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# DICE Embeddings

*Release 0.1.3.2*

**Caglar Demir**

Aug 07, 2025

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

## 1 Dicee Manual

**Version:** dicee 0.2.0

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

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

**Contact:** [caglar.demir@upb.de](mailto: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-CPU, GPUs, TPUs or computing cluster, and
3. **Huggingface**<sup>5</sup> to ease the deployment of pre-trained models.

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

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

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

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

<sup>2</sup> <https://github.com/Demirrr>

<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["Test"]["MRR"]) # => 0.8155
# See the Keci_UMLS folder embeddings and all other files
```

where the data is in the following form

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

A KGE model can also be trained from the command line

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

dicee automatically detects available GPUs and trains a model with distributed data parallels technique. Under the hood, dicee uses lightning 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 lightning 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
# {'H@1': 0.9518788343558282, 'H@3': 0.9988496932515337, 'H@10': 1.0, 'MRR': 0.
↪ 9753123402351737}
# Evaluate Keci on Validation set: Evaluate Keci on Validation set
# {'H@1': 0.6932515337423313, 'H@3': 0.9041411042944786, 'H@10': 0.9754601226993865,
↪ 'MRR': 0.8072362996241839}
# Evaluate Keci on Test set: Evaluate Keci on Test set
# {'H@1': 0.6951588502269289, 'H@3': 0.9039334341906202, 'H@10': 0.9750378214826021,
↪ 'MRR': 0.8064032293278861}

# (2)
CUDA_VISIBLE_DEVICES=0,1 python dicee/scripts/run.py --trainer PL --dataset_dir "KGs/
↪ UMLS" --model Keci --eval_model "train_val_test"
# Evaluate Keci on Train set: Evaluate Keci on Train set
# {'H@1': 0.9518788343558282, 'H@3': 0.9988496932515337, 'H@10': 1.0, 'MRR': 0.
↪ 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

```
$ head -3 KGs/Family/train.txt
_:1 <http://www.w3.org/1999/02/22-rdf-syntax-ns#type> <http://www.w3.org/2002/07/owl
→#Ontology> .
<http://www.benchmark.org/family#hasChild> <http://www.w3.org/1999/02/22-rdf-syntax-ns
→#type> <http://www.w3.org/2002/07/owl#ObjectProperty> .
<http://www.benchmark.org/family#hasParent> <http://www.w3.org/1999/02/22-rdf-syntax-
→ns#type> <http://www.w3.org/2002/07/owl#ObjectProperty> .
```

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

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

For more, please refer to examples.

## 6 Creating an Embedding Vector Database

### 6.1 Learning Embeddings

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

## 6.2 Loading Embeddings into Qdrant Vector Database

```
# Ensure that Qdrant available
# docker pull qdrant/qdrant && docker run -p 6333:6333 -p 6334:6334 -v $(pwd)/
↪qdrant_storage:/qdrant/storage:z qdrant/qdrant
diceeindex --path_model "CountryEmbeddings" --collection_name "dummy" --location
↪"localhost"
```

## 6.3 Launching Webservice

```
diceeserve --path_model "CountryEmbeddings" --collection_name "dummy" --collection_
↪location "localhost"
```

### Retrieve and Search

Get embedding of germany

```
curl -X 'GET' 'http://0.0.0.0:8000/api/get?q=germany' -H 'accept: application/json'
```

Get most similar things to europe

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

## 7 Answering Complex Queries

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

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```
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, ↵
↵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://
↵www.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/](https://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/___init___ .py	7	0	100%	
dicee/abstracts.py	338	115	66%	112-113, 115

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

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



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↪131, 154-155, 160, 173, 197, 240-254, 290, 303-306, 309-313, 353-364, 379-387, 402, ↪				
↪413-417, 427-428, 434-436, 442-445, 448-453, 576-596, 602-606, 610-612, 631, 658-696				
dicee/callbacks.py	248	103	58%	50-55, ↪
↪67-73, 76, 88-93, 98-103, 106-109, 116-133, 138-142, 146-147, 247, 281-285, 291-292, ↪				
↪310-316, 319, 324-325, 337-343, 349-358, 363-365, 410, 421-434, 438-473, 485-491				
dicee/config.py	97	2	98%	146-147
dicee/dataset_classes.py	430	146	66%	16, 44, ↪
↪57, 89-98, 104, 111-118, 121, 124, 127-151, 207-213, 216, 219-221, 324, 335-338, ↪				
↪354, 420-421, 439, 562-581, 583, 587-599, 606-615, 618, 622-636, 780-787, 790-794, ↪				
↪845, 866-878, 902-915, 937, 941-954, 964-967, 973, 985, 987, 989, 1012-1022				
dicee/eval_static_funcs.py	256	100	61%	104, 109, ↪
↪114, 261-356, 363-414, 442, 465-468				
dicee/evaluator.py	267	48	82%	48, 53, ↪
↪58, 77, 82-83, 86, 102, 119, 130, 134, 139, 173-184, 191-202, 310, 340-358, 452, ↪				
↪462, 480-485				
dicee/executer.py	134	16	88%	53-57, ↪
↪166-176, 235-236, 283				
dicee/knowledge_graph.py	82	10	88%	84, 94- ↪
↪95, 124, 128, 132-134, 137-138, 140				
dicee/knowledge_graph_embeddings.py	654	415	37%	25, 28- ↪
↪29, 37-50, 55-88, 91-125, 129-137, 171, 173-229, 261, 265, 276-277, 301-303, 311, ↪				
↪339-362, 493, 497-519, 523-547, 580, 656, 665, 710-716, 748, 806-1171, 1202-1263, ↪				
↪1267-1295, 1326, 1332				
dicee/models/___init___py	9	0	100%	
dicee/models/adopt.py	187	172	8%	50-86, ↪
↪99-110, 129-185, 195-242, 266-322, 346-448, 484-517				
dicee/models/base_model.py	240	35	85%	30-35, ↪
↪64, 66, 92, 99-116, 171, 204, 244, 250, 259, 262, 266, 273, 277, 279, 294, 307-308, ↪				
↪362, 365, 438, 450				
dicee/models/clifford.py	470	278	41%	10, 12, ↪
↪16, 24-25, 52-56, 79-87, 101-103, 108-109, 140-160, 184, 191, 195-256, 273-277, 289, ↪				
↪292, 297, 302, 346-361, 377-444, 464-470, 483, 486, 491, 496, 525-531, 544, 547, ↪				
↪552, 557, 567-576, 592-593, 613-685, 696-699, 724-749, 773-806, 842-846, 859, 869, ↪				
↪872, 877, 882, 887, 891, 895, 904-905, 935, 942, 947, 975-979, 1007-1016, 1026-1034, ↪				
↪1052-1054, 1072-1074, 1090-1092				
dicee/models/complex.py	162	25	85%	86-109, ↪
↪273-287				
dicee/models/dualE.py	59	10	83%	93-102, ↪
↪142-156				
dicee/models/ensemble.py	89	67	25%	7-29, 31, ↪
↪34, 37, 40, 43, 46, 49, 52-54, 56-58, 64-68, 71-90, 93-94, 97-112, 131				
dicee/models/function_space.py	262	221	16%	10-23, ↪
↪27-36, 39-48, 52-69, 76-87, 90-99, 102-111, 115-127, 135-157, 160-166, 169-186, 189- ↪				
↪195, 198-206, 209, 214-235, 244-247, 251-255, 259-268, 272-293, 302-308, 312-329, ↪				
↪333-336, 345-353, 356, 367-373, 393-407, 425-439, 444-454, 462-466, 475-479				
dicee/models/literal.py	33	1	97%	82
dicee/models/octonion.py	227	83	63%	21-44, ↪
↪320-329, 334-345, 348-370, 374-416, 426-474				
dicee/models/pykeen_models.py	55	5	91%	77-80, ↪
↪135				
dicee/models/quaternion.py	192	69	64%	7-21, 30- ↪
↪55, 68-72, 107, 185, 328-342, 345-364, 368-389, 399-426				

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dicee/models/real.py	61	12	80%	37-42, ↵
↪70-73, 91, 107-110				
dicee/models/static_funcs.py	10	0	100%	
dicee/models/transformers.py	234	189	19%	20-39, ↵
↪42, 56-71, 80-98, 101-112, 119-121, 124, 130-147, 151-176, 182-186, 189-193, 199-				
↪203, 206-208, 225-252, 261-264, 267-272, 275-300, 306-311, 315-368, 372-394, 400-410				
dicee/query_generator.py	374	346	7%	17-51, ↵
↪55, 61-64, 68-69, 77-91, 99-146, 154-187, 191-205, 211-268, 273-302, 306-442, 452-				
↪471, 479-502, 509-513, 518, 523-529				
dicee/read_preprocess_save_load_kg/___init___py	3	0	100%	
dicee/read_preprocess_save_load_kg/preprocess.py	243	40	84%	33, 39, ↵
↪76, 100-125, 131, 136-149, 175, 205, 380-381				
dicee/read_preprocess_save_load_kg/read_from_disk.py	36	11	69%	34, 38-
↪40, 47, 55, 58-72				
dicee/read_preprocess_save_load_kg/save_load_disk.py	53	21	60%	29-30, ↵
↪38, 47-68				
dicee/read_preprocess_save_load_kg/util.py	236	125	47%	159, 173-
↪175, 179-180, 198-204, 207-209, 214-216, 230, 244-247, 252-260, 265-271, 276-281, ↵				
↪286-291, 303-324, 330-386, 390-394, 398-399, 403, 407-408, 436, 441, 448-449				
dicee/sanity_checkers.py	47	19	60%	8-12, 21-
↪31, 46, 51, 58, 69-79				
dicee/static_funcs.py	483	194	60%	42, 52, ↵
↪58-63, 85, 92-96, 109-119, 129-131, 136, 143, 167, 172, 184, 190, 198, 202, 229-233,				
↪295, 303-309, 320-330, 341-361, 389, 413-414, 419-420, 437-438, 440-441, 443-444, ↵				
↪452, 470-474, 491-494, 498-503, 507-511, 515-516, 522-524, 539-553, 558-561, 566-				
↪569, 578-629, 634-646, 663-680, 683-691, 695-713, 724				
dicee/static_funcs_training.py	155	66	57%	7-10, ↵
↪222-319, 327-328				
dicee/static_preprocess_funcs.py	98	43	56%	17-25, ↵
↪50, 57, 59, 70, 83-107, 112-115, 120-123, 128-131				
dicee/trainer/___init___py	1	0	100%	
dicee/trainer/dice_trainer.py	151	18	88%	22, 30-
↪31, 33-35, 97, 104, 109-114, 152, 237, 280-283				
dicee/trainer/model_parallelism.py	99	87	12%	10-25, ↵
↪30-116, 121-132, 136, 141-197				
dicee/trainer/torch_trainer.py	77	6	92%	31, 102, ↵
↪168, 179-181				
dicee/trainer/torch_trainer_ddp.py	89	71	20%	11-14, ↵
↪43, 47-67, 78-94, 113-122, 126-136, 151-158, 168-191				
-----				
TOTAL	6948	3169	54%	

## 13 How to cite

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

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

(continues on next page)

```

    author={Demir, Caglar and Ngonga Ngomo, Axel-Cyrille},
    booktitle={Joint European Conference on Machine Learning and Knowledge Discovery in
↪Databases},
    pages={567--582},
    year={2023},
    organization={Springer}
}
# LitCQD
@inproceedings{demir2023litcq,
    title={LitCQD: Multi-Hop Reasoning in Incomplete Knowledge Graphs with Numeric
↪Literals},
    author={Demir, Caglar and Wiebesiek, Michel and Lu, Renzhong and Ngonga Ngomo, Axel-
↪Cyrille and Heindorf, Stefan},
    booktitle={Joint European Conference on Machine Learning and Knowledge Discovery in
↪Databases},
    pages={617--633},
    year={2023},
    organization={Springer}
}
# DICE Embedding Framework
@article{demir2022hardware,
    title={Hardware-agnostic computation for large-scale knowledge graph embeddings},
    author={Demir, Caglar and Ngomo, Axel-Cyrille Ngonga},
    journal={Software Impacts},
    year={2022},
    publisher={Elsevier}
}
# KronE
@inproceedings{demir2022kronecker,
    title={Kronecker decomposition for knowledge graph embeddings},
    author={Demir, Caglar and Lienen, Julian and Ngonga Ngomo, Axel-Cyrille},
    booktitle={Proceedings of the 33rd ACM Conference on Hypertext and Social Media},
    pages={1--10},
    year={2022}
}
# QMult, OMult, ConvQ, ConvO
@InProceedings{pmlr-v157-demir21a,
    title = {Convolutional Hypercomplex Embeddings for Link Prediction},
    author = {Demir, Caglar and Moussallem, Diego and Heindorf, Stefan and Ngonga
↪Ngomo, Axel-Cyrille},
    booktitle = {Proceedings of The 13th Asian Conference on Machine Learning},
    pages = {656--671},
    year = {2021},
    editor = {Balasubramanian, Vineeth N. and Tsang, Ivor},
    volume = {157},
    series = {Proceedings of Machine Learning Research},
    month = {17--19 Nov},
    publisher = {PMLR},
    pdf = {https://proceedings.mlr.press/v157/demir21a/demir21a.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](mailto:caglar.demir@upb.de)

## 14 dicee

### 14.1 Submodules

**dicee.\_\_main\_\_**

**dicee.abstracts**

**Classes**

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

### Module Contents

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

Abstract class for Trainer class for knowledge graph embedding models

#### Parameter

**args**

[str] ?

**callbacks:** list

?

```

attributes

callbacks

is_global_zero = True

global_rank = 0

local_rank = 0

strategy = None

on_fit_start (*args, **kwargs)
    A function to call callbacks before the training starts.

```

### Parameter

```

    args

    kwargs

    rtype
        None

on_fit_end (*args, **kwargs)
    A function to call callbacks at the ned of the training.

```

### Parameter

```

    args

    kwargs

    rtype
        None

on_train_epoch_start (*args, **kwargs)
    A function to call callbacks at the start of an epoch.

```

### Parameter

```

    args

    kwargs

    rtype
        None

on_train_epoch_end (*args, **kwargs)
    A function to call callbacks at the end of an epoch.

```

### Parameter

```

    args

    kwargs

    rtype
        None

```

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

A function to call callbacks at the end of each mini-batch during training.

### Parameter

args

kwargs

**rtype**

None

**static save\_checkpoint** (full\_path: str, model) → None

A static function to save a model into disk

### Parameter

full\_path : str

model:

**rtype**

None

**class** dicee.abstracts.**BaseInteractiveKGE** (path: str = None, url: str = None,  
construct\_ensemble: bool = False, model\_name: str = None,  
apply\_semantic\_constraint: bool = False)

Abstract/base class for using knowledge graph embedding models interactively.

### Parameter

**path\_of\_pretrained\_model\_dir**

[str] ?

**construct\_ensemble: boolean**

?

model\_name: str apply\_semantic\_constraint : boolean

**construct\_ensemble = False**

**apply\_semantic\_constraint = False**

**configs**

**get\_eval\_report** () → dict

**get\_bpe\_token\_representation** (str\_entity\_or\_relation: List[str] | str) → 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)

**get\_padded\_bpe\_triple\_representation** (triples: List[List[str]]) → Tuple[List, List, List]

### Parameters

**triples**

**set\_model\_train\_mode** () → None  
Setting the model into training mode

### Parameter

**set\_model\_eval\_mode** () → None  
Setting the model into eval mode

### Parameter

**property name**

**sample\_entity** (*n: int*) → List[str]

**sample\_relation** (*n: int*) → List[str]

**is\_seen** (*entity: str = None, relation: str = None*) → bool

**save** () → 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.**InteractiveQueryDecomposition**

**t\_norm** (*tens\_1: torch.Tensor, tens\_2: torch.Tensor, tnorm: str = 'min'*) → torch.Tensor

**tensor\_t\_norm** (*subquery\_scores: torch.FloatTensor, tnorm: str = 'min'*) → torch.FloatTensor

Compute T-norm over  $[0,1]^{n \times d}$  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'*) → torch.Tensor

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

**class** dicee.abstracts.**AbstractCallback**

Bases: abc.ABC, lightning.pytorch.callbacks.Callback

Abstract class for Callback class for knowledge graph embedding models

## Parameter

**on\_init\_start** (\*args, \*\*kwargs)

## Parameter

trainer:

model:

**rtype**

None

**on\_init\_end** (\*args, \*\*kwargs)

Call at the beginning of the training.

## Parameter

trainer:

model:

**rtype**

None

**on\_fit\_start** (trainer, model)

Call at the beginning of the training.



### Parameter

trainer:

model:

**rtype**

None

**on\_train\_epoch\_end** (*trainer, model*)

Call at the end of each epoch during training.

### Parameter

trainer:

model:

**rtype**

None

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

Call at the end of each mini-batch during the training.

### Parameter

trainer:

model:

**rtype**

None

**on\_fit\_end** (*\*args, \*\*kwargs*)

Call at the end of the training.

### Parameter

trainer:

model:

**rtype**

None

```
class dicee.abstracts.AbstractPPECallback (num_epochs, path, epoch_to_start,  
                                           last_percent_to_consider)
```

Bases: [\*AbstractCallback\*](#)

Abstract class for Callback class for knowledge graph embedding models

### Parameter

**num\_epochs**

**path**

**sample\_counter** = 0

**epoch\_count** = 0

**alphas** = None

**on\_fit\_start** (*trainer, model*)

Call at the beginning of the training.

### Parameter

trainer:

model:

**rtype**

None

**on\_fit\_end** (*trainer, model*)

Call at the end of the training.

### Parameter

trainer:

model:

**rtype**

None

**store\_ensemble** (*param\_ensemble*) → None

**class** dicee.abstracts.**BaseInteractiveTrainKGE**

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

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

**train\_k\_vs\_all** (*h, r, iteration=1, lr=0.001*)

Train k vs all :param head\_entity: :param relation: :param iteration: :param lr: :return:

**train** (*kg, lr=0.1, epoch=10, batch\_size=32, neg\_sample\_ratio=10, num\_workers=1*) → None

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

**train\_literals** (*train\_file\_path: str = None, num\_epochs: int = 100, lit\_lr: float = 0.001, lit\_normalization\_type: str = 'z-norm', batch\_size: int = 1024, sampling\_ratio: float = None, random\_seed=1, loader\_backend: str = 'pandas', freeze\_entity\_embeddings: bool = True, gate\_residual: bool = True, device: str = None, shuffle\_data: bool = True*)

Trains the Literal Embeddings model using literal data.

### Parameters

- **train\_file\_path** (*str*) – Path to the training data file.
- **num\_epochs** (*int*) – Number of training epochs.
- **lit\_lr** (*float*) – Learning rate for the literal model.
- **norm\_type** (*str*) – Normalization type to use ('z-norm', 'min-max', or None).
- **batch\_size** (*int*) – Batch size for training.
- **sampling\_ratio** (*float*) – Ratio of training triples to use.

- **loader\_backend** (*str*) – Backend for loading the dataset ('pandas' or 'rdflib').
- **freeze\_entity\_embeddings** (*bool*) – If True, freeze the entity embeddings during training.
- **gate\_residual** (*bool*) – If True, use gate residual connections in the model.
- **device** (*str*) – Device to use for training ('cuda' or 'cpu'). If None, will use available GPU or CPU.
- **suffle\_data** (*bool*) – If True, shuffle the dataset before training.

## **dicee.analyse\_experiments**

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

## **Classes**

---

*Experiment*

---

## **Functions**

---

*get\_default\_arguments()*

*analyse(args)*

---

## **Module Contents**

`dicee.analyse_experiments.get_default_arguments()`

**class** `dicee.analyse_experiments.Experiment`

```

    model_name = []
    callbacks = []
    embedding_dim = []
    num_params = []
    num_epochs = []
    batch_size = []
    lr = []
    byte_pair_encoding = []
    aswa = []
    path_dataset_folder = []

```

```

full_storage_path = []

pq = []

train_mrr = []

train_h1 = []

train_h3 = []

train_h10 = []

val_mrr = []

val_h1 = []

val_h3 = []

val_h10 = []

test_mrr = []

test_h1 = []

test_h3 = []

test_h10 = []

runtime = []

normalization = []

scoring_technique = []

save_experiment(x)

to_df()

dicee.analyse_experiments.analyse(args)

```

## **`dicee.callbacks`**

## Classes

<i>AccumulateEpochLossCallback</i>	Abstract class for Callback class for knowledge graph embedding models
<i>PrintCallback</i>	Abstract class for Callback class for knowledge graph embedding models
<i>KGESaveCallback</i>	Abstract class for Callback class for knowledge graph embedding models
<i>PseudoLabellingCallback</i>	Abstract class for Callback class for knowledge graph embedding models
<i>ASWA</i>	Adaptive stochastic weight averaging
<i>Eval</i>	Abstract class for Callback class for knowledge graph embedding models
<i>KronE</i>	Abstract class for Callback class for knowledge graph embedding models
<i>Perturb</i>	A callback for a three-Level Perturbation
<i>PeriodicEvalCallback</i>	Callback to periodically evaluate the model and optionally save checkpoints during training.
<i>LRScheduler</i>	Callback for managing learning rate scheduling and model snapshots.
<i>SWA</i>	Stochastic Weight Averaging callbacks.

## Functions

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

## Module Contents

**class** `dicee.callbacks.AccumulateEpochLossCallback` (*path: str*)

Bases: `dicee.abstracts.AbstractCallback`

Abstract class for Callback class for knowledge graph embedding models

### Parameter

**path**

**on\_fit\_end** (*trainer, model*) → None

Store epoch loss

### Parameter

trainer:

model:

**rtype**

None

**class** dicee.callbacks.**PrintCallback**

Bases: *dicee.abstracts.AbstractCallback*

Abstract class for Callback class for knowledge graph embedding models

### Parameter

**start\_time**

**on\_fit\_start** (*trainer, pl\_module*)

Call at the beginning of the training.

### Parameter

trainer:

model:

**rtype**

None

**on\_fit\_end** (*trainer, pl\_module*)

Call at the end of the training.

### Parameter

trainer:

model:

**rtype**

None

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

Call at the end of each mini-batch during the training.

### Parameter

trainer:

model:

**rtype**

None

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

Call at the end of each epoch during training.

### Parameter

trainer:

model:

**rtype**

None

```
class dicee.callbacks.KGESaveCallback (every_x_epoch: int, max_epochs: int, path: str)
```

Bases: *dicee.abstracts.AbstractCallback*

Abstract class for Callback class for knowledge graph embedding models

### Parameter

**every\_x\_epoch**

**max\_epochs**

**epoch\_counter** = 0

**path**

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

Call at the end of each mini-batch during the training.

### Parameter

trainer:

model:

**rtype**

None

**on\_fit\_start** (trainer, pl\_module)

Call at the beginning of the training.

### Parameter

trainer:

model:

**rtype**

None

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

Call at the end of each epoch during training.

### Parameter

trainer:

model:

**rtype**

None

**on\_fit\_end** (\*args, \*\*kwargs)

Call at the end of the training.

## Parameter

trainer:

model:

**rtype**

None

**on\_epoch\_end**(*model, trainer, \*\*kwargs*)

**class** `dicee.callbacks.PseudoLabellingCallback`(*data\_module, kg, batch\_size*)

Bases: `dicee.abstracts.AbstractCallback`

Abstract class for Callback class for knowledge graph embedding models

## Parameter

**data\_module**

**kg**

**num\_of\_epochs** = 0

**unlabelled\_size**

**batch\_size**

**create\_random\_data**()

**on\_epoch\_end**(*trainer, model*)

`dicee.callbacks.estimate_q`(*eps*)

estimate rate of convergence q from sequence esp

`dicee.callbacks.compute_convergence`(*seq, i*)

**class** `dicee.callbacks.ASWA`(*num\_epochs, path*)

Bases: `dicee.abstracts.AbstractCallback`

Adaptive stochastic weight averaging ASWE keeps track of the validation performance and update s the ensemble model accordingly.

**path**

**num\_epochs**

**initial\_eval\_setting** = None

**epoch\_count** = 0

**alphas** = []

**val\_aswa** = -1

**on\_fit\_end**(*trainer, model*)

Call at the end of the training.



## Parameter

trainer:

model:

**rtype**

None

**static compute\_mrr** (*trainer, model*) → 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** = None

**epoch\_counter** = 0

**on\_fit\_start** (*trainer, model*)

Call at the beginning of the training.

### Parameter

trainer:

model:

**rtype**

None

**on\_fit\_end**(*trainer, model*)

Call at the end of the training.

### Parameter

trainer:

model:

**rtype**

None

**on\_train\_epoch\_end**(*trainer, model*)

Call at the end of each epoch during training.

### Parameter

trainer:

model:

**rtype**

None

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

Call at the end of each mini-batch during the training.

### Parameter

trainer:

model:

**rtype**

None

**class** dicee.callbacks.**KronE**

Bases: *dicee.abstracts.AbstractCallback*

Abstract class for Callback class for knowledge graph embedding models

### Parameter

**f** = None

**static batch\_kronecker\_product**(*a, b*)

Kronecker product of matrices a and b with leading batch dimensions. Batch dimensions are broadcast. The number of them must be the same. :type a: torch.Tensor :type b: torch.Tensor :rtype: torch.Tensor

**get\_kronecker\_triple\_representation** (*indexed\_triple: torch.LongTensor*)

Get kronecker embeddings

**on\_fit\_start** (*trainer, model*)

Call at the beginning of the training.

### Parameter

trainer:

model:

**rtype**

None

**class** `dicce.callbacks.Perturb` (*level: str = 'input', ratio: float = 0.0, method: str = None, scaler: float = None, frequency=None*)

Bases: `dicce.abstracts.AbstractCallback`

A callback for a three-Level Perturbation

Input Perturbation: During training an input *x* is perturbed by randomly replacing its element. In the context of knowledge graph embedding models, *x* can denote a triple, a tuple of an entity and a relation, or a tuple of two entities. A perturbation means that a component of *x* is randomly replaced by an entity or a relation.

Parameter Perturbation:

Output Perturbation:

**level** = 'input'

**ratio** = 0.0

**method** = None

**scaler** = None

**frequency** = None

**on\_train\_batch\_start** (*trainer, model, batch, batch\_idx*)

Called when the train batch begins.

**class** `dicce.callbacks.PeriodicEvalCallback` (*experiment\_path: str, max\_epochs: int, eval\_every\_n\_epoch: int = 0, eval\_at\_epochs: list = None, save\_model\_every\_n\_epoch: bool = True, n\_epochs\_eval\_model: str = 'val\_test'*)

Bases: `dicce.abstracts.AbstractCallback`

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

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

**experiment\_dir**

**max\_epochs**

**epoch\_counter** = 0

**save\_model\_every\_n\_epoch** = True

**reports**

```

n_epochs_eval_model = 'val_test'

default_eval_model = None

eval_epochs

on_fit_end(trainer, model)
    Called at the end of training. Saves final evaluation report.

on_train_epoch_end(trainer, model)
    Called at the end of each training epoch. Performs evaluation and checkpointing if scheduled.

```

**class** `dicee.callbacks.LRScheduler` (*adaptive\_lr\_config: dict, total\_epochs: int, experiment\_dir: str, eta\_max: float = 0.1, snapshot\_dir: str = 'snapshots'*)

Bases: `dicee.abstracts.AbstractCallback`

Callback for managing learning rate scheduling and model snapshots.

Supports cosine annealing (“cca”), MMCCLR (“mmcclr”), and their deferred (warmup) variants: - “deferred\_cca” - “deferred\_mmcclr”

At the end of each learning rate cycle, the model can optionally be saved as a snapshot.

```

total_epochs

experiment_dir

snapshot_dir

batches_per_epoch = None

total_steps = None

cycle_length = None

warmup_steps = None

lr_lambda = None

scheduler = None

step_count = 0

snapshot_loss

on_train_start(trainer, model)
    Initialize training parameters and LR scheduler at start of training.

on_train_batch_end(trainer, model, outputs, batch, batch_idx)
    Step the LR scheduler and save model snapshot if needed after each batch.

on_fit_end(trainer, model)
    Call at the end of the training.

```

## Parameter

trainer:

model:

**rtype**

None

```

class dicee.callbacks.SWA (swa_start_epoch, swa_c_epochs: int = 1, lr_init: float = 0.1,
    swa_lr: float = 0.05, max_epochs: int = None)
    Bases: dicee.abstracts.AbstractCallback
    Stochastic Weight Averaging callbacks.

    swa_start_epoch

    swa_c_epochs = 1

    swa_lr = 0.05

    lr_init = 0.1

    max_epochs = None

    swa_model = None

    swa_n = 0

    current_epoch = -1

    moving_average (swa_model, model, alpha)
        Update SWA model with moving average of current model.

    on_fit_start (trainer, model)
        Initialize SWA model with same architecture as main model.

    on_train_epoch_start (trainer, model)
        Update learning rate according to SWA schedule.

    on_train_epoch_end (trainer, model)
        Apply SWA averaging if conditions are met.

    on_fit_end (trainer, model)
        Replace main model with SWA model at the end of training.

```

## **dicee.config**

### **Classes**

<i>Namespace</i>	Simple object for storing attributes.
------------------	---------------------------------------

### **Module Contents**

```

class dicee.config.Namespace (**kwargs)
    Bases: argparse.Namespace
    Simple object for storing attributes.
    Implements equality by attribute names and values, and provides a simple string representation.

    dataset_dir: str = None
        The path of a folder containing train.txt, and/or valid.txt and/or test.txt

    save_embeddings_as_csv: bool = False
        Embeddings of entities and relations are stored into CSV files to facilitate easy usage.

```

**storage\_path: str = 'Experiments'**

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

**path\_to\_store\_single\_run: str = None**

A single directory created that contains related data about embeddings.

**path\_single\_kg = None**

Path of a file corresponding to the input knowledge graph

**sparql\_endpoint = None**

An endpoint of a triple store.

**model: str = 'Keci'**

KGE model

**optim: str = 'Adam'**

Optimizer

**embedding\_dim: int = 64**

Size of continuous vector representation of an entity/relation

**num\_epochs: int = 150**

Number of pass over the training data

**batch\_size: int = 1024**

Mini-batch size if it is None, an automatic batch finder technique applied

**lr: float = 0.1**

Learning rate

**add\_noise\_rate: float = None**

The ratio of added random triples into training dataset

**gpus = None**

Number GPUs to be used during training

**callbacks**

10}}

**Type**

Callbacks, e.g., {"PPE"

**Type**

{ "last\_percent\_to\_consider"

**backend: str = 'pandas'**

Backend to read, process, and index input knowledge graph. pandas, polars and rdflib available

**separator: str = '\\s+'**

separator for extracting head, relation and tail from a triple

**trainer: str = 'torchCPUTrainer'**

Trainer for knowledge graph embedding model

**scoring\_technique: str = 'KvsAll'**

Scoring technique for knowledge graph embedding models

**neg\_ratio: int = 0**

Negative ratio for a true triple in NegSample training\_technique

**weight\_decay: float = 0.0**  
 Weight decay for all trainable params

**normalization: str = 'None'**  
 LayerNorm, BatchNorm1d, or None

**init\_param: str = None**  
 xavier\_normal or None

**gradient\_accumulation\_steps: int = 0**  
 Not tested e

**num\_folds\_for\_cv: int = 0**  
 Number of folds for CV

**eval\_model: str = 'train\_val\_test'**  
 ["None", "train", "train\_val", "train\_val\_test", "test"]

**Type**  
 Evaluate trained model choices

**save\_model\_at\_every\_epoch: int = None**  
 Not tested

**label\_smoothing\_rate: float = 0.0**

**num\_core: int = 0**  
 Number of CPUs to be used in the mini-batch loading process

**random\_seed: int = 0**  
 Random Seed

**sample\_triples\_ratio: float = None**  
 Read some triples that are uniformly at random sampled. Ratio being between 0 and 1

**read\_only\_few: int = None**  
 Read only first few triples

**pykeen\_model\_kwargs**  
 Additional keyword arguments for pykeen models

**kernel\_size: int = 3**  
 Size of a square kernel in a convolution operation

**num\_of\_output\_channels: int = 32**  
 Number of slices in the generated feature map by convolution.

**p: int = 0**  
 P parameter of Clifford Embeddings

**q: int = 1**  
 Q parameter of Clifford Embeddings

**input\_dropout\_rate: float = 0.0**  
 Dropout rate on embeddings of input triples

**hidden\_dropout\_rate: float = 0.0**  
 Dropout rate on hidden representations of input triples

**feature\_map\_dropout\_rate: float = 0.0**  
 Dropout rate on a feature map generated by a convolution operation

**byte\_pair\_encoding: bool = False**  
 Byte pair encoding

**Type**  
 WIP

**adaptive\_swa: bool = False**  
 Adaptive stochastic weight averaging

**swa: bool = False**  
 Stochastic weight averaging

**block\_size: int = None**  
 block size of LLM

**continual\_learning = None**  
 Path of a pretrained model size of LLM

**auto\_batch\_finding = False**  
 A flag for using auto batch finding

**eval\_every\_n\_epochs: int = 0**  
 Evaluate model every n epochs. If 0, no evaluation is applied.

**save\_every\_n\_epochs: bool = False**  
 Save model every n epochs. If True, save model at every epoch.

**eval\_at\_epochs: list = None**  
 List of epoch numbers at which to evaluate the model (e.g., 1 5 10).

**n\_epochs\_eval\_model: str = 'val\_test'**  
 Evaluating link prediction performance on data splits while performing periodic evaluation.

**adaptive\_lr**  
 0.1}

**Type**  
 Adaptive learning rate parameters, e.g., {"lr\_decay"

**swa\_start\_epoch: int = None**  
 Epoch at which to start applying stochastic weight averaging.

**\_\_iter\_\_()**

## **dicee.dataset\_classes**



## Classes

<code>BPE_NegativeSamplingDataset</code>	An abstract class representing a Dataset.
<code>MultiLabelDataset</code>	An abstract class representing a Dataset.
<code>MultiClassClassificationDataset</code>	Dataset for the 1vsALL training strategy
<code>OnevsAllDataset</code>	Dataset for the 1vsALL training strategy
<code>KvsAll</code>	Creates a dataset for KvsAll training by inheriting from <code>torch.utils.data.Dataset</code> .
<code>AllvsAll</code>	Creates a dataset for AllvsAll training by inheriting from <code>torch.utils.data.Dataset</code> .
<code>OnevsSample</code>	A custom PyTorch Dataset class for knowledge graph embeddings, which includes
<code>KvsSampleDataset</code>	KvsSample a Dataset:
<code>NegSampleDataset</code>	An abstract class representing a Dataset.
<code>TriplePredictionDataset</code>	Triple Dataset
<code>CVDDataModule</code>	Create a Dataset for cross validation
<code>LiteralDataset</code>	Dataset for loading and processing literal data for training Literal Embedding model.

## Functions

<code>reload_dataset(path, form_of_labelling, ...)</code>	Reload the files from disk to construct the Pytorch dataset
<code>construct_dataset(→ torch.utils.data.Dataset)</code>	

## Module Contents

`dicee.dataset_classes.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.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`

**class** `dicee.dataset_classes.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 `__getitems__()`, for speedup batched samples loading. This method accepts list of indices of samples of batch and returns list of samples.

### Note

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

```
train_set
ordered_bpe_entities
num_bpe_entities
neg_ratio
num_datapoints
__len__()
__getitem__(idx)
collate_fn(batch_shaped_bpe_triples: List[Tuple[torch.Tensor, torch.Tensor]])
```

```
class dicee.dataset_classes.MultiLabelDataset (train_set: torch.LongTensor,
        train_indices_target: torch.LongTensor, target_dim: int,
        torch_ordered_shaped_bpe_entities: torch.LongTensor)
```

Bases: `torch.utils.data.Dataset`

An abstract class representing a `Dataset`.

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

#### Note

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

```
train_set
train_indices_target
target_dim
num_datapoints
torch_ordered_shaped_bpe_entities
collate_fn = None
__len__()
__getitem__(idx)
```

```
class dicee.dataset_classes.MultiClassClassificationDataset (
    subword_units: numpy.ndarray, block_size: int = 8)
```

Bases: torch.utils.data.Dataset

Dataset for the 1vsALL training strategy

#### Parameters

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

#### Return type

torch.utils.data.Dataset

**train\_data**

**block\_size** = 8

**num\_of\_data\_points**

**collate\_fn** = None

**\_\_len\_\_**()

**\_\_getitem\_\_**(idx)

```
class dicee.dataset_classes.OnevsAllDataset (train_set_idx: numpy.ndarray, entity_idx
```

Bases: torch.utils.data.Dataset

Dataset for the 1vsALL training strategy

#### Parameters

- **train\_set\_idx** – Indexed triples for the training.
- **entity\_idx**s – mapping.
- **relation\_idx**s – 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.dataset_classes.KvsAll (train_set_idx: numpy.ndarray, entity_idxes, relation_idxes, 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 a 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  $[0, 1]^{|E|}$   $\{I, E\}$  is a binary label.

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

#### Note

TODO

**train\_set\_idx**

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

**entity\_idxes**

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

**relation\_idxes**

[dictionary] 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_idxes, relation_idxes,
    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  $[0, 1]^{|E|}$   $\{I, E\}$  is a binary label.

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

#### 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\_idx**

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

**relation\_idx**

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

self : torch.utils.data.Dataset

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

**train\_data** = None

**train\_target** = None

**label\_smoothing\_rate**

**collate\_fn** = None

**target\_dim**

**\_\_len\_\_**()

**\_\_getitem\_\_**(idx)

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

Bases: torch.utils.data.Dataset

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

### Parameters

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

**train\_data**

The input data converted into a PyTorch tensor.

### Type

torch.Tensor

**num\_entities**

Number of entities in the dataset.

**Type**

int

**num\_relations**

Number of relations in the dataset.

**Type**

int

**neg\_sample\_ratio**

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

**Type**

int

**label\_smoothing\_rate**

The smoothing factor applied to the labels.

**Type**

torch.Tensor

**collate\_fn**

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

**Type**

function, optional

**train\_data**

**num\_entities**

**num\_relations**

**neg\_sample\_ratio = None**

**label\_smoothing\_rate**

**collate\_fn = None**

**\_\_len\_\_()**

Returns the number of samples in the dataset.

**\_\_getitem\_\_(idx)**

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

**Parameters**

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

**Returns**

**A tuple consisting of:**

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

**Return type**  
tuple

```
class dicee.dataset_classes.KvsSampleDataset (train_set_idx: numpy.ndarray, entity_idx,
      relation_idx, 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.

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

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

$\text{new\_y} \ll |E|$  new\_y contains all 1's if  $\text{sum}(y) < \text{neg\_sample\_ratio}$  new\_y contains

**train\_set\_idx**

Indexed triples for the training.

**entity\_idx**

mapping.

**relation\_idx**

mapping.

**form**

?

**store**

?

**label\_smoothing\_rate**

?

torch.utils.data.Dataset

**train\_data** = None

**train\_target** = None

**neg\_ratio** = None

**num\_entities**

**label\_smoothing\_rate**

**collate\_fn** = None

**max\_num\_of\_classes**

**\_\_len\_\_**()

**\_\_getitem\_\_**(idx)

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

Bases: torch.utils.data.Dataset

An abstract class representing a Dataset.

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

**Note**

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

`neg_sample_ratio`

`train_set`

`length`

`num_entities`

`num_relations`

`__len__()`

`__getitem__(idx)`

```
class dicee.dataset_classes.TriplePredictionDataset (train_set: numpy.ndarray,
                                                    num_entities: int, num_relations: int, neg_sample_ratio: int = 1, label_smoothing_rate: float = 0.0)
```

Bases: `torch.utils.data.Dataset`

Triple Dataset

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

.  $x:(h,r, t)$  in KG is a unique  $h$  in  $E$  and a relation  $r$  in  $R$  and . collect\_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\_idx**

mapping.

**relation\_idx**

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.

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

For data processing use the following pattern:

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

However, the above are only necessary for distributed processing.

#### Warning

do not assign state in `prepare_data`

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

#### 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, ...).

#### Note

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

#### Parameters

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

#### Returns

A reference to the data on the new device.

Example:

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

#### See also

- `move_data_to_device()`
- `apply_to_collection()`

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

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

#### Warning

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

Example:

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

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

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

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

Example:

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

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

This is called before requesting the dataloaders:

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

```
class dicee.dataset_classes.LiteralDataset(file_path: str, ent_idx: dict = None,
                                          normalization_type: str = 'z-norm', sampling_ratio: float = None, loader_backend: str = 'pandas')
```

Bases: `torch.utils.data.Dataset`

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

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

**train\_file\_path**

Path to the training data file.

**Type**

str

**normalization**

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

**Type**

str

**normalization\_params**

Parameters used for normalization.

**Type**

dict

**sampling\_ratio**

Fraction of the training set to use for ablations.

**Type**

float

**entity\_to\_idx**

Mapping of entities to their indices.

**Type**

dict

**num\_entities**

Total number of entities.

**Type**

int

**data\_property\_to\_idx**

Mapping of data properties to their indices.

**Type**

dict

**num\_data\_properties**

Total number of data properties.

**Type**

int

**loader\_backend**

Backend to use for loading data ('pandas' or 'rdflib').

**Type**

str

**train\_file\_path**

**loader\_backend** = 'pandas'

**normalization\_type** = 'z-norm'

**normalization\_params**

**sampling\_ratio** = None

**entity\_to\_idx** = None

**num\_entities**

`__getitem__(index)`

`__len__()`

**static** `load_and_validate_literal_data` (*file\_path*: str = None, *loader\_backend*: str = 'pandas')  
→ pandas.DataFrame

Loads and validates the literal data file. :param file\_path: Path to the literal data file. :type file\_path: str

**Returns**

DataFrame containing the loaded and validated data.

**Return type**

pd.DataFrame

**static** `denormalize` (*preds\_norm*, *attributes*, *normalization\_params*) → numpy.ndarray

Denormalizes the predictions based on the normalization type.

Args: *preds\_norm* (np.ndarray): Normalized predictions to be denormalized. *attributes* (list): List of attributes corresponding to the predictions. *normalization\_params* (dict): Dictionary containing normalization parameters for each attribute.

**Returns**

Denormalized predictions.

**Return type**

np.ndarray

## dicee.eval\_static\_funcs

### Functions

`evaluate_link_prediction_performance`(→  
Dict)

`evaluate_link_prediction_performance_with_`

`evaluate_link_prediction_performance_with_`

`evaluate_link_prediction_performance_with_`  
...)

`evaluate_lp_bpe_k_vs_all`(model, triples[,  
er\_vocab, ...])

`evaluate_literal_prediction`(kge\_model[, ...]) Evaluates the trained literal prediction model on a test file.

`evaluate_ensemble_link_prediction_performance`(→ Dict) Evaluates link prediction performance of an ensemble of KGE models.

## Module Contents

`dicee.eval_static_funcs.evaluate_link_prediction_performance` (  
    *model*: `dicee.knowledge_graph_embeddings.KGE`, *triples*, *er\_vocab*: Dict[Tuple, List],  
    *re\_vocab*: Dict[Tuple, List]) → Dict

**Parameters**

- **model**
- **triples**
- **er\_vocab**

- **re\_vocab**

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

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

```
dicee.eval_static_funcs.evaluate_link_prediction_performance_with_bpe(
    model: dicee.knowledge_graph_embeddings.KGE, within_entities: List[str], triples: List[Tuple[str]],
    er_vocab: Dict[Tuple, List], re_vocab: Dict[Tuple, List])
```

### Parameters

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

```
dicee.eval_static_funcs.evaluate_lp_bpe_k_vs_all(model, triples: List[List[str]],
    er_vocab=None, batch_size=None, func_triple_to_bpe_representation: Callable = None,
    str_to_bpe_entity_to_idx=None)
```

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

Evaluates the trained literal prediction model on a test file.

### Parameters

- **eval\_file\_path** (*str*) – Path to the evaluation file.
- **store\_lit\_preds** (*bool*) – If True, stores the predictions in a CSV file.
- **eval\_literals** (*bool*) – If True, evaluates the literal predictions and prints error metrics.
- **loader\_backend** (*str*) – Backend for loading the dataset ('pandas' or 'rdflib').

### Returns

DataFrame containing error metrics for each attribute if return\_attr\_error\_metrics is True.

### Return type

pd.DataFrame

### Raises

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

```
dicee.eval_static_funcs.evaluate_ensemble_link_prediction_performance(models, triples,
    er_vocab: Dict[Tuple, List], weights: List[float] = None, batch_size: int = 512,
    weighted_averaging: bool = True) → Dict
```

Evaluates link prediction performance of an ensemble of KGE models. :param models: List of KGE models (snapshots) :param triples: np.ndarray or list of lists, shape (N,3), all integer indices (head, rel, tail) :param er\_vocab: Dict[Tuple, List]

Mapping (head\_idx, rel\_idx) → list of tail\_idx to filter (incl. target).

#### Parameters

- **weights** – Optional[List[float]] Weights for model averaging. If None, use uniform (=simple mean).
- **batch\_size** – int

#### Returns

dict of link prediction metrics (H@1, H@3, H@10, MRR)

## dicee.evaluator

### Classes

<i>Evaluator</i>	Evaluator class to evaluate KGE models in various downstream tasks
------------------	--

### Module Contents

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

Evaluator class to evaluate KGE models in various downstream tasks

Arguments

**re\_vocab** = None

**er\_vocab** = None

**ee\_vocab** = None

**func\_triple\_to\_bpe\_representation** = None

**is\_continual\_training** = None

**num\_entities** = None

**num\_relations** = None

**args**

**report**

**during\_training** = False

**vocab\_preparation** (*dataset*) → 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*)  
→ 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) → 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) → 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)
    → None
    Evaluate model after reciprocal triples are added

evaluate_lp_k_vs_all (model, triple_idx, info=None, form_of_labelling=None)
    Filtered link prediction evaluation. :param model: :param triple_idx: test triples :param info: :param
    form_of_labelling: :return:

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

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

```

#### Parameters

- **model**
- **triples** (*List of lists*)
- **info**
- **form\_of\_labelling**

```

evaluate_lp (model, triple_idx, info: str)

dummy_eval (trained_model, form_of_labelling: str)

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

```

## dicee.executer

### Classes

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

### Module Contents

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

A class for Training, Retraining and Evaluation a model.

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

**args**

**is\_continual\_training** = False

**trainer** = None

**trained\_model** = None

**knowledge\_graph** = None

**report**

**evaluator** = None

**start\_time** = None

**setup\_executor** () → None

**save\_trained\_model** () → None

Save a knowledge graph embedding model

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

### Parameter

**rtype**

None

**end** (*form\_of\_labelling: str*) → 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** () → None

Report training related information in a report.json file

**start** () → dict

Start training

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

### Parameter

**rtype**

A dict containing information about the training and/or evaluation

```
class dicee.executer.ContinuousExecute (args)
```

Bases: *Execute*

A subclass of Execute Class for retraining

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

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

**continual\_start** () → dict

Start Continual Training

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

### Parameter

**rtype**

A dict containing information about the training and/or evaluation

## dicee.knowledge\_graph

### Classes

KG	Knowledge Graph
----	-----------------

### Module Contents

```
class dicee.knowledge_graph.KG (dataset_dir: str = None, byte_pair_encoding: bool = False,
padding: bool = False, add_noise_rate: float = None, sparql_endpoint: str = None,
path_single_kg: str = None, path_for_deserialization: str = None, add_reciprocal: bool = None,
eval_model: str = None, read_only_few: int = None, sample_triples_ratio: float = None,
path_for_serialization: str = None, entity_to_idx=None, relation_to_idx=None, backend=None,
training_technique: str = None, separator: str = None)
```

Knowledge Graph

**dataset\_dir** = None

**sparql\_endpoint** = None

**path\_single\_kg** = None

**byte\_pair\_encoding** = False

**ordered\_shaped\_bpe\_tokens** = None

**add\_noise\_rate** = None

**num\_entities** = None

```

num_relations = None

path_for_deserialization = None

add_reciprocal = None

eval_model = None

read_only_few = None

sample_triples_ratio = None

path_for_serialization = None

entity_to_idx = None

relation_to_idx = None

backend = 'pandas'

training_technique = None

idx_entity_to_bpe_shaped
enc

num_tokens

num_bpe_entities = None

padding = False

dummy_id

max_length_subword_tokens = None

train_set_target = None

target_dim = None

train_target_indices = None

ordered_bpe_entities = None

separator = None

description_of_input = None

describe() → 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

<i>KGE</i>	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`, `dicee.abstracts.InteractiveQueryDecomposition`, `dicee.abstracts.BaseInteractiveTrainKGE`

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

`__str__()`

`to(device: str) → None`

`get_transductive_entity_embeddings(indices: torch.LongTensor | List[str], as_pytorch=False, as_numpy=False, as_list=True) → torch.FloatTensor | numpy.ndarray | List[float]`

`create_vector_database(collection_name: str, distance: str, location: str = 'localhost', port: int = 6333)`

`generate(h="", r="")`

`eval_lp_performance(dataset=List[Tuple[str, str, str]], filtered=True)`

`predict_missing_head_entity(relation: List[str] | str, tail_entity: List[str] | str, within=None, batch_size=2, topk=1, return_indices=False) → Tuple`

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

$\text{argmax}_{\{e \in E\}} f(e, r, t)$ , where  $r \in R$ ,  $t \in E$ .

#### Parameter

`relation`: Union[List[str], str]

String representation of selected relations.

`tail_entity`: Union[List[str], str]

String representation of selected entities.

`k`: int

Highest ranked k entities.

#### Returns: Tuple

Highest K scores and entities

`predict_missing_relations(head_entity: List[str] | str, tail_entity: List[str] | str, within=None, batch_size=2, topk=1, return_indices=False) → Tuple`

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

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

### Parameter

head\_entity: List[str]

String representation of selected entities.

tail\_entity: List[str]

String representation of selected entities.

k: int

Highest ranked k entities.

### Returns: Tuple

Highest K scores and entities

**predict\_missing\_tail\_entity** (*head\_entity: List[str] | str, relation: List[str] | str, within: List[str] = None, batch\_size=2, topk=1, return\_indices=False*) → torch.FloatTensor

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

$\text{argmax}_{\{e \in E\}} f(h, r, e)$ , 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*) → torch.FloatTensor

#### Parameters

- **logits**
- **h**
- **r**
- **t**
- **within**

**predict\_topk** (\*, *h: str | List[str] = None, r: str | List[str] = None, t: str | List[str] = None, topk: int = 10, within: List[str] = None, batch\_size: int = 1024*)

Predict missing item in a given triple.

#### Returns

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

**triple\_score** (*h: List[str] | str = None, r: List[str] | str = None, t: List[str] | str = None, logits=False*)  
→ 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

**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*) → Set

Find missing triples

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

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

Return (e,r,x)

forall 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 and (e,r,x)}

forall G

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

**predict\_literals** (*entity: List[str] | str = None, attribute: List[str] | str = None, denormalize\_preds: bool = True*) → numpy.ndarray

Predicts literal values for given entities and attributes.

#### Parameters

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

#### Returns

Predictions for the given entities and attributes.

#### Return type

numpy ndarray

## dicee.models

### Submodules

#### dicee.models.adopt

### Classes

*ADOPT*

Base class for all optimizers.



## Functions

<code>adopt(params, grads, exp_avgs, exp_avg_sqs, state_steps)</code>	Functional API that performs ADOPT algorithm computation.
---	---

## Module Contents

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

Bases: `torch.optim.optimizer.Optimizer`

Base class for all optimizers.

### Warning

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

### Parameters

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

**clip\_lambda**

**\_\_setstate\_\_** (*state*)

**step** (*closure=None*)

Perform a single optimization step.

### Parameters

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

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

Functional API that performs ADOPT algorithm computation.

## dicee.models.base\_model

### Classes

<i>BaseKGELightning</i>	Base class for all neural network modules.
<i>BaseKGE</i>	Base class for all neural network modules.
<i>IdentityClass</i>	Base class for all neural network modules.

### Module Contents

**class** dicee.models.base\_model.**BaseKGELightning** (\*args, \*\*kwargs)

Bases: lightning.LightningModule

Base class for all neural network modules.

Your models should also subclass this class.

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

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

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

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

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

#### 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.

**training\_step\_outputs** = []

**mem\_of\_model**() → Dict

Size of model in MB and number of params

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

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

#### Parameters

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

### Returns

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

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

Example:

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

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

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

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

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

### 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 `LightningModule` and access them in this hook:

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

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

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

`test_epoch_end(outputs: List[Any])`

`test_dataloader()` → 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()`

#### Note

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

#### Note

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

**`val_dataloader()`** → 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()`

#### Note

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

#### Note

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

**`predict_dataloader()`** → 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()`

#### 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()` → 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()`

#### Note

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

`configure_optimizers` (*parameters=None*)

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

#### Returns

Any of these 6 options.

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

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

```

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

```

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

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

#### Note

Some things to know:

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

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

Bases: `BaseKGELightning`

Base class for all neural network modules.

Your models should also subclass this class.

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

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

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

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

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

#### Note

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

#### Variables

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

**args**

**embedding\_dim** = None

**num\_entities** = None

**num\_relations** = None

**num\_tokens** = None

**learning\_rate** = None

**apply\_unit\_norm** = None

**input\_dropout\_rate** = None

**hidden\_dropout\_rate** = None

**optimizer\_name** = None

**feature\_map\_dropout\_rate** = None

**kernel\_size** = None

**num\_of\_output\_channels** = None

**weight\_decay** = None



```

loss

selected_optimizer = None

normalizer_class = None

normalize_head_entity_embeddings

normalize_relation_embeddings

normalize_tail_entity_embeddings

hidden_normalizer

param_init

input_dp_ent_real

input_dp_rel_real

hidden_dropout

loss_history = []

byte_pair_encoding

max_length_subword_tokens

block_size

forward_byte_pair_encoded_k_vs_all (x: torch.LongTensor)

    Parameters
         $\mathbf{x}$  ( $B \times 2 \times T$ )

forward_byte_pair_encoded_triple (x: Tuple[torch.LongTensor, torch.LongTensor])
    byte pair encoded neural link predictors

    Parameters
    -----

init_params_with_sanity_checking()

forward (x: torch.LongTensor | Tuple[torch.LongTensor, torch.LongTensor],
        y_idx: torch.LongTensor = None)

    Parameters

        •  $\mathbf{x}$ 

        •  $\mathbf{y\_idx}$ 

        • ordered_bpe_entities

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

    Parameters
         $\mathbf{x}$ 

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** ( $B \times 2 \times T$ )

```

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

```

```

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

```

Bases: torch.nn.Module

Base class for all neural network modules.

Your models should also subclass this class.

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

```

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

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

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

```

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

#### Note

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

#### Variables

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

```

args = None

__call__(x)

static forward(x)

```

## dicee.models.clifford

### Classes

<i>Keci</i>	Base class for all neural network modules.
<i>CKeci</i>	Without learning dimension scaling
<i>DeCaL</i>	Base class for all neural network modules.

### Module Contents

**class** dicee.models.clifford.**Keci**(args)

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

Base class for all neural network modules.

Your models should also subclass this class.

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

```

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

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

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

```

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

#### 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<sub>1</sub>, e<sub>2</sub>, e<sub>3</sub>, we compute interactions between e<sub>1</sub> e<sub>2</sub>, e<sub>1</sub> e<sub>3</sub>, and e<sub>2</sub> e<sub>3</sub> 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., e<sub>1</sub>e<sub>1</sub>, e<sub>1</sub>e<sub>2</sub>, e<sub>1</sub>e<sub>3</sub>,

e<sub>2</sub>e<sub>1</sub>, e<sub>2</sub>e<sub>2</sub>, e<sub>2</sub>e<sub>3</sub>, e<sub>3</sub>e<sub>1</sub>, e<sub>3</sub>e<sub>2</sub>, e<sub>3</sub>e<sub>3</sub>

Then select the triangular matrix without diagonals: e<sub>1</sub>e<sub>2</sub>, e<sub>1</sub>e<sub>3</sub>, e<sub>2</sub>e<sub>3</sub>.

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

Compute  $\sigma_{qq} = \sum_{j=1}^{p+q-1} \sum_{k=j+1}^{p+q} (h_{j,r,k} - h_{k,r,j}) e_j e_k$   $\sigma_{qq}$  captures the interactions between along q bases For instance, let q e<sub>1</sub>, e<sub>2</sub>, e<sub>3</sub>, we compute interactions between e<sub>1</sub> e<sub>2</sub>, e<sub>1</sub> e<sub>3</sub>, and e<sub>2</sub> e<sub>3</sub> 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., e<sub>1</sub>e<sub>1</sub>, e<sub>1</sub>e<sub>2</sub>, e<sub>1</sub>e<sub>3</sub>,

e<sub>2</sub>e<sub>1</sub>, e<sub>2</sub>e<sub>2</sub>, e<sub>2</sub>e<sub>3</sub>, e<sub>3</sub>e<sub>1</sub>, e<sub>3</sub>e<sub>2</sub>, e<sub>3</sub>e<sub>3</sub>

Then select the triangular matrix without diagonals: e<sub>1</sub>e<sub>2</sub>, e<sub>1</sub>e<sub>3</sub>, e<sub>2</sub>e<sub>3</sub>.

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

$\sum_{i=1}^p \sum_{j=p+1}^{p+q} (h_{i,r,j} - h_{j,r,i}) e_i e_j$

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

**for j in range(q):**

        sigma\_pq[:, :, i, j] = hp[:, :, i] \* rq[:, :, j] - hq[:, :, j] \* rp[:, :, i]

print(sigma\_pq.shape)

**apply\_coefficients**(hp, hq, rp, rq)

Multiplying a base vector with its scalar coefficient

**clifford\_multiplication**(h0, hp, hq, r0, rp, rq)

Compute our CL multiplication

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

$$e_i^2 = +1 \text{ for } i \leq p \quad e_j^2 = -1 \text{ for } p < j \leq p+q \quad e_i e_j = -e_j e_i \text{ for } i$$

eq j

$$h = \sigma_0 + \sigma_p + \sigma_q + \sigma_{pp} + \sigma_q + \sigma_{pq} \text{ where}$$

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

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

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

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

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

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

**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*) → 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, **IEI**) 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 batches 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.clifford.CKeci` ( $args$ )

Bases: `Keci`

Without learning dimension scaling

**name** = 'CKeci'

**requires\_grad\_for\_interactions** = **False**

**class** `dicee.models.clifford.DeCaL` ( $args$ )

Bases: `dicee.models.base_model.BaseKGE`

Base class for all neural network modules.

Your models should also subclass this class.

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

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

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

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

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

#### **Note**

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

#### **Variables**

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

**name** = 'DeCaL'

**entity\_embeddings**

**relation\_embeddings**

**p**

**q**

**r**

**re**

**forward\_triples** (*x: torch.Tensor*) → torch.FloatTensor

#### **Parameter**

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

**rtype**

torch.FloatTensor with (n) shape

**cl\_pqr** (*a: torch.tensor*) → torch.tensor

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

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

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

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

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

and return:

$$sigma_0 t = \sigma_0 \cdot t_0 = s0 + s1 - s2 s3, s4 \text{ and } s5$$

**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

$$\sigma_{pp} = \sum_{i=1}^{p-1} \sum_{i'=i+1}^p (h_i r_{i'} - h_{i'} r_i) (\text{model the interactions between } e_i \text{ and } e_{i'} \text{ for } 1 \leq i, i' \leq p) \sigma_{qq} = \sum_{j=p+1}^{p+q-1} \sum_{j'=j+1}^{p+q} (h_j r_{j'} - h_{j'} r_j)$$

For different base vector interactions, we have

$$\sigma_{pq} = \sum_{i=1}^p \sum_{j=p+1}^{p+q} (h_i r_j - h_j r_i) (\text{interactions between } e_i \text{ and } e_j \text{ for } 1 \leq i \leq p \text{ and } p+1 \leq j \leq p+q) \sigma_{pr} = \sum_{i=1}^p \sum_{r=p+q+1}^{p+q+r} (h_i r_r - h_r r_i)$$

**forward\_k\_vs\_all** (*x: torch.Tensor*) → 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 functions are identical Parameter ——— *x*: torch.LongTensor with (n, ) shape :rtype: torch.FloatTensor with (n, **IEI**) 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:

$$\sigma_{pp} = \sum_{i=1}^{p-1} \sum_{i'=i+1}^p (x_{i'} y_i - x_i y_{i'})$$

$\sigma_{pp}$  captures the interactions between along p bases For instance, let  $p \in e_1, e_2, e_3$ , 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

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

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\_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\_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

<i>ConEx</i>	Convolutional ComplEx Knowledge Graph Embeddings
<i>AConEx</i>	Additive Convolutional ComplEx Knowledge Graph Em- beddings
<i>Complex</i>	Base class for all neural network modules.

### Module Contents

**class** dicee.models.complex.**ConEx** (*args*)

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

Convolutional ComplEx Knowledge Graph Embeddings

**name** = 'ConEx'

**conv2d**

**fc\_num\_input**

**fc1**

**norm\_fc1**

**bn\_conv2d**

**feature\_map\_dropout**

**residual\_convolution** (*C\_1*: *Tuple[torch.Tensor, torch.Tensor]*,  
*C\_2*: *Tuple[torch.Tensor, torch.Tensor]*) → 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*) → torch.FloatTensor

**forward\_triples** (*x: torch.Tensor*) → torch.FloatTensor

#### Parameters

**x**

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

```
class dicee.models.complex.AConEx (args)
```

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

Additive Convolutional ComplEx Knowledge Graph Embeddings

**name** = 'AConEx'

**conv2d**

**fc\_num\_input**

**fc1**

**norm\_fc1**

**bn\_conv2d**

**feature\_map\_dropout**

**residual\_convolution** (*C\_1: Tuple[torch.Tensor, torch.Tensor],  
C\_2: Tuple[torch.Tensor, torch.Tensor]*) → 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*) → torch.FloatTensor

**forward\_triples** (*x: torch.Tensor*) → torch.FloatTensor

#### Parameters

**x**

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

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

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

Base class for all neural network modules.

Your models should also subclass this class.

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

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

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

(continues on next page)

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

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

### **Note**

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

### **Variables**

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

**name** = 'Complex'

**static score** (*head\_ent\_emb: torch.FloatTensor, rel\_ent\_emb: torch.FloatTensor, tail\_ent\_emb: torch.FloatTensor*)

**static k\_vs\_all\_score** (*emb\_h: torch.FloatTensor, emb\_r: torch.FloatTensor, emb\_E: torch.FloatTensor*)

### **Parameters**

- **emb\_h**
- **emb\_r**
- **emb\_E**

**forward\_k\_vs\_all** (*x: torch.LongTensor*) → *torch.FloatTensor*

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

## **dicee.models.dualE**

### **Classes**

*DualE*

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

### **Module Contents**

**class** `dicee.models.dualE.DualE` (*args*)

Bases: `dicee.models.base_model.BaseKGE`

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

**name** = 'DualE'

**entity\_embeddings**

**relation\_embeddings**

**num\_ent** = None

**kvsall\_score**(*e\_1\_h, e\_2\_h, e\_3\_h, e\_4\_h, e\_5\_h, e\_6\_h, e\_7\_h, e\_8\_h, e\_1\_t, e\_2\_t, e\_3\_t, e\_4\_t, e\_5\_t, e\_6\_t, e\_7\_t, e\_8\_t, r\_1, r\_2, r\_3, r\_4, r\_5, r\_6, r\_7, r\_8*) → torch.tensor

KvsAll scoring function

### Input

x: torch.LongTensor with (n, ) shape

### Output

torch.FloatTensor with (n) shape

**forward\_triples**(*idx\_triple: torch.tensor*) → torch.tensor

Negative Sampling forward pass:

### Input

x: torch.LongTensor with (n, ) shape

### Output

torch.FloatTensor with (n) shape

**forward\_k\_vs\_all**(*x*)

KvsAll forward pass

### Input

x: torch.LongTensor with (n, ) shape

### Output

torch.FloatTensor with (n) shape

**T**(*x: torch.tensor*) → torch.tensor

Transpose function

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

## dicee.models.ensemble

### Classes

---

*EnsembleKGE*

---

## Module Contents

```
class dicee.models.ensemble.EnsembleKGE (seed_model=None, pretrained_models: List = None)

    name

    train_mode = True

    named_children()

    property example_input_array

    parameters()

    modules()

    __iter__()

    __len__()

    eval()

    to (device)

    mem_of_model()

    __call__ (x_batch)

    step()

    get_embeddings()

    __str__()
```

## dicee.models.function\_space

### Classes

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

## Module Contents

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

    Learning Knowledge Neural Graphs

    name = 'FMult'

    entity_embeddings
```

```

relation_embeddings

k

num_sample = 50

gamma

roots

weights

compute_func(weights: torch.FloatTensor, x) → torch.FloatTensor

chain_func(weights, x: torch.FloatTensor)

forward_triples(idx_triple: torch.Tensor) → 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

    k

    num_sample = 250

    roots

    weights

    compute_func(weights: torch.FloatTensor, x) → torch.FloatTensor

    chain_func(weights, x: torch.FloatTensor)

    forward_triples(idx_triple: torch.Tensor) → torch.Tensor

    Parameters
    x

class dicee.models.function_space.FMult2(args)
    Bases: dicee.models.base_model.BaseKGE
    Learning Knowledge Neural Graphs
    name = 'FMult2'
    n_layers = 3

    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) → torch.FloatTensor

function (list_W, list_b)

trapezoid (list_W, list_b)

forward_triples (idx_triple: torch.Tensor) → torch.Tensor

```

#### Parameters

**x**

```
class dicee.models.function_space.LFMult1 (args)
```

Bases: *[dicee.models.base\\_model.BaseKGE](#)*

Embedding with trigonometric functions. We represent all entities and relations in the complex number space as:  $f(x) = \sum_{k=0}^{d-1} w_k e^{kix}$ . 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)

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.  $h = \text{sigma}(w_h^T x + b_h)$ ,  $r = \text{sigma}(w_r^T x + b_r)$ ,  
 $t = \text{sigma}(w_t^T x + b_t)$

**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:

$\text{score}(h,r,t) = \int_0^1 h(x)r(x)t(x) dx = \sum_{i,j,k=0}^{d-1} \text{dfrac}\{a_i*b_j*c_k\} \{1+(i+j+k)\%d\}$

1. generate the range for i,j and k from [0 d-1]
2. perform  $\text{dfrac}\{a_i*b_j*c_k\} \{1+(i+j+k)\%d\}$  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:

$\text{score}(h,r,t) = \int_0^1 h(x)r(x)t(x) dx = \sum_{i,j,k=0}^{d-1} \text{dfrac}\{a_i*c_j*b_k - b_i*c_j*a_k\} \{(1+(i+j)\%d)(1+k)\}$

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 ( $\text{coeff}[0][0] + \text{coeff}[0][1]x + \dots + \text{coeff}[0][d]x^d$ ,

$\text{coeff}[1][0] + \text{coeff}[1][1]x + \dots + \text{coeff}[1][d]x^d$ )

**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 ( $\text{coeff}[0][0] + \text{coeff}[0][1]x + \dots + \text{coeff}[0][d]x^d$ ,

$\text{coeff}[1][0] + \text{coeff}[1][1]x + \dots + \text{coeff}[1][d]x^d$ )

## dicee.models.literal

### Classes

*LiteralEmbeddings*

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

### Module Contents

```
class dicee.models.literal.LiteralEmbeddings (num_of_data_properties: int, embedding_dims: int,
        entity_embeddings: torch.tensor, dropout: float = 0.3, gate_residual=True,
        freeze_entity_embeddings=True)
```

Bases: `torch.nn.Module`

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

**num\_of\_data\_properties**

Number of data properties (attributes).

**Type**

int

**embedding\_dims**

Dimension of the embeddings.

**Type**

int

**entity\_embeddings**

Pre-trained entity embeddings.

**Type**

torch.tensor

**dropout**

Dropout rate for regularization.

**Type**

float

**gate\_residual**

Whether to use gated residual connections.

**Type**

bool

**freeze\_entity\_embeddings**

Whether to freeze the entity embeddings during training.

**Type**

bool

**embedding\_dim**

**num\_of\_data\_properties**

**hidden\_dim**

```

gate_residual = True

freeze_entity_embeddings = True

entity_embeddings

data_property_embeddings

fc

fc_out

dropout

gated_residual_proj

layer_norm

forward(entity_idx, attr_idx)

```

#### Parameters

- **entity\_idx** (*Tensor*) – Entity indices (batch).
- **attr\_idx** (*Tensor*) – Attribute (Data property) indices (batch).

#### Returns

scalar predictions.

#### Return type

Tensor

property device

## dicee.models.octonion

### Classes

<i>OMult</i>	Base class for all neural network modules.
<i>ConvO</i>	Base class for all neural network modules.
<i>AConvO</i>	Additive Convolutional Octonion Knowledge Graph Embeddings

### Functions

<i>octonion_mul</i> (*, O_1, O_2)
<i>octonion_mul_norm</i> (*, O_1, O_2)

### Module Contents

```

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

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

```

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

Base class for all neural network modules.

Your models should also subclass this class.

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

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

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

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

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

#### Note

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

#### Variables

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

```
name = 'OMult'
```

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

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

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

Base class for all neural network modules.

Your models should also subclass this class.

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

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

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

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

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

#### 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*)  $\rightarrow$  torch.Tensor

#### Parameters

**x**

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

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

```

class dicee.models.octonion.AConvO (args: dict)
    Bases: dicee.models.base_model.BaseKGE
    Additive Convolutional Octonion Knowledge Graph Embeddings
    name = 'AConvO'
    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)

```

## **dicee.models.pykeen\_models**

### **Classes**

<i>PykeenKGE</i>	A class for using knowledge graph embedding models implemented in Pykeen
------------------	--

### **Module Contents**

```

class dicee.models.pykeen_models.PykeenKGE (args: dict)
    Bases: dicee.models.base_model.BaseKGE
    A class for using knowledge graph embedding models implemented in Pykeen
    Notes: Pykeen_DistMult: C Pykeen_ComplEx: Pykeen_QuatE: Pykeen_MuRE: Pykeen_CP: Pykeen_HolE: Py-
    keen_HolE: Pykeen_HolE: Pykeen_TransD: Pykeen_TransE: Pykeen_TransF: Pykeen_TransH: Pykeen_TransR:

    model_kwargs
    name
    model

```

```

loss_history = []

args

entity_embeddings = None

relation_embeddings = None

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

    else:
        t = self.entity_embeddings.weight

    # (4) Call the score_t from interactions to generate triple scores. return self.interaction.score_t(h=h, r=r,
    all_entities=t, slice_size=1)

forward_triples (x: torch.LongTensor) → 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)

```

## dicke.models.quaternion

### Classes

<i>QMult</i>	Base class for all neural network modules.
<i>ConvQ</i>	Convolutional Quaternion Knowledge Graph Embeddings
<i>ACConvQ</i>	Additive Convolutional Quaternion Knowledge Graph Embeddings

### Functions

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

## Module Contents

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

**class** `dicee.models.quaternion.QMult` (*args*)

Bases: `dicee.models.base_model.BaseKGE`

Base class for all neural network modules.

Your models should also subclass this class.

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

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

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

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

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

### 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** = 'QMult'

**explicit** = True

**quaternion\_multiplication\_followed\_by\_inner\_product** (*h, r, t*)

### Parameters

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

### Returns

Triple scores.



**static quaternion\_normalizer** (*x*: torch.FloatTensor) → torch.FloatTensor

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

Absolute value of a quaternion

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

L2 norm of quaternion vector:

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

#### Parameters

**x** – The vector.

#### Returns

The normalized vector.

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

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

#### Parameters

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

**forward\_k\_vs\_all** (*x*)

#### Parameters

**x**

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

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

**class** dicee.models.quaternion.**ConvQ** (*args*)

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

Convolutional Quaternion Knowledge Graph Embeddings

**name** = 'ConvQ'

**entity\_embeddings**

**relation\_embeddings**

**conv2d**

**fc\_num\_input**

**fc1**

**bn\_conv1**

**bn\_conv2**

`feature_map_dropout`

`residual_convolution(Q_1, Q_2)`

`forward_triples(indexed_triple: torch.Tensor) → torch.Tensor`

#### Parameters

**x**

`forward_k_vs_all(x: torch.Tensor)`

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

`class dicee.models.quaternion.AConvQ(args)`

Bases: `dicee.models.base_model.BaseKGE`

Additive Convolutional Quaternion Knowledge Graph Embeddings

`name = 'AConvQ'`

`entity_embeddings`

`relation_embeddings`

`conv2d`

`fc_num_input`

`fc1`

`bn_conv1`

`bn_conv2`

`feature_map_dropout`

`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|)

## `dicee.models.real`

### Classes

<code>DistMult</code>	Embedding Entities and Relations for Learning and Inference in Knowledge Bases
<code>TransE</code>	Translating Embeddings for Modeling
<code>Shallom</code>	A shallow neural model for relation prediction ( <a href="https://arxiv.org/abs/2101.09090">https://arxiv.org/abs/2101.09090</a> )
<code>Pyke</code>	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) → 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
```

```
get_embeddings() → Tuple[numpy.ndarray, None]
```

```
forward_k_vs_all(x) → torch.FloatTensor
```

```
forward_triples(x) → torch.FloatTensor
```

### Parameters

**x**

### Returns

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

    Parameters
    x
```

## **`dicee.models.static_funcs`**

### **Functions**

<code>quaternion_mul</code> ( $\rightarrow$ Tuple[torch.Tensor, torch.Tensor, torch.Tensor, torch.Tensor], ...)	Perform quaternion multiplication
---	-----------------------------------

## **Module Contents**

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

## **`dicee.models.transformers`**

Full definition of a GPT Language Model, all of it in this single file. References: 1) the official GPT-2 TensorFlow implementation released by OpenAI: <https://github.com/openai/gpt-2/blob/master/src/model.py> 2) huggingface/transformers PyTorch implementation: [https://github.com/huggingface/transformers/blob/main/src/transformers/models/gpt2/modeling\\_gpt2.py](https://github.com/huggingface/transformers/blob/main/src/transformers/models/gpt2/modeling_gpt2.py)

## **Classes**

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

## Module Contents

**class** dicee.models.transformers.**ByteE**(\*args, \*\*kwargs)

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

Base class for all neural network modules.

Your models should also subclass this class.

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

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

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

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

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

### 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** = 'ByteE'

**config**

**temperature** = 0.5

**topk** = 2

**transformer**

**lm\_head**

**loss\_function**(*yhat\_batch*, *y\_batch*)

### Parameters

- **yhat\_batch**
- **y\_batch**

**forward** (*x*: *torch.LongTensor*)

#### Parameters

**x** (*B by T tensor*)

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

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

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

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

#### Parameters

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

#### Returns

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

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

Example:

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

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

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

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

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

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```
...  
opt2.step()
```

### Note

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

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

Bases: `torch.nn.Module`

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

**weight**

**bias**

**forward**(*input*)

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

Bases: `torch.nn.Module`

Base class for all neural network modules.

Your models should also subclass this class.

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

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

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

### Note

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

## Variables

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

```

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

```

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

Bases: torch.nn.Module

Base class for all neural network modules.

Your models should also subclass this class.

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

```

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

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

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

```

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

#### Note

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

#### Variables

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

```
c_fc
```

```
gelu
```



```

c_proj

dropout

forward(x)

```

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

Bases: torch.nn.Module

Base class for all neural network modules.

Your models should also subclass this class.

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

```

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

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

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

```

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

#### Note

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

#### Variables

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

```

ln_1

attn

ln_2

mlp

forward(x)

```

```
class dicee.models.transformers.GPTConfig
```

```
block_size: int = 1024
```

```
vocab_size: int = 50304
```

```

n_layer: int = 12

n_head: int = 12

n_embd: int = 768

dropout: float = 0.0

bias: bool = False

```

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

Bases: torch.nn.Module

Base class for all neural network modules.

Your models should also subclass this class.

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

```

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

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

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

```

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

### Note

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

### Variables

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

**config**

**transformer**

**lm\_head**

**get\_num\_params** (*non\_embedding=True*)

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

**forward** (*idx*, *targets=None*)

**crop\_block\_size** (*block\_size*)

**classmethod from\_pretrained** (*model\_type*, *override\_args=None*)

**configure\_optimizers** (*weight\_decay*, *learning\_rate*, *betas*, *device\_type*)

**estimate\_mfu** (*fwdbwd\_per\_iter*, *dt*)  
 estimate model flops utilization (MFU) in units of A100 bfloat16 peak FLOPS

## Classes

<i>ADOPT</i>	Base class for all optimizers.
<i>BaseKGELightning</i>	Base class for all neural network modules.
<i>BaseKGE</i>	Base class for all neural network modules.
<i>IdentityClass</i>	Base class for all neural network modules.
<i>BaseKGE</i>	Base class for all neural network modules.
<i>DistMult</i>	Embedding Entities and Relations for Learning and Inference in Knowledge Bases
<i>TransE</i>	Translating Embeddings for Modeling
<i>Shallom</i>	A shallow neural model for relation prediction ( <a href="https://arxiv.org/abs/2101.09090">https://arxiv.org/abs/2101.09090</a> )
<i>Pyke</i>	A Physical Embedding Model for Knowledge Graphs
<i>BaseKGE</i>	Base class for all neural network modules.
<i>ConEx</i>	Convolutional ComplEx Knowledge Graph Embeddings
<i>AConEx</i>	Additive Convolutional ComplEx Knowledge Graph Embeddings
<i>ComplEx</i>	Base class for all neural network modules.
<i>BaseKGE</i>	Base class for all neural network modules.
<i>IdentityClass</i>	Base class for all neural network modules.
<i>QMult</i>	Base class for all neural network modules.
<i>ConvQ</i>	Convolutional Quaternion Knowledge Graph Embeddings
<i>AConvQ</i>	Additive Convolutional Quaternion Knowledge Graph Embeddings
<i>BaseKGE</i>	Base class for all neural network modules.
<i>IdentityClass</i>	Base class for all neural network modules.
<i>OMult</i>	Base class for all neural network modules.
<i>ConvO</i>	Base class for all neural network modules.
<i>AConvO</i>	Additive Convolutional Octonion Knowledge Graph Embeddings
<i>Keci</i>	Base class for all neural network modules.
<i>CKeci</i>	Without learning dimension scaling
<i>DeCaL</i>	Base class for all neural network modules.
<i>BaseKGE</i>	Base class for all neural network modules.
<i>PykeenKGE</i>	A class for using knowledge graph embedding models implemented in Pykeen
<i>BaseKGE</i>	Base class for all neural network modules.
<i>FMult</i>	Learning Knowledge Neural Graphs
<i>GFMult</i>	Learning Knowledge Neural Graphs
<i>FMult2</i>	Learning Knowledge Neural Graphs

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Table 1 – continued from previous page

<i>LFMult1</i>	Embedding with trigonometric functions. We represent all entities and relations in the complex number space as:
<i>LFMult</i>	Embedding with polynomial functions. We represent all entities and relations in the polynomial space as:
<i>DualE</i>	Dual Quaternion Knowledge Graph Embeddings ( <a href="https://ojs.aaai.org/index.php/AAAI/article/download/16850/16657">https://ojs.aaai.org/index.php/AAAI/article/download/16850/16657</a> )

## Functions

```

quaternion_mul(→ Tuple[torch.Tensor, torch.Tensor, Perform quaternion multiplication
...)
quaternion_mul_with_unit_norm(*, Q_1, Q_2)

octonion_mul(*, O_1, O_2)

octonion_mul_norm(*, O_1, O_2)

```

## Package Contents

```

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

```

Bases: torch.optim.optimizer.Optimizer

Base class for all optimizers.

### Warning

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

### Parameters

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

**clip\_lambda**

**\_\_setstate\_\_** (*state*)

**step** (*closure=None*)

Perform a single optimization step.

### Parameters

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

```
class dicee.models.BaseKGE Lightning(*args, **kwargs)
```

Bases: lightning.LightningModule

Base class for all neural network modules.

Your models should also subclass this class.

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

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

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

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

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

### 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.

```
training_step_outputs = []
```

```
mem_of_model() -> Dict
```

Size of model in MB and number of params

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

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

### Parameters

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

### Returns

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

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

Example:

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

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

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

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

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

#### Note

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

`loss_function(y_hat_batch: torch.FloatTensor, y_batch: torch.FloatTensor)`

#### Parameters

- `y_hat_batch`
- `y_batch`

`on_train_epoch_end(*args, **kwargs)`

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

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

```

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

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

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

```

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

**test\_dataloader** () → 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()`

#### Note

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

#### Note

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

**val\_dataloader()** → 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()`

#### Note

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

#### Note

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

**predict\_dataloader()** → 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()`

#### 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()** → 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()`

#### **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.
```

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```
"interval": "epoch",
# How many epochs/steps should pass between calls to
# `scheduler.step()`. 1 corresponds to updating the learning
# rate after every epoch/step.
"frequency": 1,
# Metric to monitor for schedulers like `ReduceLROnPlateau`
"monitor": "val_loss",
# If set to `True`, will enforce that the value specified 'monitor'
# is available when the scheduler is updated, thus stopping
# training if not found. If set to `False`, it will only produce a warning
"strict": True,
# If using the `LearningRateMonitor` callback to monitor the
# learning rate progress, this keyword can be used to specify
# a custom logged name
"name": None,
}
```

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

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

#### Note

Some things to know:

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

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

Bases: `BaseKGELightning`

Base class for all neural network modules.

Your models should also subclass this class.

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

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

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```

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

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

```

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

### **Note**

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

### **Variables**

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

`args`

`embedding_dim = None`

`num_entities = None`

`num_relations = None`

`num_tokens = None`

`learning_rate = None`

`apply_unit_norm = None`

`input_dropout_rate = None`

`hidden_dropout_rate = None`

`optimizer_name = None`

`feature_map_dropout_rate = None`

`kernel_size = None`

`num_of_output_channels = None`

`weight_decay = None`

`loss`

`selected_optimizer = None`

```

normalizer_class = None

normalize_head_entity_embeddings

normalize_relation_embeddings

normalize_tail_entity_embeddings

hidden_normalizer

param_init

input_dp_ent_real

input_dp_rel_real

hidden_dropout

loss_history = []

byte_pair_encoding

max_length_subword_tokens

block_size

forward_byte_pair_encoded_k_vs_all (x: torch.LongTensor)

    Parameters
         $\mathbf{x}$  ( $B \times 2 \times T$ )

forward_byte_pair_encoded_triple (x: Tuple[torch.LongTensor, torch.LongTensor])
    byte pair encoded neural link predictors

    Parameters
    -----

init_params_with_sanity_checking()

forward (x: torch.LongTensor | Tuple[torch.LongTensor, torch.LongTensor],
        y_idx: torch.LongTensor = None)

    Parameters

        •  $\mathbf{x}$ 

        •  $\mathbf{y\_idx}$ 

        • ordered_bpe_entities

forward_triples (x: torch.LongTensor) → torch.Tensor

    Parameters
         $\mathbf{x}$ 

forward_k_vs_all (*args, **kwargs)

forward_k_vs_sample (*args, **kwargs)

get_triple_representation (idx_hrt)

get_head_relation_representation (indexed_triple)

```

`get_sentence_representation(x: torch.LongTensor)`

#### Parameters

- `(b (x shape)`
- `3`
- `t)`

`get_bpe_head_and_relation_representation(x: torch.LongTensor)`  
→ Tuple[torch.FloatTensor, torch.FloatTensor]

#### Parameters

`x (B x 2 x T)`

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

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

Bases: torch.nn.Module

Base class for all neural network modules.

Your models should also subclass this class.

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

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

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

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

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

#### Note

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

#### Variables

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

`args = None`

`__call__(x)`

```
static forward(x)
```

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

Bases: *BaseKGELightning*

Base class for all neural network modules.

Your models should also subclass this class.

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

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

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

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

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

#### Note

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

#### Variables

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

**args**

**embedding\_dim** = None

**num\_entities** = None

**num\_relations** = None

**num\_tokens** = None

**learning\_rate** = None

**apply\_unit\_norm** = None

**input\_dropout\_rate** = None

**hidden\_dropout\_rate** = None

**optimizer\_name** = None

```

feature_map_dropout_rate = None

kernel_size = None

num_of_output_channels = None

weight_decay = None

loss

selected_optimizer = None

normalizer_class = None

normalize_head_entity_embeddings

normalize_relation_embeddings

normalize_tail_entity_embeddings

hidden_normalizer

param_init

input_dp_ent_real

input_dp_rel_real

hidden_dropout

loss_history = []

byte_pair_encoding

max_length_subword_tokens

block_size

forward_byte_pair_encoded_k_vs_all(x: torch.LongTensor)

    Parameters
         $\mathbf{x}$  ( $B \times 2 \times T$ )

forward_byte_pair_encoded_triple(x: Tuple[torch.LongTensor, torch.LongTensor])
    byte pair encoded neural link predictors

    Parameters
    -----

init_params_with_sanity_checking()

forward(x: torch.LongTensor | Tuple[torch.LongTensor, torch.LongTensor],
        y_idx: torch.LongTensor = None)

    Parameters
        •  $\mathbf{x}$ 
        •  $\mathbf{y\_idx}$ 
        • ordered_bpe_entities

```

```

forward_triples (x: torch.LongTensor) → 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 × 2 × x T)
get_embeddings () → Tuple[numpy.ndarray, numpy.ndarray]
class dicee.models.DistMult (args)
    Bases: dicee.models.base_model.BaseKGE
    Embedding Entities and Relations for Learning and Inference in Knowledge Bases https://arxiv.org/abs/1412.6575

    name = 'DistMult'

    k_vs_all_score (emb_h: torch.FloatTensor, emb_r: torch.FloatTensor, emb_E: torch.FloatTensor)

    Parameters
    • emb_h
    • emb_r
    • emb_E
forward_k_vs_all (x: torch.LongTensor)
forward_k_vs_sample (x: torch.LongTensor, target_entity_idx: torch.LongTensor)
score (h, r, t)

class dicee.models.TransE (args)
    Bases: dicee.models.base_model.BaseKGE
    Translating Embeddings for Modeling Multi-relational Data https://proceedings.neurips.cc/paper/2013/file/1cecc7a77928ca8133fa24680a88d2f9-Paper.pdf

    name = 'TransE'

```



```

margin = 4

score(head_ent_emb, rel_ent_emb, tail_ent_emb)

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

class dicee.models.Shallom(args)
    Bases: dicee.models.base_model.BaseKGE
    A shallow neural model for relation prediction (https://arxiv.org/abs/2101.09090)
    name = 'Shallom'

    shallom

    get_embeddings() → Tuple[numpy.ndarray, None]

    forward_k_vs_all(x) → torch.FloatTensor

    forward_triples(x) → 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 them to be nested in a tree structure. You can assign the sub-
    modules as regular attributes:

```

```

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

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

```

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

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

### **Note**

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

### **Variables**

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

#### **args**

`embedding_dim = None`

`num_entities = None`

`num_relations = None`

`num_tokens = None`

`learning_rate = None`

`apply_unit_norm = None`

`input_dropout_rate = None`

`hidden_dropout_rate = None`

`optimizer_name = None`

`feature_map_dropout_rate = None`

`kernel_size = None`

`num_of_output_channels = None`

`weight_decay = None`

#### **loss**

`selected_optimizer = None`

`normalizer_class = None`

`normalize_head_entity_embeddings`

`normalize_relation_embeddings`

`normalize_tail_entity_embeddings`

```

hidden_normalizer

param_init

input_dp_ent_real

input_dp_rel_real

hidden_dropout

loss_history = []

byte_pair_encoding

max_length_subword_tokens

block_size

forward_byte_pair_encoded_k_vs_all (x: torch.LongTensor)

    Parameters
         $\mathbf{x}$  ( $B \times 2 \times T$ )

forward_byte_pair_encoded_triple (x: Tuple[torch.LongTensor, torch.LongTensor])
    byte pair encoded neural link predictors

    Parameters
    -----

init_params_with_sanity_checking ()

forward (x: torch.LongTensor | Tuple[torch.LongTensor, torch.LongTensor],
        y_idx: torch.LongTensor = None)

    Parameters

        •  $\mathbf{x}$ 

        •  $\mathbf{y\_idx}$ 

        • ordered_bpe_entities

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

    Parameters

         $\mathbf{x}$ 

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

        • ( $\mathbf{b}$  ( $x$  shape))

        • 3

        •  $\mathbf{t}$ )

```

```

get_bpe_head_and_relation_representation(x: torch.LongTensor)
    → Tuple[torch.FloatTensor, torch.FloatTensor]

    Parameters
        x (B × 2 × 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]) → 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) → torch.FloatTensor
    forward_triples(x: torch.Tensor) → torch.FloatTensor

    Parameters
        x

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

class dicee.models.AConEx(args)
    Bases: dicee.models.base_model.BaseKGE
    Additive Convolutional ComplEx Knowledge Graph Embeddings
    name = 'AConEx'
    conv2d
    fc_num_input
    fc1
    norm_fc1
    bn_conv2d
    feature_map_dropout

```

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

```
forward_triples (x: torch.Tensor) → torch.FloatTensor
```

### Parameters

**x**

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

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

Bases: `dicee.models.base_model.BaseKGE`

Base class for all neural network modules.

Your models should also subclass this class.

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

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

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

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

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

### Note

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

### Variables

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

```
name = 'Complex'
```

```
static score (head_ent_emb: torch.FloatTensor, rel_ent_emb: torch.FloatTensor,
               tail_ent_emb: torch.FloatTensor)
```

```
static k_vs_all_score(emb_h: torch.FloatTensor, emb_r: torch.FloatTensor,
emb_E: torch.FloatTensor)
```

#### Parameters

- `emb_h`
- `emb_r`
- `emb_E`

```
forward_k_vs_all(x: torch.LongTensor) → 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, torch.Tensor]
```

Perform quaternion multiplication :param Q\_1: :param Q\_2: :return:

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

Bases: *BaseKGELightning*

Base class for all neural network modules.

Your models should also subclass this class.

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

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

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

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

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

#### Note

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

#### Variables

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

`args`

`embedding_dim = None`

```

num_entities = None

num_relations = None

num_tokens = None

learning_rate = None

apply_unit_norm = None

input_dropout_rate = None

hidden_dropout_rate = None

optimizer_name = None

feature_map_dropout_rate = None

kernel_size = None

num_of_output_channels = None

weight_decay = None

loss

selected_optimizer = None

normalizer_class = None

normalize_head_entity_embeddings

normalize_relation_embeddings

normalize_tail_entity_embeddings

hidden_normalizer

param_init

input_dp_ent_real

input_dp_rel_real

hidden_dropout

loss_history = []

byte_pair_encoding

max_length_subword_tokens

block_size

forward_byte_pair_encoded_k_vs_all (x: torch.LongTensor)

```

#### Parameters

$\mathbf{x} (B \times 2 \times T)$

**forward\_byte\_pair\_encoded\_triple** (*x*: *Tuple[torch.LongTensor, torch.LongTensor]*)  
 byte pair encoded neural link predictors

**Parameters**

-----

**init\_params\_with\_sanity\_checking** ()

**forward** (*x*: *torch.LongTensor* | *Tuple[torch.LongTensor, torch.LongTensor]*,  
*y\_idx*: *torch.LongTensor* = *None*)

**Parameters**

- **x**
- **y\_idx**
- **ordered\_bpe\_entities**

**forward\_triples** (*x*: *torch.LongTensor*) → *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* × 2 × *T*)

**get\_embeddings** () → *Tuple[numpy.ndarray, numpy.ndarray]*

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

Bases: *torch.nn.Module*

Base class for all neural network modules.

Your models should also subclass this class.

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



```

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

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

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

```

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

### Note

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

### Variables

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

**args** = None

**\_\_call\_\_** (*x*)

**static forward** (*x*)

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

**class** `dicee.models.QMult` (*args*)

Bases: `dicee.models.base_model.BaseKGE`

Base class for all neural network modules.

Your models should also subclass this class.

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

```

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

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

    def forward(self, x):

```

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

### **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** = 'QMult'

**explicit** = True

**quaternion\_multiplication\_followed\_by\_inner\_product** (*h, r, t*)

### **Parameters**

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

### **Returns**

Triple scores.

**static quaternion\_normalizer** (*x: torch.FloatTensor*) → torch.FloatTensor

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

Absolute value of a quaternion

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

L2 norm of quaternion vector:

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

### **Parameters**

**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.,  
 $[\text{score}(h,r,x)|x \text{ in Entities}] \Rightarrow [0.0,0.1,\dots,0.8]$ , shape= $\Rightarrow (1, |\text{Entities}|)$  Given a batch of head entities and  
relations  $\Rightarrow$  shape (size of batch,| Entities|)

```
class dicee.models.ConvQ(args)
    Bases: dicee.models.base_model.BaseKGE
    Convolutional Quaternion Knowledge Graph Embeddings
    name = 'ConvQ'
    entity_embeddings
    relation_embeddings
    conv2d
    fc_num_input
    fc1
    bn_conv1
    bn_conv2
    feature_map_dropout
    residual_convolution(Q_1, Q_2)
    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.  $[\text{score}(h,r,x)|x \text{ in Entities}] \Rightarrow$   

 $[0.0,0.1,\dots,0.8]$ , shape= $\Rightarrow (1, |\text{Entities}|)$  Given a batch of head entities and relations  $\Rightarrow$  shape (size of batch,|  

Entities|)
```

```
class dicee.models.AConvQ(args)
    Bases: dicee.models.base_model.BaseKGE
    Additive Convolutional Quaternion Knowledge Graph Embeddings
    name = 'AConvQ'
    entity_embeddings
    relation_embeddings
    conv2d
```

```

fc_num_input

fc1

bn_conv1

bn_conv2

feature_map_dropout

residual_convolution(Q_1, Q_2)

forward_triples(indexed_triple: torch.Tensor) → torch.Tensor

```

### Parameters

**x**

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

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

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

Bases: *BaseKGELightning*

Base class for all neural network modules.

Your models should also subclass this class.

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

```

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

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

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

```

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

### Note

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

### Variables

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

```

args

embedding_dim = None

num_entities = None

num_relations = None

num_tokens = None

learning_rate = None

apply_unit_norm = None

input_dropout_rate = None

hidden_dropout_rate = None

optimizer_name = None

feature_map_dropout_rate = None

kernel_size = None

num_of_output_channels = None

weight_decay = None

loss

selected_optimizer = None

normalizer_class = None

normalize_head_entity_embeddings

normalize_relation_embeddings

normalize_tail_entity_embeddings

hidden_normalizer

param_init

input_dp_ent_real

input_dp_rel_real

hidden_dropout

loss_history = []

byte_pair_encoding

max_length_subword_tokens

block_size

forward_byte_pair_encoded_k_vs_all (x: torch.LongTensor)

```

#### Parameters

$\mathbf{x} (B \times 2 \times T)$

**forward\_byte\_pair\_encoded\_triple** (*x*: *Tuple[torch.LongTensor, torch.LongTensor]*)  
 byte pair encoded neural link predictors

**Parameters**

-----

**init\_params\_with\_sanity\_checking** ()

**forward** (*x*: *torch.LongTensor* | *Tuple[torch.LongTensor, torch.LongTensor]*,  
*y\_idx*: *torch.LongTensor* = *None*)

**Parameters**

- **x**
- **y\_idx**
- **ordered\_bpe\_entities**

**forward\_triples** (*x*: *torch.LongTensor*) → *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* × 2 × *T*)

**get\_embeddings** () → *Tuple[numpy.ndarray, numpy.ndarray]*

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

Bases: *torch.nn.Module*

Base class for all neural network modules.

Your models should also subclass this class.

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

```

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

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

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

```

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

### Note

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

### Variables

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

**args** = *None*

**\_\_call\_\_** (*x*)

**static forward** (*x*)

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

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

**class** `dicee.models.OMult` (*args*)

Bases: `dicee.models.base_model.BaseKGE`

Base class for all neural network modules.

Your models should also subclass this class.

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

```

(continues on next page)

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

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

### **Note**

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

### **Variables**

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

**name** = 'OMult'

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

**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.,  $[\text{score}(h,r,x) | x \text{ in Entities}] \Rightarrow [0.0, 0.1, \dots, 0.8]$ , shape= $\Rightarrow (1, |\text{Entities}|)$  Given a batch of head entities and relations  $\Rightarrow$  shape (size of batch, |Entities|)

**class** `dicce.models.ConvO` (*args: dict*)

Bases: `dicce.models.base_model.BaseKGE`

Base class for all neural network modules.

Your models should also subclass this class.

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

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

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

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



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

#### **Note**

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

#### **Variables**

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

**name** = 'ConvO'

**conv2d**

**fc\_num\_input**

**fc1**

**bn\_conv2d**

**norm\_fc1**

**feature\_map\_dropout**

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

**residual\_convolution** (*O\_1, O\_2*)

**forward\_triples** (*x: torch.Tensor*) → torch.Tensor

#### **Parameters**

**x**

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

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

**class** dicee.models.**AConvO** (*args: dict*)

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

Additive Convolutional Octonion Knowledge Graph Embeddings

**name** = 'AConvO'

**conv2d**

**fc\_num\_input**

**fc1**

**bn\_conv2d**

**norm\_fc1**

**feature\_map\_dropout**

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

```
residual_convolution(O_1, O_2)
```

```
forward_triples(x: torch.Tensor) → torch.Tensor
```

### Parameters

**x**

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

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

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

Bases: `dicee.models.base_model.BaseKGE`

Base class for all neural network modules.

Your models should also subclass this class.

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

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

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

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

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

### 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  $\sigma_{pp} = \sum_{i=1}^p \sum_{k=i+1}^p (h_{i,r,k} - h_{k,r,i}) e_i e_k$

$\sigma_{pp}$  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.,  $e_1 e_1, e_1 e_2, e_1 e_3$ ,

$e_2 e_1, e_2 e_2, e_2 e_3, e_3 e_1, e_3 e_2, e_3 e_3$

Then select the triangular matrix without diagonals:  $e_1 e_2, e_1 e_3, e_2 e_3$ .

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

Compute  $\sigma_{qq} = \sum_{j=1}^{p+q-1} \sum_{k=j+1}^{p+q} (h_{j,r,k} - h_{k,r,j}) e_j e_k$  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.,  $e_1 e_1, e_1 e_2, e_1 e_3$ ,

$e_2 e_1, e_2 e_2, e_2 e_3, e_3 e_1, e_3 e_2, e_3 e_3$

Then select the triangular matrix without diagonals:  $e_1 e_2, e_1 e_3, e_2 e_3$ .

**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

$h = h_0 + \sum_{i=1}^p h_{i,r} e_i + \sum_{j=p+1}^{p+q} h_{j,r} e_j$   
 $r = r_0 + \sum_{i=1}^p r_{i,r} e_i + \sum_{j=p+1}^{p+q} r_{j,r} e_j$

$e_i^2 = +1$  for  $i \leq p$   $e_j^2 = -1$  for  $p < j \leq p+q$   $e_i e_j = -e_j e_i$  for  $i$

$e_i e_j$

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

**construct\_cl\_multivector** ( $x$ : torch.FloatTensor,  $r$ : int,  $p$ : int,  $q$ : int)  
 $\rightarrow$  tuple[torch.FloatTensor, torch.FloatTensor, torch.FloatTensor]

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

### Parameter

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

#### returns

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

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

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

**forward\_k\_vs\_all** ( $x$ : torch.Tensor)  $\rightarrow$  torch.FloatTensor

Kvsall training

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

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

**construct\_batch\_selected\_cl\_multivector** ( $x$ : torch.FloatTensor,  $r$ : int,  $p$ : int,  $q$ : int)  
 $\rightarrow$  tuple[torch.FloatTensor, torch.FloatTensor, torch.FloatTensor]

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

### Parameter

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

#### returns

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

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

## Parameter

x: torch.LongTensor with (n,2) shape

target\_entity\_idx: torch.LongTensor with (n, k ) shape k denotes the selected number of examples.

**rtype**

torch.FloatTensor with (n, k) shape

**score** (h, r, t)

**forward\_triples** (x: torch.Tensor) → torch.FloatTensor

## Parameter

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

**rtype**

torch.FloatTensor with (n) shape

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

Bases: *Keci*

Without learning dimension scaling

**name** = 'CKeci'

**requires\_grad\_for\_interactions** = False

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

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

Base class for all neural network modules.

Your models should also subclass this class.

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

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

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

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

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

### Note

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

### Variables

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

**name** = 'DeCaL'

**entity\_embeddings**

**relation\_embeddings**

**p**

**q**

**r**

**re**

**forward\_triples** (*x: torch.Tensor*) → torch.FloatTensor

### Parameter

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

**rtype**

torch.FloatTensor with (n) shape

**cl\_pqr** (*a: torch.tensor*) → torch.tensor

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

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

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

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

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

and return:

$$sigma_0 t = \sigma_0 \cdot t_0 = s0 + s1 - s2 s3, s4 \text{ and } s5$$

**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

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

For different base vector interactions, we have

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

**forward\_k\_vs\_all** (*x*: torch.Tensor) → 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 functions are identical Parameter ——— *x*: torch.LongTensor with (n, ) shape :rtype: torch.FloatTensor with (n, **IEI**) 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:

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

$\sigma_{pp}$  captures the interactions between along *p* bases For instance, let  $e_1, e_2, e_3$ , 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.,  $e_1 e_1, e_1 e_2, e_1 e_3,$

$e_2 e_1, e_2 e_2, e_2 e_3, e_3 e_1, e_3 e_2, e_3 e_3$

Then select the triangular matrix without diagonals:  $e_1 e_2, e_1 e_3, e_2 e_3$ .

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

Compute

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

$\sigma_{q,q}$  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.,  $e_1 e_1, e_1 e_2, e_1 e_3,$

$e_2 e_1, e_2 e_2, e_2 e_3, e_3 e_1, e_3 e_2, e_3 e_3$

Then select the triangular matrix without diagonals:  $e_1 e_2, e_1 e_3, e_2 e_3$ .

**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.models.BaseKGE (args: dict)

```

Bases: *BaseKGELightning*

Base class for all neural network modules.

Your models should also subclass this class.

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

```

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

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

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

```

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

#### Note

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

#### Variables

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

`args`

`embedding_dim = None`

`num_entities = None`

`num_relations = None`

`num_tokens = None`

`learning_rate = None`

`apply_unit_norm = None`

`input_dropout_rate = None`

`hidden_dropout_rate = None`

```

optimizer_name = None

feature_map_dropout_rate = None

kernel_size = None

num_of_output_channels = None

weight_decay = None

loss

selected_optimizer = None

normalizer_class = None

normalize_head_entity_embeddings

normalize_relation_embeddings

normalize_tail_entity_embeddings

hidden_normalizer

param_init

input_dp_ent_real

input_dp_rel_real

hidden_dropout

loss_history = []

byte_pair_encoding

max_length_subword_tokens

block_size

forward_byte_pair_encoded_k_vs_all (x: torch.LongTensor)

    Parameters
         $\mathbf{x}$  ( $B \times 2 \times T$ )

forward_byte_pair_encoded_triple (x: Tuple[torch.LongTensor, torch.LongTensor])
    byte pair encoded neural link predictors

    Parameters
    -----

init_params_with_sanity_checking()

forward (x: torch.LongTensor | Tuple[torch.LongTensor, torch.LongTensor],
        y_idx: torch.LongTensor = None)

    Parameters
        •  $\mathbf{x}$ 
        •  $\mathbf{y\_idx}$ 
        • ordered_bpe_entities

```

**forward\_triples** (*x*: *torch.LongTensor*) → *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* × 2 × *T*)

**get\_embeddings** () → *Tuple*[*numpy.ndarray*, *numpy.ndarray*]

**class** *dicee.models.PykeenKGE* (*args*: *dict*)

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

A class for using knowledge graph embedding models implemented in Pykeen

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

**model\_kwargs**

**name**

**model**

**loss\_history** = []

**args**

**entity\_embeddings** = **None**

**relation\_embeddings** = **None**

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

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

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

**h** = **h.reshape(len(x), self.embedding\_dim, self.last\_dim)** **r** = **r.reshape(len(x), self.embedding\_dim, self.last\_dim)**

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

```

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

    else:
        t = self.entity_embeddings.weight

    # (4) Call the score_t from interactions to generate triple scores. return self.interaction.score_t(h=h, r=r,
    all_entities=t, slice_size=1)

forward_triples (x: torch.LongTensor) → torch.FloatTensor
    # => Explicit version by this we can apply bn and dropout

    # (1) Retrieve embeddings of heads, relations and tails and apply Dropout & Normalization if given. h, r, t =
    self.get_triple_representation(x) # (2) Reshape (1). if self.last_dim > 0:
        h = h.reshape(len(x), self.embedding_dim, self.last_dim) r = r.reshape(len(x), self.embedding_dim,
        self.last_dim) t = t.reshape(len(x), self.embedding_dim, self.last_dim)

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

abstract forward_k_vs_sample (x: torch.LongTensor, target_entity_idx)

```

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

Bases: *BaseKGELightning*

Base class for all neural network modules.

Your models should also subclass this class.

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

```

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

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

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

```

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

### Note

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

### Variables

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

```

args

embedding_dim = None

num_entities = None

num_relations = None

num_tokens = None

learning_rate = None

apply_unit_norm = None

input_dropout_rate = None

hidden_dropout_rate = None

optimizer_name = None

feature_map_dropout_rate = None

kernel_size = None

num_of_output_channels = None

weight_decay = None

loss

selected_optimizer = None

normalizer_class = None

normalize_head_entity_embeddings

normalize_relation_embeddings

normalize_tail_entity_embeddings

hidden_normalizer

param_init

input_dp_ent_real

input_dp_rel_real

hidden_dropout

loss_history = []

byte_pair_encoding

max_length_subword_tokens

block_size

forward_byte_pair_encoded_k_vs_all (x: torch.LongTensor)

```

#### Parameters

$\mathbf{x} (B \times 2 \times T)$

```

forward_byte_pair_encoded_triple (x: Tuple[torch.LongTensor, torch.LongTensor])
    byte pair encoded neural link predictors

    Parameters
    -----

init_params_with_sanity_checking()

forward (x: torch.LongTensor | Tuple[torch.LongTensor, torch.LongTensor],
         y_idx: torch.LongTensor = None)

    Parameters
    • x
    • y_idx
    • ordered_bpe_entities

forward_triples (x: torch.LongTensor) → torch.Tensor

    Parameters
    • x

forward_k_vs_all (*args, **kwargs)

forward_k_vs_sample (*args, **kwargs)

get_triple_representation (idx_hrt)

get_head_relation_representation (indexed_triple)

get_sentence_representation (x: torch.LongTensor)

    Parameters
    • (b (x shape)
    • 3
    • t)

get_bpe_head_and_relation_representation (x: torch.LongTensor)
    → Tuple[torch.FloatTensor, torch.FloatTensor]

    Parameters
    • x (B x 2 x T)

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

class dicke.models.FMult (args)
    Bases: dicke.models.base_model.BaseKGE
    Learning Knowledge Neural Graphs
    name = 'FMult'
    entity_embeddings
    relation_embeddings
    k

```

```

num_sample = 50

gamma

roots

weights

compute_func(weights: torch.FloatTensor, x) → torch.FloatTensor

chain_func(weights, x: torch.FloatTensor)

forward_triples(idx_triple: torch.Tensor) → torch.Tensor

```

#### Parameters

**x**

```

class dicee.models.GFMult(args)
    Bases: dicee.models.base_model.BaseKGE
    Learning Knowledge Neural Graphs
    name = 'GFMult'
    entity_embeddings
    relation_embeddings
    k
    num_sample = 250
    roots
    weights
    compute_func(weights: torch.FloatTensor, x) → torch.FloatTensor
    chain_func(weights, x: torch.FloatTensor)
    forward_triples(idx_triple: torch.Tensor) → torch.Tensor

```

#### Parameters

**x**

```

class dicee.models.FMult2(args)
    Bases: dicee.models.base_model.BaseKGE
    Learning Knowledge Neural Graphs
    name = 'FMult2'
    n_layers = 3
    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) → torch.FloatTensor

function (list_W, list_b)

trapezoid (list_W, list_b)

forward_triples (idx_triple: torch.Tensor) → 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:  $f(x) = \sum_{k=0}^{d-1} w_k e^{kix}$ . 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)
```

```
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:  $f(x) = \sum_{i=0}^{d-1} a_i x^i$  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
```

```
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.  $h = \text{sigma}(wh^T x + bh)$ ,  $r = \text{sigma}(wr^T x + br)$ ,  
 $t = \text{sigma}(wt^T x + bt)$

**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:

$$\text{score}(h,r,t) = \int_0^1 h(x)r(x)t(x) dx = \sum_{i,j,k=0}^{d-1} \text{dfrac}\{a_i*b_j*c_k\} \{1+(i+j+k)*d\}$$

1. generate the range for i,j and k from [0 d-1]
2. perform  $\text{dfrac}\{a_i*b_j*c_k\} \{1+(i+j+k)*d\}$  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:

$$\text{score}(h,r,t) = \int_0^1 h(x)r(x)t(x) dx = \sum_{i,j,k=0}^{d-1} \text{dfrac}\{a_i*c_j*b_k - b_i*c_j*a_k\} \{(1+(i+j)*d)(1+k)\}$$

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,

$$\text{coeff}[1][0] + \text{coeff}[1][1]x + \dots + \text{coeff}[1][d]x^d)$$

**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,**

$$\text{coeff}[1][0] + \text{coeff}[1][1]x + \dots + \text{coeff}[1][d]x^d)$$

**class** dicee.models.DualE (*args*)

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

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

```

name = 'DualE'

entity_embeddings

relation_embeddings

num_ent = None

kvsall_score(e_1_h, e_2_h, e_3_h, e_4_h, e_5_h, e_6_h, e_7_h, e_8_h, e_1_t, e_2_t, e_3_t, e_4_t,
            e_5_t, e_6_t, e_7_t, e_8_t, r_1, r_2, r_3, r_4, r_5, r_6, r_7, r_8) → torch.tensor
KvsAll scoring function

```

### Input

x: torch.LongTensor with (n, ) shape

### Output

torch.FloatTensor with (n) shape

**forward\_triples** (*idx\_triple: torch.tensor*) → torch.tensor  
 Negative Sampling forward pass:

### Input

x: torch.LongTensor with (n, ) shape

### Output

torch.FloatTensor with (n) shape

**forward\_k\_vs\_all** (*x*)  
 KvsAll forward pass

### Input

x: torch.LongTensor with (n, ) shape

### Output

torch.FloatTensor with (n) shape

**T** (*x: torch.tensor*) → torch.tensor  
 Transpose function

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

## dicee.query\_generator

### Classes

---

*QueryGenerator*

---

## Module Contents

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

    train_path

    val_path

    test_path

    gen_valid = False

    gen_test = True

    seed = 1

    max_ans_num = 1000000.0

    mode

    ent2id = None

    rel2id: Dict = None

    ent_in: Dict

    ent_out: Dict

    query_name_to_struct

    list2tuple(list_data)

    tuple2list(x: List | Tuple) → List | Tuple
        Convert a nested tuple to a nested list.

    set_global_seed(seed: int)
        Set seed

    construct_graph(paths: List[str]) → Tuple[Dict, Dict]
        Construct graph from triples Returns dicts with incoming and outgoing edges

    fill_query(query_structure: List[str | List], ent_in: Dict, ent_out: Dict, answer: int) → 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]]]*)  
→ None

Save Queries into Disk

**static load\_queries\_and\_answers** (*path: str*) → List[Tuple[str, Tuple[collections.defaultdict]]]

Load Queries from Disk to Memory

## **dicee.read\_preprocess\_save\_load\_kg**

### **Submodules**

#### **dicee.read\_preprocess\_save\_load\_kg.preprocess**

### **Classes**

*PreprocessKG*

Preprocess the data in memory

### **Module Contents**

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

Preprocess the data in memory

**kg**

**start** () → None

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

#### **Parameter**

**rtype**

None

**preprocess\_with\_byte\_pair\_encoding** ()

**preprocess\_with\_byte\_pair\_encoding\_with\_padding** () → None

**preprocess\_with\_pandas** () → None

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

(1) Add recipriocal or noisy triples

(2) Construct vocabulary

(3) Index datasets

## Parameter

**rtype**

None

**preprocess\_with\_polars()** → None

**sequential\_vocabulary\_construction()** → None

- (1) Read input data into memory
- (2) Remove triples with a condition
- (3) **Serialize vocabularies in a pandas dataframe where**  
=> the index is integer and => a single column is string (e.g. URI)

**dicee.read\_preprocess\_save\_load\_kg.read\_from\_disk**

## Classes

---

*ReadFromDisk*

Read the data from disk into memory

---

## Module Contents

**class** dicee.read\_preprocess\_save\_load\_kg.read\_from\_disk.**ReadFromDisk**(kg)

Read the data from disk into memory

**kg**

**start()** → 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

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

## Module Contents

```
dicee.read_preprocess_save_load_kg.util.polars_dataframe_indexer(  
    df_polars: polars.DataFrame, idx_entity: polars.DataFrame, idx_relation: polars.DataFrame)  
    → polars.DataFrame
```

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

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

### Parameters:

#### **df\_polars**

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

#### **idx\_entity**

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

#### **idx\_relation**

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

### Returns:

#### **polars.DataFrame**

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

### Example Usage:

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

### Steps:

1. Join the input DataFrame *df\_polars* on the 'relation' column with *idx\_relation* to replace the relations with their indices.
2. Join on 'subject' to replace it with the corresponding entity index using a left join on *idx\_entity*.
3. Join on 'object' to replace it with the corresponding entity index using a left join on *idx\_entity*.

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

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

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

#### Parameters:

##### df\_pandas

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

##### idx\_entity

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

##### idx\_relation

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

#### Returns:

##### pd.DataFrame

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

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

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

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

```
dicee.read_preprocess_save_load_kg.util.read_with_polars (data_path,
    read_only_few: int = None, sample_triples_ratio: float = None, separator: str = None)
    → polars.DataFrame
```

#### Load and Preprocess via Polars

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

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

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

#### Read triples from triple store into pandas dataframe

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

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

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

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

- (1) Extract domains and ranges of relations



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

`dicee.read_preprocess_save_load_kg.util.load_with_pandas(self) → None`

Deserialize data

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

`dicee.read_preprocess_save_load_kg.util.load_numpy_ndarray(*, file_path: str)`

`dicee.read_preprocess_save_load_kg.util.save_pickle(*, data: object, file_path=str)`

`dicee.read_preprocess_save_load_kg.util.load_pickle(*, file_path=str)`

`dicee.read_preprocess_save_load_kg.util.create_recipriocal_triples(x)`

Add inverse triples into dask dataframe :param x: :return:

`dicee.read_preprocess_save_load_kg.util.dataset_sanity_checking(train_set: numpy.ndarray, num_entities: int, num_relations: int) → None`

#### Parameters

- **train\_set**
- **num\_entities**
- **num\_relations**

#### Returns

## Classes

<i>PreprocessKG</i>	Preprocess the data in memory
<i>LoadSaveToDisk</i>	
<i>ReadFromDisk</i>	Read the data from disk into memory

## Package Contents

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

Preprocess the data in memory

**kg**

**start()** → None

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

#### Parameter

**rtype**  
None

**preprocess\_with\_byte\_pair\_encoding()**

**preprocess\_with\_byte\_pair\_encoding\_with\_padding()** → None

**preprocess\_with\_pandas()** → None

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

- (1) Add recipriocal or noisy triples
- (2) Construct vocabulary
- (3) Index datasets

### Parameter

**rtype**

None

**preprocess\_with\_polars()** → None

**sequential\_vocabulary\_construction()** → None

- (1) Read input data into memory
- (2) Remove triples with a condition
- (3) **Serialize vocabularies in a pandas dataframe where**  
=> the index is integer and => a single column is string (e.g. URI)

**class** dicee.read\_preprocess\_save\_load\_kg.**LoadSaveToDisk**(kg)

**kg**

**save()**

**load()**

**class** dicee.read\_preprocess\_save\_load\_kg.**ReadFromDisk**(kg)

Read the data from disk into memory

**kg**

**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.sanity\_checkers**

## Functions

<code>is_sparql_endpoint_alive([sparql_endpoint])</code>	
<code>validate_knowledge_graph(args)</code>	Validating the source of knowledge graph
<code>sanity_checking_with_arguments(args)</code>	

## Module Contents

`dicee.sanity_checkers.is_sparql_endpoint_alive (sparql_endpoint: str = None)`

`dicee.sanity_checkers.validate_knowledge_graph (args)`

Validating the source of knowledge graph

`dicee.sanity_checkers.sanity_checking_with_arguments (args)`

## `dicee.scripts`

### Submodules

#### `dicee.scripts.index_serve`

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

## Attributes

<code>app</code>
<code>neural_searcher</code>

## Classes

<code>NeuralSearcher</code>	
<code>StringListRequest</code>	!!! abstract "Usage Documentation"

## Functions

```
get_default_arguments()
```

```
index(args)
```

```
root()
```

```
search_embeddings(q)
```

```
retrieve_embeddings(q)
```

```
search_embeddings_batch(request)
```

```
serve(args)
```

```
main()
```

## Module Contents

```
dicee.scripts.index_serve.get_default_arguments()
```

```
dicee.scripts.index_serve.index(args)
```

```
dicee.scripts.index_serve.app
```

```
dicee.scripts.index_serve.neural_searcher = None
```

```
class dicee.scripts.index_serve.NeuralSearcher(args)
```

```
    collection_name
```

```
    entity_to_idx = None
```

```
    qdrant_client
```

```
    topk = 5
```

```
    retrieve_embedding(entity: str = None, entities: List[str] = None) → List
```

```
    search(entity: str)
```

```
async dicee.scripts.index_serve.root()
```

```
async dicee.scripts.index_serve.search_embeddings(q: str)
```

```
async dicee.scripts.index_serve.retrieve_embeddings(q: str)
```

```
class dicee.scripts.index_serve.StringListRequest(/, **data: Any)
```

```
    Bases: pydantic.BaseModel
```

```
    !!! abstract “Usage Documentation”
```

```
        [Models](../concepts/models.md)
```

```
    A base class for creating Pydantic models.
```

**`__class_vars__`**  
The names of the class variables defined on the model.

**`__private_attributes__`**  
Metadata about the private attributes of the model.

**`__signature__`**  
The synthesized `__init__` [*Signature*][inspect.Signature] of the model.

**`__pydantic_complete__`**  
Whether model building is completed, or if there are still undefined fields.

**`__pydantic_core_schema__`**  
The core schema of the model.

**`__pydantic_custom_init__`**  
Whether the model has a custom `__init__` function.

**`__pydantic_decorators__`**  
Metadata containing the decorators defined on the model. This replaces `Model.__validators__` and `Model.__root_validators__` from Pydantic V1.

**`__pydantic_generic_metadata__`**  
Metadata for generic models; contains data used for a similar purpose to `__args__`, `__origin__`, `__parameters__` in typing-module generics. May eventually be replaced by these.

**`__pydantic_parent_namespace__`**  
Parent namespace of the model, used for automatic rebuilding of models.

**`__pydantic_post_init__`**  
The name of the post-init method for the model, if defined.

**`__pydantic_root_model__`**  
Whether the model is a [*RootModel*][pydantic.root\_model.RootModel].

**`__pydantic_serializer__`**  
The *pydantic-core* *SchemaSerializer* used to dump instances of the model.

**`__pydantic_validator__`**  
The *pydantic-core* *SchemaValidator* used to validate instances of the model.

**`__pydantic_fields__`**  
A dictionary of field names and their corresponding [*FieldInfo*][pydantic.fields.FieldInfo] objects.

**`__pydantic_computed_fields__`**  
A dictionary of computed field names and their corresponding [*ComputedFieldInfo*][pydantic.fields.ComputedFieldInfo] objects.

**`__pydantic_extra__`**  
A dictionary containing extra values, if [*extra*][pydantic.config.ConfigDict.extra] is set to 'allow'.

**`__pydantic_fields_set__`**  
The names of fields explicitly set during instantiation.

**`__pydantic_private__`**  
Values of private attributes set on the model instance.

**`queries: List[str]`**

```
reducer: str | None = None
```

```
async dicee.scripts.index_serve.search_embeddings_batch(request: StringListRequest)
```

```
dicee.scripts.index_serve.serve(args)
```

```
dicee.scripts.index_serve.main()
```

## **dicee.scripts.run**

### **Functions**

<code>get_default_arguments([description])</code> <code>main()</code>	Extends pytorch_lightning Trainer's arguments with ours
--	---

## **Module Contents**

```
dicee.scripts.run.get_default_arguments(description=None)
```

Extends pytorch\_lightning Trainer's arguments with ours

```
dicee.scripts.run.main()
```

## **dicee.static\_funcs**

### **Functions**

<code>create_recipriocal_triples(x)</code>	Add inverse triples into dask dataframe
<code>get_er_vocab(data[, file_path])</code>	
<code>get_re_vocab(data[, file_path])</code>	
<code>get_ee_vocab(data[, file_path])</code>	
<code>timeit(func)</code>	
<code>save_pickle(*[, data, file_path])</code>	
<code>load_pickle([file_path])</code>	
<code>load_term_mapping([file_path])</code>	
<code>select_model(args[, is_continual_training, storage_path])</code>	
<code>load_model(→ Tuple[object, Tuple[dict, dict]])</code>	Load weights and initialize pytorch module from namespace arguments
<code>load_model_ensemble(...)</code>	Construct Ensemble Of weights and initialize pytorch module from namespace arguments
<code>save_numpy_ndarray(*, data, file_path)</code>	
<code>numpy_data_type_changer(→ numpy.ndarray)</code>	Detect most efficient data type for a given triples

continues on next page

Table 2 – continued from previous page

<code>save_checkpoint_model(→ None)</code>	Store Pytorch model into disk
<code>store(→ None)</code>	
<code>add_noisy_triples(→ pandas.DataFrame)</code>	Add randomly constructed triples
<code>read_or_load_kg(args, cls)</code>	
<code>intialize_model(→ Tuple[object, str])</code>	
<code>load_json(→ dict)</code>	
<code>save_embeddings(→ None)</code>	Save it as CSV if memory allows.
<code>random_prediction(pre_trained_kge)</code>	
<code>deploy_triple_prediction(pre_trained_kge, str_subject, ...)</code>	
<code>deploy_tail_entity_prediction(pre_trained_kge, ...)</code>	
<code>deploy_head_entity_prediction(pre_trained_kge, ...)</code>	
<code>deploy_relation_prediction(pre_trained_kge, ...)</code>	
<code>vocab_to_parquet(vocab_to_idx, name, ...)</code>	
<code>create_experiment_folder([folder_name])</code>	
<code>continual_training_setup_executor(→ None)</code>	
<code>exponential_function(→ torch.FloatTensor)</code>	
<code>load_numpy(→ numpy.ndarray)</code>	
<code>evaluate(entity_to_idx, scores, easy_answers, # @TODO: CD: Renamed this function hard_answers)</code>	
<code>download_file(url[, destination_folder])</code>	
<code>download_files_from_url(→ None)</code>	
<code>download_pretrained_model(→ str)</code>	
<code>write_csv_from_model_parallel(path)</code>	Create
<code>from_pretrained_model_write_embeddings_int, None)</code>	

## Module Contents

`dicee.static_funcs.create_recipriocal_triples(x)`

Add inverse triples into dask dataframe :param x: :return:

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

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

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

```

dicee.static_funcs.timeit (func)

dicee.static_funcs.save_pickle (*, data: object = None, file_path=str)

dicee.static_funcs.load_pickle (file_path=str)

dicee.static_funcs.load_term_mapping (file_path=str)

dicee.static_funcs.select_model (args: dict, is_continual_training: bool = None,
                                storage_path: str = None)

dicee.static_funcs.load_model (path_of_experiment_folder: str, model_name='model.pt', verbose=0)
    → Tuple[object, Tuple[dict, dict]]
    Load weights and initialize pytorch module from namespace arguments

dicee.static_funcs.load_model_ensemble (path_of_experiment_folder: str)
    → Tuple[dicee.models.base_model.BaseKGE, Tuple[pandas.DataFrame, pandas.DataFrame]]
    Construct Ensemble Of weights and initialize pytorch module from namespace arguments
    (1) Detect models under given path
    (2) Accumulate parameters of detected models
    (3) Normalize parameters
    (4) Insert (3) into model.

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

dicee.static_funcs.numpy_data_type_changer (train_set: numpy.ndarray, num: int)
    → numpy.ndarray
    Detect most efficient data type for a given triples :param train_set: :param num: :return:

dicee.static_funcs.save_checkpoint_model (model, path: str) → None
    Store Pytorch model into disk

dicee.static_funcs.store (trained_model, model_name: str = 'model', full_storage_path: str = None,
                        save_embeddings_as_csv=False) → None

dicee.static_funcs.add_noisy_triples (train_set: pandas.DataFrame, add_noise_rate: float)
    → pandas.DataFrame
    Add randomly constructed triples :param train_set: :param add_noise_rate: :return:

dicee.static_funcs.read_or_load_kg (args, cls)

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

dicee.static_funcs.load_json (p: str) → dict

dicee.static_funcs.save_embeddings (embeddings: numpy.ndarray, indexes, path: str) → None
    Save it as CSV if memory allows. :param embeddings: :param indexes: :param path: :return:

dicee.static_funcs.random_prediction (pre_trained_kge)

dicee.static_funcs.deploy_triple_prediction (pre_trained_kge, str_subject, str_predicate,
                                           str_object)

dicee.static_funcs.deploy_tail_entity_prediction (pre_trained_kge, str_subject, str_predicate,
                                                top_k)

```



```

dicee.static_funcs.deploy_head_entity_prediction(pre_trained_kge, str_object, str_predicate,
top_k)

dicee.static_funcs.deploy_relation_prediction(pre_trained_kge, str_subject, str_object, top_k)

dicee.static_funcs.vocab_to_parquet(vocab_to_idx, name, path_for_serialization, print_into)

dicee.static_funcs.create_experiment_folder(folder_name='Experiments')

dicee.static_funcs.continual_training_setup_executor(executor) → None

dicee.static_funcs.exponential_function(x: numpy.ndarray, lam: float, ascending_order=True)
→ torch.FloatTensor

dicee.static_funcs.load_numpy(path) → numpy.ndarray

dicee.static_funcs.evaluate(entity_to_idx, scores, easy_answers, hard_answers)
# @TODO: CD: Renamed this function Evaluate multi hop query answering on different query types

dicee.static_funcs.download_file(url, destination_folder='.')

dicee.static_funcs.download_files_from_url(base_url: str, destination_folder='.') → None

```

#### Parameters

- **base\_url** (e.g. [“https://files.dice-research.org/projects/DiceEmbeddings/KINSHIP-Keci-dim128-epoch256-KvsAll”](https://files.dice-research.org/projects/DiceEmbeddings/KINSHIP-Keci-dim128-epoch256-KvsAll))
- **destination\_folder** (e.g. `"KINSHIP-Keci-dim128-epoch256-KvsAll"`)

```

dicee.static_funcs.download_pretrained_model(url: str) → str

dicee.static_funcs.write_csv_from_model_parallel(path: str)
Create

dicee.static_funcs.from_pretrained_model_write_embeddings_into_csv(path: str) → None

```

### **dicee.static\_funcs\_training**

#### **Functions**

---

```

make_iterable_verbose(→ Iterable)

evaluate_lp([model, triple_idx, num_entities, ...])

evaluate_bpe_lp(model, triple_idx, ..., info])

efficient_zero_grad(model)

```

---

### **Module Contents**

```

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

```

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

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

```
dicee.static_funcs_training.efficient_zero_grad (model)
```

## **dicee.static\_preprocess\_funcs**

### **Attributes**

```
enable_log
```

### **Functions**

```
timeit(func)
```

```
preprocesses_input_args(args) Sanity Checking in input arguments
```

```
create_constraints(→ Tuple[dict, 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**

```
dicee.static_preprocess_funcs.enable_log = False
```

```
dicee.static_preprocess_funcs.timeit (func)
```

```
dicee.static_preprocess_funcs.preprocesses_input_args (args)
```

Sanity Checking in input arguments

```
dicee.static_preprocess_funcs.create_constraints (triples: numpy.ndarray)
      → Tuple[dict, dict, dict, dict]
```

(1) Extract domains and ranges of relations

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

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

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

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

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

## **dicee.trainer**

### **Submodules**

#### **dicee.trainer.dice\_trainer**

### **Classes**

<i>DICE_Trainer</i>	DICE_Trainer implement
---------------------	------------------------

### **Functions**

<i>load_term_mapping</i> ([file_path])
<i>initialize_trainer</i> (...)
<i>get_callbacks</i> (args)

### **Module Contents**

```
dicee.trainer.dice_trainer.load_term_mapping(file_path=str)
```

```
dicee.trainer.dice_trainer.initialize_trainer(args, callbacks)  
→ dicee.trainer.torch_trainer.TorchTrainer | dicee.trainer.model_parallelism.TensorParallel | dicee.trainer.torch_trainer_ddp
```

```
dicee.trainer.dice_trainer.get_callbacks(args)
```

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

#### **DICE\_Trainer implement**

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

args

is\_continual\_training:bool

storage\_path:str

evaluator:

report:dict

**report**

**args**

**trainer = None**

**is\_continual\_training**

**storage\_path**

**evaluator = None**

**form\_of\_labelling = None**

**continual\_start** (*knowledge\_graph*)

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

## Parameter

**returns**

- *model*
- **form\_of\_labelling** (*str*)

**initialize\_trainer** (*callbacks: List*)

→ *lightning.Trainer* | *dicke.trainer.model\_parallelism.TensorParallel* | *dicke.trainer.torch\_trainer.TorchTrainer* | *dicke.*

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: dicke.knowledge\_graph.KG* | *numpy.memmap*)

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

Start the training

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

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

**k\_fold\_cross\_validation** (*dataset*) → *Tuple[dicke.models.base\_model.BaseKGE, str]*

Perform K-fold Cross-Validation

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

## Parameters

- **self**
- **dataset**

## Returns

*model*

## dicee.trainer.model\_parallelism

### Classes

<i>TensorParallel</i>	Abstract class for Trainer class for knowledge graph embedding models
-----------------------	---

### Functions

<i>extract_input_outputs</i> (z[, device])
<i>find_good_batch_size</i> (train_loader, tp_ensemble_model)
<i>forward_backward_update_loss</i> (→ float)

### Module Contents

dicee.trainer.model\_parallelism.**extract\_input\_outputs** (z: list, device=None)

dicee.trainer.model\_parallelism.**find\_good\_batch\_size** (train\_loader, tp\_ensemble\_model)

dicee.trainer.model\_parallelism.**forward\_backward\_update\_loss** (z: Tuple, ensemble\_model)  
→ float

**class** dicee.trainer.model\_parallelism.**TensorParallel** (args, callbacks)

Bases: *dicee.abstracts.AbstractTrainer*

Abstract class for Trainer class for knowledge graph embedding models

#### Parameter

**args**

[str] ?

**callbacks: list**

?

**fit** (\*args, \*\*kwargs)

Train model

## dicee.trainer.torch\_trainer

### Classes

<i>TorchTrainer</i>	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*) → None

Training starts

Arguments

**kwargs:Tuple**

empty dictionary

**Return type**

batch loss (float)

**forward\_backward\_update** (*x\_batch*: `torch.Tensor`, *y\_batch*: `torch.Tensor`) → `torch.Tensor`

Compute forward, loss, backward, and parameter update

Arguments

**Return type**

batch loss (float)

**extract\_input\_outputs\_set\_device** (*batch*: *list*) → `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

<code>TorchDDPTrainer</code>	A Trainer based on torch.nn.parallel.DistributedDataParallel
<code>NodeTrainer</code>	

### Functions

<code>make_iterable_verbose</code> ( $\rightarrow$ 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\_idx**  
mapping.

**relation\_idx**  
mapping.

**form**  
?

**store**  
?

**label\_smoothing\_rate**  
Using hard targets (0,1) drives weights to infinity. An outlier produces enormous gradients.

**Return type**  
torch.utils.data.Dataset

**fit** (*\*args*, *\*\*kwargs*)  
Train model

**class** `dicee.trainer.torch_trainer_ddp.NodeTrainer` (*trainer*, *model*: torch.nn.Module,  
*train\_dataset\_loader*: torch.utils.data.DataLoader, *callbacks*, *num\_epochs*: int)

**trainer**

**local\_rank**

**global\_rank**

```

optimizer

train_dataset_loader

loss_func

callbacks

model

num_epochs

loss_history = []

ctx

scaler

extract_input_outputs(z: list)

train()
    Training loop for DDP

```

## Classes

*DICE\_Trainer*

DICE\_Trainer implement

## Package Contents

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

### DICE\_Trainer implement

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

args

is\_continual\_training:bool

storage\_path:str

evaluator:

report:dict

report

args

trainer = None

is\_continual\_training

storage\_path

evaluator = None

form\_of\_labelling = None



**continual\_start** (*knowledge\_graph*)

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

## Parameter

### returns

- *model*
- **form\_of\_labelling** (*str*)

**initialize\_trainer** (*callbacks: List*)

→ *lightning.Trainer* | *dicke.trainer.model\_parallelism.TensorParallel* | *dicke.trainer.torch\_trainer.TorchTrainer* | *dicke.t*

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: dicke.knowledge\_graph.KG* | *numpy.memmap*)

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

Start the training

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

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

**k\_fold\_cross\_validation** (*dataset*) → *Tuple[dicke.models.base\_model.BaseKGE, str]*

Perform K-fold Cross-Validation

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

### Parameters

- **self**
- **dataset**

### Returns

*model*

## 14.2 Attributes

`__version__`

## 14.3 Classes

<i>Pyke</i>	A Physical Embedding Model for Knowledge Graphs
<i>DistMult</i>	Embedding Entities and Relations for Learning and Inference in Knowledge Bases
<i>CKeci</i>	Without learning dimension scaling
<i>Keci</i>	Base class for all neural network modules.
<i>TransE</i>	Translating Embeddings for Modeling
<i>DeCaL</i>	Base class for all neural network modules.
<i>DualE</i>	Dual Quaternion Knowledge Graph Embeddings ( <a href="https://ojs.aaai.org/index.php/AAAI/article/download/16850/16657">https://ojs.aaai.org/index.php/AAAI/article/download/16850/16657</a> )
<i>ComplEx</i>	Base class for all neural network modules.
<i>AConEx</i>	Additive Convolutional ComplEx Knowledge Graph Embeddings
<i>AConvO</i>	Additive Convolutional Octonion Knowledge Graph Embeddings
<i>AConvQ</i>	Additive Convolutional Quaternion Knowledge Graph Embeddings
<i>ConvQ</i>	Convolutional Quaternion Knowledge Graph Embeddings
<i>ConvO</i>	Base class for all neural network modules.
<i>ConEx</i>	Convolutional ComplEx Knowledge Graph Embeddings
<i>QMult</i>	Base class for all neural network modules.
<i>OMult</i>	Base class for all neural network modules.
<i>Shallom</i>	A shallow neural model for relation prediction ( <a href="https://arxiv.org/abs/2101.09090">https://arxiv.org/abs/2101.09090</a> )
<i>LFMult</i>	Embedding with polynomial functions. We represent all entities and relations in the polynomial space as:
<i>PykeenKGE</i>	A class for using knowledge graph embedding models implemented in Pykeen
<i>Byte</i>	Base class for all neural network modules.
<i>BaseKGE</i>	Base class for all neural network modules.
<i>EnsembleKGE</i>	
<i>DICE_Trainer</i>	DICE_Trainer implement
<i>KGE</i>	Knowledge Graph Embedding Class for interactive usage of pre-trained models
<i>Execute</i>	A class for Training, Retraining and Evaluation a model.
<i>BPE_NegativeSamplingDataset</i>	An abstract class representing a Dataset.
<i>MultiLabelDataset</i>	An abstract class representing a Dataset.
<i>MultiClassClassificationDataset</i>	Dataset for the 1vsALL training strategy
<i>OnevsAllDataset</i>	Dataset for the 1vsALL training strategy
<i>KvsAll</i>	Creates a dataset for KvsAll training by inheriting from torch.utils.data.Dataset.
<i>AllvsAll</i>	Creates a dataset for AllvsAll training by inheriting from torch.utils.data.Dataset.
<i>OnevsSample</i>	A custom PyTorch Dataset class for knowledge graph embeddings, which includes
<i>KvsSampleDataset</i>	KvsSample a Dataset:
<i>NegSampleDataset</i>	An abstract class representing a Dataset.
<i>TriplePredictionDataset</i>	Triple Dataset

continues on next page

Table 3 – continued from previous page

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

## 14.4 Functions

<i>create_recipriocal_triples</i> (x)	Add inverse triples into dask dataframe
<i>get_er_vocab</i> (data[, file_path])	
<i>get_re_vocab</i> (data[, file_path])	
<i>get_ee_vocab</i> (data[, file_path])	
<i>timeit</i> (func)	
<i>save_pickle</i> (*[, data, file_path])	
<i>load_pickle</i> ([file_path])	
<i>load_term_mapping</i> ([file_path])	
<i>select_model</i> (args[, is_continual_training, storage_path])	
<i>load_model</i> (→ Tuple[object, Tuple[dict, dict]])	Load weights and initialize pytorch module from namespace arguments
<i>load_model_ensemble</i> (...)	Construct Ensemble Of weights and initialize pytorch module from namespace arguments
<i>save_numpy_ndarray</i> (*[, data, file_path])	
<i>numpy_data_type_changer</i> (→ numpy.ndarray)	Detect most efficient data type for a given triples
<i>save_checkpoint_model</i> (→ None)	Store Pytorch model into disk
<i>store</i> (→ None)	
<i>add_noisy_triples</i> (→ pandas.DataFrame)	Add randomly constructed triples
<i>read_or_load_kg</i> (args, cls)	
<i>intialize_model</i> (→ Tuple[object, str])	
<i>load_json</i> (→ dict)	
<i>save_embeddings</i> (→ None)	Save it as CSV if memory allows.
<i>random_prediction</i> (pre_trained_kge)	
<i>deploy_triple_prediction</i> (pre_trained_kge, str_subject, ...)	
<i>deploy_tail_entity_prediction</i> (pre_trained_kge, ...)	

continues on next page

Table 4 – continued from previous page

<code>deploy_head_entity_prediction(pre_trained_kge,</code>	
<code>...)</code>	
<code>deploy_relation_prediction(pre_trained_kge,</code>	
<code>...)</code>	
<code>vocab_to_parquet(vocab_to_idx, name, ...)</code>	
<code>create_experiment_folder([folder_name])</code>	
<code>continual_training_setup_executor(→ None)</code>	
<code>exponential_function(→ torch.FloatTensor)</code>	
<code>load_numpy(→ numpy.ndarray)</code>	
<code>evaluate(entity_to_idx, scores, easy_answers, # @TODO: CD: Renamed this function</code>	
<code>hard_answers)</code>	
<code>download_file(url[, destination_folder])</code>	
<code>download_files_from_url(→ None)</code>	
<code>download_pretrained_model(→ str)</code>	
<code>write_csv_from_model_parallel(path)</code>	Create
<code>from_pretrained_model_write_embeddings_into</code>	
<code>None)</code>	
<code>mapping_from_first_two_cols_to_third(train_se</code>	
<code>timeit(func)</code>	
<code>load_term_mapping([file_path])</code>	
<code>reload_dataset(path, form_of_labelling, ...)</code>	Reload the files from disk to construct the Pytorch dataset
<code>construct_dataset(→ torch.utils.data.Dataset)</code>	

## 14.5 Package Contents

**class** `dicee.Pyke` (*args*)

Bases: `dicee.models.base_model.BaseKGE`

A Physical Embedding Model for Knowledge Graphs

**name** = 'Pyke'

**dist\_func**

**margin** = 1.0

**forward\_triples** (*x*: `torch.LongTensor`)

**Parameters**

**x**

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

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

    name = 'DistMult'

    k_vs_all_score(emb_h: torch.FloatTensor, emb_r: torch.FloatTensor, emb_E: torch.FloatTensor)

        Parameters
            • emb_h
            • emb_r
            • emb_E

    forward_k_vs_all(x: torch.LongTensor)

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

    score(h, r, t)
```

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

    Without learning dimension scaling

    name = 'CKeci'

    requires_grad_for_interactions = False
```

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

Base class for all neural network modules.

Your models should also subclass this class.

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

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

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

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

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

### **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  $\sigma_{pp} = \sum_{i=1}^{p-1} \sum_{k=i+1}^p (h_{ir_k} - h_{kr_i}) e_i e_k$

$\sigma_{pp}$  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.,  $e_1 e_1, e_1 e_2, e_1 e_3$ ,

$e_2 e_1, e_2 e_2, e_2 e_3, e_3 e_1, e_3 e_2, e_3 e_3$

Then select the triangular matrix without diagonals:  $e_1 e_2, e_1 e_3, e_2 e_3$ .

`compute_sigma_qq (hq, rq)`

Compute  $\sigma_{qq} = \sum_{j=1}^{q-1} \sum_{k=j+1}^q (h_{jr_k} - h_{kr_j}) e_j e_k$   $\sigma_{qq}$  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.,  $e_1 e_1, e_1 e_2, e_1 e_3$ ,

$e_2 e_1, e_2 e_2, e_2 e_3, e_3 e_1, e_3 e_2, e_3 e_3$

Then select the triangular matrix without diagonals:  $e_1 e_2, e_1 e_3, e_2 e_3$ .

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

$\sum_{i=1}^p \sum_{j=p+1}^{p+q} (h_{ir_j} - h_{jr_i}) e_i e_j$

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

```

    for j in range(q):
        sigma_pq[:, :, i, j] = hp[:, :, i] * rq[:, :, j] - hq[:, :, j] * rp[:, :, i]
    print(sigma_pq.shape)
apply_coefficients (hp, hq, rp, rq)
    Multiplying a base vector with its scalar coefficient
clifford_multiplication (h0, hp, hq, r0, rp, rq)
    Compute our CL multiplication
    
$$h = h_0 + \sum_{i=1}^p h_i e_i + \sum_{j=p+1}^{p+q} h_j e_j$$


$$r = r_0 + \sum_{i=1}^p r_i e_i + \sum_{j=p+1}^{p+q} r_j e_j$$


$$e_i^2 = +1 \text{ for } i \leq p, e_j^2 = -1 \text{ for } p < j \leq p+q, e_i e_j = -e_j e_i \text{ for } i \neq j$$


$$h r = \sigma_0 + \sigma_p + \sigma_q + \sigma_{pp} + \sigma_{qq} + \sigma_{pq}$$

    where
    (1)  $\sigma_0 = h_0 r_0 + \sum_{i=1}^p (h_i r_i) e_i - \sum_{j=p+1}^{p+q} (h_j r_j) e_j$ 
    (2)  $\sigma_p = \sum_{i=1}^p (h_i r_0 + h_0 r_i) e_i$ 
    (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)  $\sigma_{qq} = \sum_{j=1}^{q-1} \sum_{k=j+1}^{p+q} (h_j r_k - h_k r_j) e_j e_k$ 
    (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) → 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, **IEI**) 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*) → 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*) → 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 them to be nested in a tree structure. You can assign the sub-modules as regular attributes:



```

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

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

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

```

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

### Note

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

### Variables

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

**name** = 'DeCaL'

**entity\_embeddings**

**relation\_embeddings**

**p**

**q**

**r**

**re**

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

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

and return:

$$sigma_0 t = \sigma_0 \cdot t_0 = s0 + s1 - s2 s3, s4 \text{ and } s5$$

**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

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

For different base vector interactions, we have

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

**forward\_k\_vs\_all** (*x*: *torch.Tensor*) → *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 functions are identical Parameter ——— *x*: *torch.LongTensor* with (n, ) shape :rtype: *torch.FloatTensor* with (n, **IE**) 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:

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

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

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

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

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

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

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

e2e1, e2e2, e2e3, e3e1, e3e2, e3e3

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

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

Compute

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

$\sigma_{qq}$  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\_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 = None

    kvsall_score (e_1_h, e_2_h, e_3_h, e_4_h, e_5_h, e_6_h, e_7_h, e_8_h, e_1_t, e_2_t, e_3_t, e_4_t,
        e_5_t, e_6_t, e_7_t, e_8_t, r_1, r_2, r_3, r_4, r_5, r_6, r_7, r_8) → torch.tensor

    KvsAll scoring function

```

### Input

x: torch.LongTensor with (n, ) shape

### Output

torch.FloatTensor with (n) shape

**forward\_triples** (idx\_triple: torch.tensor) → torch.tensor

Negative Sampling forward pass:

### Input

x: torch.LongTensor with (n, ) shape

### Output

torch.FloatTensor with (n) shape

**forward\_k\_vs\_all**(x)

KvsAll forward pass

### Input

x: torch.LongTensor with (n, ) shape

### Output

torch.FloatTensor with (n) shape

**T**(x: torch.tensor) → torch.tensor

Transpose function

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

**class** dicee.**Complex**(args)

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

Base class for all neural network modules.

Your models should also subclass this class.

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

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

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

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

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

### Note

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

### Variables

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

**name** = 'Complex'

**static score** (*head\_ent\_emb: torch.FloatTensor, rel\_ent\_emb: torch.FloatTensor, tail\_ent\_emb: torch.FloatTensor*)

**static k\_vs\_all\_score** (*emb\_h: torch.FloatTensor, emb\_r: torch.FloatTensor, emb\_E: torch.FloatTensor*)

### Parameters

- **emb\_h**
- **emb\_r**
- **emb\_E**

**forward\_k\_vs\_all** (*x: torch.LongTensor*) → torch.FloatTensor

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

**class** `dicee.AConEx` (*args*)

Bases: `dicee.models.base_model.BaseKGE`

Additive Convolutional Complex Knowledge Graph Embeddings

**name** = 'AConEx'

**conv2d**

**fc\_num\_input**

**fc1**

**norm\_fc1**

**bn\_conv2d**

**feature\_map\_dropout**

**residual\_convolution** (*C\_1: Tuple[torch.Tensor, torch.Tensor], C\_2: Tuple[torch.Tensor, torch.Tensor]*) → 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*) → torch.FloatTensor

**forward\_triples** (*x: torch.Tensor*) → torch.FloatTensor

### Parameters

**x**

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

**class** `dicee.AConvO` (*args: dict*)

Bases: `dicee.models.base_model.BaseKGE`

Additive Convolutional Octonion Knowledge Graph Embeddings

```

name = 'AConvO'

conv2d

fc_num_input

fc1

bn_conv2d

norm_fc1

feature_map_dropout

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

residual_convolution(O_1, O_2)

forward_triples(x: torch.Tensor) → 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.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) → 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**

**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.ConvO* (*args*: *dict*)

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

Base class for all neural network modules.

Your models should also subclass this class.

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

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

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

(continues on next page)



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

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

### **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.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]*) → *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*) → *torch.FloatTensor*

**forward\_triples** (*x*: *torch.Tensor*) → *torch.FloatTensor*

#### Parameters

**x**

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

**class** *dicee.QMult* (*args*)

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

Base class for all neural network modules.

Your models should also subclass this class.

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

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

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

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

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

#### 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 = 'QMult'`

`explicit = True`

`quaternion_multiplication_followed_by_inner_product (h, r, t)`

#### Parameters

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

#### Returns

Triple scores.

`static quaternion_normalizer (x: torch.FloatTensor) → torch.FloatTensor`

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

Absolute value of a quaternion

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

L2 norm of quaternion vector:

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

#### Parameters

**x** – The vector.

#### Returns

The normalized vector.

`score (head_ent_emb: torch.FloatTensor, rel_ent_emb: torch.FloatTensor,  
tail_ent_emb: torch.FloatTensor)`

`k_vs_all_score (bpe_head_ent_emb, bpe_rel_ent_emb, E)`

#### Parameters

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

`forward_k_vs_all (x)`

#### Parameters

**x**

`forward_k_vs_sample (x, target_entity_idx)`

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

```
class dicee.OMult (args)
```

Bases: `dicee.models.base_model.BaseKGE`

Base class for all neural network modules.

Your models should also subclass this class.

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

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

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

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

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

#### Note

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

#### Variables

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

```
name = 'OMult'
```

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

```
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 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'
```

**shallow**

**get\_embeddings** () → Tuple[numpy.ndarray, None]

**forward\_k\_vs\_all** (x) → torch.FloatTensor

**forward\_triples** (x) → 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:  $f(x) = \sum_{i=0}^{d-1} a_i x^i$  and use the three different 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.  $h = \sigma(w_h^T x + b_h)$ ,  $r = \sigma(w_r^T x + b_r)$ ,  $t = \sigma(w_t^T x + b_t)$

**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:

$$\text{score}(h,r,t) = \int_0^1 h(x)r(x)t(x) dx = \sum_{i,j,k=0}^{d-1} \text{dfrac}\{a_i*b_j*c_k\}\{1+(i+j+k)\%d\}$$

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

```

vtp_score (h, r, t)
    this part implement the vector triple product scoring techniques:

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

    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: Py-
    keen_HolE: Pykeen_HolE: Pykeen_TransD: Pykeen_TransE: Pykeen_TransF: Pykeen_TransH: Pykeen_TransR:

    model_kwargs

    name

    model

    loss_history = []

    args

    entity_embeddings = None

    relation_embeddings = None

    forward_k_vs_all (x: torch.LongTensor)
    # => Explicit version by this we can apply bn and dropout

    # (1) Retrieve embeddings of heads and relations + apply Dropout & Normalization if given. h, r =
    self.get_head_relation_representation(x) # (2) Reshape (1). if self.last_dim > 0:
        h = h.reshape(len(x), self.embedding_dim, self.last_dim) r = r.reshape(len(x), self.embedding_dim,
        self.last_dim)

```

```

# (3) Reshape all entities. if self.last_dim > 0:
    t = self.entity_embeddings.weight.reshape(self.num_entities, self.embedding_dim, self.last_dim)

else:
    t = self.entity_embeddings.weight

# (4) Call the score_t from interactions to generate triple scores. return self.interaction.score_t(h=h, r=r,
all_entities=t, slice_size=1)

forward_triples (x: torch.LongTensor) → torch.FloatTensor
# => Explicit version by this we can apply bn and dropout

# (1) Retrieve embeddings of heads, relations and tails and apply Dropout & Normalization if given. h, r, t =
self.get_triple_representation(x) # (2) Reshape (1). if self.last_dim > 0:
    h = h.reshape(len(x), self.embedding_dim, self.last_dim) r = r.reshape(len(x), self.embedding_dim,
    self.last_dim) t = t.reshape(len(x), self.embedding_dim, self.last_dim)

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

abstract forward_k_vs_sample (x: torch.LongTensor, target_entity_idx)

```

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

Bases: `dicee.models.base_model.BaseKGE`

Base class for all neural network modules.

Your models should also subclass this class.

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

```

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

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

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

```

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

#### 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 = 'ByteE'

config

temperature = 0.5

topk = 2

transformer

lm_head

loss_function(yhat_batch, y_batch)

```

#### Parameters

- **yhat\_batch**
- **y\_batch**

**forward** (*x: torch.LongTensor*)

#### Parameters

**x** (*B by T tensor*)

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

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

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

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

#### Parameters

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

#### Returns

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

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

Example:

```

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

```



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

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

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

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

#### **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: `BaseKGE Lightning`

Base class for all neural network modules.

Your models should also subclass this class.

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

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

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

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

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

#### **Note**

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

child.

### Variables

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

#### args

**embedding\_dim** = None

**num\_entities** = None

**num\_relations** = None

**num\_tokens** = None

**learning\_rate** = None

**apply\_unit\_norm** = None

**input\_dropout\_rate** = None

**hidden\_dropout\_rate** = None

**optimizer\_name** = None

**feature\_map\_dropout\_rate** = None

**kernel\_size** = None

**num\_of\_output\_channels** = None

**weight\_decay** = None

#### loss

**selected\_optimizer** = None

**normalizer\_class** = None

**normalize\_head\_entity\_embeddings**

**normalize\_relation\_embeddings**

**normalize\_tail\_entity\_embeddings**

**hidden\_normalizer**

**param\_init**

**input\_dp\_ent\_real**

**input\_dp\_rel\_real**

**hidden\_dropout**

**loss\_history** = []

**byte\_pair\_encoding**

```

max_length_subword_tokens

block_size

forward_byte_pair_encoded_k_vs_all (x: torch.LongTensor)

    Parameters
         $\mathbf{x}$  ( $B \times 2 \times T$ )

forward_byte_pair_encoded_triple (x: Tuple[torch.LongTensor, torch.LongTensor])
    byte pair encoded neural link predictors

    Parameters
        -----

init_params_with_sanity_checking()

forward (x: torch.LongTensor | Tuple[torch.LongTensor, torch.LongTensor],
        y_idx: torch.LongTensor = None)

    Parameters
        •  $\mathbf{x}$ 
        •  $\mathbf{y\_idx}$ 
        • ordered_bpe_entities

forward_triples (x: torch.LongTensor) → torch.Tensor

    Parameters
         $\mathbf{x}$ 

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
        • ( $\mathbf{b}$  ( $x$  shape)
        • 3
        •  $\mathbf{t}$ )

get_bpe_head_and_relation_representation (x: torch.LongTensor)
    → Tuple[torch.FloatTensor, torch.FloatTensor]

    Parameters
         $\mathbf{x}$  ( $B \times 2 \times T$ )

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

class dicee.EnsembleKGE (seed_model=None, pretrained_models: List = None)

    name

```

```

train_mode = True

named_children()

property example_input_array

parameters()

modules()

__iter__()

__len__()

eval()

to(device)

mem_of_model()

__call__(x_batch)

step()

get_embeddings()

__str__()

```

`dicee.create_recipriocal_triples(x)`  
 Add inverse triples into dask dataframe :param x: :return:

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

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

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

`dicee.timeit(func)`

`dicee.save_pickle(*, data: object = None, file_path=str)`

`dicee.load_pickle(file_path=str)`

`dicee.load_term_mapping(file_path=str)`

`dicee.select_model(args: dict, is_continual_training: bool = None, storage_path: str = None)`

`dicee.load_model(path_of_experiment_folder: str, model_name='model.pt', verbose=0)`  
 → Tuple[object, Tuple[dict, dict]]  
 Load weights and initialize pytorch module from namespace arguments

`dicee.load_model_ensemble(path_of_experiment_folder: str)`  
 → Tuple[dicee.models.base\_model.BaseKGE, Tuple[pandas.DataFrame, pandas.DataFrame]]  
 Construct Ensemble Of weights and initialize pytorch module from namespace arguments

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

```

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

dicee.numpy_data_type_changer(train_set: numpy.ndarray, num: int) → numpy.ndarray
    Detect most efficient data type for a given triples :param train_set: :param num: :return:

dicee.save_checkpoint_model(model, path: str) → None
    Store Pytorch model into disk

dicee.store(trained_model, model_name: str = 'model', full_storage_path: str = None,
    save_embeddings_as_csv=False) → None

dicee.add_noisy_triples(train_set: pandas.DataFrame, add_noise_rate: float) → pandas.DataFrame
    Add randomly constructed triples :param train_set: :param add_noise_rate: :return:

dicee.read_or_load_kg(args, cls)

dicee.intialize_model(args: dict, verbose=0) → Tuple[object, str]

dicee.load_json(p: str) → dict

dicee.save_embeddings(embeddings: numpy.ndarray, indexes, path: str) → None
    Save it as CSV if memory allows. :param embeddings: :param indexes: :param path: :return:

dicee.random_prediction(pre_trained_kge)

dicee.deploy_triple_prediction(pre_trained_kge, str_subject, str_predicate, str_object)

dicee.deploy_tail_entity_prediction(pre_trained_kge, str_subject, str_predicate, top_k)

dicee.deploy_head_entity_prediction(pre_trained_kge, str_object, str_predicate, top_k)

dicee.deploy_relation_prediction(pre_trained_kge, str_subject, str_object, top_k)

dicee.vocab_to_parquet(vocab_to_idx, name, path_for_serialization, print_into)

dicee.create_experiment_folder(folder_name='Experiments')

dicee.continual_training_setup_executor(executor) → None

dicee.exponential_function(x: numpy.ndarray, lam: float, ascending_order=True) → torch.FloatTensor

dicee.load_numpy(path) → 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='.') → None

```

### Parameters

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

```

dicee.download_pretrained_model(url: str) → str

```

```

dicee.write_csv_from_model_parallel(path: str)

```

Create

`dicee.from_pretrained_model_write_embeddings_into_csv(path: str) → None`

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

#### DICE\_Trainer implement

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

args

is\_continual\_training:bool

storage\_path:str

evaluator:

report:dict

report

args

trainer = None

is\_continual\_training

storage\_path

evaluator = None

form\_of\_labelling = None

continual\_start(*knowledge\_graph*)

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

#### Parameter

returns

- *model*
- **form\_of\_labelling** (*str*)

**initialize\_trainer** (*callbacks: List*)

→ `lightning.Trainer` | `dicee.trainer.model_parallelism.TensorParallel` | `dicee.trainer.torch_trainer.TorchTrainer` | `dicee.`

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]

Start the training

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

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

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

Perform K-fold Cross-Validation

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

#### Parameters

- **self**
- **dataset**

#### Returns

model

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

Bases: *dicee.abstracts.BaseInteractiveKGE*, *dicee.abstracts.InteractiveQueryDecomposition*, *dicee.abstracts.BaseInteractiveTrainKGE*

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

**\_\_str\_\_** ()

**to** (*device: str*) → None

**get\_transductive\_entity\_embeddings** (*indices: torch.LongTensor | List[str], as\_pytorch=False, as\_numpy=False, as\_list=True*) → torch.FloatTensor | numpy.ndarray | List[float]

**create\_vector\_database** (*collection\_name: str, distance: str, location: str = 'localhost', port: int = 6333*)

**generate** (*h="", r=""*)

**eval\_lp\_performance** (*dataset=List[Tuple[str, str, str]], filtered=True*)

**predict\_missing\_head\_entity** (*relation: List[str] | str, tail\_entity: List[str] | str, within=None, batch\_size=2, topk=1, return\_indices=False*) → Tuple

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

$\text{argmax}_{\{e \in E\}} f(e, r, t)$ , where  $r \in R$ ,  $t \in E$ .

### Parameter

relation: Union[List[str], str]

String representation of selected relations.

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

String representation of selected entities.

k: int

Highest ranked k entities.

### Returns: Tuple

Highest K scores and entities

**predict\_missing\_relations** (*head\_entity: List[str] | str, tail\_entity: List[str] | str, within=None, batch\_size=2, topk=1, return\_indices=False*) → Tuple

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

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

### Parameter

head\_entity: List[str]

String representation of selected entities.

tail\_entity: List[str]

String representation of selected entities.

k: int

Highest ranked k entities.

### Returns: Tuple

Highest K scores and entities

**predict\_missing\_tail\_entity** (*head\_entity: List[str] | str, relation: List[str] | str, within: List[str] = None, batch\_size=2, topk=1, return\_indices=False*) → torch.FloatTensor

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

$\operatorname{argmax}_{\{e \in E\}} f(h, r, e)$ , 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) → torch.FloatTensor

#### Parameters

- **logits**
- **h**
- **r**
- **t**
- **within**

**predict\_topk** (\*, *h*: str | List[str] = None, *r*: str | List[str] = None, *t*: str | List[str] = None, *topk*: int = 10, *within*: List[str] = None, *batch\_size*: int = 1024)

Predict missing item in a given triple.

#### Returns

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

**triple\_score** (*h*: List[str] | *str* = None, *r*: List[str] | *str* = None, *t*: List[str] | *str* = None, *logits*=False) → 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

**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*) → Set

Find missing triples

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

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

Return (e,r,x)

return 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 and (e,r,x)

return G

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

**predict\_literals** (*entity: List[str] | str = None, attribute: List[str] | str = None, denormalize\_preds: bool = True*) → numpy.ndarray

Predicts literal values for given entities and attributes.

### Parameters

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

### Returns

Predictions for the given entities and attributes.

### Return type

numpy ndarray

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

A class for Training, Retraining and Evaluation a model.

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

**args**

**is\_continual\_training** = False

**trainer** = None

**trained\_model** = None

**knowledge\_graph** = None

**report**

**evaluator** = None

**start\_time** = None

**setup\_executor** () → None

**save\_trained\_model** () → None

Save a knowledge graph embedding model

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

### Parameter

**rtype**

None

**end** (*form\_of\_labelling: str*) → 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** () → None

Report training related information in a report.json file

**start** () → dict

Start training

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

## Parameter

**rtype**

A dict containing information about the training and/or evaluation

`dicee.mapping_from_first_two_cols_to_third(train_set_idx)`

`dicee.timeit(func)`

`dicee.load_term_mapping(file_path=str)`

`dicee.reload_dataset(path: str, form_of_labelling, scoring_technique, neg_ratio, label_smoothing_rate)`

Reload the files from disk to construct the Pytorch dataset

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

**class** `dicee.BPE_NegativeSamplingDataset(train_set: torch.LongTensor, ordered_shaped_bpe_entities: torch.LongTensor, neg_ratio: int)`

Bases: torch.utils.data.Dataset

An abstract class representing a Dataset.

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

### Note

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

**train\_set**

**ordered\_bpe\_entities**

**num\_bpe\_entities**

**neg\_ratio**

**num\_datapoints**

**\_\_len\_\_()**

`__getitem__(idx)`

`collate_fn(batch_shaped_bpe_triples: List[Tuple[torch.Tensor, torch.Tensor]])`

```
class dicee.MultiLabelDataset (train_set: torch.LongTensor, train_indices_target: torch.LongTensor,
                               target_dim: int, torch_ordered_shaped_bpe_entities: torch.LongTensor)
```

Bases: `torch.utils.data.Dataset`

An abstract class representing a Dataset.

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

#### Note

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

`train_set`

`train_indices_target`

`target_dim`

`num_datapoints`

`torch_ordered_shaped_bpe_entities`

`collate_fn = None`

`__len__()`

`__getitem__(idx)`

```
class dicee.MultiClassClassificationDataset (subword_units: numpy.ndarray, block_size: int = 8)
```

Bases: `torch.utils.data.Dataset`

Dataset for the 1vsALL training strategy

#### Parameters

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

#### Return type

`torch.utils.data.Dataset`

`train_data`

```

block_size = 8

num_of_data_points

collate_fn = None

__len__()

__getitem__(idx)

```

```
class dicee.OnevsAllDataset (train_set_idx: numpy.ndarray, entity_idx)
```

Bases: torch.utils.data.Dataset

Dataset for the 1vsALL training strategy

#### Parameters

- **train\_set\_idx** – Indexed triples for the training.
- **entity\_idx** – mapping.
- **relation\_idx** – 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_idx, relation_idx, 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 a 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

#### Note

TODO

**train\_set\_idx**

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

**entity\_idx**

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

**relation\_idxxs**

[dictionary] 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\_idxxs, relation\_idxxs, 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.  $(h, r) \in KG$

#### 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\_idxxs**

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

**relation\_idxxs**

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

self : torch.utils.data.Dataset

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

**train\_data** = None

**train\_target** = None

**label\_smoothing\_rate**

**collate\_fn** = None

**target\_dim**

**\_\_len\_\_**()

**\_\_getitem\_\_**(idx)

```
class dicee.OnevsSample(train_set: numpy.ndarray, num_entities, num_relations,  
                        neg_sample_ratio: int = None, label_smoothing_rate: float = 0.0)
```

Bases: torch.utils.data.Dataset

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

#### Parameters

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

**train\_data**

The input data converted into a PyTorch tensor.

#### Type

torch.Tensor

**num\_entities**

Number of entities in the dataset.

#### Type

int

**num\_relations**

Number of relations in the dataset.

#### Type

int

**neg\_sample\_ratio**

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

#### Type

int

**label\_smoothing\_rate**

The smoothing factor applied to the labels.

#### Type

torch.Tensor



**collate\_fn**

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

**Type**

function, optional

**train\_data**

**num\_entities**

**num\_relations**

**neg\_sample\_ratio = None**

**label\_smoothing\_rate**

**collate\_fn = None**

**\_\_len\_\_()**

Returns the number of samples in the dataset.

**\_\_getitem\_\_(idx)**

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

**Parameters**

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

**Returns**

**A tuple consisting of:**

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

**Return type**

tuple

```
class dicee.KvsSampleDataset (train_set_idx: numpy.ndarray, entity_idxxs, relation_idxxs, 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

**train\_set\_idx**

Indexed triples for the training.

**entity\_idxxs**

mapping.

```

    relation_idx
    mapping.

    form
    ?

    store
    ?

    label_smoothing_rate
    ?

    torch.utils.data.Dataset

```

```

train_data = None

train_target = None

neg_ratio = None

num_entities

label_smoothing_rate

collate_fn = None

max_num_of_classes

__len__()

__getitem__(idx)

```

```

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

```

Bases: torch.utils.data.Dataset

An abstract class representing a Dataset.

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

#### Note

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

```

neg_sample_ratio

train_set

length

num_entities

num_relations

```

```

__len__()

__getitem__(idx)

class dicee.TriplePredictionDataset (train_set: numpy.ndarray, num_entities: int, num_relations: int,
    neg_sample_ratio: int = 1, label_smoothing_rate: float = 0.0)
    Bases: torch.utils.data.Dataset
        Triple Dataset
            D:= {(x)_i}_i ^N, where
                . x:(h,r, t) in KG is a unique h in E and a relation r in R and . collect_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_idx
                mapping.

            relation_idx
                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.CVDDataModule (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.

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

For data processing use the following pattern:

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

However, the above are only necessary for distributed processing.

### Warning

do not assign state in `prepare_data`

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

### 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, ...).

### Note

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

#### Parameters

- **batch** – A batch of data that needs to be transferred to a new device.

- **device** – The target device as defined in PyTorch.
- **dataloader\_idx** – The index of the dataloader to which the batch belongs.

### Returns

A reference to the data on the new device.

Example:

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

### See also

- `move_data_to_device()`
- `apply_to_collection()`

### `prepare_data(*args, **kwargs)`

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

### Warning

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

Example:

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

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

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

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

Example:

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

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

This is called before requesting the dataloaders:

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

```
class dicee.LiteralDataset (file_path: str, ent_idx: dict = None, normalization_type: str = 'z-norm',
                           sampling_ratio: float = None, loader_backend: str = 'pandas')
```

Bases: torch.utils.data.Dataset

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

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

**train\_file\_path**

Path to the training data file.

**Type**

str

**normalization**

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

**Type**

str

**normalization\_params**

Parameters used for normalization.

**Type**

dict

**sampling\_ratio**

Fraction of the training set to use for ablations.

**Type**

float

**entity\_to\_idx**

Mapping of entities to their indices.

**Type**

dict

**num\_entities**

Total number of entities.

**Type**

int

**data\_property\_to\_idx**

Mapping of data properties to their indices.

**Type**

dict

**num\_data\_properties**

Total number of data properties.

**Type**

int

**loader\_backend**

Backend to use for loading data ('pandas' or 'rdflib').

**Type**

str

**train\_file\_path**

**loader\_backend** = 'pandas'

**normalization\_type** = 'z-norm'

**normalization\_params**

**sampling\_ratio** = None

**entity\_to\_idx** = None

**num\_entities**

**\_\_getitem\_\_** (*index*)

**\_\_len\_\_** ()

**static load\_and\_validate\_literal\_data** (*file\_path: str = None, loader\_backend: str = 'pandas'*)  
→ pandas.DataFrame

Loads and validates the literal data file. :param file\_path: Path to the literal data file. :type file\_path: str

**Returns**

DataFrame containing the loaded and validated data.

**Return type**

pd.DataFrame



**static denormalize** (*preds\_norm, attributes, normalization\_params*) → numpy.ndarray

Denormalizes the predictions based on the normalization type.

Args: *preds\_norm* (np.ndarray): Normalized predictions to be denormalized. *attributes* (list): List of attributes corresponding to the predictions. *normalization\_params* (dict): Dictionary containing normalization parameters for each attribute.

**Returns**

Denormalized predictions.

**Return type**

np.ndarray

**class** dicee.**QueryGenerator** (*train\_path, val\_path: str, test\_path: str, ent2id: Dict = None, rel2id: Dict = None, seed: int = 1, gen\_valid: bool = False, gen\_test: bool = True*)

**train\_path**

**val\_path**

**test\_path**

**gen\_valid** = False

**gen\_test** = True

**seed** = 1

**max\_ans\_num** = 1000000.0

**mode**

**ent2id** = None

**rel2id**: Dict = None

**ent\_in**: Dict

**ent\_out**: Dict

**query\_name\_to\_struct**

**list2tuple** (*list\_data*)

**tuple2list** (*x: List | Tuple*) → List | Tuple

Convert a nested tuple to a nested list.

**set\_global\_seed** (*seed: int*)

Set seed

**construct\_graph** (*paths: List[str]*) → Tuple[Dict, Dict]

Construct graph from triples Returns dicts with incoming and outgoing edges

**fill\_query** (*query\_structure: List[str | List], ent\_in: Dict, ent\_out: Dict, answer: int*) → 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]]])
    → None
    Save Queries into Disk

static load_queries_and_answers (path: str) → List[Tuple[str, Tuple[collections.defaultdict]]]
    Load Queries from Disk to Memory

dicee.__version__ = '0.1.5'

```

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