DICE Embeddings

Release 0.1.3.2

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DICE Embeddings[1]: 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

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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**[3] **& Co.** to use parallelism at preprocessing a large knowledge graph,

2. **PyTorch**[4] **& Co.** to learn knowledge graph embeddings via multi-CPUs, GPUs, TPUs or computing cluster, and

3. **Huggingface**[5] to ease the deployment of pre-trained models.

Why Pandas[6] **& 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[7] **& 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[8] & PytorchLightning[9]. 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[10]**?** Deploy a pre-trained embedding model without writing a single line of code.

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

2 Installation

2.1 Installation from Source

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

or

```
pip install dicee
```

3 Download Knowledge Graphs

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

To test the Installation

```
python -m pytest -p no:warnings -x # Runs >114 tests leading to > 15 mins
python -m pytest -p no:warnings --lf # run only the last failed test
python -m pytest -p no:warnings --ff # to run the failures first and then the rest of↵
↪the tests.
```

4 Knowledge Graph Embedding Models

1. TransE, DistMult, ComplEx, ConEx, QMult, OMult, ConvO, ConvQ, Keci

2. All 44 models available in https://github.com/pykeen/pykeen#models

   For more, please refer to `examples`.

5 How to Train

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

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

```
# Train a model by only using the GPU-0
CUDA_VISIBLE_DEVICES=0 dicee --dataset_dir "KGs/UMLS" --model Keci --eval_model
↪"train_val_test"
# Train a model by only using GPU-1
CUDA_VISIBLE_DEVICES=1 dicee --dataset_dir "KGs/UMLS" --model Keci --eval_model
↪"train_val_test"
NCCL_P2P_DISABLE=1 CUDA_VISIBLE_DEVICES=0,1 python dicee/scripts/run.py --trainer PL -
↪-dataset_dir "KGs/UMLS" --model Keci --eval_model "train_val_test"
```

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

```
# Two equivalent executions
# (1)
dicee --dataset_dir "KGs/UMLS" --model Keci --eval_model "train_val_test"
# Evaluate Keci on Train set: Evaluate Keci on Train set
# {'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
```

```python
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.

7

8 Predicting Missing Links

```python
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

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

- For more please look at dice-research.org/projects/DiceEmbeddings/[11]

10 How to Deploy

```python
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[12]:

Name	Stmts	Miss	Cover	Missing
dicee/__init__.py	7	0	100%	
dicee/abstracts.py	338	115	66%	112-113,␣

<div align="right">(continues on next page)</div>

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

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

```
→131, 154-155, 160, 173, 197, 240-254, 290, 303-306, 309-313, 353-364, 379-387, 402,␣
→413-417, 427-428, 434-436, 442-445, 448-453, 576-596, 602-606, 610-612, 631, 658-696
dicee/callbacks.py                                        248    103    58%    50-55,␣
→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
```

```
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}
→,
```

```
  author={Demir, Caglar and Ngonga Ngomo, Axel-Cyrille},
  booktitle={Joint European Conference on Machine Learning and Knowledge Discovery in␣
→Databases},
  pages={567--582},
  year={2023},
  organization={Springer}
}
# LitCQD
@inproceedings{demir2023litcqd,
  title={LitCQD: Multi-Hop Reasoning in Incomplete Knowledge Graphs with Numeric␣
→Literals},
  author={Demir, Caglar and Wiebesiek, Michel and Lu, Renzhong and Ngonga Ngomo, Axel-
→Cyrille and Heindorf, Stefan},
  booktitle={Joint European Conference on Machine Learning and Knowledge Discovery in␣
→Databases},
  pages={617--633},
  year={2023},
  organization={Springer}
}
# DICE Embedding Framework
@article{demir2022hardware,
  title={Hardware-agnostic computation for large-scale knowledge graph embeddings},
  author={Demir, Caglar and Ngomo, Axel-Cyrille Ngonga},
  journal={Software Impacts},
  year={2022},
  publisher={Elsevier}
}
# KronE
@inproceedings{demir2022kronecker,
  title={Kronecker decomposition for knowledge graph embeddings},
  author={Demir, Caglar and Lienen, Julian and Ngonga Ngomo, Axel-Cyrille},
  booktitle={Proceedings of the 33rd ACM Conference on Hypertext and Social Media},
  pages={1--10},
  year={2022}
}
# QMult, OMult, ConvQ, ConvO
@InProceedings{pmlr-v157-demir21a,
  title =         {Convolutional Hypercomplex Embeddings for Link Prediction},
  author =        {Demir, Caglar and Moussallem, Diego and Heindorf, Stefan and Ngonga␣
→Ngomo, Axel-Cyrille},
  booktitle =         {Proceedings of The 13th Asian Conference on Machine Learning},
  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

14 dicee

14.1 Submodules

dicee.__main__

dicee.abstracts

Classes

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

Module Contents

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

    Abstract class for Trainer class for knowledge graph embedding models

    Parameter

    args
        [str] ?

    callbacks: list
        ?

attributes

callbacks

is_global_zero = True

global_rank = 0

local_rank = 0

strategy = None

on_fit_start(**args*, ***kwargs*)

A function to call callbacks before the training starts.

Parameter

args

kwargs

> **rtype**
> None

on_fit_end(**args*, ***kwargs*)

A function to call callbacks at the ned of the training.

Parameter

args

kwargs

> **rtype**
> None

on_train_epoch_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**

14

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 imes d} where n denotes the number of hops and d denotes number of entities

t_conorm (*tens_1: torch.Tensor*, *tens_2: torch.Tensor*, *tconorm: str = 'min'*) → 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.

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*, *suffle_data: bool = True*)

    Trains the Literal Embeddings model using literal data.

        Parameters

            • **train_file_path** (*str*) – Path to the training data file.

            • **num_epochs** (*int*) – Number of training epochs.

            • **lit_lr** (*float*) – Learning rate for the literal model.

            • **norm_type** (*str*) – Normalization type to use ('z-norm', 'min-max', or None).

            • **batch_size** (*int*) – Batch size for training.

            • **sampling_ratio** (*float*) – Ratio of training triples to use.

- **loader_backend** (`str`) – Backend for loading the dataset ('pandas' or 'rdflib').

- **freeze_entity_embeddings** (`bool`) – If True, freeze the entity embeddings during training.

- **gate_residual** (`bool`) – If True, use gate residual connections in the model.

- **device** (`str`) – Device to use for training ('cuda' or 'cpu'). If None, will use available GPU or CPU.

- **suffle_data** (`bool`) – If True, shuffle the dataset before training.

dicee.analyse_experiments

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

Classes

Experiment

Functions

get_default_arguments()
analyse(args)

Module Contents

dicee.analyse_experiments.**get_default_arguments**()

class dicee.analyse_experiments.**Experiment**

    model_name = []

    callbacks = []

    embedding_dim = []

    num_params = []

    num_epochs = []

    batch_size = []

    lr = []

    byte_pair_encoding = []

    aswa = []

    path_dataset_folder = []

```
full_storage_path = []

pq = []

train_mrr = []

train_h1 = []

train_h3 = []

train_h10 = []

val_mrr = []

val_h1 = []

val_h3 = []

val_h10 = []

test_mrr = []

test_h1 = []

test_h3 = []

test_h10 = []

runtime = []

normalization = []

scoring_technique = []

save_experiment(x)

to_df()
```

dicee.analyse_experiments.**analyse**(*args*)

dicee.callbacks

Classes

AccumulateEpochLossCallback	Abstract class for Callback class for knowledge graph embedding models
PrintCallback	Abstract class for Callback class for knowledge graph embedding models
KGESaveCallback	Abstract class for Callback class for knowledge graph embedding models
PseudoLabellingCallback	Abstract class for Callback class for knowledge graph embedding models
Eval	Abstract class for Callback class for knowledge graph embedding models
KronE	Abstract class for Callback class for knowledge graph embedding models
Perturb	A callback for a three-Level Perturbation
PeriodicEvalCallback	Callback to periodically evaluate the model and optionally save checkpoints during training.
LRScheduler	Callback for managing learning rate scheduling and model snapshots.

Functions

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

Module Contents

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

Bases: *dicee.abstracts.AbstractCallback*

Abstract class for Callback class for knowledge graph embedding models

Parameter

path

on_fit_end(*trainer*, *model*) → 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.**Eval**(*path*, *epoch_ratio: int = None*)

Bases: *dicee.abstracts.AbstractCallback*

Abstract class for Callback class for knowledge graph embedding models

Parameter

path

reports = []

epoch_ratio = None

epoch_counter = 0

on_fit_start(*trainer*, *model*)

Call at the beginning of the training.

Parameter

trainer:

model:

>   **rtype**
>   None

on_fit_end(*trainer*, *model*)

Call at the end of the training.

> **Parameter**

trainer:

model:

> **rtype**
>> None

on_train_epoch_end(*trainer*, *model*)

    Call at the end of each epoch during training.

> **Parameter**

trainer:

model:

> **rtype**
>> None

on_train_batch_end(**args*, ***kwargs*)

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

> **Parameter**

trainer:

model:

> **rtype**
>> None

class dicee.callbacks.**KronE**

    Bases: *dicee.abstracts.AbstractCallback*

Abstract class for Callback class for knowledge graph embedding models

> **Parameter**

f = None

static batch_kronecker_product(*a*, *b*)

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

get_kronecker_triple_representation(*indexed_triple: torch.LongTensor*)

    Get kronecker embeddings

on_fit_start(*trainer*, *model*)

    Call at the beginning of the training.

> **Parameter**

trainer:

model:

> **rtype**
>> None

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

Bases: *dicee.abstracts.AbstractCallback*

A callback for a three-Level Perturbation

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

Parameter Perturbation:

Output Perturbation:

level = 'input'

ratio = 0.0

method = None

scaler = None

frequency = None

on_train_batch_start(*trainer*, *model*, *batch*, *batch_idx*)

> Called when the train batch begins.

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

Bases: *dicee.abstracts.AbstractCallback*

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

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

experiment_dir

max_epochs

epoch_counter = 0

save_model_every_n_epoch = True

reports

n_epochs_eval_model = 'val_test'

default_eval_model = None

eval_epochs

on_fit_end(*trainer*, *model*)

> Called at the end of training. Saves final evaluation report.

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

dicee.config

Classes

Namespace	Simple object for storing attributes.

Module Contents

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

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

`backend: str = 'pandas'`

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

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

    separator for extracting head, relation and tail from a triple

`trainer: str = 'torchCPUTrainer'`

    Trainer for knowledge graph embedding model

`scoring_technique: str = 'KvsAll'`

    Scoring technique for knowledge graph embedding models

`neg_ratio: int = 0`

    Negative ratio for a true triple in NegSample training_technique

`weight_decay: float = 0.0`

    Weight decay for all trainable params

`normalization: str = 'None'`

    LayerNorm, BatchNorm1d, or None

`init_param: str = None`

    xavier_normal or None

`gradient_accumulation_steps: int = 0`

    Not tested e

`num_folds_for_cv: int = 0`

    Number of folds for CV

`eval_model: str = 'train_val_test'`

    ["None", "train", "train_val", "train_val_test", "test"]

        Type

            Evaluate trained model choices

`save_model_at_every_epoch: int = None`

    Not tested

`label_smoothing_rate: float = 0.0`

`num_core: int = 0`

    Number of CPUs to be used in the mini-batch loading process

`random_seed: int = 0`

    Random Seed

`sample_triples_ratio: float = None`

    Read some triples that are uniformly at random sampled. Ratio being between 0 and 1

`read_only_few: int = None`

    Read only first few triples

`pykeen_model_kwargs`

    Additional keyword arguments for pykeen models

`kernel_size: int = 3`

    Size of a square kernel in a convolution operation

`num_of_output_channels: int = 32`

>   Number of slices in the generated feature map by convolution.

`p: int = 0`

>   P parameter of Clifford Embeddings

`q: int = 1`

>   Q parameter of Clifford Embeddings

`input_dropout_rate: float = 0.0`

>   Dropout rate on embeddings of input triples

`hidden_dropout_rate: float = 0.0`

>   Dropout rate on hidden representations of input triples

`feature_map_dropout_rate: float = 0.0`

>   Dropout rate on a feature map generated by a convolution operation

`byte_pair_encoding: bool = False`

>   Byte pair encoding

>   **Type**
>   >   WIP

`adaptive_swa: bool = False`

>   Adaptive stochastic weight averaging

`swa: bool = False`

>   Stochastic weight averaging

`swag: bool = False`

>   Stochastic weight averaging - Gaussian

`ema: bool = False`

>   Exponential Moving Average

`twa: bool = False`

>   Trainable 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

    "cca"}'

        Type

            Adaptive learning rate parameters, e.g., '{"scheduler_name"

swa_start_epoch: int = None

    Epoch at which to start applying stochastic weight averaging.

swa_c_epochs: int = 1

    Number of epochs to average over for SWA, SWAG, EMA, TWA.

__iter__()

dicee.dataset_classes

Classes

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

Functions

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

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_idxs** – mapping.

- **relation_idxs** – mapping.

- **form** – ?

- **num_workers** – int for https://pytorch.org/docs/stable/data.html#torch.utils.data. DataLoader

Return type
torch.utils.data.Dataset

train_data

block_size = 8

num_of_data_points

collate_fn = None

__len__()

__getitem__(*idx*)

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

Bases: torch.utils.data.Dataset

Dataset for the 1vsALL training strategy

Parameters

- **train_set_idx** – Indexed triples for the training.

- **entity_idxs** – mapping.

- **relation_idxs** – mapping.

- **form** – ?

- **num_workers** – int for https://pytorch.org/docs/stable/data.html#torch.utils.data. DataLoader

Return type
   torch.utils.data.Dataset

train_data

target_dim

collate_fn = None

__len__()

__getitem__(*idx*)

class dicee.dataset_classes.**KvsAll**(*train_set_idx: numpy.ndarray*, *entity_idxs*, *relation_idxs*, *form*,
   store=None, *label_smoothing_rate: float = 0.0*)

Bases: torch.utils.data.Dataset

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

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

> ℹ **Note**
>
> TODO

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

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

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

self : torch.utils.data.Dataset

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

train_data = None

train_target = None

label_smoothing_rate

collate_fn = None

__len__()

__getitem__(*idx*)

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

    Bases: `torch.utils.data.Dataset`

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

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

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

> ℹ **Note**
>
> **AllvsAll extends KvsAll via none existing (h,r). Hence, it adds data points that are labelled without 1s,**
>   only with 0s.

    train_set_idx

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

    entity_idxs

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

    relation_idxs

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

    self : torch.utils.data.Dataset

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

    train_data = None

    train_target = None

    label_smoothing_rate

    collate_fn = None

    target_dim

    __len__()

    __getitem__(*idx*)

class dicee.dataset_classes.**OnevsSample**(*train_set: numpy.ndarray*, *num_entities*, *num_relations*,
      neg_sample_ratio: int = None, *label_smoothing_rate: float = 0.0*)

    Bases: `torch.utils.data.Dataset`

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

        Parameters

            • **train_set** (*np.ndarray*) – A numpy array containing triples of knowledge graph data. Each triple consists of (head_entity, relation, tail_entity).

- **num_entities** (`int`) – The number of unique entities in the knowledge graph.

- **num_relations** (`int`) – The number of unique relations in the knowledge graph.

- **neg_sample_ratio** (`int, optional`) – The number of negative samples to be generated per positive sample. Must be a positive integer and less than num_entities.

- **label_smoothing_rate** (`float, optional`) – A label smoothing rate to apply to the positive and negative labels. Defaults to 0.0.

train_data

    The input data converted into a PyTorch tensor.

        Type

            torch.Tensor

num_entities

    Number of entities in the dataset.

        Type

            int

num_relations

    Number of relations in the dataset.

        Type

            int

neg_sample_ratio

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

        Type

            int

label_smoothing_rate

    The smoothing factor applied to the labels.

        Type

            torch.Tensor

collate_fn

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

        Type

            function, optional

train_data

num_entities

num_relations

neg_sample_ratio = None

label_smoothing_rate

collate_fn = None

__len__()

    Returns the number of samples in the dataset.

__getitem__(*idx*)

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

> **Parameters**
>> **idx** (*int*) – The index of the sample to retrieve.
>
> **Returns**
>> **A tuple consisting of:**
>>> - x (torch.Tensor): The head and relation part of the triple.
>>>
>>> - y_idx (torch.Tensor): The concatenated indices of the true object (tail entity) and the indices of the negative samples.
>>>
>>> - y_vec (torch.Tensor): A vector containing the labels for the positive and negative samples, with label smoothing applied.
>
> **Return type**
>> tuple

class dicee.dataset_classes.**KvsSampleDataset**(*train_set_idx: numpy.ndarray*, *entity_idxs*, *relation_idxs*, *form*, *store=None*, *neg_ratio=None*, *label_smoothing_rate: float = 0.0*)

> Bases: torch.utils.data.Dataset

>> **KvsSample a Dataset:**

>>> **D:= {(x,y)_i}_i ^N, where**
>>>> . x:(h,r) is a unique h in E and a relation r in R and . y in [0,1]^{|**E**|} is a binary label.

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

>>> **At each mini-batch construction, we subsample(y), hence n**
>>>> |**new_y**| << |**E**| new_y contains all 1's if sum(y)< neg_sample ratio new_y contains

>> **train_set_idx**
>>> Indexed triples for the training.

>> **entity_idxs**
>>> mapping.

>> **relation_idxs**
>>> mapping.

>> **form**
>>> ?

>> **store**
>>> ?

>> **label_smoothing_rate**
>>> ?

>> torch.utils.data.Dataset

> **train_data = None**

> **train_target = None**

> **neg_ratio = None**

num_entities

label_smoothing_rate

collate_fn = None

max_num_of_classes

__len__()

__getitem__(*idx*)

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

Bases: torch.utils.data.Dataset

An abstract class representing a Dataset.

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

> **ⓘ 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_triples

length

num_entities

num_relations

labels

train_set = []

__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 . collact_fn => Generates negative triples

collect_fn:

orall (h,r,t) in G obtain, create negative triples{(h,r,x),(,r,t),(h,m,t)}

y:labels are represented in torch.float16

train_set_idx
　　Indexed triples for the training.

entity_idxs
　　mapping.

relation_idxs
　　mapping.

form
　　　?

store
　　　?

label_smoothing_rate

collate_fn: batch:List[torch.IntTensor] Returns ———- torch.utils.data.Dataset

`label_smoothing_rate`

`neg_sample_ratio`

`train_set`

`length`

`num_entities`

`num_relations`

`__len__()`

`__getitem__`(*idx*)

`collate_fn`(*batch: List[torch.Tensor]*)

class dicee.dataset_classes.**CVDataModule**(*train_set_idx: numpy.ndarray*, *num_entities*, *num_relations*, *neg_sample_ratio*, *batch_size*, *num_workers*)

　　Bases: pytorch_lightning.LightningDataModule

　　Create a Dataset for cross validation

　　Parameters

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

　　Return type

　　　?

`train_set_idx`

`num_entities`

`num_relations`

`neg_sample_ratio`

`batch_size`

`num_workers`

`train_dataloader`() → torch.utils.data.DataLoader

> An iterable or collection of iterables specifying training samples.
>
> For more information about multiple dataloaders, see this section.
>
> 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()`*

> > ℹ️ **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:

```python
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, …).

> ℹ **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:

```python
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)
```

```python
class LitDataModule(LightningDataModule):
    def __init__(self):
        super().__init__()
        self.prepare_data_per_node = False
```

This is called before requesting the dataloaders:

```python
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

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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_performa. 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, normalize_scores: 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

[Evaluator]()	Evaluator class to evaluate KGE models in various downstream tasks

Module Contents

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

      Evaluator class to evaluate KGE models in various downstream tasks

      Arguments

    re_vocab = None

    er_vocab = None

    ee_vocab = None

    func_triple_to_bpe_representation = None

    is_continual_training = None

    num_entities = None

    num_relations = None

    args

    report

    during_training = False

    vocab_preparation(*dataset*) → 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

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

Module Contents

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

> A class for Training, Retraining and Evaluation a model.
>
> (1) Loading & Preprocessing & Serializing input data.
>
> (2) Training & Validation & Testing
>
> (3) Storing all necessary info
>
> **distributed**
>
> **args**
>
> **is_continual_training = False**
>
> **trainer = None**
>
> **trained_model = None**
>
> **knowledge_graph = None**
>
> **report**
>
> **evaluator = None**
>
> **start_time = None**
>
> **is_rank_zero**() → bool
>
> **cleanup**()
>
> **setup_executor**() → None

create_and_store_kg()

load_from_memmap()

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

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

Module Contents

class `dicee.knowledge_graph_embeddings.`**`KGE`**(*path=None*, *url=None*, *construct_ensemble=False*, *model_name=None*)

    Bases: *dicee.abstracts.BaseInteractiveKGE*,   *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.

    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.

    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.

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

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 :

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

Return (e,r,x)

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

confidence: float

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

topk: int

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

at_most: int

Stop after finding at_most missing triples

{(e,r,x) | f(e,r,x) > confidence land (e,r,x)}

otin G

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

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

ADOPT Optimizer Implementation.

This module implements the ADOPT (Adaptive Optimization with Precise Tracking) algorithm, an advanced optimization method for training neural networks.

ADOPT Overview:

ADOPT is an adaptive learning rate optimization algorithm that combines the benefits of momentum-based methods with per-parameter learning rate adaptation. Unlike Adam, which applies momentum to raw gradients, ADOPT normalizes gradients first and then applies momentum, leading to more stable training dynamics.

Key Features: - Gradient normalization before momentum application - Adaptive per-parameter learning rates - Optional gradient clipping that grows with training steps - Support for decoupled weight decay (AdamW-style) - Multiple execution modes: single-tensor, multi-tensor (foreach), and fused (planned)

Algorithm Comparison:

Adam: $m = \beta_1 * m + (1-\beta_1) * g$, $\theta = \theta - \alpha * m / \sqrt{v}$ ADOPT: $m = \beta_1 * m + (1-\beta_1) * g / \sqrt{v}$, $\theta = \theta - \alpha * m$

The key difference is that ADOPT normalizes gradients before momentum, which provides better stability and can lead to improved convergence.

Classes:

- ADOPT: Main optimizer class (extends torch.optim.Optimizer)

Functions:

- adopt: Functional API for ADOPT algorithm computation
- _single_tensor_adopt: Single-tensor implementation (TorchScript compatible)
- _multi_tensor_adopt: Multi-tensor implementation using foreach operations

Performance:

- Single-tensor: Default, compatible with torch.jit.script
- Multi-tensor (foreach): 2-3x faster on GPU through vectorization
- Fused (planned): Would provide maximum performance via specialized kernels

Example:

```python
>>> import torch
>>> from dicee.models.adopt import ADOPT
>>>
>>> model = torch.nn.Linear(10, 1)
>>> optimizer = ADOPT(model.parameters(), lr=0.001, weight_decay=0.01, decouple=True)
>>>
>>> # Training loop
>>> for epoch in range(num_epochs):
...     optimizer.zero_grad()
...     output = model(input)
...     loss = criterion(output, target)
...     loss.backward()
...     optimizer.step()
```

References:

Original implementation: https://github.com/iShohei220/adopt

Notes:

This implementation is based on the original ADOPT implementation and adapted to work with the PyTorch optimizer interface and the dicee framework.

Classes

ADOPT	ADOPT Optimizer.

Functions

adopt(params, grads, exp_avgs, exp_avg_sqs, state_steps)	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

ADOPT Optimizer.

ADOPT is an adaptive learning rate optimization algorithm that combines momentum-based updates with adaptive per-parameter learning rates. It uses exponential moving averages of gradients and squared gradients, with gradient clipping for stability.

The algorithm performs the following key operations: 1. Normalizes gradients by the square root of the second moment estimate 2. Applies optional gradient clipping based on the training step 3. Updates parameters using momentum-smoothed normalized gradients 4. Supports decoupled weight decay (AdamW-style) or L2 regularization

Mathematical formulation:

$m_t = \beta_1 * m_{t-1} + (1 - \beta_1) * \text{clip}(g_t / \sqrt{v_t})$ $v_t = \beta_2 * v_{t-1} + (1 - \beta_2) * g_t^2$ $\theta_t = \theta_{t-1} - \alpha * m_t$

where:

- θ_t: parameter at step t

- g_t: gradient at step t

- m_t: first moment estimate (momentum)

- v_t: second moment estimate (variance)

- α: learning rate

- β_1, β_2: exponential decay rates

- clip(): optional gradient clipping function

Reference:
Original implementation: https://github.com/iShohei220/adopt

Parameters

- **params** (*ParamsT*) – Iterable of parameters to optimize or dicts defining parameter groups.

- **lr** (*float or Tensor, optional*) – Learning rate. Can be a float or 1-element Tensor. Default: 1e-3

- **betas** (*Tuple[float, float], optional*) – Coefficients (β_1, β_2) for computing running averages of gradient and its square. β_1 controls momentum, β_2 controls variance. Default: (0.9, 0.9999)

- **eps** (*float, optional*) – Term added to denominator to improve numerical stability. Default: 1e-6

- **clip_lambda** (*Callable[[int], float], optional*) – Function that takes the step number and returns the gradient clipping threshold. Common choices: - lambda step: step**0.25 (default, gradually increases clipping threshold) - lambda step: 1.0 (constant clipping) - None (no clipping) Default: lambda step: step**0.25

- **weight_decay** (*float, optional*) – Weight decay coefficient (L2 penalty). Default: 0.0

- **decouple** (*bool, optional*) – If True, uses decoupled weight decay (AdamW-style), applying weight decay directly to parameters. If False, adds weight decay to gradients (L2 regularization). Default: False

- **foreach** (*bool, optional*) – If True, uses the faster foreach implementation for multi-tensor operations. Default: None (auto-select)

- **maximize** (*bool, optional*) – If True, maximizes parameters instead of minimizing. Useful for reinforcement learning. Default: False

- **capturable** (*bool, optional*) – If True, the optimizer is safe to capture in a CUDA graph. Requires learning rate as Tensor. Default: False

- **differentiable** (*bool, optional*) – If True, the optimization step can be differentiated. Useful for meta-learning. Default: False

- **fused** (*bool, optional*) – If True, uses fused kernel implementation (currently not supported). Default: None

Raises

- **ValueError** – If learning rate, epsilon, betas, or weight_decay are invalid.

- **RuntimeError** – If fused is enabled (not currently supported).

- **RuntimeError** – If lr is a Tensor with foreach=True and capturable=False.

Example

```
>>> # Basic usage
>>> optimizer = ADOPT(model.parameters(), lr=0.001)
>>> optimizer.zero_grad()
>>> loss.backward()
>>> optimizer.step()
```

```
>>> # With decoupled weight decay
>>> optimizer = ADOPT(model.parameters(), lr=0.001, weight_decay=0.01,
→decouple=True)
```

```
>>> # Custom gradient clipping
>>> optimizer = ADOPT(model.parameters(), clip_lambda=lambda step: max(1.0,
→step**0.5))
```

> **ⓘ Note**
>
> - For most use cases, the default hyperparameters work well
>
> - Consider using decouple=True for better generalization (similar to AdamW)
>
> - The clip_lambda function helps stabilize training in early steps

`clip_lambda`

`__setstate__`(*state*)

    Restore optimizer state from a checkpoint.

    This method handles backward compatibility when loading optimizer state from older versions. It ensures all required fields are present with default values and properly converts step counters to tensors if needed.

    Key responsibilities: 1. Set default values for newly added hyperparameters 2. Convert old-style scalar step counters to tensor format 3. Place step tensors on appropriate devices based on capturable/fused modes

    Parameters

        `state` (*`dict`*) – Optimizer state dictionary (typically from torch.load()).

> **ⓘ Note**
>
> - This enables loading checkpoints saved with older ADOPT versions
>
> - Step counters are converted to appropriate device/dtype for compatibility
>
> - Capturable and fused modes require step tensors on parameter devices

`step`(*closure=None*)

    Perform a single optimization step.

    This method executes one iteration of the ADOPT optimization algorithm across all parameter groups. It orchestrates the following workflow:

    1. Optionally evaluates a closure to recompute the loss (useful for algorithms like LBFGS or when loss needs multiple evaluations)

    2. For each parameter group: - Collects parameters with gradients and their associated state - Extracts hyperparameters (betas, learning rate, etc.) - Calls the functional adopt() API to perform the actual update

    3. Returns the loss value if a closure was provided

    The functional API (adopt()) handles three execution modes: - Single-tensor: Updates one parameter at a time (default, JIT-compatible) - Multi-tensor (foreach): Batches operations for better performance - Fused: Uses fused CUDA kernels (not yet implemented)

    Gradient scaling support: This method is compatible with automatic mixed precision (AMP) training. It can access grad_scale and found_inf attributes for gradient unscaling and inf/nan detection when used with GradScaler.

    Parameters

        `closure` (*`Callable, optional`*) – A callable that reevaluates the model and returns the loss. The closure should: - Enable gradients (torch.enable_grad()) - Compute forward pass - Compute loss - Compute backward pass - Return the loss value Example: lambda: (loss := model(x), loss.backward(), loss)[-1] Default: None

Returns

The loss value returned by the closure, or None if no
    closure was provided.

Return type

Optional[Tensor]

Example

```
>>> # Standard usage
>>> loss = criterion(model(input), target)
>>> loss.backward()
>>> optimizer.step()
```

```
>>> # With closure (e.g., for line search)
>>> def closure():
...     optimizer.zero_grad()
...     output = model(input)
...     loss = criterion(output, target)
...     loss.backward()
...     return loss
>>> loss = optimizer.step(closure)
```

> ℹ **Note**
>
> - Call zero_grad() before computing gradients for the next step
>
> - CUDA graph capture is checked for safety when capturable=True
>
> - The method is thread-safe for different parameter groups

`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.

This is the main functional interface for the ADOPT optimization algorithm. It dispatches to one of three implementations based on the execution mode:

1. **Single-tensor mode** (default): Updates parameters one at a time - Compatible with torch.jit.script - More flexible but slower - Used when foreach=False or automatically for small models

2. **Multi-tensor (foreach) mode**: Batches operations across tensors - 2-3x faster on GPU through vectorization - Groups tensors by device/dtype automatically - Used when foreach=True

3. **Fused mode**: Uses specialized fused kernels (not yet implemented) - Would provide maximum performance - Currently raises RuntimeError if enabled

Algorithm overview (ADOPT):

ADOPT adapts learning rates per-parameter while using momentum on normalized gradients. The key innovation is normalizing gradients before momentum, which provides more stable training than standard Adam.

Mathematical formulation:

Normalize gradient by its historical variance normed_g_t = g_t / $\sqrt{(v\_t + \varepsilon)}$

Optional gradient clipping for stability normed_g_t = clip(normed_g_t, threshold(t))

Momentum on normalized gradients (key difference from Adam) m_t = β_1 * m_{t-1} + (1 - β_1) * normed_g_t

Parameter update θ_t = θ_{t-1} - α * m_t

Update variance estimate v_t = β_2 * v_{t-1} + (1 - β_2) * g_t^2

where:

- θ: parameters
- g: gradients
- m: first moment (momentum of normalized gradients)
- v: second moment (variance of raw gradients)
- α: learning rate
- β_1, β_2: exponential decay rates
- ε: numerical stability constant
- clip(): gradient clipping function based on step

Automatic mode selection:

When foreach and fused are both None (default), the function automatically selects the best implementation based on: - Parameter types and devices - Whether differentiable mode is enabled - Learning rate type (float vs Tensor) - Capturable mode requirements

param params
Parameters to optimize.

type params
List[Tensor]

param grads
Gradients for each parameter.

type grads
List[Tensor]

param exp_avgs
First moment estimates (momentum).

type exp_avgs
List[Tensor]

param exp_avg_sqs
Second moment estimates (variance).

type exp_avg_sqs
List[Tensor]

param state_steps
    Step counters (must be singleton tensors).

type state_steps
    List[Tensor]

param foreach
    Whether to use multi-tensor implementation. None: auto-select based on configuration (default).

type foreach
    Optional[bool]

param capturable
    If True, ensure CUDA graph capture safety.

type capturable
    bool

param differentiable
    If True, allow gradients through optimization step.

type differentiable
    bool

param fused
    If True, use fused kernels (not implemented).

type fused
    Optional[bool]

param grad_scale
    Gradient scaler for AMP training.

type grad_scale
    Optional[Tensor]

param found_inf
    Flag for inf/nan detection in AMP.

type found_inf
    Optional[Tensor]

param has_complex
    Whether any parameters are complex-valued.

type has_complex
    bool

param beta1
    Exponential decay rate for first moment (momentum). Typical range: 0.9-0.95.

type beta1
    float

param beta2
    Exponential decay rate for second moment (variance). Typical range: 0.999-0.9999 (higher than Adam).

type beta2
    float

param lr
    Learning rate. Can be a scalar Tensor for dynamic learning rate with capturable=True.

type lr
> Union[float, Tensor]

param clip_lambda
> Function that maps step number to gradient clipping threshold. None disables clipping.

type clip_lambda
> Optional[Callable[[int], float]]

param weight_decay
> Weight decay coefficient (L2 penalty).

type weight_decay
> float

param decouple
> If True, use decoupled weight decay (AdamW-style). Recommended for better generalization.

type decouple
> bool

param eps
> Small constant for numerical stability in normalization.

type eps
> float

param maximize
> If True, maximize objective instead of minimize.

type maximize
> bool

raises RuntimeError
> If torch.jit.script is used with foreach or fused.

raises RuntimeError
> If state_steps contains non-tensor elements.

raises RuntimeError
> If fused=True (not yet implemented).

raises RuntimeError
> If lr is Tensor with foreach=True and capturable=False.

Example

```
>>> # Typically called by ADOPT optimizer, not directly
>>> adopt(
...     params=[p1, p2],
...     grads=[g1, g2],
...     exp_avgs=[m1, m2],
...     exp_avg_sqs=[v1, v2],
...     state_steps=[step1, step2],
...     beta1=0.9,
...     beta2=0.9999,
...     lr=0.001,
...     clip_lambda=lambda s: s**0.25,
...     weight_decay=0.01,
...     decouple=True,
```

```
...         eps=1e-6,
...         maximize=False,
... )
```

> ℹ️ **Note**
>
> - For distributed training, this API is compatible with torch/distributed/optim
>
> - The foreach mode is generally preferred for GPU training
>
> - Complex parameters are handled transparently by viewing as real
>
> - First optimization step only initializes variance, doesn't update parameters

> ↪ **See also**
>
> - ADOPT class: High-level optimizer interface
>
> - _single_tensor_adopt: Single-tensor implementation details
>
> - _multi_tensor_adopt: Multi-tensor implementation details

dicee.models.base_model

Classes

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

Module Contents

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

Bases: `lightning.LightningModule`

Base class for all neural network modules.

Your models should also subclass this class.

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

```python
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.

> **ℹ 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:

```python
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 `Light-ningModule` and access them in this hook:

```python
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()`
>
>> ℹ️ **Note**
>>
>> Lightning tries to add the correct sampler for distributed and arbitrary hardware. There is no need to set it yourself.
>
>> ℹ️ **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()`
>
>> ℹ️ **Note**
>>
>> Lightning tries to add the correct sampler for distributed and arbitrary hardware There is no need to set it yourself.

> **ℹ 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()`

> **ℹ 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()`

> **ℹ 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:

```python
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**
> > **x** (*B x 2 x T*)

forward_byte_pair_encoded_triple(*x: Tuple[torch.LongTensor, torch.LongTensor]*)

    byte pair encoded neural link predictors

       Parameters

          ----

init_params_with_sanity_checking()

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

       Parameters

- **x**

- **y_idx**

- **ordered_bpe_entities**

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

       Parameters

          x

forward_k_vs_all(**args*, ***kwargs*)

forward_k_vs_sample(**args*, ***kwargs*)

get_triple_representation(*idx_hrt*)

get_head_relation_representation(*indexed_triple*)

get_sentence_representation(*x: torch.LongTensor*)

       Parameters

- **(b** (*x shape*)

- **3**

- **t)**

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

       Parameters

         x (*B x 2 x T*)

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

class dicee.models.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:

```python
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

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

Module Contents

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

    Bases: *dicee.models.base_model.BaseKGE*

    Base class for all neural network modules.

    Your models should also subclass this class.

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

```python
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_1, e_2, e_3, we compute interactions between e_1 e_2, e_1 e_3 , and e_2 e_3 This can be implemented with a nested two for loops

> results = [] for i in range(p - 1):
>
> > **for k in range(i + 1, p):**
> > results.append(hp[:, :, i] * rp[:, :, k] - hp[:, :, k] * rp[:, :, i])
>
> sigma_pp = torch.stack(results, dim=2) assert sigma_pp.shape == (b, r, int((p * (p - 1)) / 2))

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

> e2e1, e2e2, e2e3, e3e1, e3e2, e3e3

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

compute_sigma_qq (*hq*, *rq*)

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

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

for k in range(j + 1, q):
results.append(hq[:, :, j] * rq[:, :, k] - hq[:, :, k] * rq[:, :, j])

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

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

e2e1, e2e2, e2e3, e3e1, e3e2, e3e3

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

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

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

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

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

print(sigma_pq.shape)

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

Multiplying a base vector with its scalar coefficient

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

Compute our CL multiplication

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

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

eq j

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

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

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

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

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

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

(6) sigma_{pq} = sum_{i=1}^{p} sum_{j=p+1}^{p+q} (h_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 funcitons are identical Parameter ——— x: torch.LongTensor with (n,2) shape :rtype: torch.FloatTensor with (n, **|E|**) shape

construct_batch_selected_cl_multivector(*x: torch.FloatTensor*, *r: int*, *p: int*, *q: int*)
    → tuple[torch.FloatTensor, torch.FloatTensor, torch.FloatTensor]

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

Parameter

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

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

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

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:

```python
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.

> ℹ **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,

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

and return:

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

`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

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

For different base vector interactions, we have

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

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

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

Multiplying a base vector with its scalar coefficient

construct_cl_multivector(*x: torch.FloatTensor*, *re: int*, *p: int*, *q: int*, *r: int*) → tuple[torch.FloatTensor, torch.FloatTensor, torch.FloatTensor]

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

Parameter

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

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

compute_sigma_pp(*hp, rp*)

Compute .. math:

```
\sigma_{p,p}^* = \sum_{i=1}^{p-1}\sum_{i'=i+1}^{p}(x_iy_{i'}-x_{i'}y_i)
```

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

> results = [] for i in range(p - 1):
>
> > **for k in range(i + 1, p):**
> > results.append(hp[:, :, i] * rp[:, :, k] - hp[:, :, k] * rp[:, :, i])
>
> sigma_pp = torch.stack(results, dim=2) assert sigma_pp.shape == (b, r, int((p * (p - 1)) / 2))

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

> e2e1, e2e2, e2e3, e3e1, e3e2, e3e3

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

compute_sigma_qq(*hq, rq*)

Compute

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

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

> results = [] for j in range(q - 1):
>
> > **for k in range(j + 1, q):**
> > results.append(hq[:, :, j] * rq[:, :, k] - hq[:, :, k] * rq[:, :, j])

```
sigma_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

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

Module Contents

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

    Bases: *dicee.models.base_model.BaseKGE*

    Convolutional ComplEx Knowledge Graph Embeddings

    name = 'ConEx'

    conv2d

    fc_num_input

    fc1

    norm_fc1

    bn_conv2d

    feature_map_dropout

    residual_convolution(*C_1: Tuple[torch.Tensor, torch.Tensor]*,
        C_2: Tuple[torch.Tensor, torch.Tensor]) → 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 submodules as regular attributes:

```python
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.

> **ℹ 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**(*models: list = None*, *seed_model=None*, *pretrained_models: List = None*)

    name

    train_mode = True

    args

    named_children()

    property example_input_array

    parameters()

    modules()

    __iter__()

    __len__()

    eval()

to(*device*)

state_dict()
>   Return the state dict of the ensemble.

load_state_dict(*state_dict*, *strict=True*)
>   Load the state dict into the ensemble.

mem_of_model()

__call__(*x_batch*)

step()

get_embeddings()

__str__()

dicee.models.function_space

Classes

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

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}^{k=d-1}wk e^{kix}. and use the three differents scoring function as in the paper to evaluate the score

name = 'LFMult1'

entity_embeddings

relation_embeddings

forward_triples(*idx_triple*)

> **Parameters**
>> **x**

tri_score(*h*, *r*, *t*)

vtp_score(*h*, *r*, *t*)

class dicee.models.function_space.**LFMult**(*args*)

> Bases: *dicee.models.base_model.BaseKGE*

Embedding with polynomial functions. We represent all entities and relations in the polynomial space as: f(x) = sum_{i=0}^{d-1} a_k x^{i%d} and use the three differents scoring function as in the paper to evaluate the score. We also consider combining with Neural Networks.

name = 'LFMult'

entity_embeddings

relation_embeddings

degree

m

x_values

forward_triples(*idx_triple*)

> **Parameters**
>> **x**

construct_multi_coeff(*x*)

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

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

linear(*x*, *w*, *b*)

scalar_batch_NN (*a*, *b*, *c*)

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

tri_score (*coeff_h*, *coeff_r*, *coeff_t*)

    this part implement the trilinear scoring techniques:

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

    1. generate the range for i,j and k from [0 d-1]

    2. perform dfrac{a_i*b_j*c_k}{1+(i+j+k)%d} in parallel for every batch

    3. take the sum over each batch

vtp_score (*h*, *r*, *t*)

    this part implement the vector triple product scoring techniques:

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

    1. generate the range for i,j and k from [0 d-1]

    2. Compute the first and second terms of the sum

    3. Multiply with then denominator and take the sum

    4. take the sum over each batch

comp_func (*h*, *r*, *t*)

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

polynomial (*coeff*, *x*, *degree*)

    This function takes a matrix tensor of coefficients (coeff), a tensor vector of points x and range of integer [0,1,…d] and return a vector tensor (coeff[0][0] + coeff[0][1]x +…+ coeff[0][d]x^d,

        coeff[1][0] + coeff[1][1]x +…+ coeff[1][d]x^d)

pop (*coeff*, *x*, *degree*)

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

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

        coeff[1][0] + coeff[1][1]x +…+ coeff[1][d]x^d)

dicee.models.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

Classes

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

Functions

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

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
```

(continues on next page)

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```python
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 submodules as regular attributes:

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


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

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```python
        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.

> ### ℹ 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.octonion.**AConvO**(*args: dict*)

> Bases: *dicee.models.base_model.BaseKGE*

Additive Convolutional Octonion Knowledge Graph Embeddings

name = 'AConvO'

conv2d

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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

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

Module Contents

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

> Bases: *dicee.models.base_model.BaseKGE*

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

> Notes: Pykeen_DistMult: C Pykeen_ComplEx: Pykeen_QuatE: Pykeen_MuRE: Pykeen_CP: Pykeen_HolE: Pykeen_HolE: Pykeen_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*)

dicee.models.quaternion

Classes

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

Functions

quaternion_mul_with_unit_norm(*, Q_1, Q_2)	

Module Contents

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

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

> Bases: *dicee.models.base_model.BaseKGE*

Base class for all neural network modules.

Your models should also subclass this class.

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

```python
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

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

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**

class dicee.models.real.**CoKEConfig**

> Configuration for the CoKE (Contextualized Knowledge Graph Embedding) model.
>
> **block_size**
>> Sequence length for transformer (3 for triples: head, relation, tail)
>
> **vocab_size**
>> Total vocabulary size (num_entities + num_relations)
>
> **n_layer**
>> Number of transformer layers
>
> **n_head**
>> Number of attention heads per layer
>
> **n_embd**
>> Embedding dimension (set to match model embedding_dim)
>
> **dropout**
>> Dropout rate applied throughout the model
>
> **bias**
>> Whether to use bias in linear layers
>
> **causal**
>> Whether to use causal masking (False for bidirectional attention)
>
> **block_size: int = 3**
>
> **vocab_size: int = None**
>
> **n_layer: int = 6**
>
> **n_head: int = 8**
>
> **n_embd: int = None**
>
> **dropout: float = 0.3**
>
> **bias: bool = True**
>
> **causal: bool = False**

class dicee.models.real.**CoKE**(*args*, *config: CoKEConfig = CoKEConfig()*)

> Bases: *dicee.models.base_model.BaseKGE*
>
> Contextualized Knowledge Graph Embedding (CoKE) model. Based on: https://arxiv.org/pdf/1911.02168.
>
> CoKE uses a transformer encoder to learn contextualized representations of entities and relations. For link prediction, it predicts masked elements in (head, relation, tail) triples using bidirectional attention, similar to BERT's masked language modeling approach.
>
> The model creates a sequence [head_emb, relation_emb, mask_emb], adds positional embeddings, and processes it through transformer layers to predict the tail entity.

```
name = 'CoKE'

config

pos_emb

mask_emb

blocks

ln_f

coke_dropout
```

forward_k_vs_all(*x: torch.Tensor*)

score(*emb_h*, *emb_r*, *emb_t*)

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

dicee.models.static_funcs

Functions

quaternion_mul(→ Tuple[torch.Tensor, torch.Tensor, ...)	Perform quaternion multiplication

Module Contents

dicee.models.static_funcs.**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:

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

Classes

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

Module Contents

class dicee.models.transformers.**BytE**(**args*, ***kwargs*)

> Bases: *dicee.models.base_model.BaseKGE*
>
> Base class for all neural network modules.
>
> Your models should also subclass this class.
>
> Modules can also contain other Modules, allowing them to be nested in a tree structure. You can assign the submodules as regular attributes:

```python
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 = 'BytE'

config

temperature = 0.5

topk = 2

transformer

lm_head

loss_function(*yhat_batch*, *y_batch*)

> > **Parameters**
> > > - **yhat_batch**
> > > - **y_batch**

forward(*x: torch.LongTensor*)

        Parameters

                x (`B by T tensor`)

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

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

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

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

        Parameters

- **batch** – The output of your data iterable, normally a `DataLoader`.

- **batch_idx** – The index of this batch.

- **dataloader_idx** – The index of the dataloader that produced this batch. (only if multiple dataloaders used)

        Returns

- `Tensor` - The loss tensor

- `dict` - A dictionary which can include any keys, but must include the key `'loss'` in the case of automatic optimization.

- `None` - In automatic optimization, this will skip to the next batch (but is not supported for multi-GPU, TPU, or DeepSpeed). For manual optimization, this has no special meaning, as returning the loss is not required.

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

Example:

```python
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:

```python
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.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.**SelfAttention**(*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:

```python
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.

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c_attn

c_proj

attn_dropout

resid_dropout

n_head

n_embd

dropout

causal

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 submodules as regular attributes:

```python
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:

```python
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

causal: bool = True
```

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

> Bases: torch.nn.Module
>
> Base class for all neural network modules.
>
> Your models should also subclass this class.
>
> Modules can also contain other Modules, allowing them to be nested in a tree structure. You can assign the sub-modules as regular attributes:

```python
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

ADOPT	ADOPT Optimizer.
BaseKGELightning	Base class for all neural network modules.
BaseKGE	Base class for all neural network modules.
IdentityClass	Base class for all neural network modules.
BaseKGE	Base class for all neural network modules.
Block	Base class for all neural network modules.
DistMult	Embedding Entities and Relations for Learning and Inference in Knowledge Bases
TransE	Translating Embeddings for Modeling
Shallom	A shallow neural model for relation prediction (https://arxiv.org/abs/2101.09090)
Pyke	A Physical Embedding Model for Knowledge Graphs
CoKEConfig	Configuration for the CoKE (Contextualized Knowledge Graph Embedding) model.
CoKE	Contextualized Knowledge Graph Embedding (CoKE) model.
BaseKGE	Base class for all neural network modules.
ConEx	Convolutional ComplEx Knowledge Graph Embeddings
AConEx	Additive Convolutional ComplEx Knowledge Graph Embeddings
ComplEx	Base class for all neural network modules.
BaseKGE	Base class for all neural network modules.
IdentityClass	Base class for all neural network modules.
QMult	Base class for all neural network modules.
ConvQ	Convolutional Quaternion Knowledge Graph Embeddings
AConvQ	Additive Convolutional Quaternion Knowledge Graph Embeddings
BaseKGE	Base class for all neural network modules.
IdentityClass	Base class for all neural network modules.
OMult	Base class for all neural network modules.
ConvO	Base class for all neural network modules.
AConvO	Additive Convolutional Octonion Knowledge Graph Embeddings
Keci	Base class for all neural network modules.

Table 1 – continued from previous page

CKeci	Without learning dimension scaling
DeCaL	Base class for all neural network modules.
BaseKGE	Base class for all neural network modules.
PykeenKGE	A class for using knowledge graph embedding models implemented in Pykeen
BaseKGE	Base class for all neural network modules.
FMult	Learning Knowledge Neural Graphs
GFMult	Learning Knowledge Neural Graphs
FMult2	Learning Knowledge Neural Graphs
LFMult1	Embedding with trigonometric functions. We represent all entities and relations in the complex number space as:
LFMult	Embedding with polynomial functions. We represent all entities and relations in the polynomial space as:
DualE	Dual Quaternion Knowledge Graph Embeddings (https://ojs.aaai.org/index.php/AAAI/article/download/16850/16657)

Functions

quaternion_mul($\rightarrow$ 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

ADOPT Optimizer.

ADOPT is an adaptive learning rate optimization algorithm that combines momentum-based updates with adaptive per-parameter learning rates. It uses exponential moving averages of gradients and squared gradients, with gradient clipping for stability.

The algorithm performs the following key operations: 1. Normalizes gradients by the square root of the second moment estimate 2. Applies optional gradient clipping based on the training step 3. Updates parameters using momentum-smoothed normalized gradients 4. Supports decoupled weight decay (AdamW-style) or L2 regularization

Mathematical formulation:

$m_t = \beta_1 * m_{t-1} + (1 - \beta_1) * \text{clip}(g_t / \sqrt{(v_t)})$ $v_t = \beta_2 * v_{t-1} + (1 - \beta_2) * g_t^2$ $\theta_t = \theta_{t-1} - \alpha * m_t$

where:

- θ_t: parameter at step t

- g_t: gradient at step t

- m_t: first moment estimate (momentum)

- v_t: second moment estimate (variance)

- α: learning rate

- β_1, β_2: exponential decay rates

- clip(): optional gradient clipping function

Reference:

Original implementation: https://github.com/iShohei220/adopt

Parameters

- **params** (`ParamsT`) – Iterable of parameters to optimize or dicts defining parameter groups.

- **lr** (`float or Tensor, optional`) – Learning rate. Can be a float or 1-element Tensor. Default: 1e-3

- **betas** (`Tuple[float, float], optional`) – Coefficients (β_1, β_2) for computing running averages of gradient and its square. β_1 controls momentum, β_2 controls variance. Default: (0.9, 0.9999)

- **eps** (`float, optional`) – Term added to denominator to improve numerical stability. Default: 1e-6

- **clip_lambda** (`Callable[[int], float], optional`) – Function that takes the step number and returns the gradient clipping threshold. Common choices: - lambda step: step**0.25 (default, gradually increases clipping threshold) - lambda step: 1.0 (constant clipping) - None (no clipping) Default: lambda step: step**0.25

- **weight_decay** (`float, optional`) – Weight decay coefficient (L2 penalty). Default: 0.0

- **decouple** (`bool, optional`) – If True, uses decoupled weight decay (AdamW-style), applying weight decay directly to parameters. If False, adds weight decay to gradients (L2 regularization). Default: False

- **foreach** (`bool, optional`) – If True, uses the faster foreach implementation for multi-tensor operations. Default: None (auto-select)

- **maximize** (`bool, optional`) – If True, maximizes parameters instead of minimizing. Useful for reinforcement learning. Default: False

- **capturable** (`bool, optional`) – If True, the optimizer is safe to capture in a CUDA graph. Requires learning rate as Tensor. Default: False

- **differentiable** (`bool, optional`) – If True, the optimization step can be differentiated. Useful for meta-learning. Default: False

- **fused** (`bool, optional`) – If True, uses fused kernel implementation (currently not supported). Default: None

Raises

- **ValueError** – If learning rate, epsilon, betas, or weight_decay are invalid.

- **RuntimeError** – If fused is enabled (not currently supported).

- **RuntimeError** – If lr is a Tensor with foreach=True and capturable=False.

Example

```
>>> # Basic usage
>>> optimizer = ADOPT(model.parameters(), lr=0.001)
>>> optimizer.zero_grad()
>>> loss.backward()
>>> optimizer.step()
```

```
>>> # With decoupled weight decay
>>> optimizer = ADOPT(model.parameters(), lr=0.001, weight_decay=0.01,␣
↪decouple=True)
```

```
>>> # Custom gradient clipping
>>> optimizer = ADOPT(model.parameters(), clip_lambda=lambda step: max(1.0,␣
↪step**0.5))
```

> **ⓘ Note**
>
> - For most use cases, the default hyperparameters work well
> - Consider using decouple=True for better generalization (similar to AdamW)
> - The clip_lambda function helps stabilize training in early steps

clip_lambda

__setstate__(*state*)

Restore optimizer state from a checkpoint.

This method handles backward compatibility when loading optimizer state from older versions. It ensures all required fields are present with default values and properly converts step counters to tensors if needed.

Key responsibilities: 1. Set default values for newly added hyperparameters 2. Convert old-style scalar step counters to tensor format 3. Place step tensors on appropriate devices based on capturable/fused modes

> **Parameters**
> **state** (*dict*) – Optimizer state dictionary (typically from torch.load()).

> **ⓘ Note**
>
> - This enables loading checkpoints saved with older ADOPT versions
> - Step counters are converted to appropriate device/dtype for compatibility
> - Capturable and fused modes require step tensors on parameter devices

step(*closure=None*)

Perform a single optimization step.

This method executes one iteration of the ADOPT optimization algorithm across all parameter groups. It orchestrates the following workflow:

1. Optionally evaluates a closure to recompute the loss (useful for algorithms like LBFGS or when loss needs multiple evaluations)

2. For each parameter group: - Collects parameters with gradients and their associated state - Extracts hyperparameters (betas, learning rate, etc.) - Calls the functional adopt() API to perform the actual update

3. Returns the loss value if a closure was provided

The functional API (adopt()) handles three execution modes: - Single-tensor: Updates one parameter at a time (default, JIT-compatible) - Multi-tensor (foreach): Batches operations for better performance - Fused: Uses fused CUDA kernels (not yet implemented)

Gradient scaling support: This method is compatible with automatic mixed precision (AMP) training. It can access grad_scale and found_inf attributes for gradient unscaling and inf/nan detection when used with GradScaler.

Parameters

closure (*Callable, optional*) – A callable that reevaluates the model and returns the loss. The closure should: - Enable gradients (torch.enable_grad()) - Compute forward pass - Compute loss - Compute backward pass - Return the loss value Example: lambda: (loss := model(x), loss.backward(), loss)[-1] Default: None

Returns

The loss value returned by the closure, or None if no
closure was provided.

Return type

Optional[Tensor]

Example

```
>>> # Standard usage
>>> loss = criterion(model(input), target)
>>> loss.backward()
>>> optimizer.step()
```

```
>>> # With closure (e.g., for line search)
>>> def closure():
...     optimizer.zero_grad()
...     output = model(input)
...     loss = criterion(output, target)
...     loss.backward()
...     return loss
>>> loss = optimizer.step(closure)
```

> ⓘ **Note**
>
> - Call zero_grad() before computing gradients for the next step
>
> - CUDA graph capture is checked for safety when capturable=True
>
> - The method is thread-safe for different parameter groups

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

Bases: lightning.LightningModule

Base class for all neural network modules.

Your models should also subclass this class.

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

```python
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.

> **ℹ 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:

```python
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:

```python
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()
```

> **ℹ 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:

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

    def training_step(self):
        loss = ...
```

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```python
        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()`

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

> ℹ️ **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()`

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

> ℹ️ **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()`

> ℹ️ **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()`

> ℹ️ **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.

```python
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`.

> **ℹ 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 submodules as regular attributes:

```python
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**
> **x** (`B x 2 x T`)

forward_byte_pair_encoded_triple(*x: Tuple[torch.LongTensor, torch.LongTensor]*)

> byte pair encoded neural link predictors

> **Parameters**
> `-------`

init_params_with_sanity_checking()

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

> **Parameters**
>
> - **x**
>
> - **y_idx**
>
> - **ordered_bpe_entities**

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

> **Parameters**
> **x**

forward_k_vs_all(**args, **kwargs*)

forward_k_vs_sample(**args, **kwargs*)

get_triple_representation(*idx_hrt*)

get_head_relation_representation(*indexed_triple*)

get_sentence_representation(*x: torch.LongTensor*)

> **Parameters**
>
> - **(b** (`x shape`)
>
> - **3**
>
> - **t)**

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

> **Parameters**
>> **x** (`B x 2 x T`)

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

class dicee.models.**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 submodules as regular attributes:

```python
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 submodules as regular attributes:

```python
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.

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

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

args

embedding_dim = None

num_entities = None

num_relations = None

num_tokens = None

learning_rate = None

apply_unit_norm = None

input_dropout_rate = None

hidden_dropout_rate = None

optimizer_name = None

feature_map_dropout_rate = None

kernel_size = None

num_of_output_channels = None

weight_decay = None

loss

```
selected_optimizer = None
```

```
normalizer_class = None
```

normalize_head_entity_embeddings

normalize_relation_embeddings

normalize_tail_entity_embeddings

hidden_normalizer

param_init

input_dp_ent_real

input_dp_rel_real

hidden_dropout

```
loss_history = []
```

byte_pair_encoding

max_length_subword_tokens

block_size

forward_byte_pair_encoded_k_vs_all(*x: torch.LongTensor*)

>   **Parameters**
>   **x** (`B x 2 x T`)

forward_byte_pair_encoded_triple(*x: Tuple[torch.LongTensor, torch.LongTensor]*)

>   byte pair encoded neural link predictors

>   **Parameters**
>   `-------`

init_params_with_sanity_checking()

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

>   **Parameters**
>
>   • **x**
>
>   • **y_idx**
>
>   • **ordered_bpe_entities**

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

>   **Parameters**
>   **x**

forward_k_vs_all(**args*, ***kwargs*)

forward_k_vs_sample(**args*, ***kwargs*)

get_triple_representation(*idx_hrt*)

get_head_relation_representation(*indexed_triple*)

get_sentence_representation(*x: torch.LongTensor*)

> **Parameters**
>
> - **(b** (*x shape*)
>
> - **3**
>
> - **t)**

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

> **Parameters**
> **x** (*B x 2 x T*)

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

class dicee.models.**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:

```python
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.**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.**CoKEConfig**

> Configuration for the CoKE (Contextualized Knowledge Graph Embedding) model.

> **block_size**
>> Sequence length for transformer (3 for triples: head, relation, tail)

> **vocab_size**
>> Total vocabulary size (num_entities + num_relations)

> **n_layer**
>> Number of transformer layers

> **n_head**
>> Number of attention heads per layer

> **n_embd**
>> Embedding dimension (set to match model embedding_dim)

> **dropout**
>> Dropout rate applied throughout the model

> **bias**
>> Whether to use bias in linear layers

> **causal**
>> Whether to use causal masking (False for bidirectional attention)

> **block_size: int = 3**

> **vocab_size: int = None**

> **n_layer: int = 6**

> **n_head: int = 8**

> **n_embd: int = None**

```
dropout: float = 0.3

bias: bool = True

causal: bool = False
```

class dicee.models.**CoKE**(*args*, *config: CoKEConfig = CoKEConfig()*)

Bases: *dicee.models.base_model.BaseKGE*

Contextualized Knowledge Graph Embedding (CoKE) model. Based on: https://arxiv.org/pdf/1911.02168.

CoKE uses a transformer encoder to learn contextualized representations of entities and relations. For link prediction, it predicts masked elements in (head, relation, tail) triples using bidirectional attention, similar to BERT's masked language modeling approach.

The model creates a sequence [head_emb, relation_emb, mask_emb], adds positional embeddings, and processes it through transformer layers to predict the tail entity.

name = 'CoKE'

config

pos_emb

mask_emb

blocks

ln_f

coke_dropout

forward_k_vs_all(*x: torch.Tensor*)

score(*emb_h*, *emb_r*, *emb_t*)

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

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 submodules as regular attributes:

```python
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**
> > **x** (`B x 2 x T`)

forward_byte_pair_encoded_triple(*x: Tuple[torch.LongTensor, torch.LongTensor]*)

> byte pair encoded neural link predictors

> **Parameters**
> > -------

init_params_with_sanity_checking()

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

> **Parameters**
> > - **x**
> > - **y_idx**
> > - **ordered_bpe_entities**

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

> **Parameters**
> > **x**

forward_k_vs_all(**args*, ***kwargs*)

forward_k_vs_sample(**args*, ***kwargs*)

get_triple_representation(*idx_hrt*)

get_head_relation_representation(*indexed_triple*)

get_sentence_representation(*x: torch.LongTensor*)

> **Parameters**
> > - **(b** (`x shape`)
> > - **3**
> > - **t)**

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

> **Parameters**
> > **x** (`B x 2 x T`)

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

class dicee.models.**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:

```python
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 submodules as regular attributes:

```python
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.

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

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

args

embedding_dim = None

num_entities = None

num_relations = None

num_tokens = None

learning_rate = None

```
apply_unit_norm = None

input_dropout_rate = None

hidden_dropout_rate = None

optimizer_name = None

feature_map_dropout_rate = None

kernel_size = None

num_of_output_channels = None

weight_decay = None

loss

selected_optimizer = None

normalizer_class = None

normalize_head_entity_embeddings

normalize_relation_embeddings

normalize_tail_entity_embeddings

hidden_normalizer

param_init

input_dp_ent_real

input_dp_rel_real

hidden_dropout

loss_history = []

byte_pair_encoding

max_length_subword_tokens

block_size
```

forward_byte_pair_encoded_k_vs_all(*x: torch.LongTensor*)

> **Parameters**
> **x** (*B x 2 x T*)

forward_byte_pair_encoded_triple(*x: Tuple[torch.LongTensor, torch.LongTensor]*)

> byte pair encoded neural link predictors

> **Parameters**
> -------

init_params_with_sanity_checking()

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

> **Parameters**
>
> - **x**
>
> - **y_idx**
>
> - **ordered_bpe_entities**

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

> **Parameters**
>
> **x**

forward_k_vs_all(**args, **kwargs*)

forward_k_vs_sample(**args, **kwargs*)

get_triple_representation(*idx_hrt*)

get_head_relation_representation(*indexed_triple*)

get_sentence_representation(*x: torch.LongTensor*)

> **Parameters**
>
> - **(b** (*x shape*)
>
> - **3**
>
> - **t)**

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

> **Parameters**
>
> **x** (*B x 2 x T*)

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

class dicee.models.**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:

```python
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)
```

```python
    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 submodules as regular attributes:

```python
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.**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.**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:

```python
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**
> > **x** (*B x 2 x T*)

forward_byte_pair_encoded_triple(*x: Tuple[torch.LongTensor, torch.LongTensor]*)

> byte pair encoded neural link predictors

> > **Parameters**
> > > -------

init_params_with_sanity_checking()

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

>   **Parameters**
>
>   - **x**
>
>   - **y_idx**
>
>   - **ordered_bpe_entities**

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

>   **Parameters**
>   **x**

forward_k_vs_all(**args, **kwargs*)

forward_k_vs_sample(**args, **kwargs*)

get_triple_representation(*idx_hrt*)

get_head_relation_representation(*indexed_triple*)

get_sentence_representation(*x: torch.LongTensor*)

>   **Parameters**
>
>   - **(b** (*x shape*)
>
>   - **3**
>
>   - **t)**

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

>   **Parameters**
>   **x** (*B x 2 x T*)

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

class dicee.models.**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:

```python
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)

    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.**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:

```python
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 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_i r_k - h_k r_i) e_i e_k
>
> sigma_{pp} captures the interactions between along p bases For instance, let p e_1, e_2, e_3, we compute interactions between e_1 e_2, e_1 e_3 , and e_2 e_3 This can be implemented with a nested two for loops
>
>> results = [] for i in range(p - 1):

> **for k in range(i + 1, p):**
>> results.append(hp[:, :, i] * rp[:, :, k] - hp[:, :, k] * rp[:, :, i])

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

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

> e2e1, e2e2, e2e3, e3e1, e3e2, e3e3

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

compute_sigma_qq (*hq*, *rq*)

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

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

>> **for k in range(j + 1, q):**
>>> results.append(hq[:, :, j] * rq[:, :, k] - hq[:, :, k] * rq[:, :, j])

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

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

> e2e1, e2e2, e2e3, e3e1, e3e2, e3e3

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

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

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

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

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

print(sigma_pq.shape)

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

Multiplying a base vector with its scalar coefficient

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

Compute our CL multiplication

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

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

eq j

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

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

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

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

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

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

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

construct_cl_multivector (*x: torch.FloatTensor*, *r: int*, *p: int*, *q: int*)
$\rightarrow$ tuple[torch.FloatTensor, torch.FloatTensor, torch.FloatTensor]

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

Parameter

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

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

forward_k_vs_with_explicit (*x: torch.Tensor*)

k_vs_all_score (*bpe_head_ent_emb*, *bpe_rel_ent_emb*, *E*)

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

Kvsall training

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

(2) Construct head entity and relation embeddings according to Cl_{p,q}(mathbb{R}^d) .

(3) Perform Cl multiplication

(4) Inner product of (3) and all entity embeddings

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

construct_batch_selected_cl_multivector (*x: torch.FloatTensor*, *r: int*, *p: int*, *q: int*)
$\rightarrow$ 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 submodules as regular attributes:

```python
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.

> **ℹ 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,

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

and return:

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

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

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

For different base vector interactions, we have

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

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

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

    Multiplying a base vector with its scalar coefficient

construct_cl_multivector(*x: torch.FloatTensor, re: int, p: int, q: int, r: int*)
        → tuple[torch.FloatTensor, torch.FloatTensor, torch.FloatTensor]

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

    Parameter

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

        returns

            • **a0** (*torch.FloatTensor*)

            • **ap** (*torch.FloatTensor*)

            • **aq** (*torch.FloatTensor*)

            • **ar** (*torch.FloatTensor*)

compute_sigma_pp(*hp, rp*)

    Compute .. math:

```
\sigma_{p,p}^* = \sum_{i=1}^{p-1}\sum_{i'=i+1}^{p}(x_iy_{i'}-x_{i'}y_i)
```

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

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

        for k in range(i + 1, p):
            results.append(hp[:, :, i] * rp[:, :, k] - hp[:, :, k] * rp[:, :, i])

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

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

    e2e1, e2e2, e2e3, e3e1, e3e2, e3e3

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

compute_sigma_qq(*hq, rq*)

    Compute

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

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

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

    for k in range(j + 1, q):
        results.append(hq[:, :, j] * rq[:, :, k] - hq[:, :, k] * rq[:, :, j])

sigma_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.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:

```python
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**
> > **x** (`B x 2 x T`)

forward_byte_pair_encoded_triple(*x: Tuple[torch.LongTensor, torch.LongTensor]*)

> byte pair encoded neural link predictors

> > **Parameters**
> > > **-------**

init_params_with_sanity_checking()

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

> **Parameters**

> > - **x**

> > - **y_idx**

> > - **ordered_bpe_entities**

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

> **Parameters**
> > **x**

forward_k_vs_all (**args, **kwargs*)

forward_k_vs_sample (**args, **kwargs*)

get_triple_representation (*idx_hrt*)

get_head_relation_representation (*indexed_triple*)

get_sentence_representation (*x: torch.LongTensor*)

> **Parameters**
> > - **(b** (*x shape*)
> > - **3**
> > - **t)**

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

> **Parameters**
> > **x** (*B x 2 x T*)

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

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

> Bases: *dicee.models.base_model.BaseKGE*
>
> A class for using knowledge graph embedding models implemented in Pykeen
>
> Notes: Pykeen_DistMult: C Pykeen_ComplEx: Pykeen_QuatE: Pykeen_MuRE: Pykeen_CP: Pykeen_HolE: 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:

```python
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**
> > **x** (*B x 2 x T*)

forward_byte_pair_encoded_triple(*x: Tuple[torch.LongTensor, torch.LongTensor]*)

> byte pair encoded neural link predictors

> > **Parameters**
> > -------

init_params_with_sanity_checking()

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

> > **Parameters**

> > > • **x**

> > > • **y_idx**

> > > • **ordered_bpe_entities**

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

> > **Parameters**
> > **x**

forward_k_vs_all(**args, **kwargs*)

forward_k_vs_sample(**args, **kwargs*)

get_triple_representation(*idx_hrt*)

get_head_relation_representation(*indexed_triple*)

get_sentence_representation(*x: torch.LongTensor*)

> > **Parameters**

> > > • **(b** (`x shape`)

> > > • **3**

> > > • **t)**

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

> > **Parameters**
> > **x** (`B x 2 x T`)

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

class dicee.models.**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.**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}^{k=d-1}wk e^{kix}. and use the three differents scoring function as in the paper to evaluate the score

> **name = 'LFMult1'**

> **entity_embeddings**

> **relation_embeddings**

> **forward_triples**(*idx_triple*)

>> **Parameters**
>>> **x**

> **tri_score**(*h*, *r*, *t*)

> **vtp_score**(*h*, *r*, *t*)

class dicee.models.**LFMult**(*args*)

> Bases: *dicee.models.base_model.BaseKGE*

> Embedding with polynomial functions. We represent all entities and relations in the polynomial space as: f(x) = sum_{i=0}^{d-1} a_k x^{i%d} and use the three differents scoring function as in the paper to evaluate the score. We also consider combining with Neural Networks.

> **name = 'LFMult'**

> **entity_embeddings**

> **relation_embeddings**

> **degree**

> **m**

> **x_values**

forward_triples(*idx_triple*)

> **Parameters**
> **x**

construct_multi_coeff(*x*)

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

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

linear(*x*, *w*, *b*)

scalar_batch_NN(*a*, *b*, *c*)

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

tri_score(*coeff_h*, *coeff_r*, *coeff_t*)

> this part implement the trilinear scoring techniques:
>
> score(h,r,t) = int_{0}{1} h(x)r(x)t(x) dx = sum_{i,j,k = 0}^{d-1} dfrac{a_i*b_j*c_k}{1+(i+j+k)%d}
>
> 1. generate the range for i,j and k from [0 d-1]
>
> 2. perform dfrac{a_i*b_j*c_k}{1+(i+j+k)%d} in parallel for every batch
>
> 3. take the sum over each batch

vtp_score(*h*, *r*, *t*)

> this part implement the vector triple product scoring techniques:
>
> score(h,r,t) = int_{0}{1} h(x)r(x)t(x) dx = sum_{i,j,k = 0}^{d-1} dfrac{a_i*c_j*b_k - b_i*c_j*a_k}{(1+(i+j)%d)(1+k)}
>
> 1. generate the range for i,j and k from [0 d-1]
>
> 2. Compute the first and second terms of the sum
>
> 3. Multiply with then denominator and take the sum
>
> 4. take the sum over each batch

comp_func(*h*, *r*, *t*)

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

polynomial(*coeff*, *x*, *degree*)

> This function takes a matrix tensor of coefficients (coeff), a tensor vector of points x and range of integer [0,1,…d] and return a vector tensor (coeff[0][0] + coeff[0][1]x +…+ coeff[0][d]x^d,
>
> > **coeff[1][0] + coeff[1][1]x +…+ coeff[1][d]x^d)**

pop(*coeff*, *x*, *degree*)

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

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

> Bases: *dicee.models.base_model.BaseKGE*

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

name = 'DualE'

entity_embeddings

relation_embeddings

num_ent = None

kvsall_score(*e_1_h, e_2_h, e_3_h, e_4_h, e_5_h, e_6_h, e_7_h, e_8_h, e_1_t, e_2_t, e_3_t, e_4_t, e_5_t, e_6_t, e_7_t, e_8_t, r_1, r_2, r_3, r_4, r_5, r_6, r_7, r_8*) → 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*, *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 byte pair encoding and add padding
>
> **preprocess_with_pandas**() → None
>
> > Preprocess with pandas: add reciprocal triples, construct vocabulary, and index datasets
>
> **preprocess_with_polars**() → None
>
> > Preprocess with polars: add reciprocal triples and create indexed datasets

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

polars_dataframe_indexer(→ polars.DataFrame)	Replaces 'subject', 'relation', and 'object' columns in the input Polars DataFrame with their corresponding index values
pandas_dataframe_indexer(→ pandas.DataFrame)	Replaces 'subject', 'relation', and 'object' columns in the input Pandas DataFrame with their corresponding index values
apply_reciprocal_or_noise(add_reciprocal, eval_model)	Add reciprocal triples if conditions are met
timeit(func)	
read_with_polars(→ polars.DataFrame)	Load and Preprocess via Polars
read_with_pandas(data_path[, read_only_few, ...])	Load and Preprocess via Pandas
read_from_disk(→ Tuple[polars.DataFrame, pandas.DataFrame])	
count_triples(→ int)	Returns the total number of triples in the triple store.
fetch_worker(endpoint, offsets, chunk_size, ...)	Worker process: fetch assigned chunks and save to disk with per-worker tqdm.
read_from_triple_store_with_polars(endpoint[, ...])	Main function to read all triples in parallel, save as Parquet, and load into Polars dataframe.
read_from_triple_store_with_pandas([endpoint])	Read triples from triple store into pandas dataframe
get_er_vocab(data[, file_path])	
get_re_vocab(data[, file_path])	
get_ee_vocab(data[, file_path])	
create_constraints(triples[, file_path])	
load_with_pandas(→ None)	Deserialize data
save_numpy_ndarray(*, data, file_path)	
load_numpy_ndarray(*, file_path)	
save_pickle(*, data[, file_path])	
load_pickle(*[, file_path])	
create_repriocal_triples(x)	Add inverse triples into dask dataframe
dataset_sanity_checking(→ None)	

Module Contents

dicee.read_preprocess_save_load_kg.util.**polars_dataframe_indexer**(
        df_polars: polars.DataFrame, *idx_entity: polars.DataFrame*, *idx_relation: polars.DataFrame*)
        → 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_reciprocal_or_noise`**(*add_reciprocal: bool*, *eval_model: str*, *df: object = None*, *info: str = None*)

Add reciprocal triples if conditions are met

`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*)

Load and Preprocess via Pandas

`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.`**`count_triples`**(*endpoint: str*) → int

Returns the total number of triples in the triple store.

`dicee.read_preprocess_save_load_kg.util.`**`fetch_worker`**(*endpoint: str*, *offsets: list[int]*, *chunk_size: int*, *output_dir: str*, *worker_id: int*)

Worker process: fetch assigned chunks and save to disk with per-worker tqdm.

`dicee.read_preprocess_save_load_kg.util.`**`read_from_triple_store_with_polars`**(
endpoint: str, *chunk_size: int = 500000*, *output_dir: str = 'triples_parquet'*)

Main function to read all triples in parallel, save as Parquet, and load into Polars dataframe.

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

Read triples from triple store into pandas dataframe

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

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

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

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

>   (1) Extract domains and ranges of relations

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

dicee.read_preprocess_save_load_kg.util.**load_with_pandas**(*self*) → 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

PreprocessKG	Preprocess the data in memory
LoadSaveToDisk	
ReadFromDisk	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 byte pair encoding and add padding

preprocess_with_pandas() → None

    Preprocess with pandas: add reciprocal triples, construct vocabulary, and index datasets

preprocess_with_polars() → None

    Preprocess with polars: add reciprocal triples and create indexed datasets

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

is_sparql_endpoint_alive([sparql_endpoint])	
validate_knowledge_graph(args)	Validating the source of knowledge graph
sanity_checking_with_arguments(args)	
sanity_check_callback_args(args)	Perform sanity checks on callback-related arguments.

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.sanity_checkers.**sanity_check_callback_args**(*args*)

> Perform sanity checks on callback-related arguments.

dicee.scripts

Submodules

dicee.scripts.index_serve

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

Attributes

app
neural_searcher

Classes

NeuralSearcher
StringListRequest

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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**

    Bases: pydantic.BaseModel

    queries: List[str]

    reducer: str | None = None

async dicee.scripts.index_serve.**search_embeddings_batch**(*request: StringListRequest*)

dicee.scripts.index_serve.**serve**(*args*)

dicee.scripts.index_serve.**main**()

dicee.scripts.run

Functions

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

Module Contents

dicee.scripts.run.**get_default_arguments**(*description=None*)

    Extends pytorch_lightning Trainer's arguments with ours

dicee.scripts.run.**main**()

dicee.static_funcs

Functions

create_recipriocal_triples(x)	Add inverse triples into dask dataframe
get_er_vocab(data[, file_path])	
get_re_vocab(data[, file_path])	
get_ee_vocab(data[, file_path])	
timeit(func)	
save_pickle(*[, data, file_path])	
load_pickle([file_path])	
load_term_mapping([file_path])	
select_model(args[, is_continual_training, storage_path])	
load_model(→ Tuple[object, Tuple[dict, dict]])	Load weights and initialize pytorch module from namespace arguments
load_model_ensemble(...)	Construct Ensemble Of weights and initialize pytorch module from namespace arguments
save_numpy_ndarray(*, data, file_path)	
numpy_data_type_changer(→ numpy.ndarray)	Detect most efficient data type for a given triples
save_checkpoint_model(→ None)	Store Pytorch model into disk

Table 2 – continued from previous page

store(→ None)	
add_noisy_triples(→ pandas.DataFrame)	Add randomly constructed triples
read_or_load_kg(args, cls)	
intialize_model(→ Tuple[object, str])	
load_json(→ dict)	
save_embeddings(→ None)	Save it as CSV if memory allows.
random_prediction(pre_trained_kge)	
deploy_triple_prediction(pre_trained_kge, str_subject, ...)	
deploy_tail_entity_prediction(pre_trained_kge, ...)	
deploy_head_entity_prediction(pre_trained_kge, ...)	
deploy_relation_prediction(pre_trained_kge, ...)	
vocab_to_parquet(vocab_to_idx, name, ...)	
create_experiment_folder([folder_name])	
continual_training_setup_executor(→ None)	
exponential_function(→ torch.FloatTensor)	
load_numpy(→ numpy.ndarray)	
evaluate(entity_to_idx, scores, easy_answers, hard_answers)	# @TODO: CD: Renamed this function
download_file(url[, destination_folder])	
download_files_from_url(→ None)	
download_pretrained_model(→ str)	
write_csv_from_model_parallel(path)	Create
from_pretrained_model_write_embeddings_into None)	

Module Contents

dicee.static_funcs.**create_recipriocal_triples**(*x*)

    Add inverse triples into dask dataframe :param x: :return:

dicee.static_funcs.**get_er_vocab**(*data*, *file_path: str = None*)

dicee.static_funcs.**get_re_vocab**(*data*, *file_path: str = None*)

dicee.static_funcs.**get_ee_vocab**(*data*, *file_path: str = None*)

`dicee.static_funcs.`**`timeit`**(*func*)

`dicee.static_funcs.`**`save_pickle`**(***, *data: object = None*, *file_path=str*)

`dicee.static_funcs.`**`load_pickle`**(*file_path=str*)

`dicee.static_funcs.`**`load_term_mapping`**(*file_path=str*)

`dicee.static_funcs.`**`select_model`**(*args: dict*, *is_continual_training: bool = None*, *storage_path: str = None*)

`dicee.static_funcs.`**`load_model`**(*path_of_experiment_folder: str*, *model_name='model.pt'*, *verbose=0*) → Tuple[object, Tuple[dict, dict]]

Load weights and initialize pytorch module from namespace arguments

`dicee.static_funcs.`**`load_model_ensemble`**(*path_of_experiment_folder: str*) → Tuple[*dicee.models.base_model.BaseKGE*, Tuple[pandas.DataFrame, pandas.DataFrame]]

Construct Ensemble Of weights and initialize pytorch module from namespace arguments

(1) Detect models under given path

(2) Accumulate parameters of detected models

(3) Normalize parameters

(4) Insert (3) into model.

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

`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")
>
>   • **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

DICE_Trainer	DICE_Trainer implement

Functions

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

Module Contents

```
dicee.trainer.dice_trainer.load_term_mapping(file_path=str)
```

```
dicee.trainer.dice_trainer.initialize_trainer(args, callbacks)
        → 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 | *dicee.trainer.model_parallelism.TensorParallel* | *dicee.trainer.torch_trainer.TorchTrainer* | *dicee.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: 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

dicee.trainer.model_parallelism

Classes

TensorParallel	Abstract class for Trainer class for knowledge graph embedding models

Functions

extract_input_outputs(z[, device])	
find_good_batch_size(train_loader, tp_ensemble_model)	
forward_backward_update_loss(→ 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

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

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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

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

Functions

make_iterable_verbose(→ Iterable)	

Module Contents

dicee.trainer.torch_trainer_ddp.**make_iterable_verbose**(*iterable_object*, *verbose*, *desc='Default'*, *position=None*, *leave=True*) → Iterable

class dicee.trainer.torch_trainer_ddp.**TorchDDPTrainer**(*args*, *callbacks*)

Bases: *dicee.abstracts.AbstractTrainer*

A Trainer based on torch.nn.parallel.DistributedDataParallel

Arguments

entity_idxs
mapping.

relation_idxs
mapping.

form
?

store
?

label_smoothing_rate
Using hard targets (0,1) drives weights to infinity. An outlier produces enormous gradients.

Return type
torch.utils.data.Dataset

fit(**args*, ***kwargs*)
Train model

class dicee.trainer.torch_trainer_ddp.**NodeTrainer**(*trainer*, *model: torch.nn.Module*, *train_dataset_loader: torch.utils.data.DataLoader*, *callbacks*, *num_epochs: int*)

trainer

local_rank

global_rank

optimizer

train_dataset_loader

loss_func

callbacks

model

num_epochs

loss_history = []

ctx

scaler

extract_input_outputs(*z: list*)

train()
> Training loop for DDP

Classes

DICE_Trainer	DICE_Trainer implement

Package Contents

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

> **DICE_Trainer implement**
> > 1- Pytorch Lightning trainer (https://pytorch-lightning.readthedocs.io/en/stable/common/trainer.html)
> > 2- Multi-GPU Trainer(https://pytorch.org/docs/stable/generated/torch.nn.parallel.DistributedDataParallel.html) 3- CPU Trainer
> >
> > args
> >
> > is_continual_training:bool
> >
> > storage_path:str
> >
> > evaluator:
> >
> > report:dict
>
> **report**
>
> **args**
>
> **trainer = None**
>
> **is_continual_training**
>
> **storage_path**
>
> **evaluator = None**
>
> **form_of_labelling = None**

continual_start(*knowledge_graph*)

    (1) Initialize training.

    (2) Load model

    (3) Load trainer (3) Fit model

    Parameter

        returns

            • *model*

            • **form_of_labelling** (*str*)

initialize_trainer(*callbacks: List*)

          → lightning.Trainer | *dicee.trainer.model_parallelism.TensorParallel* | *dicee.trainer.torch_trainer.TorchTrainer* | *dicee.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: 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

dicee.weight_averaging

Classes

ASWA	Adaptive stochastic weight averaging
SWA	Stochastic Weight Averaging callback.
SWAG	Stochastic Weight Averaging - Gaussian (SWAG).
EMA	Exponential Moving Average (EMA) callback.
TWA	Train with Weight Averaging (TWA) using subspace projection + averaging.

Module Contents

class dicee.weight_averaging.**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.weight_averaging.**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 callback.

Initialize SWA callback.

> **swa_start_epoch: int**
> The epoch at which to start SWA.

> **swa_c_epochs: int**
> The number of epochs to use for SWA.

> **lr_init: float**
> The initial learning rate.

> **swa_lr: float**
> The learning rate to use during SWA.

> **max_epochs: int**
> The maximum number of epochs. args.num_epochs

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

static moving_average(*swa_model*, *running_model*, *alpha*)

Update SWA model with moving average of current model. Math: # SWA update: # $\theta\_swa \leftarrow (1 - alpha) * \theta\_swa + alpha * \theta$ # alpha = 1 / (n + 1), where n = number of models already averaged # alpha is tracked via self.swa_n in code

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.

class dice.weight_averaging.**SWAG**(*swa_start_epoch*, *swa_c_epochs: int = 1*, *lr_init: float = 0.1*, *swa_lr: float = 0.05*, *max_epochs: int = None*, *max_num_models: int = 20*, *var_clamp: float = 1e-30*)

Bases: *dicee.abstracts.AbstractCallback*

Stochastic Weight Averaging - Gaussian (SWAG). Parameters

    swa_start_epoch

        [int] Epoch at which to start collecting weights.

    swa_c_epochs

        [int] Interval of epochs between updates.

    lr_init

        [float] Initial LR.

    swa_lr

        [float] LR in SWA / GSWA phase.

    max_epochs

        [int] Total number of epochs.

    max_num_models

        [int] Number of models to keep for low-rank covariance approx.

    var_clamp

        [float] Clamp low variance for stability.

swa_start_epoch

swa_c_epochs = 1

swa_lr = 0.05

lr_init = 0.1

max_epochs = None

max_num_models = 20

var_clamp = 1e-30

mean = None

sq_mean = None

deviations = []

gswa_n = 0

current_epoch = -1

get_mean_and_var()

    Return mean + variance (diagonal part).

sample (*base_model*, *scale=0.5*)

    Sample new model from SWAG posterior distribution.

    Math: # From SWAG, posterior is approximated as: # θ ~ N(mean, Σ) # where $\Sigma \approx$ diag(var) + (1/(K-1)) * D D^T # - mean = running average of weights # - var = elementwise variance (sq_mean - mean^2) # - D = [dev_1, dev_2, …, dev_K], deviations from mean (low-rank approx) # - K = number of collected models

    # Sampling step: # 1. θ_diag = mean + scale * std $\odot$ ϵ, where ϵ ~ N(0, I) # 2. θ_lowrank = θ_diag + (D z) / sqrt(K-1), where z ~ N(0, I_K) # Final sample = θ_lowrank

on_train_epoch_start (*trainer*, *model*)

    Update LR schedule (same as SWA).

on_train_epoch_end (*trainer*, *model*)

    Collect Gaussian stats at the end of epochs after swa_start.

on_fit_end (*trainer*, *model*)

    Set model weights to the collected SWAG mean at the end of training.

class dicee.weight_averaging.**EMA** (*ema_start_epoch: int*, *decay: float = 0.999*, *max_epochs: int = None*, *ema_c_epochs: int = 1*)

Bases: *dicee.abstracts.AbstractCallback*

Exponential Moving Average (EMA) callback.

    Parameters

- **ema_start_epoch** (*int*) – Epoch to start EMA.

- **decay** (*float*) – EMA decay rate (typical: 0.99 - 0.9999) Math: θ_ema <- decay * θ_ema + (1 - decay) * θ

- **max_epochs** (*int*) – Maximum number of epochs.

ema_start_epoch

decay = 0.999

max_epochs = None

ema_c_epochs = 1

ema_model = None

current_epoch = −1

static ema_update (*ema_model*, *running_model*, *decay: float*)

    Update EMA model with exponential moving average of current model. Math: # EMA update: # θ_ema ← (1 - alpha) * θ_ema + alpha * θ # alpha = 1 - decay, where decay is the EMA smoothing factor (typical 0.99 - 0.999) # alpha controls how much of the current model θ contributes to the EMA # decay is fixed in code –> can be extended to scheduled

on_train_epoch_start (*trainer*, *model*)

    Track current epoch.

on_train_epoch_end (*trainer*, *model*)

    Update EMA if past start epoch.

on_fit_end (*trainer*, *model*)

    Replace main model with EMA model at the end of training.

class dicee.weight_averaging.**TWA**(*twa_start_epoch: int*, *lr_init: float*, *num_samples: int = 5*,
    reg_lambda: float = 0.0, *max_epochs: int = None*, *twa_c_epochs: int = 1*)

Bases: *dicee.abstracts.AbstractCallback*

Train with Weight Averaging (TWA) using subspace projection + averaging.

Parameters

twa_start_epoch
    [int] Epoch to start TWA.

lr_init
    [float] Learning rate used for β updates.

num_samples
    [int] Number of sampled weight snapshots to build projection subspace.

reg_lambda
    [float] Regularization coefficient for β updates.

max_epochs
    [int] Total number of training epochs.

twa_c_epochs
    [int] Interval of epochs between TWA updates.

twa_start_epoch

num_samples = 5

reg_lambda = 0.0

max_epochs = None

lr_init

twa_c_epochs = 1

current_epoch = −1

weight_samples = []

twa_model = None

base_weights = None

P = None

beta = None

sample_weights(*model*)
    Collect sampled weights from the current model and maintain rolling buffer.

build_projection(*weight_samples*, *k=None*)
    Build projection subspace from collected weight samples. :param weight_samples: list of flat weight tensors
    [(D,), …] :param k: number of basis vectors to keep. Defaults to min(N, D).

    Returns
        (D,) base weight vector (average) P: (D, k) projection matrix with top-k basis directions

    Return type
        mean_w

on_train_epoch_start (*trainer*, *model*)

    Track epoch.

on_train_epoch_end (*trainer*, *model*)

    Main TWA logic: build subspace and update in β space.

    # Math: # TWA weight update: # w_twa = mean_w + P * beta # mean_w = (1/n) * sum_i w_i (SWA baseline) # beta <- (1 - eta * lambda) * beta - eta * P^T * g # g = gradient of training loss w.r.t. full model weights # eta = learning rate, lambda = ridge regularization # P = orthonormal basis spanning sampled checkpoints {w_i}

on_fit_end (*trainer*, *model*)

    Replace with TWA model at the end.

14.2 Attributes

`__version__`

14.3 Classes

Pyke	A Physical Embedding Model for Knowledge Graphs
DistMult	Embedding Entities and Relations for Learning and Inference in Knowledge Bases
CKeci	Without learning dimension scaling
Keci	Base class for all neural network modules.
TransE	Translating Embeddings for Modeling
DeCaL	Base class for all neural network modules.
DualE	Dual Quaternion Knowledge Graph Embeddings (https://ojs.aaai.org/index.php/AAAI/article/download/16850/16657)
ComplEx	Base class for all neural network modules.
AConEx	Additive Convolutional ComplEx Knowledge Graph Embeddings
AConvO	Additive Convolutional Octonion Knowledge Graph Embeddings
AConvQ	Additive Convolutional Quaternion Knowledge Graph Embeddings
ConvQ	Convolutional Quaternion Knowledge Graph Embeddings
ConvO	Base class for all neural network modules.
ConEx	Convolutional ComplEx Knowledge Graph Embeddings
QMult	Base class for all neural network modules.
OMult	Base class for all neural network modules.
Shallom	A shallow neural model for relation prediction (https://arxiv.org/abs/2101.09090)
LFMult	Embedding with polynomial functions. We represent all entities and relations in the polynomial space as:
CoKE	Contextualized Knowledge Graph Embedding (CoKE) model.

Table 3 – continued from previous page

PykeenKGE	A class for using knowledge graph embedding models implemented in Pykeen
BytE	Base class for all neural network modules.
BaseKGE	Base class for all neural network modules.
EnsembleKGE	
DICE_Trainer	DICE_Trainer implement
KGE	Knowledge Graph Embedding Class for interactive usage of pre-trained models
BPE_NegativeSamplingDataset	An abstract class representing a `Dataset`.
MultiLabelDataset	An abstract class representing a `Dataset`.
MultiClassClassificationDataset	Dataset for the 1vsALL training strategy
OnevsAllDataset	Dataset for the 1vsALL training strategy
KvsAll	Creates a dataset for KvsAll training by inheriting from torch.utils.data.Dataset.
AllvsAll	Creates a dataset for AllvsAll training by inheriting from torch.utils.data.Dataset.
OnevsSample	A custom PyTorch Dataset class for knowledge graph embeddings, which includes
KvsSampleDataset	KvsSample a Dataset:
NegSampleDataset	An abstract class representing a `Dataset`.
TriplePredictionDataset	Triple Dataset
CVDataModule	Create a Dataset for cross validation
LiteralDataset	Dataset for loading and processing literal data for training Literal Embedding model.
QueryGenerator	

14.4 Functions

create_recipriocal_triples(x)	Add inverse triples into dask dataframe
get_er_vocab(data[, file_path])	
get_re_vocab(data[, file_path])	
get_ee_vocab(data[, file_path])	
timeit(func)	
save_pickle(*[, data, file_path])	
load_pickle([file_path])	
load_term_mapping([file_path])	
select_model(args[, is_continual_training, storage_path])	
load_model(→ Tuple[object, Tuple[dict, dict]])	Load weights and initialize pytorch module from namespace arguments

Table 4 – continued from previous page

load_model_ensemble(...)	Construct Ensemble Of weights and initialize pytorch module from namespace arguments
save_numpy_ndarray(*, data, file_path)	
numpy_data_type_changer(→ numpy.ndarray)	Detect most efficient data type for a given triples
save_checkpoint_model(→ None)	Store Pytorch model into disk
store(→ None)	
add_noisy_triples(→ pandas.DataFrame)	Add randomly constructed triples
read_or_load_kg(args, cls)	
intialize_model(→ Tuple[object, str])	
load_json(→ dict)	
save_embeddings(→ None)	Save it as CSV if memory allows.
random_prediction(pre_trained_kge)	
deploy_triple_prediction(pre_trained_kge, str_subject, ...)	
deploy_tail_entity_prediction(pre_trained_kge, ...)	
deploy_head_entity_prediction(pre_trained_kge, ...)	
deploy_relation_prediction(pre_trained_kge, ...)	
vocab_to_parquet(vocab_to_idx, name, ...)	
create_experiment_folder([folder_name])	
continual_training_setup_executor(→ None)	
exponential_function(→ torch.FloatTensor)	
load_numpy(→ numpy.ndarray)	
evaluate(entity_to_idx, scores, easy_answers, hard_answers)	# @TODO: CD: Renamed this function
download_file(url[, destination_folder])	
download_files_from_url(→ None)	
download_pretrained_model(→ str)	
write_csv_from_model_parallel(path)	Create
from_pretrained_model_write_embeddings_int None)	
mapping_from_first_two_cols_to_third(train_se	
timeit(func)	

Table 4 – continued from previous page

load_term_mapping([file_path])	
reload_dataset(path, form_of_labelling, ...)	Reload the files from disk to construct the Pytorch dataset
construct_dataset(→ torch.utils.data.Dataset)	

14.5 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 sub-modules as regular attributes:

```python
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_1, e_2, e_3, we compute interactions between e_1 e_2, e_1 e_3 , and e_2 e_3 This can be implemented with a nested two for loops

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

> > > **for k in range(i + 1, p):**
> > > results.append(hp[:, :, i] * rp[:, :, k] - hp[:, :, k] * rp[:, :, i])

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

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

e2e1, e2e2, e2e3, e3e1, e3e2, e3e3

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

`compute_sigma_qq` *(hq, rq)*

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

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

   for k in range(j + 1, q):
      results.append(hq[:, :, j] * rq[:, :, k] - hq[:, :, k] * rq[:, :, j])

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

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

e2e1, e2e2, e2e3, e3e1, e3e2, e3e3

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

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

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

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

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

print(sigma_pq.shape)

`apply_coefficients` *(hp, hq, rp, rq)*

Multiplying a base vector with its scalar coefficient

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

Compute our CL multiplication

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

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

eq j

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

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

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

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

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

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

(6) sigma_{pq} = sum_{i=1}^{p} sum_{j=p+1}^{p+q} (h_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 funcitons are identical Parameter ——— x: torch.LongTensor with (n,2) shape :rtype: torch.FloatTensor with (n, **|E|**) shape

`construct_batch_selected_cl_multivector` (*x: torch.FloatTensor*, *r: int*, *p: int*, *q: int*)
→ tuple[torch.FloatTensor, torch.FloatTensor, torch.FloatTensor]

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

Parameter

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

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

`forward_k_vs_sample` (*x: torch.LongTensor*, *target_entity_idx: torch.LongTensor*) → 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 submodules as regular attributes:

```python
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,

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

and return:

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

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

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

For different base vector interactions, we have

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

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

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

> Multiplying a base vector with its scalar coefficient

construct_cl_multivector(*x: torch.FloatTensor, re: int, p: int, q: int, r: int*)
    → tuple[torch.FloatTensor, torch.FloatTensor, torch.FloatTensor]

> Construct a batch of multivectors Cl_{p,q,r}(mathbb{R}^d)
>
> ### Parameter
>
> x: torch.FloatTensor with (n,d) shape
>
> > **returns**
> >
> > - **a0** (*torch.FloatTensor*)
> > - **ap** (*torch.FloatTensor*)
> > - **aq** (*torch.FloatTensor*)
> > - **ar** (*torch.FloatTensor*)

compute_sigma_pp(*hp, rp*)

> Compute .. math:

```
\sigma_{p,p}^* = \sum_{i=1}^{p-1}\sum_{i'=i+1}^{p}(x_iy_{i'}-x_{i'}y_i)
```

> sigma_{pp} captures the interactions between along p bases For instance, let p e_1, e_2, e_3, we compute interactions between e_1 e_2, e_1 e_3 , and e_2 e_3 This can be implemented with a nested two for loops
>
> > results = [] for i in range(p - 1):
> >
> > > **for k in range(i + 1, p):**
> > > results.append(hp[:, :, i] * rp[:, :, k] - hp[:, :, k] * rp[:, :, i])
> >
> > sigma_pp = torch.stack(results, dim=2) assert sigma_pp.shape == (b, r, int((p * (p - 1)) / 2))
>
> Yet, this computation would be quite inefficient. Instead, we compute interactions along all p, e.g., e1e1, e1e2, e1e3,
>
> > e2e1, e2e2, e2e3, e3e1, e3e2, e3e3
>
> Then select the triangular matrix without diagonals: e1e2, e1e3, e2e3.

compute_sigma_qq(*hq, rq*)

> Compute

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

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

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

    for k in range(j + 1, q):
        results.append(hq[:, :, j] * rq[:, :, k] - hq[:, :, k] * rq[:, :, j])

sigma_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:

```python
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:

```python
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.**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:

```python
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.

> **ℹ 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:

```python
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'

shallom

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_k x^{i%d} and use the three differents scoring function as in the paper to evaluate the score. We also consider combining with Neural Networks.

name = 'LFMult'

entity_embeddings

relation_embeddings

degree

m

x_values

forward_triples(*idx_triple*)

Parameters

x

construct_multi_coeff(*x*)

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

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

linear(*x*, *w*, *b*)

scalar_batch_NN(*a*, *b*, *c*)

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

tri_score(*coeff_h*, *coeff_r*, *coeff_t*)

this part implement the trilinear scoring techniques:

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

1. generate the range for i,j and k from [0 d-1]

2. perform dfrac{a_i*b_j*c_k}{1+(i+j+k)%d} in parallel for every batch

3. take the sum over each batch

vtp_score(*h*, *r*, *t*)

this part implement the vector triple product scoring techniques:

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

1. generate the range for i,j and k from [0 d-1]

2. Compute the first and second terms of the sum

3. Multiply with then denominator and take the sum

4. take the sum over each batch

comp_func(*h*, *r*, *t*)

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

polynomial(*coeff*, *x*, *degree*)

This function takes a matrix tensor of coefficients (coeff), a tensor vector of points x and range of integer [0,1,…d] and return a vector tensor (coeff[0][0] + 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.**CoKE**(*args*, *config:* *CoKEConfig* = *CoKEConfig()*)

Bases: *dicee.models.base_model.BaseKGE*

Contextualized Knowledge Graph Embedding (CoKE) model. Based on: https://arxiv.org/pdf/1911.02168.

CoKE uses a transformer encoder to learn contextualized representations of entities and relations. For link prediction, it predicts masked elements in (head, relation, tail) triples using bidirectional attention, similar to BERT's masked language modeling approach.

The model creates a sequence [head_emb, relation_emb, mask_emb], adds positional embeddings, and processes it through transformer layers to predict the tail entity.

`name = 'CoKE'`

`config`

`pos_emb`

`mask_emb`

`blocks`

`ln_f`

`coke_dropout`

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

`score`(*emb_h*, *emb_r*, *emb_t*)

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

`class` dicee.**`PykeenKGE`**(*args: dict*)

Bases: *dicee.models.base_model.BaseKGE*

A class for using knowledge graph embedding models implemented in Pykeen

Notes: Pykeen_DistMult: C Pykeen_ComplEx: Pykeen_QuatE: Pykeen_MuRE: Pykeen_CP: Pykeen_HolE: Pykeen_HolE: Pykeen_HolE: 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.**BytE** (**args*, ***kwargs*)

Bases: *dicee.models.base_model.BaseKGE*

Base class for all neural network modules.

Your models should also subclass this class.

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

```python
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 = 'BytE'

config

temperature = 0.5

`topk = 2`

`transformer`

`lm_head`

`loss_function`(*yhat_batch*, *y_batch*)

>   **Parameters**

>   • **`yhat_batch`**

>   • **`y_batch`**

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

>   **Parameters**
>   **`x`**(*B by T tensor*)

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

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

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

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

>   **Parameters**

>   • **`batch`** – The output of your data iterable, normally a `DataLoader`.

>   • **`batch_idx`** – The index of this batch.

>   • **`dataloader_idx`** – The index of the dataloader that produced this batch. (only if multiple dataloaders used)

>   **Returns**

>   • `Tensor` - The loss tensor

>   • `dict` - A dictionary which can include any keys, but must include the key `'loss'` in the case of automatic optimization.

>   • `None` - In automatic optimization, this will skip to the next batch (but is not supported for multi-GPU, TPU, or DeepSpeed). For manual optimization, this has no special meaning, as returning the loss is not required.

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

> Example:

```python
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()
```

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

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

Bases: `BaseKGELightning`

Base class for all neural network modules.

Your models should also subclass this class.

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

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


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

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

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

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

Variables

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

args

embedding_dim = None

num_entities = None

num_relations = None

num_tokens = None

learning_rate = None

apply_unit_norm = None

input_dropout_rate = None

hidden_dropout_rate = None

optimizer_name = None

feature_map_dropout_rate = None

kernel_size = None

num_of_output_channels = None

weight_decay = None

loss

selected_optimizer = None

normalizer_class = None

normalize_head_entity_embeddings

normalize_relation_embeddings

normalize_tail_entity_embeddings

hidden_normalizer

param_init

input_dp_ent_real

input_dp_rel_real

hidden_dropout

loss_history = []

byte_pair_encoding

max_length_subword_tokens

block_size

`forward_byte_pair_encoded_k_vs_all`(*x: torch.LongTensor*)

> **Parameters**
>> **`x`**(`B x 2 x T`)

`forward_byte_pair_encoded_triple`(*x: Tuple[torch.LongTensor, torch.LongTensor]*)

> byte pair encoded neural link predictors

> **Parameters**
>> `-------`

`init_params_with_sanity_checking`()

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

> **Parameters**
>> - **`x`**
>> - **`y_idx`**
>> - **`ordered_bpe_entities`**

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

> **Parameters**
>> **`x`**

`forward_k_vs_all`(**args*, ***kwargs*)

`forward_k_vs_sample`(**args*, ***kwargs*)

`get_triple_representation`(*idx_hrt*)

`get_head_relation_representation`(*indexed_triple*)

`get_sentence_representation`(*x: torch.LongTensor*)

> **Parameters**
>> - **`(b`**(`x shape`)
>> - **`3`**
>> - **`t)`**

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

> **Parameters**
>> **`x`**(`B x 2 x T`)

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

class dicee.**EnsembleKGE**(*models: list = None*, *seed_model=None*, *pretrained_models: List = None*)

> **`name`**

> **`train_mode = True`**

> **`args`**

named_children()

property example_input_array

parameters()

modules()

__iter__()

__len__()

eval()

to(*device*)

state_dict()

      Return the state dict of the ensemble.

load_state_dict(*state_dict*, *strict=True*)

      Load the state dict into the ensemble.

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.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: [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.

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.

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

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 :

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

> Return (e,r,x)

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

> confidence: float
>
> A threshold for an output of a sigmoid function given a triple.
>
> topk: int
>
> Highest ranked k item to select triples with f(e,r,x) > confidence .
>
> at_most: int
>
> Stop after finding at_most missing triples
>
> {(e,r,x) | f(e,r,x) > confidence land (e,r,x)}

otin G

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

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.**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_idxs*)

> Bases: `torch.utils.data.Dataset`
>
> Dataset for the 1vsALL training strategy
>
> > **Parameters**
> >
> > - **train_set_idx** – Indexed triples for the training.
> >
> > - **entity_idxs** – mapping.
> >
> > - **relation_idxs** – mapping.
> >
> > - **form** – ?
> >
> > - **num_workers** – int for https://pytorch.org/docs/stable/data.html#torch.utils.data.DataLoader
> >
> > **Return type**
> >
> > torch.utils.data.Dataset
>
> **train_data**
>
> **target_dim**
>
> **collate_fn = None**
>
> **__len__**()
>
> **__getitem__**(*idx*)

class dicee.**KvsAll**(*train_set_idx: numpy.ndarray*, *entity_idxs*, *relation_idxs*, *form*, *store=None*, *label_smoothing_rate: float = 0.0*)

> Bases: `torch.utils.data.Dataset`
>
> **Creates a dataset for KvsAll training by inheriting from torch.utils.data.Dataset.**
>
> > Let D denote a dataset for KvsAll training and be defined as D:= {(x,y)_i}_i ^N, where x: (h,r) is an unique tuple of an entity h in E and a relation r in R that has been seed in the input graph. y: denotes a multi-label vector in [0,1]^{|E|} is a binary label.
>
> orall y_i =1 s.t. (h r E_i) in KG
>
> > ℹ️ **Note**
> >
> > TODO
>
> **train_set_idx**
>
> > [numpy.ndarray] n by 3 array representing n triples
>
> **entity_idxs**
>
> > [dictonary] string representation of an entity to its integer id
>
> **relation_idxs**
>
> > [dictonary] string representation of a relation to its integer id
>
> self : torch.utils.data.Dataset
>
> ```
> >>> a = KvsAll()
> >>> a
> ? array([0, 1, 2, 3, 4, 5, 6, 7, 8, 9])
> ```

```
train_data = None

train_target = None

label_smoothing_rate

collate_fn = None
```

__len__()

__getitem__(*idx*)

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

Bases: `torch.utils.data.Dataset`

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

Let D denote a dataset for AllvsAll training and be defined as D:= {(x,y)_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| x |R| y: denotes a multi-label vector in [0,1]^{|E|} is a binary label.

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

> **ⓘ Note**
>
> **AllvsAll extends KvsAll via none existing (h,r). Hence, it adds data points that are labelled without 1s,**
> only with 0s.

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

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

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

self : torch.utils.data.Dataset

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

```
train_data = None

train_target = None

label_smoothing_rate

collate_fn = None

target_dim
```

__len__()

__getitem__(*idx*)

class dicee.**OnevsSample**(*train_set: numpy.ndarray*, *num_entities*, *num_relations*,
       neg_sample_ratio: int = None, *label_smoothing_rate: float = 0.0*)

Bases: `torch.utils.data.Dataset`

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

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

train_data

> The input data converted into a PyTorch tensor.
>
> > **Type**
> >
> > torch.Tensor

num_entities

> Number of entities in the dataset.
>
> > **Type**
> >
> > int

num_relations

> Number of relations in the dataset.
>
> > **Type**
> >
> > int

neg_sample_ratio

> Ratio of negative samples to be drawn for each positive sample.
>
> > **Type**
> >
> > int

label_smoothing_rate

> The smoothing factor applied to the labels.
>
> > **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_idxs*, *relation_idxs*, *form*, *store=None*, *neg_ratio=None*, *label_smoothing_rate: float = 0.0*)

> Bases: `torch.utils.data.Dataset`
>
> > **KvsSample a Dataset:**
> >
> > > **D:= {(x,y)_i}_i ^N, where**
> > > > . x:(h,r) is a unique h in E and a relation r in R and . y in [0,1]^{|E|} is a binary label.
> >
> > **orall y_i =1 s.t. (h r E_i) in KG**
> >
> > > **At each mini-batch construction, we subsample(y), hence n**
> > > > |new_y| << |E| new_y contains all 1's if sum(y)< neg_sample ratio new_y contains
> >
> > **train_set_idx**
> > > Indexed triples for the training.
> >
> > **entity_idxs**
> > > mapping.
> >
> > **relation_idxs**
> > > mapping.
> >
> > **form**
> > > ?
> >
> > **store**
> > > ?
> >
> > **label_smoothing_rate**
> > > ?

torch.utils.data.Dataset

train_data = None

train_target = None

neg_ratio = None

num_entities

label_smoothing_rate

collate_fn = None

max_num_of_classes

__len__()

__getitem__(*idx*)

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

Bases: torch.utils.data.Dataset

An abstract class representing a Dataset.

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

> **ⓘ 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_triples

length

num_entities

num_relations

labels

train_set = []

__len__()

__getitem__(*idx*)

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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 . collact_fn => Generates negative triples

collect_fn:

orall (h,r,t) in G obtain, create negative triples{(h,r,x),(,r,t),(h,m,t)}

y:labels are represented in torch.float16

train_set_idx
Indexed triples for the training.

entity_idxs
mapping.

relation_idxs
mapping.

form
?

store
?

label_smoothing_rate

collate_fn: batch:List[torch.IntTensor] Returns ———- torch.utils.data.Dataset

label_smoothing_rate

neg_sample_ratio

train_set

length

num_entities

num_relations

__len__()

__getitem__(*idx*)

collate_fn(*batch: List[torch.Tensor]*)

class dicee.**CVDataModule**(*train_set_idx: numpy.ndarray*, *num_entities*, *num_relations*, *neg_sample_ratio*, *batch_size*, *num_workers*)

Bases: `pytorch_lightning.LightningDataModule`

Create a Dataset for cross validation

Parameters

- **train_set_idx** – Indexed triples for the training.

- **num_entities** – entity to index mapping.

- **num_relations** – relation to index mapping.

- **batch_size** – int

- **form** – ?

- **num_workers** – 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()*

> ℹ **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:

```python
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):
```

```python
        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

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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]]]*)
        $\rightarrow$ None
    Save Queries into Disk

static load_queries_and_answers(*path: str*) $\rightarrow$ List[Tuple[str, Tuple[collections.defaultdict]]]
    Load Queries from Disk to Memory

dicee.**__version__ = '0.1.5'**

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