocess_with_pandas() (dicee.read_preprocess_save_load_kg.preprocess.PreprocessKG method), 98
preprocess_with_polars() (dicee.read_preprocess_save_load_kg.PreprocessKG method), 103
preprocess_with_polars() (dicee.read_preprocess_save_load_kg.preprocess.PreprocessKG method), 98
preprocesses_input_args() (in module dicee.static_preprocess_funcs), 156
PreprocessKG (class in dicee.read_preprocess_save_load_kg), 103
```

```
PreprocessKG (class in dicee.read_preprocess_save_load_kg.preprocess), 98
previous_args (dicee.executer.ContinuousExecute attribute), 144
PrintCallback (class in dicee.callbacks), 119
process (dicee.trainer.torch_trainer.TorchTrainer attribute), 108
PseudoLabellingCallback (class in dicee.callbacks), 122
ptdtype (dicee.trainer.torch_trainer_ddp.NodeTrainer attribute), 110
Pyke (class in dicee), 159
Pyke (class in dicee.models), 64
Pyke (class in dicee.models.real), 43
pykeen_model_kwargs (dicee.config.Namespace attribute), 127
PykeenKGE (class in dicee), 176
PykeenKGE (class in dicee.models), 90
PykeenKGE (class in dicee.models.pykeen_models), 38
Q
q (dicee.config.Namespace attribute), 127
q (dicee.DeCaL attribute), 164
q (dicee.Keci attribute), 160
g (dicee.models.clifford.DeCaL attribute), 25
q (dicee.models.clifford.Keci attribute), 22
q (dicee.models.DeCaL attribute), 85
q (dicee.models.Keci attribute), 81
qdrant_client (dicee.scripts.serve.NeuralSearcher attribute), 106
QMult (class in dicee), 172
QMult (class in dicee.models), 72
QMult (class in dicee.models.quaternion), 40
quaternion_mul() (in module dicee.models), 69
quaternion_mul() (in module dicee.models.static_funcs), 44
quaternion_mul_with_unit_norm() (in module dicee.models), 72
\verb"quaternion_mul_with_unit_norm"() \textit{ (in module dicee.models.quaternion)}, 40
\verb"quaternion_multiplication_followed_by_inner_product() \textit{ (dicee.models.QMult method)}, 73
quaternion_multiplication_followed_by_inner_product() (dicee.models.quaternion.QMult method), 40
quaternion_multiplication_followed_by_inner_product() (dicee.QMult method), 173
quaternion_normalizer() (dicee.models.QMult static method), 73
\verb"quaternion_normalizer"() \textit{ (dicee.models.quaternion.QMult static method)}, 40
quaternion_normalizer() (dicee.QMult static method), 173
query_name_to_struct (dicee.query_generator.QueryGenerator attribute), 151
query_name_to_struct (dicee.QueryGenerator attribute), 201
QueryGenerator (class in dicee), 201
QueryGenerator (class in dicee.query_generator), 150
r (dicee.DeCaL attribute), 164
r (dicee Keci attribute), 160
r (dicee.models.clifford.DeCaL attribute), 25
r (dicee.models.clifford.Keci attribute), 22
r (dicee.models.DeCaL attribute), 85
r (dicee.models.Keci attribute), 81
random_prediction() (in module dicee), 183
random_prediction() (in module dicee.static_funcs), 154
random_seed (dicee.config.Namespace attribute), 127
ratio (dicee.callbacks.Perturb attribute), 125
re (dicee.DeCaL attribute), 164
re (dicee.models.clifford.DeCaL attribute), 25
re (dicee.models.DeCaL attribute), 85
re_vocab (dicee.evaluator.Evaluator attribute), 141
read_from_disk() (in module dicee.read_preprocess_save_load_kg.util), 102
read_from_triple_store() (in module dicee.read_preprocess_save_load_kg.util), 102
read_only_few (dicee.config.Namespace attribute), 127
read_only_few (dicee.knowledge_graph.KG attribute), 145
read_or_load_kg() (in module dicee), 183
read_or_load_kg() (in module dicee.static_funcs), 154
read_preprocess_index_serialize_data() (dicee.Execute method), 189
read_preprocess_index_serialize_data() (dicee.executer.Execute method), 143
read_with_pandas() (in module dicee.read_preprocess_save_load_kg.util), 102
read_with_polars() (in module dicee.read_preprocess_save_load_kg.util), 101
ReadFromDisk (class in dicee.read_preprocess_save_load_kg), 104
```

```
ReadFromDisk (class in dicee.read_preprocess_save_load_kg.read_from_disk), 98
rel2id (dicee.query_generator.QueryGenerator attribute), 150
rel2id (dicee.QueryGenerator attribute), 201
relation_embeddings (dicee.AConvQ attribute), 170
relation_embeddings (dicee.ConvQ attribute), 170
relation_embeddings (dicee.DeCaL attribute), 164
relation_embeddings (dicee.DualE attribute), 167
relation embeddings (dicee.LFMult attribute), 175
relation_embeddings (dicee.models.AConvQ attribute), 74
relation_embeddings (dicee.models.clifford.DeCaL attribute), 25
relation_embeddings (dicee.models.ConvQ attribute), 74
relation_embeddings (dicee.models.DeCaL attribute), 85
relation_embeddings (dicee.models.DualE attribute), 97
relation_embeddings (dicee.models.dualE.DualE attribute), 31
relation_embeddings (dicee.models.FMult attribute), 93
relation_embeddings (dicee.models.FMult2 attribute), 95
relation_embeddings (dicee.models.function_space.FMult attribute), 32
relation_embeddings (dicee.models.function_space.FMult2 attribute), 33
relation_embeddings (dicee.models.function_space.GFMult attribute), 32
relation_embeddings (dicee.models.function_space.LFMult attribute), 34
relation_embeddings (dicee.models.function_space.LFMult1 attribute), 33
relation_embeddings (dicee.models.GFMult attribute), 94
relation_embeddings (dicee.models.LFMult attribute), 95
relation_embeddings (dicee.models.LFMult1 attribute), 95
relation_embeddings (dicee.models.pykeen_models.PykeenKGE attribute), 39
relation_embeddings (dicee.models.PykeenKGE attribute), 90
relation_embeddings (dicee.models.quaternion.AConvQ attribute), 42
relation_embeddings (dicee.models.quaternion.ConvQ attribute), 41
{\tt relation\_embeddings}~(\textit{dicee.PykeenKGE attribute}),~177
relation_to_idx (dicee.knowledge_graph.KG attribute), 145
relations_str (dicee.knowledge_graph.KG property), 146
reload dataset () (in module dicee), 190
reload_dataset() (in module dicee.dataset_classes), 129
report (dicee.DICE_Trainer attribute), 184
report (dicee.evaluator.Evaluator attribute), 141
report (dicee.Execute attribute), 189
report (dicee.executer.Execute attribute), 143
report (dicee.trainer.DICE_Trainer attribute), 110
report (dicee.trainer.dice_trainer.DICE_Trainer attribute), 106
reports (dicee.callbacks.Eval attribute), 123
requires_grad_for_interactions (dicee.Keci attribute), 161
requires_grad_for_interactions (dicee.KeciBase attribute), 160
requires_grad_for_interactions (dicee.models.clifford.Keci attribute), 22
requires_grad_for_interactions (dicee.models.clifford.KeciBase attribute), 24
requires_grad_for_interactions (dicee.models.Keci attribute), 81
requires_grad_for_interactions (dicee.models.KeciBase attribute), 84
resid_dropout (dicee.models.transformers.CausalSelfAttention attribute), 48
residual_convolution() (dicee.AConEx method), 169
residual_convolution() (dicee.AConvO method), 169
residual_convolution() (dicee.AConvQ method), 170
residual_convolution() (dicee.ConEx method), 172
residual_convolution() (dicee.ConvO method), 172
residual_convolution() (dicee.ConvQ method), 171
residual_convolution() (dicee.models.AConEx method), 68
residual_convolution() (dicee.models.AConvO method), 80
residual_convolution() (dicee.models.AConvQ method), 75
residual_convolution() (dicee.models.complex.AConEx method), 29
\verb"residual_convolution"() \textit{ (dicee.models.complex.ConEx method)}, 28
residual_convolution() (dicee.models.ConEx method), 67
residual_convolution() (dicee.models.ConvO method), 80
residual convolution() (dicee.models.ConvO method), 74
residual_convolution() (dicee.models.octonion.AConvO method), 38
residual_convolution() (dicee.models.octonion.ConvO method), 37
residual_convolution() (dicee.models.quaternion.AConvQ method), 42
residual_convolution() (dicee.models.quaternion.ConvQ method), 42
retrieve_embeddings() (in module dicee.scripts.serve), 105
return_multi_hop_query_results() (dicee.KGE method), 187
return_multi_hop_query_results() (dicee.knowledge_graph_embeddings.KGE method), 149
```

```
root () (in module dicee.scripts.serve), 105
roots (dicee.models.FMult attribute), 94
roots (dicee.models.function_space.FMult attribute), 32
roots (dicee.models.function_space.GFMult attribute), 32
roots (dicee.models.GFMult attribute), 94
runtime (dicee.analyse_experiments.Experiment attribute), 118
S
sample_counter (dicee.abstracts.AbstractPPECallback attribute), 117
sample_entity() (dicee.abstracts.BaseInteractiveKGE method), 114
sample_relation() (dicee.abstracts.BaseInteractiveKGE method), 114
sample_triples_ratio (dicee.config.Namespace attribute), 127
sample_triples_ratio (dicee.knowledge_graph.KG attribute), 145
sanity_checking_with_arguments() (in module dicee.sanity_checkers), 152
save() (dicee.abstracts.BaseInteractiveKGE method), 114
save() (dicee.read_preprocess_save_load_kg.LoadSaveToDisk method), 103
save() (dicee.read_preprocess_save_load_kg.save_load_disk.LoadSaveToDisk method), 99
save_checkpoint() (dicee.abstracts.AbstractTrainer static method), 113
save checkpoint model () (in module dicee), 182
save_checkpoint_model() (in module dicee.static_funcs), 154
save_embeddings() (in module dicee), 183
save_embeddings() (in module dicee.static_funcs), 154
save_embeddings_as_csv (dicee.config.Namespace attribute), 126
save_experiment() (dicee.analyse_experiments.Experiment method), 118
save_model_at_every_epoch (dicee.config.Namespace attribute), 127
{\tt save\_numpy\_ndarray()} \ \textit{(in module dicee)}, 182
save_numpy_ndarray() (in module dicee.read_preprocess_save_load_kg.util), 102
save_numpy_ndarray() (in module dicee.static_funcs), 154
save_pickle() (in module dicee), 182
save_pickle() (in module dicee.read_preprocess_save_load_kg.util), 102
save_pickle() (in module dicee.static_funcs), 153
save_queries() (dicee.query_generator.QueryGenerator method), 151
save_queries() (dicee.QueryGenerator method), 202
save_queries_and_answers() (dicee.query_generator.QueryGenerator static method), 151
save_queries_and_answers() (dicee.QueryGenerator static method), 202
save_trained_model() (dicee.Execute method), 189
save_trained_model() (dicee.executer.Execute method), 143
scalar_batch_NN() (dicee.LFMult method), 176
scalar_batch_NN() (dicee.models.function_space.LFMult method), 34
scalar_batch_NN() (dicee.models.LFMult method), 96
scaler (dicee.callbacks.Perturb attribute), 125
score () (dicee.ComplEx static method), 168
score () (dicee.DistMult method), 160
score () (dicee. Keci method), 163
score () (dicee.models.clifford.Keci method), 24
score() (dicee.models.ComplEx static method), 69
score () (dicee.models.complex.ComplEx static method), 30
score () (dicee.models.DistMult method), 64
score () (dicee.models.Keci method), 84
score () (dicee.models.octonion.OMult method), 36
score () (dicee.models.OMult method), 79
score () (dicee.models.QMult method), 73
score () (dicee.models.quaternion.QMult method), 41
score() (dicee.models.real.DistMult method), 43
score() (dicee.models.real.TransE method), 43
score() (dicee.models.TransE method), 64
score() (dicee.OMult method), 175
score () (dicee.QMult method), 174
score () (dicee. TransE method), 163
score_func (dicee.models.FMult2 attribute), 94
score_func (dicee.models.function_space.FMult2 attribute), 33
\verb|scoring_technique| (\textit{dicee.analyse\_experiments.Experiment attribute}), 118
scoring_technique (dicee.config.Namespace attribute), 126
search() (dicee.scripts.serve.NeuralSearcher method), 106
search_embeddings() (in module dicee.scripts.serve), 105
seed (dicee.query_generator.QueryGenerator attribute), 150
seed (dicee.QueryGenerator attribute), 201
```

```
select model() (in module dicee), 182
select_model() (in module dicee.static_funcs), 153
selected_optimizer (dicee.BaseKGE attribute), 180
selected_optimizer (dicee.models.base_model.BaseKGE attribute), 19
selected_optimizer (dicee.models.BaseKGE attribute), 59, 62, 65, 70, 76, 89, 92
separator (dicee.config.Namespace attribute), 126
{\tt separator}~(\textit{dicee.knowledge\_graph.KG~attribute}),~146
sequential_vocabulary_construction() (dicee.read_preprocess_save_load_kg.PreprocessKG method), 103
sequential_vocabulary_construction() (dicee.read_preprocess_save_load_kg.preprocess.PreprocessKG method), 98
set_global_seed() (dicee.query_generator.QueryGenerator method), 151
set_global_seed() (dicee.QueryGenerator method), 202
\verb|set_model_eval_mode()| \textit{(dicee.abstracts.BaseInteractiveKGE method)}, 114
set_model_train_mode() (dicee.abstracts.BaseInteractiveKGE method), 114
setup() (dicee.CVDataModule method), 199
setup() (dicee.dataset_classes.CVDataModule method), 137
Shallom (class in dicee), 175
Shallom (class in dicee.models), 64
Shallom (class in dicee.models.real), 43
shallom (dicee.models.real.Shallom attribute), 43
shallom (dicee.models.Shallom attribute), 64
shallom (dicee.Shallom attribute), 175
shallom width (dicee.models.real.Shallom attribute), 43
shallom_width (dicee.models.Shallom attribute), 64
shallom_width (dicee.Shallom attribute), 175
single_hop_query_answering() (dicee.KGE method), 187
single_hop_query_answering() (dicee.knowledge_graph_embeddings.KGE method), 149
sparql_endpoint (dicee.config.Namespace attribute), 126
sparql_endpoint (dicee.knowledge_graph.KG attribute), 145
start() (dicee.DICE_Trainer method), 184
start () (dicee. Execute method), 190
start () (dicee.executer.Execute method), 144
start() (dicee.read_preprocess_save_load_kg.PreprocessKG method), 103
start() (dicee.read_preprocess_save_load_kg.preprocess.PreprocessKG method), 98
\verb|start|| (\textit{dicee.read\_preprocess\_save\_load\_kg.read\_from\_disk.ReadFromDisk\ method)}, 98
start() (dicee.read_preprocess_save_load_kg.ReadFromDisk method), 104
start () (dicee.trainer.DICE_Trainer method), 111
start () (dicee.trainer.dice trainer.DICE Trainer method), 107
start_time (dicee.callbacks.PrintCallback attribute), 120
start_time (dicee.Execute attribute), 189
start_time (dicee.executer.Execute attribute), 143
storage_path (dicee.config.Namespace attribute), 126
storage_path (dicee.DICE_Trainer attribute), 184
storage_path (dicee.Execute attribute), 189
storage_path (dicee.executer.Execute attribute), 143
storage_path (dicee.trainer.DICE_Trainer attribute), 110
storage_path (dicee.trainer.dice_trainer.DICE_Trainer attribute), 107
store (dicee. Allvs All attribute), 194
store (dicee.dataset_classes.AllvsAll attribute), 132
store (dicee.dataset_classes.KvsSampleDataset attribute), 135
store (dicee.KvsSampleDataset attribute), 196
store () (in module dicee), 182
store() (in module dicee.static_funcs), 154
\verb|store_ensemble()| \textit{(dicee.abstracts.AbstractPPECallback method)}, 117
strategy (dicee.abstracts.AbstractTrainer attribute), 112
swa (dicee.config.Namespace attribute), 128
Т
T() (dicee.DualE method), 167
T() (dicee.models.DualE method), 97
T() (dicee.models.dualE.DualE method), 31
t_conorm() (dicee.KGE method), 187
t_conorm() (dicee.knowledge_graph_embeddings.KGE method), 149
t_norm() (dicee.KGE method), 187
t_norm() (dicee.knowledge_graph_embeddings.KGE method), 149
target_dim (dicee.AllvsAll attribute), 194
target_dim (dicee.dataset_classes.AllvsAll attribute), 132
target_dim (dicee.dataset_classes.MultiLabelDataset attribute), 130
```

```
target dim (dicee.dataset classes.OnevsAllDataset attribute), 131
target_dim (dicee.knowledge_graph.KG attribute), 146
target_dim (dicee.MultiLabelDataset attribute), 191
target_dim (dicee.OnevsAllDataset attribute), 192
temperature (dicee. BytE attribute), 178
temperature (dicee.models.transformers.BytE attribute), 45
tensor_t_norm() (dicee.KGE method), 187
tensor_t_norm() (dicee.knowledge_graph_embeddings.KGE method), 149
test_dataloader() (dicee.models.base_model.BaseKGELightning method), 14
test_dataloader() (dicee.models.BaseKGELightning method), 54
test_epoch_end() (dicee.models.base_model.BaseKGELightning method), 14
test_epoch_end() (dicee.models.BaseKGELightning method), 54
test_h1 (dicee.analyse_experiments.Experiment attribute), 118
test_h3 (dicee.analyse_experiments.Experiment attribute), 118
test_h10 (dicee.analyse_experiments.Experiment attribute), 118
test_mrr (dicee.analyse_experiments.Experiment attribute), 118
test_path (dicee.query_generator.QueryGenerator attribute), 150
test_path (dicee.QueryGenerator attribute), 201
timeit() (in module dicee), 182, 190
timeit() (in module dicee.read_preprocess_save_load_kg.util), 101
timeit() (in module dicee.static_funcs), 153
timeit() (in module dicee.static_preprocess_funcs), 156
to() (dicee.KGE method), 185
to() (dicee.knowledge_graph_embeddings.KGE method), 146
to_df() (dicee.analyse_experiments.Experiment method), 118
topk (dicee.BytE attribute), 178
topk (dicee.models.transformers.BytE attribute), 45
torch_ordered_shaped_bpe_entities (dicee.dataset_classes.MultiLabelDataset attribute), 130
{\tt torch\_ordered\_shaped\_bpe\_entities}~(\textit{dicee.MultiLabelDataset attribute}),~191
TorchDDPTrainer (class in dicee.trainer.torch_trainer_ddp), 109
TorchTrainer (class in dicee.trainer.torch_trainer), 108
train() (dicee.KGE method), 188
train() (dicee.knowledge_graph_embeddings.KGE method), 150
train() (dicee.trainer.torch_trainer_ddp.NodeTrainer method), 110
train_data (dicee. Allvs All attribute), 193
train_data (dicee.dataset_classes.AllvsAll attribute), 132
train data (dicee.dataset classes.KvsAll attribute), 131
train_data (dicee.dataset_classes.KvsSampleDataset attribute), 135
train_data (dicee.dataset_classes.MultiClassClassificationDataset attribute), 130
train_data (dicee.dataset_classes.OnevsAllDataset attribute), 131
train_data (dicee.dataset_classes.OnevsSample attribute), 133
train_data (dicee.KvsAll attribute), 193
train_data (dicee.KvsSampleDataset attribute), 196
train_data (dicee.MultiClassClassificationDataset attribute), 192
train_data (dicee.OnevsAllDataset attribute), 192
train_data (dicee.OnevsSample attribute), 194, 195
train_dataloader() (dicee.CVDataModule method), 198
train_dataloader() (dicee.dataset_classes.CVDataModule method), 137
train_dataloader() (dicee.models.base_model.BaseKGELightning method), 16
train_dataloader() (dicee.models.BaseKGELightning method), 56
train_dataloaders (dicee.trainer.torch_trainer.TorchTrainer attribute), 108
train_dataset_loader (dicee.trainer.torch_trainer_ddp.NodeTrainer attribute), 110
train_h1 (dicee.analyse_experiments.Experiment attribute), 118
train_h3 (dicee.analyse_experiments.Experiment attribute), 118
train_h10 (dicee.analyse_experiments.Experiment attribute), 118
train_indices_target (dicee.dataset_classes.MultiLabelDataset attribute), 130
train_indices_target (dicee.MultiLabelDataset attribute), 191
{\tt train\_k\_vs\_all()} \ (\textit{dicee.KGE method}), \, 188
train_k_vs_all() (dicee.knowledge_graph_embeddings.KGE method), 150
train_mrr (dicee.analyse_experiments.Experiment attribute), 118
train path (dicee.query generator.QueryGenerator attribute), 150
train_path (dicee.QueryGenerator attribute), 201
train_set (dicee.BPE_NegativeSamplingDataset attribute), 190
train_set (dicee.dataset_classes.BPE_NegativeSamplingDataset attribute), 129
train_set (dicee.dataset_classes.MultiLabelDataset attribute), 130
train_set (dicee.dataset_classes.NegSampleDataset attribute), 135
train_set (dicee.dataset_classes.TriplePredictionDataset attribute), 136
train_set (dicee.MultiLabelDataset attribute), 191
```

```
train set (dicee.NegSampleDataset attribute), 196
train_set (dicee. TriplePredictionDataset attribute), 197
train_set_idx (dicee.CVDataModule attribute), 198
train_set_idx (dicee.dataset_classes.CVDataModule attribute), 137
train_set_target (dicee.knowledge_graph.KG attribute), 145
train_target (dicee.AllvsAll attribute), 194
train_target (dicee.dataset_classes.AllvsAll attribute), 132
train target (dicee.dataset classes.KvsAll attribute), 131
train_target (dicee.dataset_classes.KvsSampleDataset attribute), 135
train_target (dicee.KvsAll attribute), 193
train_target (dicee.KvsSampleDataset attribute), 196
\verb|train_target_indices|| \textit{dicee.knowledge\_graph.KG attribute}||, 146
train_triples() (dicee.KGE method), 188
train_triples() (dicee.knowledge_graph_embeddings.KGE method), 150
trained_model (dicee.Execute attribute), 189
trained_model (dicee.executer.Execute attribute), 143
trainer (dicee.config.Namespace attribute), 126
trainer (dicee.DICE_Trainer attribute), 184
trainer (dicee. Execute attribute), 189
trainer (dicee.executer.Execute attribute), 143
trainer (dicee.trainer.DICE_Trainer attribute), 110
trainer (dicee.trainer.dice_trainer.DICE_Trainer attribute), 107
trainer (dicee.trainer.torch_trainer_ddp.NodeTrainer attribute), 109
training_step (dicee.trainer.torch_trainer.TorchTrainer attribute), 108
training_step() (dicee.BytE method), 178
training_step() (dicee.models.base_model.BaseKGELightning method), 13
training_step() (dicee.models.BaseKGELightning method), 53
training_step() (dicee.models.transformers.BytE method), 46
training_step_outputs (dicee.models.base_model.BaseKGELightning attribute), 13
training_step_outputs (dicee.models.BaseKGELightning attribute), 53
training_technique (dicee.knowledge_graph.KG attribute), 145
TransE (class in dicee), 163
TransE (class in dicee.models), 64
TransE (class in dicee.models.real), 43
transfer_batch_to_device() (dicee.CVDataModule method), 199
transfer_batch_to_device() (dicee.dataset_classes.CVDataModule method), 138
transformer (dicee.BytE attribute), 178
transformer (dicee.models.transformers.BytE attribute), 45
transformer (dicee.models.transformers.GPT attribute), 50
trapezoid() (dicee.models.FMult2 method), 95
trapezoid() (dicee.models.function_space.FMult2 method), 33
tri_score() (dicee.LFMult method), 176
tri_score() (dicee.models.function_space.LFMult method), 34
tri_score() (dicee.models.function_space.LFMult1 method), 34
tri_score() (dicee.models.LFMult method), 96
tri_score() (dicee.models.LFMult1 method), 95
triple_score() (dicee.KGE method), 187
triple_score() (dicee.knowledge_graph_embeddings.KGE method), 148
TriplePredictionDataset (class in dicee), 197
TriplePredictionDataset (class in dicee.dataset_classes), 135
{\tt tuned\_embedding\_dim}~(\textit{dicee.models.FMult2 attribute}), 94
tuned_embedding_dim (dicee.models.function_space.FMult2 attribute), 33
tuple2list() (dicee.query_generator.QueryGenerator method), 151
tuple2list() (dicee.QueryGenerator method), 201
unlabelled_size (dicee.callbacks.PseudoLabellingCallback attribute), 122
unmap() (dicee.query_generator.QueryGenerator method), 151
unmap () (dicee.QueryGenerator method), 202
unmap_query() (dicee.query_generator.QueryGenerator method), 151
unmap_query() (dicee.QueryGenerator method), 202
val_aswa (dicee.callbacks.ASWA attribute), 122
val_dataloader() (dicee.models.base_model.BaseKGELightning method), 15
val_dataloader() (dicee.models.BaseKGELightning method), 55
val_h1 (dicee.analyse_experiments.Experiment attribute), 118
```

```
val h3 (dicee.analyse experiments.Experiment attribute), 118
val_h10 (dicee.analyse_experiments.Experiment attribute), 118
val_mrr (dicee.analyse_experiments.Experiment attribute), 118
val_path (dicee.query_generator.QueryGenerator attribute), 150
val_path (dicee.QueryGenerator attribute), 201
validate_knowledge_graph() (in module dicee.sanity_checkers), 152
vocab_preparation() (dicee.evaluator.Evaluator method), 141
vocab_size (dicee.models.transformers.GPTConfig attribute), 49
vocab_to_parquet() (in module dicee), 183
vocab_to_parquet() (in module dicee.static_funcs), 154
vtp_score() (dicee.LFMult method), 176
vtp_score() (dicee.models.function_space.LFMult method), 34
vtp_score() (dicee.models.function_space.LFMult1 method), 34
\verb|vtp_score|()| \textit{(dicee.models.LFMult method)}, 96
vtp_score() (dicee.models.LFMult1 method), 95
W
weight (dicee.BytE attribute), 178
weight (dicee.models.transformers.BytE attribute), 45
weight (dicee.models.transformers.GPT attribute), 50
weight (dicee.models.transformers.LayerNorm attribute), 47
weight_decay (dicee.BaseKGE attribute), 180
weight_decay (dicee.config.Namespace attribute), 127
weight_decay (dicee.models.base_model.BaseKGE attribute), 19
weight_decay (dicee.models.BaseKGE attribute), 59, 62, 65, 70, 76, 89, 92
weights (dicee.models.FMult attribute), 94
weights (dicee.models.function_space.FMult attribute), 32
weights (dicee.models.function_space.GFMult attribute), 33
weights (dicee.models.GFMult attribute), 94
write_links() (dicee.query_generator.QueryGenerator method), 151
write_links() (dicee.QueryGenerator method), 202
write_report() (dicee.Execute method), 190
write_report() (dicee.executer.Execute method), 144
X
x_values (dicee.LFMult attribute), 175
x_values (dicee.models.function_space.LFMult attribute), 34
x_values (dicee.models.LFMult attribute), 95
```