
DICE Embeddings

Release 0.1.3.2

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Contents:

1	Dicee Manual	2
2	Installation	3
2.1	Installation from Source	3
3	Download Knowledge Graphs	3
4	Knowledge Graph Embedding Models	3
5	How to Train	3
6	Creating an Embedding Vector Database	5
6.1	Learning Embeddings	5
6.2	Loading Embeddings into Qdrant Vector Database	6
6.3	Launching Webservice	6
7	Answering Complex Queries	6
8	Predicting Missing Links	8
9	Downloading Pretrained Models	8
10	How to Deploy	8
11	Docker	8
12	Coverage Report	8
13	How to cite	10
14	dicee	12
14.1	Submodules	12
14.2	Attributes	167
14.3	Classes	168
14.4	Functions	169
14.5	Package Contents	170
	Python Module Index	217

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

1 Dicee Manual

Version: dicee 0.2.0

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

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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-CPU, GPUs, TPUs or computing cluster, and
3. **Huggingface**⁵ to ease the deployment of pre-trained models.

Why Pandas⁶ & Co. ? A large knowledge graph can be read and preprocessed (e.g. removing literals) by pandas, modin, or polars in parallel. Through polars, a knowledge graph having more than 1 billion triples can be read in parallel fashion. Importantly, using these frameworks allow us to perform all necessary computations on a single CPU as well as a cluster of computers.

Why PyTorch⁷ & Co. ? PyTorch is one of the most popular machine learning frameworks available at the time of writing. PytorchLightning facilitates scaling the training procedure of PyTorch without boilerplate. In our framework, we combine **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 Gradio¹⁰? Deploy a pre-trained embedding model without writing a single line of code.

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

² <https://github.com/Demirrr>

³ <https://pandas.pydata.org/>

⁴ <https://pytorch.org/>

⁵ <https://huggingface.co/>

⁶ <https://pandas.pydata.org/>

⁷ <https://pytorch.org/>

⁸ <https://pytorch.org/>

⁹ <https://www.pytorchlightning.ai/>

¹⁰ <https://huggingface.co/gradio>

2 Installation

2.1 Installation from Source

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

or

```
pip install dicee
```

3 Download Knowledge Graphs

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

To test the Installation

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

4 Knowledge Graph Embedding Models

1. TransE, DistMult, ComplEx, ConEx, QMult, OMult, ConvO, ConvQ, Keci
2. All 44 models available in <https://github.com/pykeen/pykeen#models>

For more, please refer to examples.

5 How to Train

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

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

where the data is in the following form

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

A KGE model can also be trained from the command line

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

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

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

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

```
# Two equivalent executions
# (1)
dicee --dataset_dir "KGs/UMLS" --model Keci --eval_model "train_val_test"
# Evaluate Keci on Train set: Evaluate Keci on Train set
# {'H@1': 0.9518788343558282, 'H@3': 0.9988496932515337, 'H@10': 1.0, 'MRR': 0.
↪ 9753123402351737}
# Evaluate Keci on Validation set: Evaluate Keci on Validation set
# {'H@1': 0.6932515337423313, 'H@3': 0.9041411042944786, 'H@10': 0.9754601226993865,
↪ 'MRR': 0.8072362996241839}
# Evaluate Keci on Test set: Evaluate Keci on Test set
# {'H@1': 0.6951588502269289, 'H@3': 0.9039334341906202, 'H@10': 0.9750378214826021,
↪ 'MRR': 0.8064032293278861}

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

Similarly, models can be easily trained with torchrun

```
torchrun --standalone --nnodes=1 --nproc_per_node=gpu dicee/scripts/run.py --trainer_
→torchDDP --dataset_dir "KGs/UMLS" --model Keci --eval_model "train_val_test"
# Evaluate Keci on Train set: Evaluate Keci on Train set: Evaluate Keci on Train set
# {'H@1': 0.9518788343558282, 'H@3': 0.9988496932515337, 'H@10': 1.0, 'MRR': 0.
→9753123402351737}
# Evaluate Keci on Validation set: Evaluate Keci on Validation set
# {'H@1': 0.6932515337423313, 'H@3': 0.9041411042944786, 'H@10': 0.9754601226993865,
→'MRR': 0.8072499937521418}
# Evaluate Keci on Test set: Evaluate Keci on Test set
{'H@1': 0.6951588502269289, 'H@3': 0.9039334341906202, 'H@10': 0.9750378214826021,
→'MRR': 0.8064032293278861}
```

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

```
torchrun --nnodes 2 --nproc_per_node=gpu --node_rank 0 --rdzv_id 455 --rdzv_backend_
→c10d --rdzv_endpoint=nebula dicee/scripts/run.py --trainer torchDDP --dataset_dir_
→KGs/UMLS
torchrun --nnodes 2 --nproc_per_node=gpu --node_rank 1 --rdzv_id 455 --rdzv_backend_
→c10d --rdzv_endpoint=nebula dicee/scripts/run.py --trainer torchDDP --dataset_dir_
→KGs/UMLS
```

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

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

where the data is in the following form

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

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

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

For more, please refer to examples.

6 Creating an Embedding Vector Database

6.1 Learning Embeddings

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

6.2 Loading Embeddings into Qdrant Vector Database

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

6.3 Launching Webservice

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

Retrieve and Search

Get embedding of germany

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

Get most similar things to europe

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

7 Answering Complex Queries

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

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

For more, please refer to examples/multi_hop_query_answering.

8 Predicting Missing Links

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

9 Downloading Pretrained Models

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

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

10 How to Deploy

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

11 Docker

To build the Docker image:

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

To test the Docker image:

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

12 Coverage Report

The coverage report is generated using `coverage.py`¹²:

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

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

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

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

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

TOTAL	6948	3169	54%	

13 How to cite

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

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

(continues on next page)

```

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

```

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

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

14 dicee

14.1 Submodules

dicee.__main__

dicee.abstracts

Classes

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

Module Contents

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

Abstract class for Trainer class for knowledge graph embedding models

Parameter

args

[str] ?

callbacks: list

?

attributes

callbacks

is_global_zero = True

global_rank = 0

local_rank = 0

strategy = None

on_fit_start (*args, **kwargs)

A function to call callbacks before the training starts.

Parameter

args

kwargs

rtype

None

on_fit_end (*args, **kwargs)

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

Parameter

args

kwargs

rtype

None

on_train_epoch_end (*args, **kwargs)

A function to call callbacks at the end of an epoch.

Parameter

args

kwargs

rtype

None

on_train_batch_end (*args, **kwargs)

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

Parameter

args

kwargs

rtype

None

static save_checkpoint (*full_path: str, model*) → None

A static function to save a model into disk

Parameter

full_path : str

model:

rtype

None

class dicee.abstracts.**BaseInteractiveKGE** (*path: str = None, url: str = None,*
construct_ensemble: bool = False, model_name: str = None,
apply_semantic_constraint: bool = False)

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

Parameter

path_of_pretrained_model_dir
[str] ?

construct_ensemble: boolean
?

model_name: str *apply_semantic_constraint* : boolean

construct_ensemble = False

apply_semantic_constraint = False

configs

get_eval_report () → dict

get_bpe_token_representation (*str_entity_or_relation: List[str] | str*) → List[List[int]] | List[int]

Parameters

str_entity_or_relation (*corresponds to a str or a list of strings to be tokenized via BPE and shaped.*)

Return type

A list integer(s) or a list of lists containing integer(s)

get_padded_bpe_triple_representation (*triples: List[List[str]]*) → Tuple[List, List, List]

Parameters

triples

set_model_train_mode () → None

Setting the model into training mode

Parameter

set_model_eval_mode () → None

Setting the model into eval mode

Parameter

property name

sample_entity (*n: int*) → List[str]

sample_relation (*n: int*) → List[str]

is_seen (*entity: str = None, relation: str = None*) → bool

save () → None

get_entity_index (*x: str*)

get_relation_index (*x: str*)

index_triple (*head_entity: List[str], relation: List[str], tail_entity: List[str]*)
→ Tuple[torch.LongTensor, torch.LongTensor, torch.LongTensor]

Index Triple

Parameter

head_entity: List[str]

String representation of selected entities.

relation: List[str]

String representation of selected relations.

tail_entity: List[str]

String representation of selected entities.

Returns: Tuple

pytorch tensor of triple score

add_new_entity_embeddings (*entity_name: str = None, embeddings: torch.FloatTensor = None*)

get_entity_embeddings (*items: List[str]*)

Return embedding of an entity given its string representation

Parameter

items:

entities

get_relation_embeddings (*items: List[str]*)

Return embedding of a relation given its string representation

Parameter

items:

relations

construct_input_and_output (*head_entity: List[str], relation: List[str], tail_entity: List[str], labels*)

Construct a data point :param head_entity: :param relation: :param tail_entity: :param labels: :return:

```

parameters ()

class dicee.abstracts.InteractiveQueryDecomposition

    t_norm (tens_1: torch.Tensor, tens_2: torch.Tensor, tnorm: str = 'min') → torch.Tensor

    tensor_t_norm (subquery_scores: torch.FloatTensor, tnorm: str = 'min') → torch.FloatTensor
        Compute T-norm over  $[0,1]^{n \times d}$  where n denotes the number of hops and d denotes number of
        entities

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

    negnorm (tens_1: torch.Tensor, lambda_: float, neg_norm: str = 'standard') → torch.Tensor

class dicee.abstracts.AbstractCallback
    Bases: abc.ABC, lightning.pytorch.callbacks.Callback
    Abstract class for Callback class for knowledge graph embedding models

```

Parameter

```
on_init_start (*args, **kwargs)
```

Parameter

trainer:

model:

rtype

None

```
on_init_end (*args, **kwargs)
```

Call at the beginning of the training.

Parameter

trainer:

model:

rtype

None

```
on_fit_start (trainer, model)
```

Call at the beginning of the training.

Parameter

trainer:

model:

rtype

None

```
on_train_epoch_end (trainer, model)
```

Call at the end of each epoch during training.

Parameter

trainer:

model:

rtype

None

on_train_batch_end (*args, **kwargs)

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

Parameter

trainer:

model:

rtype

None

on_fit_end (*args, **kwargs)

Call at the end of the training.

Parameter

trainer:

model:

rtype

None

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

Bases: [AbstractCallback](#)

Abstract class for Callback class for knowledge graph embedding models

Parameter

num_epochs

path

sample_counter = 0

epoch_count = 0

alphas = None

on_fit_start (trainer, model)

Call at the beginning of the training.

Parameter

trainer:

model:

rtype
None

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

Parameter

trainer:

model:

rtype
None

store_ensemble (*param_ensemble*) → None

class dicee.abstracts.**BaseInteractiveTrainKGE**

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

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

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

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

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

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

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

Trains the Literal Embeddings model using literal data.

Parameters

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

dicee.analyse_experiments

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

Classes

Experiment

Functions

*get_default_arguments()**analyse(args)*

Module Contents

```
dicee.analyse_experiments.get_default_arguments()
```

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

```
    model_name = []
    callbacks = []
    embedding_dim = []
    num_params = []
    num_epochs = []
    batch_size = []
    lr = []
    byte_pair_encoding = []
    aswa = []
    path_dataset_folder = []
    full_storage_path = []
    pq = []
    train_mrr = []
    train_h1 = []
    train_h3 = []
    train_h10 = []
```

```

val_mrr = []
val_h1 = []
val_h3 = []
val_h10 = []
test_mrr = []
test_h1 = []
test_h3 = []
test_h10 = []
runtime = []
normalization = []
scoring_technique = []
save_experiment(x)
to_df()

```

```
dicee.analyse_experiments.analyse(args)
```

dicee.callbacks

Classes

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

Functions

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

Module Contents

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

Bases: `dicee.abstracts.AbstractCallback`

Abstract class for Callback class for knowledge graph embedding models

Parameter

path

on_fit_end (*trainer, model*) → None

Store epoch loss

Parameter

trainer:

model:

rtype

None

class `dicee.callbacks.PrintCallback`

Bases: `dicee.abstracts.AbstractCallback`

Abstract class for Callback class for knowledge graph embedding models

Parameter

start_time

on_fit_start (*trainer, pl_module*)

Call at the beginning of the training.

Parameter

trainer:

model:

rtype

None

on_fit_end (*trainer, pl_module*)

Call at the end of the training.

Parameter

trainer:

model:

rtype

None

on_train_batch_end (**args, **kwargs*)

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

Parameter

trainer:

model:

rtype

None

on_train_epoch_end (*args, **kwargs)

Call at the end of each epoch during training.

Parameter

trainer:

model:

rtype

None

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

Bases: *dicee.abstracts.AbstractCallback*

Abstract class for Callback class for knowledge graph embedding models

Parameter

every_x_epoch

max_epochs

epoch_counter = 0

path

on_train_batch_end (*args, **kwargs)

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

Parameter

trainer:

model:

rtype

None

on_fit_start (trainer, pl_module)

Call at the beginning of the training.

Parameter

trainer:

model:

rtype

None

on_train_epoch_end (*args, **kwargs)
Call at the end of each epoch during training.

Parameter

trainer:

model:

rtype
None

on_fit_end (*args, **kwargs)
Call at the end of the training.

Parameter

trainer:

model:

rtype
None

on_epoch_end (model, trainer, **kwargs)

class dicee.callbacks.**PseudoLabellingCallback** (data_module, kg, batch_size)

Bases: *dicee.abstracts.AbstractCallback*

Abstract class for Callback class for knowledge graph embedding models

Parameter

data_module

kg

num_of_epochs = 0

unlabelled_size

batch_size

create_random_data ()

on_epoch_end (trainer, model)

estimate_q (eps)

estimate rate of convergence q from sequence esp

compute_convergence (seq, i)

class dicee.callbacks.**ASWA** (num_epochs, path)

Bases: *dicee.abstracts.AbstractCallback*

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

path

```

num_epochs

initial_eval_setting = None

epoch_count = 0

alphas = []

val_aswa = -1

```

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

Parameter

trainer:
 model:

rtype
 None

static compute_mrr (*trainer*, *model*) → float

get_aswa_state_dict (*model*)

decide (*running_model_state_dict*, *ensemble_state_dict*, *val_running_model*,
mrr_updated_ensemble_model)

Perform Hard Update, software or rejection

Parameters

- **running_model_state_dict**
- **ensemble_state_dict**
- **val_running_model**
- **mrr_updated_ensemble_model**

on_train_epoch_end (*trainer*, *model*)
 Call at the end of each epoch during training.

Parameter

trainer:
 model:

rtype
 None

class `dicee.callbacks.Eval` (*path*, *epoch_ratio*: *int* = *None*)

Bases: `dicee.abstracts.AbstractCallback`

Abstract class for Callback class for knowledge graph embedding models

Parameter

`path`

`reports = []`

`epoch_ratio = None`

`epoch_counter = 0`

`on_fit_start (trainer, model)`

Call at the beginning of the training.

Parameter

trainer:

model:

rtype

None

`on_fit_end (trainer, model)`

Call at the end of the training.

Parameter

trainer:

model:

rtype

None

`on_train_epoch_end (trainer, model)`

Call at the end of each epoch during training.

Parameter

trainer:

model:

rtype

None

`on_train_batch_end (*args, **kwargs)`

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

Parameter

trainer:

model:

rtype

None

```
class dicee.callbacks.KronE
```

Bases: *dicee.abstracts.AbstractCallback*

Abstract class for Callback class for knowledge graph embedding models

Parameter

f = None

static batch_kronecker_product (*a, b*)

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

get_kronecker_triple_representation (*indexed_triple: torch.LongTensor*)

Get kronecker embeddings

on_fit_start (*trainer, model*)

Call at the beginning of the training.

Parameter

trainer:

model:

rtype

None

```
class 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.

Parameters

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

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

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

Module Contents

```

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

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

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

    storage_path: str = 'Experiments'
        A directory named with time of execution under –storage_path that contains related data about embeddings.

    path_to_store_single_run: str = None
        A single directory created that contains related data about embeddings.

    path_single_kg = None
        Path of a file corresponding to the input knowledge graph

    sparql_endpoint = None
        An endpoint of a triple store.

```

model: str = 'Keci'
KGE model

optim: str = 'Adam'
Optimizer

embedding_dim: int = 64
Size of continuous vector representation of an entity/relation

num_epochs: int = 150
Number of pass over the training data

batch_size: int = 1024
Mini-batch size if it is None, an automatic batch finder technique applied

lr: float = 0.1
Learning rate

add_noise_rate: float = None
The ratio of added random triples into training dataset

gpus = None
Number GPUs to be used during training

callbacks
10}}

Type
Callbacks, e.g., {"PPE"

Type
{ "last_percent_to_consider"

backend: str = 'pandas'
Backend to read, process, and index input knowledge graph. pandas, polars and rdflib available

separator: str = '\\s+'
separator for extracting head, relation and tail from a triple

trainer: str = 'torchCPUTrainer'
Trainer for knowledge graph embedding model

scoring_technique: str = 'KvsAll'
Scoring technique for knowledge graph embedding models

neg_ratio: int = 0
Negative ratio for a true triple in NegSample training_technique

weight_decay: float = 0.0
Weight decay for all trainable params

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

init_param: str = None
xavier_normal or None

gradient_accumulation_steps: int = 0
Not tested e

num_folds_for_cv: int = 0
 Number of folds for CV

eval_model: str = 'train_val_test'
 ["None", "train", "train_val", "train_val_test", "test"]

Type
 Evaluate trained model choices

save_model_at_every_epoch: int = None
 Not tested

label_smoothing_rate: float = 0.0

num_core: int = 0
 Number of CPUs to be used in the mini-batch loading process

random_seed: int = 0
 Random Seed

sample_triples_ratio: float = None
 Read some triples that are uniformly at random sampled. Ratio being between 0 and 1

read_only_few: int = None
 Read only first few triples

pykeen_model_kwargs
 Additional keyword arguments for pykeen models

kernel_size: int = 3
 Size of a square kernel in a convolution operation

num_of_output_channels: int = 32
 Number of slices in the generated feature map by convolution.

p: int = 0
 P parameter of Clifford Embeddings

q: int = 1
 Q parameter of Clifford Embeddings

input_dropout_rate: float = 0.0
 Dropout rate on embeddings of input triples

hidden_dropout_rate: float = 0.0
 Dropout rate on hidden representations of input triples

feature_map_dropout_rate: float = 0.0
 Dropout rate on a feature map generated by a convolution operation

byte_pair_encoding: bool = False
 Byte pair encoding

Type
 WIP

adaptive_swa: bool = False
 Adaptive stochastic weight averaging

swa: bool = False
Stochastic weight averaging

block_size: int = None
block size of LLM

continual_learning = None
Path of a pretrained model size of LLM

auto_batch_finding = False
A flag for using auto batch finding

eval_every_n_epochs: int = 0
Evaluate model every n epochs. If 0, no evaluation is applied.

save_every_n_epochs: bool = False
Save model every n epochs. If True, save model at every epoch.

eval_at_epochs: list = None
List of epoch numbers at which to evaluate the model (e.g., 1 5 10).

n_epochs_eval_model: str = 'val_test'
Evaluating link prediction performance on data splits while performing periodic evaluation.

adaptive_lr
0.1}

Type
Adaptive learning rate parameters, e.g., {"lr_decay"

swa_start_epoch: int = None
Epoch at which to start applying stochastic weight averaging.

__iter__()

dicee.dataset_classes

Classes

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

Functions

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

Module Contents

`dicee.dataset_classes.reload_dataset` (*path: str, form_of_labelling, scoring_technique, neg_ratio, label_smoothing_rate*)

Reload the files from disk to construct the Pytorch dataset

`dicee.dataset_classes.construct_dataset` (*, *train_set: numpy.ndarray | list, valid_set=None, test_set=None, ordered_bpe_entities=None, train_target_indices=None, target_dim: int = None, entity_to_idx: dict, relation_to_idx: dict, form_of_labelling: str, scoring_technique: str, neg_ratio: int, label_smoothing_rate: float, byte_pair_encoding=None, block_size: int = None*)
→ `torch.utils.data.Dataset`

class `dicee.dataset_classes.BPE_NegativeSamplingDataset` (*train_set: torch.LongTensor, ordered_shaped_bpe_entities: torch.LongTensor, neg_ratio: int*)

Bases: `torch.utils.data.Dataset`

An abstract class representing a Dataset.

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

Note

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

`train_set`

`ordered_bpe_entities`

`num_bpe_entities`

`neg_ratio`

`num_datapoints`

`__len__()`

`__getitem__(idx)`

`collate_fn` (*batch_shaped_bpe_triples: List[Tuple[torch.Tensor, torch.Tensor]]*)

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

Bases: `torch.utils.data.Dataset`

An abstract class representing a `Dataset`.

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

Note

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

`train_set`

`train_indices_target`

`target_dim`

`num_datapoints`

`torch_ordered_shaped_bpe_entities`

`collate_fn = None`

`__len__()`

`__getitem__(idx)`

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

Bases: `torch.utils.data.Dataset`

Dataset for the 1vsALL training strategy

Parameters

- `train_set_idx` – Indexed triples for the training.
- `entity_idx`s – mapping.
- `relation_idx`s – mapping.
- `form` – ?
- `num_workers` – int for <https://pytorch.org/docs/stable/data.html#torch.utils.data.DataLoader>

Return type

`torch.utils.data.Dataset`

`train_data`

`block_size = 8`

`num_of_data_points`

```
collate_fn = None
```

```
__len__()
```

```
__getitem__(idx)
```

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

Bases: torch.utils.data.Dataset

Dataset for the 1vsALL training strategy

Parameters

- **train_set_idx** – Indexed triples for the training.
- **entity_idx** – mapping.
- **relation_idx** – mapping.
- **form** – ?
- **num_workers** – int for <https://pytorch.org/docs/stable/data.html#torch.utils.data.DataLoader>

Return type

torch.utils.data.Dataset

```
train_data
```

```
target_dim
```

```
collate_fn = None
```

```
__len__()
```

```
__getitem__(idx)
```

```
class dicee.dataset_classes.KvsAll (train_set_idx: numpy.ndarray, entity_idx, relation_idx, form,  
store=None, label_smoothing_rate: float = 0.0)
```

Bases: torch.utils.data.Dataset

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

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

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

Note

TODO

train_set_idx

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

entity_idx

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

relation_idx

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

self : torch.utils.data.Dataset

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

train_data = None

train_target = None

label_smoothing_rate

collate_fn = None

__len__()

__getitem__(idx)

```
class dicee.dataset_classes.AllvsAll (train_set_idx: numpy.ndarray, entity_idxes, relation_idxes,
    label_smoothing_rate=0.0)
```

Bases: torch.utils.data.Dataset

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

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

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

Note

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

train_set_idx

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

entity_idxes

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

relation_idxes

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

self : torch.utils.data.Dataset

```
>>> a = 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_idxes,
relation_idxes, form, store=None, neg_ratio=None, label_smoothing_rate: float = 0.0)
```

Bases: torch.utils.data.Dataset

KvsSample a Dataset:

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

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

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

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

|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_idxes

mapping.

```

    relation_idx
    mapping.

    form
    ?

    store
    ?

    label_smoothing_rate
    ?

    torch.utils.data.Dataset

```

```

train_data = None

train_target = None

neg_ratio = None

num_entities

label_smoothing_rate

collate_fn = None

max_num_of_classes

__len__()

__getitem__(idx)

```

```

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

```

Bases: torch.utils.data.Dataset

An abstract class representing a Dataset.

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

Note

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

```

neg_sample_ratio

train_set

length

num_entities

num_relations

```

```

__len__()

__getitem__(idx)

class dicee.dataset_classes.TriplePredictionDataset (train_set: numpy.ndarray,
    num_entities: int, num_relations: int, neg_sample_ratio: int = 1, label_smoothing_rate: float = 0.0)
Bases: torch.utils.data.Dataset
    Triple Dataset
        D:= {(x)_i}_i ^N, where
            . x:(h,r, t) in KG is a unique h in E and a relation r in R and . collect_fn => Generates
            negative triples
        collect_fn:
orall (h,r,t) in G obtain, create negative triples {(h,r,x),(r,t),(h,m,t)}
        y:labels are represented in torch.float16

    train_set_idx
        Indexed triples for the training.

    entity_idxxs
        mapping.

    relation_idxxs
        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.CVDDataModule (train_set_idx: numpy.ndarray, num_entities,
    num_relations, neg_sample_ratio, batch_size, num_workers)
Bases: pytorch_lightning.LightningDataModule
    Create a Dataset for cross validation

```

Parameters

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

Return type

?

train_set_idx

num_entities

num_relations

neg_sample_ratio

batch_size

num_workers

train_dataloader() → torch.utils.data.DataLoader

An iterable or collection of iterables specifying training samples.

For more information about multiple dataloaders, see this section.

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

For data processing use the following pattern:

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

However, the above are only necessary for distributed processing.

Warning

do not assign state in `prepare_data`

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

Note

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

setup(*args, **kwargs)

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

Parameters

stage – either 'fit', 'validate', 'test', or 'predict'

Example:

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

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

        # don't do this
        self.something = else

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

transfer_batch_to_device(*args, **kwargs)

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

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

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

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

Note

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

Parameters

- **batch** – A batch of data that needs to be transferred to a new device.

- **device** – The target device as defined in PyTorch.
- **dataloader_idx** – The index of the dataloader to which the batch belongs.

Returns

A reference to the data on the new device.

Example:

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

See also

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

`prepare_data(*args, **kwargs)`

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

Warning

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

Example:

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

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

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

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

Example:

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

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

This is called before requesting the dataloaders:

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

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

Bases: torch.utils.data.Dataset

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

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

train_file_path

Path to the training data file.

Type

str

normalization

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

Type

str

normalization_params

Parameters used for normalization.

Type

dict

sampling_ratio

Fraction of the training set to use for ablations.

Type

float

entity_to_idx

Mapping of entities to their indices.

Type

dict

num_entities

Total number of entities.

Type

int

data_property_to_idx

Mapping of data properties to their indices.

Type

dict

num_data_properties

Total number of data properties.

Type

int

loader_backend

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

Type

str

train_file_path

loader_backend = 'pandas'

normalization_type = 'z-norm'

normalization_params

sampling_ratio = None

entity_to_idx = None

num_entities

__getitem__ (*index*)

__len__ ()

static load_and_validate_literal_data (*file_path: str = None, loader_backend: str = 'pandas'*)
→ pandas.DataFrame

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

Returns

DataFrame containing the loaded and validated data.

Return type

pd.DataFrame

static denormalize (*preds_norm, attributes, normalization_params*) → numpy.ndarray

Denormalizes the predictions based on the normalization type.

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

Returns

Denormalized predictions.

Return type

np.ndarray

dicee.eval_static_funcs

Functions

<code>evaluate_link_prediction_performance(→</code>	
<code>Dict)</code>	
<code>evaluate_link_prediction_performance_with_</code>	
<code>evaluate_link_prediction_performance_with_</code>	
<code>evaluate_link_prediction_performance_with_</code>	
<code>...)</code>	
<code>evaluate_lp_bpe_k_vs_all(model, triples[,</code>	
<code>er_vocab, ...])</code>	
<code>evaluate_literal_prediction(kge_model[, ...])</code>	Evaluates the trained literal prediction model on a test file.
<code>evaluate_ensemble_link_prediction_performai</code>	Evaluates link prediction performance of an ensemble of
<code>Dict)</code>	KGE models.

Module Contents

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

Parameters

- **model**
- **triples**
- **er_vocab**
- **re_vocab**

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

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

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

Parameters

- **model**
- **triples**
- **within_entities**
- **er_vocab**
- **re_vocab**

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

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

Evaluates the trained literal prediction model on a test file.

Parameters

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

Returns

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

Return type

pd.DataFrame

Raises

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

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

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

Mapping (head_idx, rel_idx) → list of tail_idx to filter (incl. target).

Parameters

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

Returns

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

dicee.evaluator

Classes

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

Module Contents

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

Evaluator class to evaluate KGE models in various downstream tasks

Arguments

re_vocab = None

er_vocab = None

ee_vocab = None

func_triple_to_bpe_representation = None

is_continual_training = None

num_entities = None

num_relations = None

args

report

during_training = False

vocab_preparation (*dataset*) → None

A function to wait future objects for the attributes of executor

Return type

None

eval (*dataset*: `dicee.knowledge_graph.KG`, *trained_model*, *form_of_labelling*, *during_training=False*)
→ None

eval_rank_of_head_and_tail_entity (*, *train_set*, *valid_set=None*, *test_set=None*, *trained_model*)

eval_rank_of_head_and_tail_byte_pair_encoded_entity (*, *train_set=None*, *valid_set=None*,
test_set=None, *ordered_bpe_entities*, *trained_model*)

eval_with_byte (*, *raw_train_set*, *raw_valid_set=None*, *raw_test_set=None*, *trained_model*,
form_of_labelling) → None

Evaluate model after reciprocal triples are added

eval_with_bpe_vs_all (*, *raw_train_set*, *raw_valid_set=None*, *raw_test_set=None*, *trained_model*,
form_of_labelling) → None

Evaluate model after reciprocal triples are added

```

eval_with_vs_all (*, train_set, valid_set=None, test_set=None, trained_model, form_of_labelling)
    → None
    Evaluate model after reciprocal triples are added

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

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

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

    Parameters

    • model

    • triples (List of lists)

    • info

    • form_of_labelling

evaluate_lp (model, triple_idx, info: str)

dummy_eval (trained_model, form_of_labelling: str)

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

```

dicee.executer

Classes

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

Module Contents

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

A class for Training, Retraining and Evaluation a model.

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

args

is_continual_training = **False**

trainer = **None**

trained_model = **None**

knowledge_graph = **None**

report

evaluator = **None**

start_time = None

setup_executor() → None

save_trained_model() → None

Save a knowledge graph embedding model

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

Parameter

rtype

None

end(*form_of_labelling: str*) → dict

End training

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

Parameter

rtype

A dict containing information about the training and/or evaluation

write_report() → None

Report training related information in a report.json file

start() → dict

Start training

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

Parameter

rtype

A dict containing information about the training and/or evaluation

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

Bases: *Execute*

A subclass of Execute Class for retraining

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

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

continual_start() → dict
 Start Continual Training

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

Parameter

rtype
 A dict containing information about the training and/or evaluation

dicee.knowledge_graph

Classes

<i>KG</i>	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.

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

Parameter

relation: Union[List[str], str]

String representation of selected relations.

tail_entity: Union[List[str], str]

String representation of selected entities.

k: int

Highest ranked k entities.

Returns: Tuple

Highest K scores and entities

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

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

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

Parameter

head_entity: List[str]

String representation of selected entities.

tail_entity: List[str]

String representation of selected entities.

k: int

Highest ranked k entities.

Returns: Tuple

Highest K scores and entities

predict_missing_tail_entity (*head_entity: List[str] | str, relation: List[str] | str,*
within: List[str] = None, batch_size=2, topk=1, return_indices=False) → torch.FloatTensor

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

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 $f(e,r,x) > \text{confidence}$.

at_most: int

Stop after finding at_most missing triples

$\{(e,r,x) \mid f(e,r,x) > \text{confidence} \text{ and } (e,r,x)$

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*) \rightarrow numpy.ndarray

Predicts literal values for given entities and attributes.

Parameters

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

Returns

Predictions for the given entities and attributes.

Return type

numpy ndarray

dicee.models

Submodules

dicee.models.adopt

Classes

ADOPT

Base class for all optimizers.

Functions

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`

Base class for all optimizers.

Warning

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

Parameters

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

clip_lambda

__setstate__ (*state*)

step (*closure=None*)

Perform a single optimization step.

Parameters

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

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

Functional API that performs ADOPT algorithm computation.

dicee.models.base_model

Classes

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

Module Contents

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

Bases: `lightning.LightningModule`

Base class for all neural network modules.

Your models should also subclass this class.

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

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

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

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

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

Note

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

Variables

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

training_step_outputs = []

mem_of_model() → Dict

Size of model in MB and number of params

training_step (*batch, batch_idx=None*)

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

Parameters

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

Returns

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

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

Example:

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

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

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

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

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

Note

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

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

Parameters

- **yhat_batch**
- **y_batch**

on_train_epoch_end (**args, **kwargs*)

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

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

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

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

    def on_train_epoch_end(self):
```

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

test_epoch_end(*outputs: List[Any]*)

test_dataloader() → None

An iterable or collection of iterables specifying test samples.

For more information about multiple dataloaders, see this section.

For data processing use the following pattern:

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

However, the above are only necessary for distributed processing.

Warning

do not assign state in `prepare_data`

- `test()`
- `prepare_data()`
- `setup()`

Note

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

Note

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

val_dataloader() → None

An iterable or collection of iterables specifying validation samples.

For more information about multiple dataloaders, see this section.

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

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

- `fit()`
- `validate()`

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

Note

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

Note

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

`predict_dataloader()` → None

An iterable or collection of iterables specifying prediction samples.

For more information about multiple dataloaders, see this section.

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

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

Note

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

Returns

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

`train_dataloader()` → None

An iterable or collection of iterables specifying training samples.

For more information about multiple dataloaders, see this section.

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

For data processing use the following pattern:

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

However, the above are only necessary for distributed processing.

Warning

do not assign state in `prepare_data`

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

Note

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

configure_optimizers (*parameters=None*)

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

Returns

Any of these 6 options.

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

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

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

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

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

Note

Some things to know:

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

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

Bases: *BaseKGELightning*

Base class for all neural network modules.

Your models should also subclass this class.

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

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

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

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

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

Note

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

Variables

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

`args`

`embedding_dim` = None

`num_entities` = None

`num_relations` = None

`num_tokens` = None

`learning_rate` = None

`apply_unit_norm` = None

`input_dropout_rate` = None

`hidden_dropout_rate` = None

`optimizer_name` = None

`feature_map_dropout_rate` = None

`kernel_size` = None

`num_of_output_channels` = None

`weight_decay` = None

`loss`

`selected_optimizer` = None

`normalizer_class` = None

`normalize_head_entity_embeddings`

`normalize_relation_embeddings`

`normalize_tail_entity_embeddings`

`hidden_normalizer`

`param_init`

`input_dp_ent_real`

`input_dp_rel_real`

`hidden_dropout`

`loss_history` = []

`byte_pair_encoding`

`max_length_subword_tokens`

`block_size`

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

Parameters

x (*B* × 2 × *T*)

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

byte pair encoded neural link predictors

Parameters

init_params_with_sanity_checking ()

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

Parameters

- **x**
- **y_idx**
- **ordered_bpe_entities**

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

Parameters

x

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

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

get_triple_representation (*idx_hrt*)

get_head_relation_representation (*indexed_triple*)

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

Parameters

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

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

Parameters

x (*B* × 2 × *T*)

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

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

Bases: *torch.nn.Module*

Base class for all neural network modules.

Your models should also subclass this class.

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


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

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

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

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

Note

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

Variables

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

args = *None*

__call__ (*x*)

static forward (*x*)

dicee.models.clifford

Classes

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

Module Contents

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

Bases: `dicee.models.base_model.BaseKGE`

Base class for all neural network modules.

Your models should also subclass this class.

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

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

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

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

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

Note

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

Variables

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

name = 'Keci'

p

q

r

requires_grad_for_interactions = True

compute_sigma_pp (*hp, rp*)

Compute $\sigma_{pp} = \sum_{i=1}^{p-1} \sum_{k=i+1}^p (h_{ir_k} - h_{kr_i}) e_i e_k$

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

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

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

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

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

Yet, this computation would be quite inefficient. Instead, we compute interactions along all p, e.g., $e_1 e_1, e_1 e_2, e_1 e_3$,

$e_2 e_1, e_2 e_2, e_2 e_3, e_3 e_1, e_3 e_2, e_3 e_3$

Then select the triangular matrix without diagonals: $e_1 e_2, e_1 e_3, e_2 e_3$.

compute_sigma_qq (*hq, rq*)

Compute $\sigma_{qq} = \sum_{j=1}^{p+q-1} \sum_{k=j+1}^{p+q} (h_{jr_k} - h_{kr_j}) e_j e_k \sigma_q$ 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., e_1e_1 , e_1e_2 , e_1e_3 ,

e_2e_1 , e_2e_2 , e_2e_3 , e_3e_1 , e_3e_2 , e_3e_3

Then select the triangular matrix without diagonals: e_1e_2 , e_1e_3 , e_2e_3 .

```

compute_sigma_pq(*, hp, hq, rp, rq)
sum_{i=1}^p sum_{j=p+1}^{p+q} (h_i r_j - h_j r_i) e_i e_j
results = [] sigma_pq = torch.zeros(b, r, p, q) for i in range(p):
    for j in range(q):
        sigma_pq[:, :, i, j] = hp[:, :, i] * rq[:, :, j] - hq[:, :, j] * rp[:, :, i]
print(sigma_pq.shape)

```

apply_coefficients (hp, hq, rp, rq)

Multiplying a base vector with its scalar coefficient

clifford_multiplication (h_0, hp, hq, r_0, rp, rq)

Compute our CL multiplication

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

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

eq j

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

- (1) $\sigma_0 = h_0 r_0 + \sum_{i=1}^p (h_0 r_i - h_i r_0) e_i - \sum_{j=p+1}^{p+q} (h_j r_j) e_j$
- (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 functions are identical Parameter ——— *x: torch.LongTensor* with (n,2) shape :rtype: torch.FloatTensor with (n, **IEI**) shape

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

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

Parameter

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

returns

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

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

Parameter

x: torch.LongTensor with (n,2) shape

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

rtype

torch.FloatTensor with (n, k) shape

score (*h, r, t*)

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

Parameter

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

rtype

torch.FloatTensor with (n) shape

class `dicee.models.clifford.CKeci` (*args*)

Bases: *Keci*

Without learning dimension scaling

name = 'CKeci'

```
requires_grad_for_interactions = False
```

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

Bases: `dicee.models.base_model.BaseKGE`

Base class for all neural network modules.

Your models should also subclass this class.

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

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

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

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

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

Note

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

Variables

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

name = 'DeCaL'

entity_embeddings

relation_embeddings

p

q

r

re

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

Parameter

x: torch.LongTensor with (n,) shape

rtype

torch.FloatTensor with (n) shape

cl_pqr (a: torch.tensor) → torch.tensor

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

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

compute_sigmas_single (list_h_emb, list_r_emb, list_t_emb)

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

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

and return:

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

compute_sigmas_multivect (list_h_emb, list_r_emb)

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

For same bases vectors interaction we have

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

For different base vector interactions, we have

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

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

Kvsall training

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

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

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

Multiplying a base vector with its scalar coefficient

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

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

Parameter

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

returns

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

compute_sigma_pp (hp, rp)

Compute .. math:

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

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

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

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

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

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

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

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

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

e2e1, e2e2, e2e3, e3e1, e3e2, e3e3

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

compute_sigma_rr (hk, rk)

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

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

Compute

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

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

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

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

```
    print(sigma_pq.shape)
```

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

Compute

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

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

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

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

```
    print(sigma_pq.shape)
```

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

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

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

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

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

```
    print(sigma_pq.shape)
```

dicee.models.complex

Classes

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

Module Contents

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

Bases: *dicee.models.base_model.BaseKGE*

Convolutional ComplEx Knowledge Graph Embeddings

```
name = 'ConEx'
```



```

conv2d

fc_num_input

fc1

norm_fc1

bn_conv2d

feature_map_dropout

residual_convolution (C_1: Tuple[torch.Tensor, torch.Tensor],
                      C_2: Tuple[torch.Tensor, torch.Tensor]) → torch.FloatTensor
    Compute residual score of two complex-valued embeddings. :param C_1: a tuple of two pytorch tensors
    that corresponds complex-valued embeddings :param C_2: a tuple of two pytorch tensors that corresponds
    complex-valued embeddings :return:

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

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

    Parameters
    x

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

class dicee.models.complex.AConEx (args)
    Bases: dicee.models.base_model.BaseKGE
    Additive Convolutional ComplEx Knowledge Graph Embeddings
    name = 'AConEx'

conv2d

fc_num_input

fc1

norm_fc1

bn_conv2d

feature_map_dropout

residual_convolution (C_1: Tuple[torch.Tensor, torch.Tensor],
                      C_2: Tuple[torch.Tensor, torch.Tensor]) → torch.FloatTensor
    Compute residual score of two complex-valued embeddings. :param C_1: a tuple of two pytorch tensors
    that corresponds complex-valued embeddings :param C_2: a tuple of two pytorch tensors that corresponds
    complex-valued embeddings :return:

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

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

    Parameters
    x

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

```

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

Base class for all neural network modules.

Your models should also subclass this class.

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

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

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

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

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

Note

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

Variables

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

`name = 'Complex'`

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

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

Parameters

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

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

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

dicee.models.dualE

Classes

<i>DualE</i>	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

$\mathbf{T}(x: \text{torch.tensor}) \rightarrow \text{torch.tensor}$

Transpose function

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

dicее.models.ensemble

Classes

EnsembleKGE

Module Contents

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

```
    name
```

```
    train_mode = True
```

```
    named_children()
```

```
    property example_input_array
```

```
    parameters()
```

```
    modules()
```

```
    __iter__()
```

```
    __len__()
```

```
    eval()
```

```
    to (device)
```

```
    mem_of_model()
```

```
    __call__ (x_batch)
```

```
    step()
```

```
    get_embeddings()
```

```
    __str__()
```

dicee.models.function_space

Classes

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

Module Contents

```
class dicee.models.function_space.FMult (args)
    Bases: dicee.models.base_model.BaseKGE
    Learning Knowledge Neural Graphs
    name = 'FMult'
    entity_embeddings
    relation_embeddings
    k
    num_sample = 50
    gamma
    roots
    weights
    compute_func (weights: torch.FloatTensor, x) → torch.FloatTensor
    chain_func (weights, x: torch.FloatTensor)
    forward_triples (idx_triple: torch.Tensor) → torch.Tensor
```

Parameters

x

```
class dicee.models.function_space.GFMult (args)
    Bases: dicee.models.base_model.BaseKGE
    Learning Knowledge Neural Graphs
    name = 'GFMult'
    entity_embeddings
    relation_embeddings
    k
    num_sample = 250
```

```

roots

weights

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

chain_func (weights, x: torch.FloatTensor)

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

```

Parameters

x

```

class dicee.models.function_space.FMult2 (args)
    Bases: dicee.models.base_model.BaseKGE
    Learning Knowledge Neural Graphs
    name = 'FMult2'
    n_layers = 3
    k
    n = 50
    score_func = 'compositional'
    discrete_points
    entity_embeddings
    relation_embeddings
    build_func (Vec)
    build_chain_funcs (list_Vec)
    compute_func (W, b, x) → torch.FloatTensor
    function (list_W, list_b)
    trapezoid (list_W, list_b)
    forward_triples (idx_triple: torch.Tensor) → torch.Tensor

```

Parameters

x

```

class dicee.models.function_space.LFMult1 (args)
    Bases: dicee.models.base_model.BaseKGE

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

    name = 'LFMult1'
    entity_embeddings
    relation_embeddings

```

forward_triples (*idx_triple*)

Parameters

x

tri_score (*h, r, t*)

vtp_score (*h, r, t*)

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

Bases: *dicee.models.base_model.BaseKGE*

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

name = 'LFMult'

entity_embeddings

relation_embeddings

degree

m

x_values

forward_triples (*idx_triple*)

Parameters

x

construct_multi_coeff (*x*)

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

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

linear (*x, w, b*)

scalar_batch_NN (*a, b, c*)

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

tri_score (*coeff_h, coeff_r, coeff_t*)

this part implement the trilinear scoring techniques:

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

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

vtp_score (*h, r, t*)

this part implement the vector triple product scoring techniques:

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

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

comp_func (*h, r, t*)

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

polynomial (*coeff, x, degree*)

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

coeff[1][0] + *coeff*[1][1]*x* +...+ *coeff*[1][*d*]*x*^{*d*})

pop (*coeff, x, degree*)

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

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

coeff[1][0] + *coeff*[1][1]*x* +...+ *coeff*[1][*d*]*x*^{*d*})

dicee.models.literal

Classes

LiteralEmbeddings

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

Module Contents

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

Bases: `torch.nn.Module`

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

num_of_data_properties

Number of data properties (attributes).

Type

`int`

embedding_dims

Dimension of the embeddings.

Type

`int`

entity_embeddings

Pre-trained entity embeddings.

Type

`torch.tensor`

dropout

Dropout rate for regularization.

Type

float

gate_residual

Whether to use gated residual connections.

Type

bool

freeze_entity_embeddings

Whether to freeze the entity embeddings during training.

Type

bool

embedding_dim

num_of_data_properties

hidden_dim

gate_residual = True

freeze_entity_embeddings = True

entity_embeddings

data_property_embeddings

fc

fc_out

dropout

gated_residual_proj

layer_norm

forward (*entity_idx*, *attr_idx*)

Parameters

- **entity_idx** (*Tensor*) – Entity indices (batch).
- **attr_idx** (*Tensor*) – Attribute (Data property) indices (batch).

Returns

scalar predictions.

Return type

Tensor

property device

dicee.models.octonion

Classes

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

Functions

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

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

Module Contents

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

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

```
class dicee.models.octonion.OMult(args)
```

Bases: *dicee.models.base_model.BaseKGE*

Base class for all neural network modules.

Your models should also subclass this class.

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

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

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

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

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

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:

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

    conv2d

    fc_num_input

    fc1

    bn_conv2d

    norm_fc1

    feature_map_dropout

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

    residual_convolution(O_1, O_2)

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

    Parameters
    x

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

```

dicee.models.pykeen_models

Classes

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)
```

dicее.models.quaternion

Classes

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

Functions

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

Module Contents

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

```
class dicее.models.quaternion.QMult (args)
```

Bases: *dicее.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 = '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

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

Module Contents

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

Bases: `dicee.models.base_model.BaseKGE`

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

`name = 'DistMult'`

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

Parameters

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

`forward_k_vs_all(x: torch.LongTensor)`

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

`score(h, r, t)`

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

Bases: `dicee.models.base_model.BaseKGE`

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

```

    name = 'TransE'

    margin = 4

    score(head_ent_emb, rel_ent_emb, tail_ent_emb)

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

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

    shallom

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

    forward_k_vs_all(x) → torch.FloatTensor

    forward_triples(x) → torch.FloatTensor

```

Parameters

x

Returns

```

class dicee.models.real.Pyke(args)
    Bases: dicee.models.base_model.BaseKGE
    A Physical Embedding Model for Knowledge Graphs
    name = 'Pyke'

    dist_func

    margin = 1.0

    forward_triples(x: torch.LongTensor)

```

Parameters

x

`dicee.models.static_funcs`

Functions

```

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:

```

dicее.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

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

Module Contents

```
class dicее.models.transformers.ByteE(*args, **kwargs)
```

Bases: *dicее.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 = 'BytE'

config

temperature = 0.5

topk = 2

transformer

lm_head

loss_function (*yhat_batch, y_batch*)

Parameters

- **yhat_batch**
- **y_batch**

forward (*x: torch.LongTensor*)

Parameters

x (*B by T tensor*)

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

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

training_step (*batch, batch_idx=None*)

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

Parameters

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

Returns

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

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

Example:

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

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

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

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

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

Note

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

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

Bases: torch.nn.Module

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

weight

bias

forward(*input*)

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

Bases: torch.nn.Module

Base class for all neural network modules.

Your models should also subclass this class.

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

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

class Model(nn.Module):
```

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(continued from previous page)

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

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

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

Note

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

Variables

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

c_attn

c_proj

attn_dropout

resid_dropout

n_head

n_embd

dropout

flash = True

forward (*x*)

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

Bases: `torch.nn.Module`

Base class for all neural network modules.

Your models should also subclass this class.

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

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

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

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(continued from previous page)

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

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

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

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 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.

`ln_1`

`attn`

`ln_2`

`mlp`

`forward(x)`

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

```
    block_size: int = 1024
```

```
    vocab_size: int = 50304
```

```
    n_layer: int = 12
```

```
    n_head: int = 12
```

```
    n_embd: int = 768
```

```
    dropout: float = 0.0
```

```
    bias: bool = False
```

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

```
    Bases: torch.nn.Module
```

Base class for all neural network modules.

Your models should also subclass this class.

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

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

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

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


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

Note

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

Variables

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

config

transformer

lm_head

get_num_params (*non_embedding=True*)

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

forward (*idx, targets=None*)

crop_block_size (*block_size*)

classmethod from_pretrained (*model_type, override_args=None*)

configure_optimizers (*weight_decay, learning_rate, betas, device_type*)

estimate_mfu (*fwdbwd_per_iter, dt*)

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

Classes

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

continues on next page

Table 1 – continued from previous page

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

Functions

```

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

octonion_mul(*, O_1, O_2)

octonion_mul_norm(*, O_1, O_2)

```

Package Contents

```

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

```

Bases: torch.optim.optimizer.Optimizer

Base class for all optimizers.

Warning

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

Parameters

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

`clip_lambda`

`__setstate__` (*state*)

`step` (*closure=None*)

Perform a single optimization step.

Parameters

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

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

Bases: `lightning.LightningModule`

Base class for all neural network modules.

Your models should also subclass this class.

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

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

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

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

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

Note

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

Variables

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

training_step_outputs = []

mem_of_model() → Dict

Size of model in MB and number of params

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

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

Parameters

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

Returns

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

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

Example:

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

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

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

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

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

Note

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

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

Parameters

- `yhat_batch`
- `y_batch`

`on_train_epoch_end(*args, **kwargs)`

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

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

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

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

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

`test_epoch_end(outputs: List[Any])`

`test_dataloader()` → None

An iterable or collection of iterables specifying test samples.

For more information about multiple dataloaders, see this section.

For data processing use the following pattern:

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

However, the above are only necessary for distributed processing.

Warning

do not assign state in `prepare_data`

- `test()`

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

Note

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

Note

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

`val_dataloader()` → None

An iterable or collection of iterables specifying validation samples.

For more information about multiple dataloaders, see this section.

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

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

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

Note

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

Note

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

`predict_dataloader()` → None

An iterable or collection of iterables specifying prediction samples.

For more information about multiple dataloaders, see this section.

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

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

Note

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

Returns

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

`train_dataloader()` → None

An iterable or collection of iterables specifying training samples.

For more information about multiple dataloaders, see this section.

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

For data processing use the following pattern:

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

However, the above are only necessary for distributed processing.

Warning

do not assign state in `prepare_data`

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

Note

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

`configure_optimizers(parameters=None)`

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

Returns

Any of these 6 options.

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

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

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

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

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

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

Note

Some things to know:

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


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

Bases: *BaseKGELightning*

Base class for all neural network modules.

Your models should also subclass this class.

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

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

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

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

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

Note

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

Variables

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

`args`

`embedding_dim = None`

`num_entities = None`

`num_relations = None`

`num_tokens = None`

`learning_rate = None`

`apply_unit_norm = None`

`input_dropout_rate = None`

`hidden_dropout_rate = None`

`optimizer_name = None`

`feature_map_dropout_rate = None`

```

kernel_size = None

num_of_output_channels = None

weight_decay = None

loss

selected_optimizer = None

normalizer_class = None

normalize_head_entity_embeddings

normalize_relation_embeddings

normalize_tail_entity_embeddings

hidden_normalizer

param_init

input_dp_ent_real

input_dp_rel_real

hidden_dropout

loss_history = []

byte_pair_encoding

max_length_subword_tokens

block_size

forward_byte_pair_encoded_k_vs_all (x: torch.LongTensor)

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

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

    Parameters
    -----

init_params_with_sanity_checking()

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

    Parameters
        •  $\mathbf{x}$ 
        •  $\mathbf{y\_idx}$ 
        •  $\mathbf{ordered\_bpe\_entities}$ 

```

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

Parameters

x

forward_k_vs_all (*args, **kwargs)

forward_k_vs_sample (*args, **kwargs)

get_triple_representation (idx_hrt)

get_head_relation_representation (indexed_triple)

get_sentence_representation (x : torch.LongTensor)

Parameters

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

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

Parameters

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

get_embeddings () \rightarrow Tuple[numpy.ndarray, numpy.ndarray]

class dicee.models.IdentityClass (args=None)

Bases: torch.nn.Module

Base class for all neural network modules.

Your models should also subclass this class.

Modules can also contain other Modules, allowing them to be nested in a tree structure. You can assign the 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.

args = None

__call__(*x*)

static forward(*x*)

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

Bases: *BaseKGELightning*

Base class for all neural network modules.

Your models should also subclass this class.

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

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

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

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

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

Note

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

Variables

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

args

embedding_dim = None

num_entities = None

```

num_relations = None

num_tokens = None

learning_rate = None

apply_unit_norm = None

input_dropout_rate = None

hidden_dropout_rate = None

optimizer_name = None

feature_map_dropout_rate = None

kernel_size = None

num_of_output_channels = None

weight_decay = None

loss

selected_optimizer = None

normalizer_class = None

normalize_head_entity_embeddings

normalize_relation_embeddings

normalize_tail_entity_embeddings

hidden_normalizer

param_init

input_dp_ent_real

input_dp_rel_real

hidden_dropout

loss_history = []

byte_pair_encoding

max_length_subword_tokens

block_size

forward_byte_pair_encoded_k_vs_all (x: torch.LongTensor)

```

Parameters

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

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

byte pair encoded neural link predictors

Parameters

```
init_params_with_sanity_checking()
```

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

Parameters

- **x**
- **y_idx**
- **ordered_bpe_entities**

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

Parameters

x

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

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

```
get_triple_representation(idx_hrt)
```

```
get_head_relation_representation(indexed_triple)
```

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

Parameters

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

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

Parameters

x (*B* × 2 × *T*)

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

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

Bases: `dicee.models.base_model.BaseKGE`

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

```
name = 'DistMult'
```

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

Parameters

- **emb_h**
- **emb_r**
- **emb_E**

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

```

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

score (h, r, t)

class dicee.models.TransE(args)
    Bases: dicee.models.base_model.BaseKGE

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

    name = 'TransE'

    margin = 4

    score (head_ent_emb, rel_ent_emb, tail_ent_emb)

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

class dicee.models.Shallom(args)
    Bases: dicee.models.base_model.BaseKGE

    A shallow neural model for relation prediction (https://arxiv.org/abs/2101.09090)

    name = 'Shallom'

    shallom

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

    forward_k_vs_all (x) → torch.FloatTensor

    forward_triples (x) → torch.FloatTensor

        Parameters
        x

        Returns

class dicee.models.Pyke(args)
    Bases: dicee.models.base_model.BaseKGE

    A Physical Embedding Model for Knowledge Graphs

    name = 'Pyke'

    dist_func

    margin = 1.0

    forward_triples (x: torch.LongTensor)

        Parameters
        x

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

    Base class for all neural network modules.

    Your models should also subclass this class.

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

```

```

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

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

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

```

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

Note

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

Variables

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

`args`

`embedding_dim = None`

`num_entities = None`

`num_relations = None`

`num_tokens = None`

`learning_rate = None`

`apply_unit_norm = None`

`input_dropout_rate = None`

`hidden_dropout_rate = None`

`optimizer_name = None`

`feature_map_dropout_rate = None`

`kernel_size = None`

`num_of_output_channels = None`

`weight_decay = None`

`loss`

`selected_optimizer = None`


```

normalizer_class = None

normalize_head_entity_embeddings

normalize_relation_embeddings

normalize_tail_entity_embeddings

hidden_normalizer

param_init

input_dp_ent_real

input_dp_rel_real

hidden_dropout

loss_history = []

byte_pair_encoding

max_length_subword_tokens

block_size

forward_byte_pair_encoded_k_vs_all (x: torch.LongTensor)

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

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

    Parameters
    -----

init_params_with_sanity_checking()

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

    Parameters

        •  $\mathbf{x}$ 

        •  $\mathbf{y\_idx}$ 

        • ordered_bpe_entities

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

    Parameters
         $\mathbf{x}$ 

forward_k_vs_all (*args, **kwargs)

forward_k_vs_sample (*args, **kwargs)

get_triple_representation (idx_hrt)

get_head_relation_representation (indexed_triple)

```

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

Parameters

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

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

Parameters

x (*B* × 2 × *T*)

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

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

Bases: *dicee.models.base_model.BaseKGE*

Convolutional ComplEx Knowledge Graph Embeddings

name = 'ConEx'

conv2d

fc_num_input

fc1

norm_fc1

bn_conv2d

feature_map_dropout

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

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

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

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

Parameters

x

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

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

Bases: *dicee.models.base_model.BaseKGE*

Additive Convolutional ComplEx Knowledge Graph Embeddings

name = 'AConEx'

conv2d

fc_num_input

fc1

norm_fc1

bn_conv2d

feature_map_dropout

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

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

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

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

Parameters

x

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

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

Bases: *dicee.models.base_model.BaseKGE*

Base class for all neural network modules.

Your models should also subclass this class.

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

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

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

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

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

Note

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

Variables

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

```
name = 'Complex'
```

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

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

Parameters

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

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

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

```
dicee.models.quaternion_mul(*, Q_1, Q_2)  
→ Tuple[torch.Tensor, torch.Tensor, torch.Tensor, torch.Tensor]
```

Perform quaternion multiplication :param Q_1: :param Q_2: :return:

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

Bases: `BaseKGELightning`

Base class for all neural network modules.

Your models should also subclass this class.

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

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

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

Note

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

Variables

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

```

args

embedding_dim = None

num_entities = None

num_relations = None

num_tokens = None

learning_rate = None

apply_unit_norm = None

input_dropout_rate = None

hidden_dropout_rate = None

optimizer_name = None

feature_map_dropout_rate = None

kernel_size = None

num_of_output_channels = None

weight_decay = None

loss

selected_optimizer = None

normalizer_class = None

normalize_head_entity_embeddings

normalize_relation_embeddings

normalize_tail_entity_embeddings

hidden_normalizer

param_init

input_dp_ent_real

input_dp_rel_real

hidden_dropout

loss_history = []

byte_pair_encoding

max_length_subword_tokens

block_size

forward_byte_pair_encoded_k_vs_all (x: torch.LongTensor)

```

Parameters

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

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

Parameters

init_params_with_sanity_checking ()

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

Parameters

- **x**
- **y_idx**
- **ordered_bpe_entities**

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

Parameters

x

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

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

get_triple_representation (*idx_hrt*)

get_head_relation_representation (*indexed_triple*)

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

Parameters

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

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

Parameters

x (*B* × 2 × *T*)

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

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

Bases: *torch.nn.Module*

Base class for all neural network modules.

Your models should also subclass this class.

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

```

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

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

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

```

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

Note

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

Variables

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

args = *None*

__call__ (*x*)

static forward (*x*)

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

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

Bases: `dicee.models.base_model.BaseKGE`

Base class for all neural network modules.

Your models should also subclass this class.

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

```

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

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

    def forward(self, x):
        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:

```

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

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

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

```

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

Note

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

Variables

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

args

embedding_dim = None

```

num_entities = None

num_relations = None

num_tokens = None

learning_rate = None

apply_unit_norm = None

input_dropout_rate = None

hidden_dropout_rate = None

optimizer_name = None

feature_map_dropout_rate = None

kernel_size = None

num_of_output_channels = None

weight_decay = None

loss

selected_optimizer = None

normalizer_class = None

normalize_head_entity_embeddings

normalize_relation_embeddings

normalize_tail_entity_embeddings

hidden_normalizer

param_init

input_dp_ent_real

input_dp_rel_real

hidden_dropout

loss_history = []

byte_pair_encoding

max_length_subword_tokens

block_size

forward_byte_pair_encoded_k_vs_all (x: torch.LongTensor)

```

Parameters

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

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

Parameters

init_params_with_sanity_checking ()

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

Parameters

- **x**
- **y_idx**
- **ordered_bpe_entities**

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

Parameters

x

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

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

get_triple_representation (*idx_hrt*)

get_head_relation_representation (*indexed_triple*)

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

Parameters

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

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

Parameters

x (*B* × 2 × *T*)

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

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

Bases: *torch.nn.Module*

Base class for all neural network modules.

Your models should also subclass this class.

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

```

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

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

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

```

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

Note

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

Variables

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

args = None

__call__(*x*)

static forward(*x*)

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

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

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

Bases: `dicee.models.base_model.BaseKGE`

Base class for all neural network modules.

Your models should also subclass this class.

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

```

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

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

    def forward(self, x):

```

(continues on next page)

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

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

Note

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

Variables

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

name = 'OMult'

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

score (*head_ent_emb: torch.FloatTensor, rel_ent_emb: torch.FloatTensor, tail_ent_emb: torch.FloatTensor*)

k_vs_all_score (*bpe_head_ent_emb, bpe_rel_ent_emb, E*)

forward_k_vs_all (*x*)

Completed. Given a head entity and a relation (h,r), we compute scores for all possible triples, i.e., $[\text{score}(h,r,x) | x \text{ in Entities}] \Rightarrow [0.0, 0.1, \dots, 0.8]$, shape $\Rightarrow (1, \text{Entities})$ Given a batch of head entities and relations \Rightarrow shape (size of batch, l Entities)

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

Bases: `dicee.models.base_model.BaseKGE`

Base class for all neural network modules.

Your models should also subclass this class.

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

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

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

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

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

Note

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

Variables

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

name = 'ConvO'

conv2d

fc_num_input

fc1

bn_conv2d

norm_fc1

feature_map_dropout

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

residual_convolution (*O_1, O_2*)

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

Parameters

x

forward_k_vs_all (*x: torch.Tensor*)

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

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

Bases: *dicee.models.base_model.BaseKGE*

Additive Convolutional Octonion Knowledge Graph Embeddings

name = 'AConvO'

conv2d

fc_num_input

fc1

bn_conv2d

norm_fc1

feature_map_dropout

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

```
residual_convolution(O_1, O_2)
```

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

Parameters

x

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

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

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

Bases: `dicee.models.base_model.BaseKGE`

Base class for all neural network modules.

Your models should also subclass this class.

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

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

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

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

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

Note

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

Variables

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

```
name = 'Keci'
```

```
p
```

```
q
```

```
r
```

```
requires_grad_for_interactions = True
```


compute_sigma_pp (*hp, rp*)

Compute $\sigma_{pp} = \sum_{i=1}^{p-1} \sum_{k=i+1}^p (h_{i,r_k} - h_{k,r_i}) e_i e_k$

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

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

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

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

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

Yet, this computation would be quite inefficient. Instead, we compute interactions along all p , e.g., $e_1 e_1, e_1 e_2, e_1 e_3$,

$e_2 e_1, e_2 e_2, e_2 e_3, e_3 e_1, e_3 e_2, e_3 e_3$

Then select the triangular matrix without diagonals: $e_1 e_2, e_1 e_3, e_2 e_3$.

compute_sigma_qq (*hq, rq*)

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

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

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

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

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

Yet, this computation would be quite inefficient. Instead, we compute interactions along all p , e.g., $e_1 e_1, e_1 e_2, e_1 e_3$,

$e_2 e_1, e_2 e_2, e_2 e_3, e_3 e_1, e_3 e_2, e_3 e_3$

Then select the triangular matrix without diagonals: $e_1 e_2, e_1 e_3, e_2 e_3$.

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

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

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

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

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

e_j

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

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

- (2) $\sigma_p = \sum_{i=1}^p (h_{0r_i} + h_{ir_0}) e_i$
- (3) $\sigma_q = \sum_{j=p+1}^{p+q} (h_{0r_j} + h_{jr_0}) e_j$
- (4) $\sigma_{pp} = \sum_{i=1}^{p-1} \sum_{k=i+1}^p (h_{ir_k} - h_{kr_i}) e_i e_k$
- (5) $\sigma_{qq} = \sum_{j=1}^{p+q-1} \sum_{k=j+1}^{p+q} (h_{jr_k} - h_{kr_j}) e_j e_k$
- (6) $\sigma_{pq} = \sum_{i=1}^p \sum_{j=p+1}^{p+q} (h_{ir_j} - h_{jr_i}) e_i e_j$

construct_cl_multivector (*x: torch.FloatTensor, r: int, p: int, q: int*)
 \rightarrow tuple[torch.FloatTensor, torch.FloatTensor, torch.FloatTensor]
Construct a batch of multivectors $Cl_{\{p,q\}}(\mathbb{R}^d)$

Parameter

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

returns

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

forward_k_vs_with_explicit (*x: torch.Tensor*)
k_vs_all_score (*bpe_head_ent_emb, bpe_rel_ent_emb, E*)

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

Kvsall training

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

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

construct_batch_selected_cl_multivector (*x: torch.FloatTensor, r: int, p: int, q: int*)
 \rightarrow tuple[torch.FloatTensor, torch.FloatTensor, torch.FloatTensor]
Construct a batch of batchs multivectors $Cl_{\{p,q\}}(\mathbb{R}^d)$

Parameter

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

returns

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

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

Parameter

x: torch.LongTensor with (n,2) shape

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

rtype

torch.FloatTensor with (n, k) shape

score (*h, r, t*)

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

Parameter

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

rtype

torch.FloatTensor with (n) shape

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

Bases: *Keci*

Without learning dimension scaling

name = 'CKeci'

requires_grad_for_interactions = False

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

Bases: *dicee.models.base_model.BaseKGE*

Base class for all neural network modules.

Your models should also subclass this class.

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

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

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

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

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

Note

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

Variables

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

name = 'DeCaL'

entity_embeddings

relation_embeddings

p

q

r

re

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

Parameter

x: torch.LongTensor with (n,) shape

rtype

torch.FloatTensor with (n) shape

cl_pqr (*a: torch.tensor*) → torch.tensor

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

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

compute_sigmas_single (*list_h_emb, list_r_emb, list_t_emb*)

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

$$s_0 = h_0 r_0 t_0 s_1 = \sum_{i=1}^p h_i r_i t_0 s_2 = \sum_{j=p+1}^{p+q} h_j r_j t_0 s_3 = \sum_{i=1}^q (h_0 r_i t_i + h_i r_0 t_i) s_4 = \sum_{i=p+1}^{p+q} (h_0 r_i t_i + h_i r_0 t_i) s_5 = \sum_{i=p+q+1}^{p+q+r} (h_0 r_i t_i + h_i r_0 t_i)$$

and return:

$$\sigma_0 t = \sigma_0 \cdot t_0 = s_0 + s_1 - s_2 s_3, s_4 \text{ and } s_5$$

compute_sigmas_multivect (*list_h_emb, list_r_emb*)

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

For same bases vectors interaction we have

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

For different base vector interactions, we have

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

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

Kvsall training

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

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

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

Multiplying a base vector with its scalar coefficient

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

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

Parameter

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

returns

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

compute_sigma_pp (*hp, rp*)

Compute .. math:

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

$\sigma_{\{pp\}}$ captures the interactions between along *p* bases For instance, let *p* e₁, e₂, e₃, we compute interactions between e₁ e₂, e₁ e₃, and e₂ e₃ 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., $e_1 e_1, e_1 e_2, e_1 e_3$,

$e_2 e_1, e_2 e_2, e_2 e_3, e_3 e_1, e_3 e_2, e_3 e_3$

Then select the triangular matrix without diagonals: $e_1 e_2, e_1 e_3, e_2 e_3$.

compute_sigma_rr (hk, rk)

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

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

Compute

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

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

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

print(sigma_pq.shape)

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

Compute

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

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

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

print(sigma_pq.shape)

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

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

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

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

print(sigma_pq.shape)

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

Bases: *BaseKGELightning*

Base class for all neural network modules.

Your models should also subclass this class.

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

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

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

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

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

Note

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

Variables

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

`args`

`embedding_dim = None`

`num_entities = None`

`num_relations = None`

`num_tokens = None`

`learning_rate = None`

`apply_unit_norm = None`

`input_dropout_rate = None`

`hidden_dropout_rate = None`

`optimizer_name = None`

`feature_map_dropout_rate = None`

```

kernel_size = None

num_of_output_channels = None

weight_decay = None

loss

selected_optimizer = None

normalizer_class = None

normalize_head_entity_embeddings

normalize_relation_embeddings

normalize_tail_entity_embeddings

hidden_normalizer

param_init

input_dp_ent_real

input_dp_rel_real

hidden_dropout

loss_history = []

byte_pair_encoding

max_length_subword_tokens

block_size

forward_byte_pair_encoded_k_vs_all (x: torch.LongTensor)

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

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

    Parameters
    -----

init_params_with_sanity_checking()

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

    Parameters
        •  $\mathbf{x}$ 
        •  $\mathbf{y\_idx}$ 
        •  $\mathbf{ordered\_bpe\_entities}$ 

```


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:

```

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

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

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

```

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

Note

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

Variables

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

args

```

embedding_dim = None

num_entities = None

num_relations = None

num_tokens = None

learning_rate = None

apply_unit_norm = None

input_dropout_rate = None

hidden_dropout_rate = None

optimizer_name = None

feature_map_dropout_rate = None

kernel_size = None

num_of_output_channels = None

weight_decay = None

loss

selected_optimizer = None

normalizer_class = None

normalize_head_entity_embeddings

normalize_relation_embeddings

normalize_tail_entity_embeddings

hidden_normalizer

param_init

input_dp_ent_real

input_dp_rel_real

hidden_dropout

loss_history = []

byte_pair_encoding

max_length_subword_tokens

block_size

forward_byte_pair_encoded_k_vs_all (x: torch.LongTensor)

```

Parameters

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

```

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

    Parameters
    -----

init_params_with_sanity_checking()

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

    Parameters
    • x
    • y_idx
    • ordered_bpe_entities

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

    Parameters
    • x

forward_k_vs_all (*args, **kwargs)

forward_k_vs_sample (*args, **kwargs)

get_triple_representation (idx_hrt)

get_head_relation_representation (indexed_triple)

get_sentence_representation (x: torch.LongTensor)

    Parameters
    • (b (x shape)
    • 3
    • t)

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

    Parameters
    • x (B x 2 x T)

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

class 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: $f(x) = \sum_{k=0}^{d-1} w_k e^{kix}$. and use the three differents scoring function as in the paper to evaluate the score

```
name = 'LFMult1'
```

```
entity_embeddings
```

```
relation_embeddings
```

```
forward_triples (idx_triple)
```

Parameters

x

```
tri_score (h, r, t)
```

```
vtp_score (h, r, t)
```

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

Bases: *[dicee.models.base_model.BaseKGE](#)*

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

```
name = 'LFMult'
```

```
entity_embeddings
```

```
relation_embeddings
```

```
degree
```

```
m
```

```
x_values
```

forward_triples (*idx_triple*)

Parameters

x

construct_multi_coeff (*x*)

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

Constructing a 2 layers NN to represent the embeddings. $h = \text{sigma}(w_h^T x + b_h)$, $r = \text{sigma}(w_r^T x + b_r)$, $t = \text{sigma}(w_t^T x + b_t)$

linear (*x, w, b*)

scalar_batch_NN (*a, b, c*)

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

tri_score (*coeff_h, coeff_r, coeff_t*)

this part implement the trilinear scoring techniques:

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

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

vtp_score (*h, r, t*)

this part implement the vector triple product scoring techniques:

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

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

comp_func (*h, r, t*)

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

polynomial (*coeff, x, degree*)

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

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

pop (*coeff, x, degree*)

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

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

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

class dicee.models.DualE (*args*)

Bases: *dicee.models.base_model.BaseKGE*

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

```

name = 'DualE'

entity_embeddings

relation_embeddings

num_ent = None

kvsall_score(e_1_h, e_2_h, e_3_h, e_4_h, e_5_h, e_6_h, e_7_h, e_8_h, e_1_t, e_2_t, e_3_t, e_4_t,
            e_5_t, e_6_t, e_7_t, e_8_t, r_1, r_2, r_3, r_4, r_5, r_6, r_7, r_8) → torch.tensor
KvsAll scoring function

```

Input

x: torch.LongTensor with (n,) shape

Output

torch.FloatTensor with (n) shape

forward_triples (*idx_triple: torch.tensor*) → torch.tensor
 Negative Sampling forward pass:

Input

x: torch.LongTensor with (n,) shape

Output

torch.FloatTensor with (n) shape

forward_k_vs_all (*x*)
 KvsAll forward pass

Input

x: torch.LongTensor with (n,) shape

Output

torch.FloatTensor with (n) shape

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

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

dicee.query_generator

Classes

QueryGenerator

Module Contents

```
class dicee.query_generator.QueryGenerator(train_path, val_path: str, test_path: str,
    ent2id: Dict = None, rel2id: Dict = None, seed: int = 1, gen_valid: bool = False,
    gen_test: bool = True)

    train_path

    val_path

    test_path

    gen_valid = False

    gen_test = True

    seed = 1

    max_ans_num = 1000000.0

    mode

    ent2id = None

    rel2id: Dict = None

    ent_in: Dict

    ent_out: Dict

    query_name_to_struct

    list2tuple(list_data)

    tuple2list(x: List | Tuple) → List | Tuple
        Convert a nested tuple to a nested list.

    set_global_seed(seed: int)
        Set seed

    construct_graph(paths: List[str]) → Tuple[Dict, Dict]
        Construct graph from triples Returns dicts with incoming and outgoing edges

    fill_query(query_structure: List[str | List], ent_in: Dict, ent_out: Dict, answer: int) → bool
        Private method for fill_query logic.

    achieve_answer(query: List[str | List], ent_in: Dict, ent_out: Dict) → set
        Private method for achieve_answer logic. @TODO: Document the code

    write_links(ent_out, small_ent_out)

    ground_queries(query_structure: List[str | List], ent_in: Dict, ent_out: Dict, small_ent_in: Dict,
        small_ent_out: Dict, gen_num: int, query_name: str)
        Generating queries and achieving answers

    unmap(query_type, queries, tp_answers, fp_answers, fn_answers)

    unmap_query(query_structure, query, id2ent, id2rel)
```

generate_queries (*query_struct: List, gen_num: int, query_type: str*)

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

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

abstract load_queries (*path*)

get_queries (*query_type: str, gen_num: int*)

static save_queries_and_answers (*path: str, data: List[Tuple[str, Tuple[collections.defaultdict]]]*)
→ None

Save Queries into Disk

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

Load Queries from Disk to Memory

dicee.read_preprocess_save_load_kg

Submodules

dicee.read_preprocess_save_load_kg.preprocess

Classes

PreprocessKG

Preprocess the data in memory

Module Contents

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

Preprocess the data in memory

kg

start () → None

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

Parameter

rtype

None

preprocess_with_byte_pair_encoding ()

preprocess_with_byte_pair_encoding_with_padding () → None

preprocess_with_pandas () → None

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

(1) Add recipriocal or noisy triples

(2) Construct vocabulary

(3) Index datasets

Parameter

rtype
None

preprocess_with_polars() → None

sequential_vocabulary_construction() → None

- (1) Read input data into memory
- (2) Remove triples with a condition
- (3) **Serialize vocabularies in a pandas dataframe where**
=> the index is integer and => a single column is string (e.g. URI)

dicee.read_preprocess_save_load_kg.read_from_disk

Classes

ReadFromDisk

Read the data from disk into memory

Module Contents

class dicee.read_preprocess_save_load_kg.read_from_disk.**ReadFromDisk**(kg)

Read the data from disk into memory

kg

start() → None

Read a knowledge graph from disk into memory

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

Parameter

None

rtype
None

add_noisy_triples_into_training()

dicee.read_preprocess_save_load_kg.save_load_disk

Classes

LoadSaveToDisk

Module Contents

class `dicee.read_preprocess_save_load_kg.save_load_disk.LoadSaveToDisk` (*kg*)

kg

save ()

load ()

dicee.read_preprocess_save_load_kg.util

Functions

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

Module Contents

```
dicee.read_preprocess_save_load_kg.util.polars_dataframe_indexer(  
    df_polars: polars.DataFrame, idx_entity: polars.DataFrame, idx_relation: polars.DataFrame)  
    → polars.DataFrame
```

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

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

Parameters:

df_polars

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

idx_entity

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

idx_relation

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

Returns:

polars.DataFrame

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

Example Usage:

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

Steps:

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

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

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

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

Parameters:

df_pandas

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

idx_entity

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

idx_relation

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

Returns:

pd.DataFrame

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

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

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

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

```
dicee.read_preprocess_save_load_kg.util.read_with_polars(data_path,  
    read_only_few: int = None, sample_triples_ratio: float = None, separator: str = None)  
    → polars.DataFrame
```

Load and Preprocess via Polars

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

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

```
dicee.read_preprocess_save_load_kg.util.read_from_triple_store(endpoint: str = None)
```

Read triples from triple store into pandas dataframe

```
dicee.read_preprocess_save_load_kg.util.get_er_vocab(data, file_path: str = None)
```

```
dicee.read_preprocess_save_load_kg.util.get_re_vocab(data, file_path: str = None)
```

```
dicee.read_preprocess_save_load_kg.util.get_ee_vocab(data, file_path: str = None)
```

```
dicee.read_preprocess_save_load_kg.util.create_constraints(triples, file_path: str = None)
```

- (1) Extract domains and ranges of relations

(2) Store a mapping from relations to entities that are outside of the domain and range. Create constrained entities based on the range of relations :param triples: :return: Tuple[dict, dict]

`dicee.read_preprocess_save_load_kg.util.load_with_pandas(self) → None`

Deserialize data

`dicee.read_preprocess_save_load_kg.util.save_numpy_ndarray(*, data: numpy.ndarray, file_path: str)`

`dicee.read_preprocess_save_load_kg.util.load_numpy_ndarray(*, file_path: str)`

`dicee.read_preprocess_save_load_kg.util.save_pickle(*, data: object, file_path=str)`

`dicee.read_preprocess_save_load_kg.util.load_pickle(*, file_path=str)`

`dicee.read_preprocess_save_load_kg.util.create_recipriocal_triples(x)`

Add inverse triples into dask dataframe :param x: :return:

`dicee.read_preprocess_save_load_kg.util.dataset_sanity_checking(train_set: numpy.ndarray, num_entities: int, num_relations: int) → None`

Parameters

- **train_set**
- **num_entities**
- **num_relations**

Returns

Classes

<i>PreprocessKG</i>	Preprocess the data in memory
<i>LoadSaveToDisk</i>	
<i>ReadFromDisk</i>	Read the data from disk into memory

Package Contents

class `dicee.read_preprocess_save_load_kg.PreprocessKG(kg)`

Preprocess the data in memory

kg

start() → None

Preprocess train, valid and test datasets stored in knowledge graph instance

Parameter

rtype
None

preprocess_with_byte_pair_encoding()

preprocess_with_byte_pair_encoding_with_padding() → None

preprocess_with_pandas() → None

Preprocess train, valid and test datasets stored in knowledge graph instance with pandas

- (1) Add recipriocal or noisy triples
- (2) Construct vocabulary
- (3) Index datasets

Parameter

rtype

None

preprocess_with_polars() → None

sequential_vocabulary_construction() → None

- (1) Read input data into memory
- (2) Remove triples with a condition
- (3) **Serialize vocabularies in a pandas dataframe where**
=> the index is integer and => a single column is string (e.g. URI)

class dicee.read_preprocess_save_load_kg.**LoadSaveToDisk**(kg)

kg

save()

load()

class dicee.read_preprocess_save_load_kg.**ReadFromDisk**(kg)

Read the data from disk into memory

kg

start() → None

Read a knowledge graph from disk into memory

Data will be available at the train_set, test_set, valid_set attributes.

Parameter

None

rtype

None

add_noisy_triples_into_training()

dicee.sanity_checkers

Functions

<code>is_sparql_endpoint_alive([sparql_endpoint])</code>	
<code>validate_knowledge_graph(args)</code>	Validating the source of knowledge graph
<code>sanity_checking_with_arguments(args)</code>	

Module Contents

`dicee.sanity_checkers.is_sparql_endpoint_alive (sparql_endpoint: str = None)`

`dicee.sanity_checkers.validate_knowledge_graph (args)`

Validating the source of knowledge graph

`dicee.sanity_checkers.sanity_checking_with_arguments (args)`

`dicee.scripts`

Submodules

`dicee.scripts.index_serve`

```
$ docker pull qdrant/qdrant && docker run -p 6333:6333 -p 6334:6334 -v $(pwd)/qdrant_storage:/qdrant/storage:z  
qdrant/qdrant $ dicee_vector_db -index -serve -path CountryEmbeddings -collection "countries_vdb"
```

Attributes

<code>app</code>
<code>neural_searcher</code>

Classes

<code>NeuralSearcher</code>	
<code>StringListRequest</code>	!!! abstract "Usage Documentation"

Functions

```
get_default_arguments()
```

```
index(args)
```

```
root()
```

```
search_embeddings(q)
```

```
retrieve_embeddings(q)
```

```
search_embeddings_batch(request)
```

```
serve(args)
```

```
main()
```

Module Contents

```
dicee.scripts.index_serve.get_default_arguments()
```

```
dicee.scripts.index_serve.index(args)
```

```
dicee.scripts.index_serve.app
```

```
dicee.scripts.index_serve.neural_searcher = None
```

```
class dicee.scripts.index_serve.NeuralSearcher(args)
```

```
    collection_name
```

```
    entity_to_idx = None
```

```
    qdrant_client
```

```
    topk = 5
```

```
    retrieve_embedding(entity: str = None, entities: List[str] = None) → List
```

```
    search(entity: str)
```

```
async dicee.scripts.index_serve.root()
```

```
async dicee.scripts.index_serve.search_embeddings(q: str)
```

```
async dicee.scripts.index_serve.retrieve_embeddings(q: str)
```

```
class dicee.scripts.index_serve.StringListRequest(/, **data: Any)
```

```
    Bases: pydantic.BaseModel
```

```
    !!! abstract “Usage Documentation”
```

```
        [Models](../concepts/models.md)
```

```
    A base class for creating Pydantic models.
```

`__class_vars__`

The names of the class variables defined on the model.

`__private_attributes__`

Metadata about the private attributes of the model.

`__signature__`

The synthesized `__init__` [*Signature*][inspect.Signature] of the model.

`__pydantic_complete__`

Whether model building is completed, or if there are still undefined fields.

`__pydantic_core_schema__`

The core schema of the model.

`__pydantic_custom_init__`

Whether the model has a custom `__init__` function.

`__pydantic_decorators__`

Metadata containing the decorators defined on the model. This replaces `Model.__validators__` and `Model.__root_validators__` from Pydantic V1.

`__pydantic_generic_metadata__`

Metadata for generic models; contains data used for a similar purpose to `__args__`, `__origin__`, `__parameters__` in typing-module generics. May eventually be replaced by these.

`__pydantic_parent_namespace__`

Parent namespace of the model, used for automatic rebuilding of models.

`__pydantic_post_init__`

The name of the post-init method for the model, if defined.

`__pydantic_root_model__`

Whether the model is a [*RootModel*][pydantic.root_model.RootModel].

`__pydantic_serializer__`

The *pydantic-core* *SchemaSerializer* used to dump instances of the model.

`__pydantic_validator__`

The *pydantic-core* *SchemaValidator* used to validate instances of the model.

`__pydantic_fields__`

A dictionary of field names and their corresponding [*FieldInfo*][pydantic.fields.FieldInfo] objects.

`__pydantic_computed_fields__`

A dictionary of computed field names and their corresponding [*ComputedFieldInfo*][pydantic.fields.ComputedFieldInfo] objects.

`__pydantic_extra__`

A dictionary containing extra values, if [*extra*][pydantic.config.ConfigDict.extra] is set to 'allow'.

`__pydantic_fields_set__`

The names of fields explicitly set during instantiation.

`__pydantic_private__`

Values of private attributes set on the model instance.

`queries: List[str]`

```
reducer: str | None = None
```

```
async dicee.scripts.index_serve.search_embeddings_batch(request: StringListRequest)
```

```
dicee.scripts.index_serve.serve(args)
```

```
dicee.scripts.index_serve.main()
```

dicee.scripts.run

Functions

<code>get_default_arguments([description])</code> <code>main()</code>	Extends pytorch_lightning Trainer's arguments with ours
--	---

Module Contents

```
dicee.scripts.run.get_default_arguments(description=None)
```

Extends pytorch_lightning Trainer's arguments with ours

```
dicee.scripts.run.main()
```

dicee.static_funcs

Functions

<code>create_recipriocal_triples(x)</code>	Add inverse triples into dask dataframe
<code>get_er_vocab(data[, file_path])</code>	
<code>get_re_vocab(data[, file_path])</code>	
<code>get_ee_vocab(data[, file_path])</code>	
<code>timeit(func)</code>	
<code>save_pickle(*[, data, file_path])</code>	
<code>load_pickle([file_path])</code>	
<code>load_term_mapping([file_path])</code>	
<code>select_model(args[, is_continual_training, storage_path])</code>	
<code>load_model(→ Tuple[object, Tuple[dict, dict]])</code>	Load weights and initialize pytorch module from namespace arguments
<code>load_model_ensemble(...)</code>	Construct Ensemble Of weights and initialize pytorch module from namespace arguments
<code>save_numpy_ndarray(*, data, file_path)</code>	
<code>numpy_data_type_changer(→ numpy.ndarray)</code>	Detect most efficient data type for a given triples

continues on next page

Table 2 – continued from previous page

<code>save_checkpoint_model(→ None)</code>	Store Pytorch model into disk
<code>store(→ None)</code>	
<code>add_noisy_triples(→ pandas.DataFrame)</code>	Add randomly constructed triples
<code>read_or_load_kg(args, cls)</code>	
<code>intialize_model(→ Tuple[object, str])</code>	
<code>load_json(→ dict)</code>	
<code>save_embeddings(→ None)</code>	Save it as CSV if memory allows.
<code>random_prediction(pre_trained_kge)</code>	
<code>deploy_triple_prediction(pre_trained_kge, str_subject, ...)</code>	
<code>deploy_tail_entity_prediction(pre_trained_kge, ...)</code>	
<code>deploy_head_entity_prediction(pre_trained_kge, ...)</code>	
<code>deploy_relation_prediction(pre_trained_kge, ...)</code>	
<code>vocab_to_parquet(vocab_to_idx, name, ...)</code>	
<code>create_experiment_folder([folder_name])</code>	
<code>continual_training_setup_executor(→ None)</code>	
<code>exponential_function(→ torch.FloatTensor)</code>	
<code>load_numpy(→ numpy.ndarray)</code>	
<code>evaluate(entity_to_idx, scores, easy_answers, # @TODO: CD: Renamed this function hard_answers)</code>	
<code>download_file(url[, destination_folder])</code>	
<code>download_files_from_url(→ None)</code>	
<code>download_pretrained_model(→ str)</code>	
<code>write_csv_from_model_parallel(path)</code>	Create
<code>from_pretrained_model_write_embeddings_int, None)</code>	

Module Contents

`dicee.static_funcs.create_recipriocal_triples(x)`

Add inverse triples into dask dataframe :param x: :return:

`dicee.static_funcs.get_er_vocab(data, file_path: str = None)`

`dicee.static_funcs.get_re_vocab(data, file_path: str = None)`

`dicee.static_funcs.get_ee_vocab(data, file_path: str = None)`

```

dicee.static_funcs.timeit (func)

dicee.static_funcs.save_pickle (*, data: object = None, file_path=str)

dicee.static_funcs.load_pickle (file_path=str)

dicee.static_funcs.load_term_mapping (file_path=str)

dicee.static_funcs.select_model (args: dict, is_continual_training: bool = None,
                                storage_path: str = None)

dicee.static_funcs.load_model (path_of_experiment_folder: str, model_name='model.pt', verbose=0)
    → Tuple[object, Tuple[dict, dict]]
    Load weights and initialize pytorch module from namespace arguments

dicee.static_funcs.load_model_ensemble (path_of_experiment_folder: str)
    → Tuple[dicee.models.base_model.BaseKGE, Tuple[pandas.DataFrame, pandas.DataFrame]]
    Construct Ensemble Of weights and initialize pytorch module from namespace arguments
    (1) Detect models under given path
    (2) Accumulate parameters of detected models
    (3) Normalize parameters
    (4) Insert (3) into model.

dicee.static_funcs.save_numpy_ndarray (*, data: numpy.ndarray, file_path: str)

dicee.static_funcs.numpy_data_type_changer (train_set: numpy.ndarray, num: int)
    → numpy.ndarray
    Detect most efficient data type for a given triples :param train_set: :param num: :return:

dicee.static_funcs.save_checkpoint_model (model, path: str) → None
    Store Pytorch model into disk

dicee.static_funcs.store (trained_model, model_name: str = 'model', full_storage_path: str = None,
                        save_embeddings_as_csv=False) → None

dicee.static_funcs.add_noisy_triples (train_set: pandas.DataFrame, add_noise_rate: float)
    → pandas.DataFrame
    Add randomly constructed triples :param train_set: :param add_noise_rate: :return:

dicee.static_funcs.read_or_load_kg (args, cls)

dicee.static_funcs.intialize_model (args: dict, verbose=0) → Tuple[object, str]

dicee.static_funcs.load_json (p: str) → dict

dicee.static_funcs.save_embeddings (embeddings: numpy.ndarray, indexes, path: str) → None
    Save it as CSV if memory allows. :param embeddings: :param indexes: :param path: :return:

dicee.static_funcs.random_prediction (pre_trained_kge)

dicee.static_funcs.deploy_triple_prediction (pre_trained_kge, str_subject, str_predicate,
                                           str_object)

dicee.static_funcs.deploy_tail_entity_prediction (pre_trained_kge, str_subject, str_predicate,
                                                top_k)

```

```

dicee.static_funcs.deploy_head_entity_prediction(pre_trained_kge, str_object, str_predicate,
top_k)

dicee.static_funcs.deploy_relation_prediction(pre_trained_kge, str_subject, str_object, top_k)

dicee.static_funcs.vocab_to_parquet(vocab_to_idx, name, path_for_serialization, print_into)

dicee.static_funcs.create_experiment_folder(folder_name='Experiments')

dicee.static_funcs.continual_training_setup_executor(executor) → None

dicee.static_funcs.exponential_function(x: numpy.ndarray, lam: float, ascending_order=True)
→ torch.FloatTensor

dicee.static_funcs.load_numpy(path) → numpy.ndarray

dicee.static_funcs.evaluate(entity_to_idx, scores, easy_answers, hard_answers)
# @TODO: CD: Renamed this function Evaluate multi hop query answering on different query types

dicee.static_funcs.download_file(url, destination_folder='.')

dicee.static_funcs.download_files_from_url(base_url: str, destination_folder='.') → None

```

Parameters

- **base_url** (e.g. [“https://files.dice-research.org/projects/DiceEmbeddings/KINSHIP-Keci-dim128-epoch256-KvsAll”](https://files.dice-research.org/projects/DiceEmbeddings/KINSHIP-Keci-dim128-epoch256-KvsAll))
- **destination_folder** (e.g. `"KINSHIP-Keci-dim128-epoch256-KvsAll"`)

```

dicee.static_funcs.download_pretrained_model(url: str) → str

```

```

dicee.static_funcs.write_csv_from_model_parallel(path: str)

```

Create

```

dicee.static_funcs.from_pretrained_model_write_embeddings_into_csv(path: str) → None

```

dicee.static_funcs_training

Functions

```

make_iterable_verbose(→ Iterable)

evaluate_lp([model, triple_idx, num_entities, ...])

evaluate_bpe_lp(model, triple_idx, ..., info])

efficient_zero_grad(model)

```

Module Contents

```

dicee.static_funcs_training.make_iterable_verbose(iterable_object, verbose, desc='Default',
position=None, leave=True) → Iterable

```

```
dicee.static_funcs_training.evaluate_lp (model=None, triple_idx=None, num_entities=None,
      er_vocab: Dict[Tuple, List] = None, re_vocab: Dict[Tuple, List] = None, info='Eval Starts',
      batch_size=128, chunk_size=1000)
```

```
dicee.static_funcs_training.evaluate_bpe_lp (model, triple_idx: List[Tuple],
      all_bpe_shaped_entities, er_vocab: Dict[Tuple, List], re_vocab: Dict[Tuple, List],
      info='Eval Starts')
```

```
dicee.static_funcs_training.efficient_zero_grad (model)
```

dicee.static_preprocess_funcs

Attributes

```
enable_log
```

Functions

```
timeit(func)
```

```
preprocesses_input_args(args) Sanity Checking in input arguments
```

```
create_constraints(→ Tuple[dict, dict, dict, dict])
```

```
get_er_vocab(data)
```

```
get_re_vocab(data)
```

```
get_ee_vocab(data)
```

```
mapping_from_first_two_cols_to_third(train_se
```

Module Contents

```
dicee.static_preprocess_funcs.enable_log = False
```

```
dicee.static_preprocess_funcs.timeit (func)
```

```
dicee.static_preprocess_funcs.preprocesses_input_args (args)
```

Sanity Checking in input arguments

```
dicee.static_preprocess_funcs.create_constraints (triples: numpy.ndarray)
      → Tuple[dict, dict, dict, dict]
```

(1) Extract domains and ranges of relations

(2) Store a mapping from relations to entities that are outside of the domain and range. Create constraints entities based on the range of relations :param triples: :return:

```
dicee.static_preprocess_funcs.get_er_vocab (data)
```

```
dicee.static_preprocess_funcs.get_re_vocab (data)
```



```
dicee.static_preprocess_funcs.get_ee_vocab(data)
```

```
dicee.static_preprocess_funcs.mapping_from_first_two_cols_to_third(train_set_idx)
```

dicee.trainer

Submodules

dicee.trainer.dice_trainer

Classes

<i>DICE_Trainer</i>	DICE_Trainer implement
---------------------	------------------------

Functions

<i>load_term_mapping</i> ([file_path])
<i>initialize_trainer</i> (...)
<i>get_callbacks</i> (args)

Module Contents

```
dicee.trainer.dice_trainer.load_term_mapping(file_path=str)
```

```
dicee.trainer.dice_trainer.initialize_trainer(args, callbacks)  
→ dicee.trainer.torch_trainer.TorchTrainer | dicee.trainer.model_parallelism.TensorParallel | dicee.trainer.torch_trainer_ddp
```

```
dicee.trainer.dice_trainer.get_callbacks(args)
```

```
class dicee.trainer.dice_trainer.DICE_Trainer(args, is_continual_training: bool, storage_path,  
        evaluator=None)
```

DICE_Trainer implement

- 1- Pytorch Lightning trainer (<https://pytorch-lightning.readthedocs.io/en/stable/common/trainer.html>)
- 2- Multi-GPU Trainer(<https://pytorch.org/docs/stable/generated/torch.nn.parallel.DistributedDataParallel.html>)
- 3- CPU Trainer

args

is_continual_training:bool

storage_path:str

evaluator:

report:dict

report

args

trainer = None

is_continual_training

storage_path

evaluator = None

form_of_labelling = None

continual_start (*knowledge_graph*)

- (1) Initialize training.
- (2) Load model
- (3) Load trainer (3) Fit model

Parameter

returns

- *model*
- **form_of_labelling** (*str*)

initialize_trainer (*callbacks: List*)

→ *lightning.Trainer* | *dicее.trainer.model_parallelism.TensorParallel* | *dicее.trainer.torch_trainer.TorchTrainer* | *dicее.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: dicее.knowledge_graph.KG* | *numpy.memmap*)

→ *Tuple[dicее.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[dicее.models.base_model.BaseKGE, str]*

Perform K-fold Cross-Validation

1. Obtain K train and test splits.
2. **For each split,**
 - 2.1 initialize trainer and model
 - 2.2. Train model with configuration provided in args.
 - 2.3. Compute the mean reciprocal rank (MRR) score of the model on the test respective split.
3. Report the mean and average MRR .

Parameters

- **self**
- **dataset**

Returns

model

dicee.trainer.model_parallelism

Classes

<i>TensorParallel</i>	Abstract class for Trainer class for knowledge graph embedding models
-----------------------	---

Functions

<i>extract_input_outputs</i> (z[, device])
<i>find_good_batch_size</i> (train_loader, tp_ensemble_model)
<i>forward_backward_update_loss</i> (→ float)

Module Contents

dicee.trainer.model_parallelism.**extract_input_outputs** (z: list, device=None)

dicee.trainer.model_parallelism.**find_good_batch_size** (train_loader, tp_ensemble_model)

dicee.trainer.model_parallelism.**forward_backward_update_loss** (z: Tuple, ensemble_model)
→ float

class dicee.trainer.model_parallelism.**TensorParallel** (args, callbacks)

Bases: *dicee.abstracts.AbstractTrainer*

Abstract class for Trainer class for knowledge graph embedding models

Parameter

args

[str] ?

callbacks: list

?

fit (*args, **kwargs)

Train model

dicee.trainer.torch_trainer

Classes

<i>TorchTrainer</i>	TorchTrainer for using single GPU or multi CPUs on a single node
---------------------	--

Module Contents

class `dicee.trainer.torch_trainer.TorchTrainer` (*args*, *callbacks*)

Bases: `dicee.abstracts.AbstractTrainer`

TorchTrainer for using single GPU or multi CPUs on a single node

Arguments

`callbacks`: list of Abstract callback instances

`loss_function` = None

`optimizer` = None

`model` = None

`train_dataloaders` = None

`training_step` = None

`process`

`fit` (**args*, *train_dataloaders*, ***kwargs*) → None

Training starts

Arguments

kwargs:Tuple

empty dictionary

Return type

batch loss (float)

forward_backward_update (*x_batch: torch.Tensor*, *y_batch: torch.Tensor*) → torch.Tensor

Compute forward, loss, backward, and parameter update

Arguments

Return type

batch loss (float)

extract_input_outputs_set_device (*batch: list*) → Tuple

Construct inputs and outputs from a batch of inputs with outputs From a batch of inputs and put

Arguments

Return type

(tuple) mini-batch on select device

dicee.trainer.torch_trainer_ddp

Classes

<code>TorchDDPTrainer</code>	A Trainer based on torch.nn.parallel.DistributedDataParallel
<code>NodeTrainer</code>	

Functions

<code>make_iterable_verbose</code> (\rightarrow Iterable)
--

Module Contents

`dicee.trainer.torch_trainer_ddp.make_iterable_verbose` (*iterable_object*, *verbose*,
desc='Default', *position*=None, *leave*=True) \rightarrow Iterable

class `dicee.trainer.torch_trainer_ddp.TorchDDPTrainer` (*args*, *callbacks*)

Bases: `dicee.abstracts.AbstractTrainer`

A Trainer based on torch.nn.parallel.DistributedDataParallel

Arguments

entity_idx
mapping.

relation_idx
mapping.

form
?

store
?

label_smoothing_rate
Using hard targets (0,1) drives weights to infinity. An outlier produces enormous gradients.

Return type
torch.utils.data.Dataset

fit (**args*, ***kwargs*)
Train model

class `dicee.trainer.torch_trainer_ddp.NodeTrainer` (*trainer*, *model*: torch.nn.Module,
train_dataset_loader: torch.utils.data.DataLoader, *callbacks*, *num_epochs*: int)

trainer

local_rank

global_rank

```

optimizer

train_dataset_loader

loss_func

callbacks

model

num_epochs

loss_history = []

ctx

scaler

extract_input_outputs(z: list)

train()
    Training loop for DDP

```

Classes

<i>DICE_Trainer</i>	DICE_Trainer implement
---------------------	------------------------

Package Contents

```
class dicee.trainer.DICE_Trainer(args, is_continual_training: bool, storage_path, evaluator=None)
```

DICE_Trainer implement

- 1- Pytorch Lightning trainer (<https://pytorch-lightning.readthedocs.io/en/stable/common/trainer.html>)
- 2- Multi-GPU Trainer(<https://pytorch.org/docs/stable/generated/torch.nn.parallel.DistributedDataParallel.html>)
- 3- CPU Trainer

args

is_continual_training:bool

storage_path:str

evaluator:

report:dict

report

args

trainer = None

is_continual_training

storage_path

evaluator = None

form_of_labelling = None

continual_start (*knowledge_graph*)

- (1) Initialize training.
- (2) Load model
- (3) Load trainer (3) Fit model

Parameter

returns

- *model*
- **form_of_labelling** (*str*)

initialize_trainer (*callbacks: List*)

→ *lightning.Trainer* | *dicke.trainer.model_parallelism.TensorParallel* | *dicke.trainer.torch_trainer.TorchTrainer* | *dicke.t*

Initialize Trainer from input arguments

initialize_or_load_model ()

init_dataloader (*dataset: torch.utils.data.Dataset*) → *torch.utils.data.DataLoader*

init_dataset () → *torch.utils.data.Dataset*

start (*knowledge_graph: dicke.knowledge_graph.KG* | *numpy.memmap*)

→ *Tuple[dicke.models.base_model.BaseKGE, str]*

Start the training

- (1) Initialize Trainer
- (2) Initialize or load a pretrained KGE model

in DDP setup, we need to load the memory map of already read/index KG.

k_fold_cross_validation (*dataset*) → *Tuple[dicke.models.base_model.BaseKGE, str]*

Perform K-fold Cross-Validation

1. Obtain K train and test splits.
2. **For each split,**
 - 2.1 initialize trainer and model
 - 2.2. Train model with configuration provided in args.
 - 2.3. Compute the mean reciprocal rank (MRR) score of the model on the test respective split.
3. Report the mean and average MRR .

Parameters

- **self**
- **dataset**

Returns

model

14.2 Attributes

`__version__`

14.3 Classes

<i>Pyke</i>	A Physical Embedding Model for Knowledge Graphs
<i>DistMult</i>	Embedding Entities and Relations for Learning and Inference in Knowledge Bases
<i>CKeci</i>	Without learning dimension scaling
<i>Keci</i>	Base class for all neural network modules.
<i>TransE</i>	Translating Embeddings for Modeling
<i>DeCaL</i>	Base class for all neural network modules.
<i>DualE</i>	Dual Quaternion Knowledge Graph Embeddings (https://ojs.aaai.org/index.php/AAAI/article/download/16850/16657)
<i>ComplEx</i>	Base class for all neural network modules.
<i>AConEx</i>	Additive Convolutional ComplEx Knowledge Graph Embeddings
<i>AConvO</i>	Additive Convolutional Octonion Knowledge Graph Embeddings
<i>AConvQ</i>	Additive Convolutional Quaternion Knowledge Graph Embeddings
<i>ConvQ</i>	Convolutional Quaternion Knowledge Graph Embeddings
<i>ConvO</i>	Base class for all neural network modules.
<i>ConEx</i>	Convolutional ComplEx Knowledge Graph Embeddings
<i>QMult</i>	Base class for all neural network modules.
<i>OMult</i>	Base class for all neural network modules.
<i>Shallom</i>	A shallow neural model for relation prediction (https://arxiv.org/abs/2101.09090)
<i>LFMult</i>	Embedding with polynomial functions. We represent all entities and relations in the polynomial space as:
<i>PykeenKGE</i>	A class for using knowledge graph embedding models implemented in Pykeen
<i>Byte</i>	Base class for all neural network modules.
<i>BaseKGE</i>	Base class for all neural network modules.
<i>EnsembleKGE</i>	
<i>DICE_Trainer</i>	DICE_Trainer implement
<i>KGE</i>	Knowledge Graph Embedding Class for interactive usage of pre-trained models
<i>Execute</i>	A class for Training, Retraining and Evaluation a model.
<i>BPE_NegativeSamplingDataset</i>	An abstract class representing a Dataset.
<i>MultiLabelDataset</i>	An abstract class representing a Dataset.
<i>MultiClassClassificationDataset</i>	Dataset for the 1vsALL training strategy
<i>OnevsAllDataset</i>	Dataset for the 1vsALL training strategy
<i>KvsAll</i>	Creates a dataset for KvsAll training by inheriting from torch.utils.data.Dataset.
<i>AllvsAll</i>	Creates a dataset for AllvsAll training by inheriting from torch.utils.data.Dataset.
<i>OnevsSample</i>	A custom PyTorch Dataset class for knowledge graph embeddings, which includes
<i>KvsSampleDataset</i>	KvsSample a Dataset:
<i>NegSampleDataset</i>	An abstract class representing a Dataset.
<i>TriplePredictionDataset</i>	Triple Dataset

continues on next page

Table 3 – continued from previous page

<i>CVDataModule</i>	Create a Dataset for cross validation
<i>LiteralDataset</i>	Dataset for loading and processing literal data for training Literal Embedding model.
<i>QueryGenerator</i>	

14.4 Functions

<i>create_recipriocal_triples</i> (x)	Add inverse triples into dask dataframe
<i>get_er_vocab</i> (data[, file_path])	
<i>get_re_vocab</i> (data[, file_path])	
<i>get_ee_vocab</i> (data[, file_path])	
<i>timeit</i> (func)	
<i>save_pickle</i> (*[, data, file_path])	
<i>load_pickle</i> ([file_path])	
<i>load_term_mapping</i> ([file_path])	
<i>select_model</i> (args[, is_continual_training, storage_path])	
<i>load_model</i> (→ Tuple[object, Tuple[dict, dict]])	Load weights and initialize pytorch module from namespace arguments
<i>load_model_ensemble</i> (...)	Construct Ensemble Of weights and initialize pytorch module from namespace arguments
<i>save_numpy_ndarray</i> (*[, data, file_path])	
<i>numpy_data_type_changer</i> (→ numpy.ndarray)	Detect most efficient data type for a given triples
<i>save_checkpoint_model</i> (→ None)	Store Pytorch model into disk
<i>store</i> (→ None)	
<i>add_noisy_triples</i> (→ pandas.DataFrame)	Add randomly constructed triples
<i>read_or_load_kg</i> (args, cls)	
<i>intialize_model</i> (→ Tuple[object, str])	
<i>load_json</i> (→ dict)	
<i>save_embeddings</i> (→ None)	Save it as CSV if memory allows.
<i>random_prediction</i> (pre_trained_kge)	
<i>deploy_triple_prediction</i> (pre_trained_kge, str_subject, ...)	
<i>deploy_tail_entity_prediction</i> (pre_trained_kge, ...)	

continues on next page

Table 4 – continued from previous page

<code>deploy_head_entity_prediction(pre_trained_kge,</code>	
<code>...)</code>	
<code>deploy_relation_prediction(pre_trained_kge,</code>	
<code>...)</code>	
<code>vocab_to_parquet(vocab_to_idx, name, ...)</code>	
<code>create_experiment_folder([folder_name])</code>	
<code>continual_training_setup_executor(→ None)</code>	
<code>exponential_function(→ torch.FloatTensor)</code>	
<code>load_numpy(→ numpy.ndarray)</code>	
<code>evaluate(entity_to_idx, scores, easy_answers, # @TODO: CD: Renamed this function</code>	
<code>hard_answers)</code>	
<code>download_file(url[, destination_folder])</code>	
<code>download_files_from_url(→ None)</code>	
<code>download_pretrained_model(→ str)</code>	
<code>write_csv_from_model_parallel(path)</code>	Create
<code>from_pretrained_model_write_embeddings_into</code>	
<code>None)</code>	
<code>mapping_from_first_two_cols_to_third(train_se</code>	
<code>timeit(func)</code>	
<code>load_term_mapping([file_path])</code>	
<code>reload_dataset(path, form_of_labelling, ...)</code>	Reload the files from disk to construct the Pytorch dataset
<code>construct_dataset(→ torch.utils.data.Dataset)</code>	

14.5 Package Contents

class `dicee.Pyke` (*args*)

Bases: `dicee.models.base_model.BaseKGE`

A Physical Embedding Model for Knowledge Graphs

name = 'Pyke'

dist_func

margin = 1.0

forward_triples (*x*: `torch.LongTensor`)

Parameters

x

```
class dicee.DistMult (args)
    Bases: dicee.models.base_model.BaseKGE

    Embedding Entities and Relations for Learning and Inference in Knowledge Bases https://arxiv.org/abs/1412.6575

    name = 'DistMult'

    k_vs_all_score (emb_h: torch.FloatTensor, emb_r: torch.FloatTensor, emb_E: torch.FloatTensor)

        Parameters
            • emb_h
            • emb_r
            • emb_E

    forward_k_vs_all (x: torch.LongTensor)

    forward_k_vs_sample (x: torch.LongTensor, target_entity_idx: torch.LongTensor)

    score (h, r, t)
```

```
class dicee.CKeci (args)
    Bases: Keci

    Without learning dimension scaling

    name = 'CKeci'

    requires_grad_for_interactions = False
```

```
class dicee.Keci (args)
    Bases: dicee.models.base_model.BaseKGE

    Base class for all neural network modules.

    Your models should also subclass this class.
```

Modules can also contain other Modules, allowing them to be nested in a tree structure. You can assign the sub-modules as regular attributes:

```
import torch.nn as nn
import torch.nn.functional as F

class Model(nn.Module):
    def __init__(self) -> None:
        super().__init__()
        self.conv1 = nn.Conv2d(1, 20, 5)
        self.conv2 = nn.Conv2d(20, 20, 5)

    def forward(self, x):
        x = F.relu(self.conv1(x))
        return F.relu(self.conv2(x))
```

Submodules assigned in this way will be registered, and will also have their parameters converted when you call `to()`, etc.

Note

As per the example above, an `__init__()` call to the parent class must be made before assignment on the child.

Variables

`training (bool)` – Boolean represents whether this module is in training or evaluation mode.

`name = 'Keci'`

`p`

`q`

`r`

`requires_grad_for_interactions = True`

`compute_sigma_pp (hp, rp)`

Compute $\sigma_{pp} = \sum_{i=1}^{p-1} \sum_{k=i+1}^p (h_i r_k - h_k r_i) e_i e_k$

σ_{pp} captures the interactions between along p bases For instance, let $p = e_1, e_2, e_3$, we compute interactions between $e_1 e_2, e_1 e_3$, and $e_2 e_3$ This can be implemented with a nested two for loops

`results = []` for i in `range(p - 1)`:

for k in `range(i + 1, p)`:

`results.append(hp[:, :, i] * rp[:, :, k] - hp[:, :, k] * rp[:, :, i])`

`sigma_pp = torch.stack(results, dim=2)` assert `sigma_pp.shape == (b, r, int((p * (p - 1)) / 2))`

Yet, this computation would be quite inefficient. Instead, we compute interactions along all p , e.g., $e_1 e_1, e_1 e_2, e_1 e_3$,

$e_2 e_1, e_2 e_2, e_2 e_3, e_3 e_1, e_3 e_2, e_3 e_3$

Then select the triangular matrix without diagonals: $e_1 e_2, e_1 e_3, e_2 e_3$.

`compute_sigma_qq (hq, rq)`

Compute $\sigma_{qq} = \sum_{j=1}^{q-1} \sum_{k=j+1}^q (h_j r_k - h_k r_j) e_j e_k$ σ_{qq} captures the interactions between along q bases For instance, let $q = e_1, e_2, e_3$, we compute interactions between $e_1 e_2, e_1 e_3$, and $e_2 e_3$ This can be implemented with a nested two for loops

`results = []` for j in `range(q - 1)`:

for k in `range(j + 1, q)`:

`results.append(hq[:, :, j] * rq[:, :, k] - hq[:, :, k] * rq[:, :, j])`

`sigma_qq = torch.stack(results, dim=2)` assert `sigma_qq.shape == (b, r, int((q * (q - 1)) / 2))`

Yet, this computation would be quite inefficient. Instead, we compute interactions along all p , e.g., $e_1 e_1, e_1 e_2, e_1 e_3$,

$e_2 e_1, e_2 e_2, e_2 e_3, e_3 e_1, e_3 e_2, e_3 e_3$

Then select the triangular matrix without diagonals: $e_1 e_2, e_1 e_3, e_2 e_3$.

`compute_sigma_pq (*, hp, hq, rp, rq)`

$\sum_{i=1}^p \sum_{j=p+1}^{p+q} (h_i r_j - h_j r_i) e_i e_j$

`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
    
$$h = h_0 + \sum_{i=1}^p h_i e_i + \sum_{j=p+1}^{p+q} h_j e_j$$


$$r = r_0 + \sum_{i=1}^p r_i e_i + \sum_{j=p+1}^{p+q} r_j e_j$$


$$e_i^2 = +1 \text{ for } i \leq p, e_j^2 = -1 \text{ for } p < j \leq p+q, e_i e_j = -e_j e_i \text{ for } i \neq j$$


$$h r = \sigma_0 + \sigma_p + \sigma_q + \sigma_{pp} + \sigma_{qq} + \sigma_{pq}$$

    where
    (1)  $\sigma_0 = h_0 r_0 + \sum_{i=1}^p (h_i r_i) e_i - \sum_{j=p+1}^{p+q} (h_j r_j) e_j$ 
    (2)  $\sigma_p = \sum_{i=1}^p (h_i r_0 + h_0 r_i) e_i$ 
    (3)  $\sigma_q = \sum_{j=p+1}^{p+q} (h_0 r_j + h_j r_0) e_j$ 
    (4)  $\sigma_{pp} = \sum_{i=1}^{p-1} \sum_{k=i+1}^p (h_i r_k - h_k r_i) e_i e_k$ 
    (5)  $\sigma_{qq} = \sum_{j=1}^{q-1} \sum_{k=j+1}^{p+q} (h_j r_k - h_k r_j) e_j e_k$ 
    (6)  $\sigma_{pq} = \sum_{i=1}^p \sum_{j=p+1}^{p+q} (h_i r_j - h_j r_i) e_i e_j$ 
construct_cl_multivector (x: torch.FloatTensor, r: int, p: int, q: int)
    → tuple[torch.FloatTensor, torch.FloatTensor, torch.FloatTensor]
    Construct a batch of multivectors  $Cl_{\{p,q\}}(\mathbb{R}^d)$ 

```

Parameter

x: torch.FloatTensor with (n,d) shape

returns

- **a0** (torch.FloatTensor with (n,r) shape)
- **ap** (torch.FloatTensor with (n,r,p) shape)
- **aq** (torch.FloatTensor with (n,r,q) shape)

```

forward_k_vs_with_explicit (x: torch.Tensor)
k_vs_all_score (bpe_head_ent_emb, bpe_rel_ent_emb, E)
forward_k_vs_all (x: torch.Tensor) → torch.FloatTensor
    Kvsall training

```

- (1) Retrieve real-valued embedding vectors for heads and relations \mathbb{R}^d .
- (2) Construct head entity and relation embeddings according to $Cl_{\{p,q\}}(\mathbb{R}^d)$.
- (3) Perform CL multiplication
- (4) Inner product of (3) and all entity embeddings

forward_k_vs_with_explicit and this functions are identical **Parameter** ——— x: torch.LongTensor with (n,2) shape :rtype: torch.FloatTensor with (n, **IEI**) shape

construct_batch_selected_cl_multivector (*x: torch.FloatTensor, r: int, p: int, q: int*)
 → tuple[torch.FloatTensor, torch.FloatTensor, torch.FloatTensor]

Construct a batch of batchs multivectors $CL_{\{p,q\}}(\mathbb{R}^d)$

Parameter

x: torch.FloatTensor with (n,k, d) shape

returns

- **a0** (*torch.FloatTensor with (n,k, m) shape*)
- **ap** (*torch.FloatTensor with (n,k, m, p) shape*)
- **aq** (*torch.FloatTensor with (n,k, m, q) shape*)

forward_k_vs_sample (*x: torch.LongTensor, target_entity_idx: torch.LongTensor*) → torch.FloatTensor

Parameter

x: torch.LongTensor with (n,2) shape

target_entity_idx: torch.LongTensor with (n, k) shape k denotes the selected number of examples.

rtype

torch.FloatTensor with (n, k) shape

score (*h, r, t*)

forward_triples (*x: torch.Tensor*) → torch.FloatTensor

Parameter

x: torch.LongTensor with (n,3) shape

rtype

torch.FloatTensor with (n) shape

class `dicee.TransE` (*args*)

Bases: `dicee.models.base_model.BaseKGE`

Translating Embeddings for Modeling Multi-relational Data <https://proceedings.neurips.cc/paper/2013/file/1cecc7a77928ca8133fa24680a88d2f9-Paper.pdf>

name = 'TransE'

margin = 4

score (*head_ent_emb, rel_ent_emb, tail_ent_emb*)

forward_k_vs_all (*x: torch.Tensor*) → torch.FloatTensor

class `dicee.DeCaL` (*args*)

Bases: `dicee.models.base_model.BaseKGE`

Base class for all neural network modules.

Your models should also subclass this class.

Modules can also contain other Modules, allowing them to be nested in a tree structure. You can assign the sub-modules as regular attributes:

```

import torch.nn as nn
import torch.nn.functional as F

class Model(nn.Module):
    def __init__(self) -> None:
        super().__init__()
        self.conv1 = nn.Conv2d(1, 20, 5)
        self.conv2 = nn.Conv2d(20, 20, 5)

    def forward(self, x):
        x = F.relu(self.conv1(x))
        return F.relu(self.conv2(x))

```

Submodules assigned in this way will be registered, and will also have their parameters converted when you call `to()`, etc.

Note

As per the example above, an `__init__()` call to the parent class must be made before assignment on the child.

Variables

training (*bool*) – Boolean represents whether this module is in training or evaluation mode.

name = 'DeCaL'

entity_embeddings

relation_embeddings

p

q

r

re

forward_triples (*x: torch.Tensor*) \rightarrow torch.FloatTensor

Parameter

x: torch.LongTensor with (n,) shape

rtype

torch.FloatTensor with (n) shape

cl_pqr (*a: torch.tensor*) \rightarrow torch.tensor

Input: tensor(batch_size, emb_dim) \rightarrow output: tensor with 1+p+q+r components with size (batch_size, emb_dim/(1+p+q+r)) each.

1) takes a tensor of size (batch_size, emb_dim), split it into 1 + p + q + r components, hence 1+p+q+r must be a divisor of the emb_dim. 2) Return a list of the 1+p+q+r components vectors, each are tensors of size (batch_size, emb_dim/(1+p+q+r))

compute_sigmas_single (*list_h_emb, list_r_emb, list_t_emb*)

here we compute all the sums with no others vectors interaction taken with the scalar product with t, that is,

$$s0 = h_0 r_0 t_0 s1 = \sum_{i=1}^p h_i r_i t_0 s2 = \sum_{j=p+1}^{p+q} h_j r_j t_0 s3 = \sum_{i=1}^q (h_0 r_i t_i + h_i r_0 t_i) s4 = \sum_{i=p+1}^{p+q} (h_0 r_i t_i + h_i r_0 t_i) s5 = \sum_{i=p+q+1}^{p+q+r} (h_0 r_i t_i + h_i r_0 t_i)$$

and return:

$$sigma_0 t = \sigma_0 \cdot t_0 = s0 + s1 - s2 s3, s4 \text{ and } s5$$

compute_sigmas_multivect (*list_h_emb, list_r_emb*)

Here we compute and return all the sums with vectors interaction for the same and different bases.

For same bases vectors interaction we have

$$\sigma_p p = \sum_{i=1}^{p-1} \sum_{i'=i+1}^p (h_i r_{i'} - h_{i'} r_i) (\text{model the interactions between } e_i \text{ and } e_{i'} \text{ for } 1 \leq i, i' \leq p) \sigma_q q = \sum_{j=p+1}^{p+q-1} \sum_{j'=j+1}^{p+q} (h_j r_{j'} - h_{j'} r_j)$$

For different base vector interactions, we have

$$\sigma_p q = \sum_{i=1}^p \sum_{j=p+1}^{p+q} (h_i r_j - h_j r_i) (\text{interactions between } e_i \text{ and } e_j \text{ for } 1 \leq i \leq p \text{ and } p+1 \leq j \leq p+q) \sigma_p r = \sum_{i=1}^p \sum_{r=p+q+1}^{p+q+r} (h_i r_r - h_r r_i)$$

forward_k_vs_all (*x: torch.Tensor*) → torch.FloatTensor

Kvsall training

- (1) Retrieve real-valued embedding vectors for heads and relations
- (2) Construct head entity and relation embeddings according to $Cl_{\{p,q,r\}}(\mathbb{R}^d)$.
- (3) Perform Cl multiplication
- (4) Inner product of (3) and all entity embeddings

forward_k_vs_with_explicit and this functions are identical Parameter ——— x: torch.LongTensor with (n,) shape :rtype: torch.FloatTensor with (n, **IE**) shape

apply_coefficients (*h0, hp, hq, hk, r0, rp, rq, rk*)

Multiplying a base vector with its scalar coefficient

construct_cl_multivector (*x: torch.FloatTensor, re: int, p: int, q: int, r: int*)
→ tuple[torch.FloatTensor, torch.FloatTensor, torch.FloatTensor]

Construct a batch of multivectors $Cl_{\{p,q,r\}}(\mathbb{R}^d)$

Parameter

x: torch.FloatTensor with (n,d) shape

returns

- **a0** (*torch.FloatTensor*)
- **ap** (*torch.FloatTensor*)
- **aq** (*torch.FloatTensor*)
- **ar** (*torch.FloatTensor*)

compute_sigma_pp (*hp, rp*)

Compute .. math:

$$\sigma_{p,p}^* = \sum_{i=1}^{p-1} \sum_{i'=i+1}^p (x_{i'} y_i - x_i y_{i'})$$

σ_{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

$$\sigma_{q,q}^* = \sum_{j=p+1}^{p+q-1} \sum_{j'=j+1}^{p+q} (x_j y_{j'} - x_{j'} y_j) Eq.16$$

σ_{qq} captures the interactions between along q bases For instance, let q e_1, e_2, e_3, we compute interactions between e_1 e_2, e_1 e_3, and e_2 e_3 This can be implemented with a nested two for loops

results = [] for j in range(q - 1):

for k in range(j + 1, q):

 results.append(hq[:, :, j] * rq[:, :, k] - hq[:, :, k] * rq[:, :, j])

sigma_qq = torch.stack(results, dim=2) assert sigma_qq.shape == (b, r, int((q * (q - 1)) / 2))

Yet, this computation would be quite inefficient. Instead, we compute interactions along all p , e.g., e1e1, e1e2, e1e3,

e2e1, e2e2, e2e3, e3e1, e3e2, e3e3

Then select the triangular matrix without diagonals: e1e2, e1e3, e2e3.

compute_sigma_rr (*hk, rk*)

$$\sigma_{r,r}^* = \sum_{k=p+q+1}^{p+q+r-1} \sum_{k'=k+1}^p (x_k y_{k'} - x_{k'} y_k)$$

compute_sigma_pq (*, *hp, hq, rp, rq*)

Compute

$$\sum_{i=1}^p \sum_{j=p+1}^{p+q} (h_i r_j - h_j r_i) e_i e_j$$

results = [] sigma_pq = torch.zeros(b, r, p, q) for i in range(p):

for j in range(q):

 sigma_pq[:, :, i, j] = hp[:, :, i] * rq[:, :, j] - hq[:, :, j] * rp[:, :, i]

```

print(sigma_pq.shape)
compute_sigma_pr (*, hp, hk, rp, rk)
    Compute

```

$$\sum_{i=1}^p \sum_{j=p+1}^{p+q} (h_i r_j - h_j r_i) e_i e_j$$

```

results = []
sigma_pq = torch.zeros(b, r, p, q)
for i in range(p):
    for j in range(q):
        sigma_pq[:, :, i, j] = hp[:, :, i] * rq[:, :, j] - hq[:, :, j] * rp[:, :, i]
print(sigma_pq.shape)
compute_sigma_qr (*, hq, hk, rq, rk)

```

$$\sum_{i=1}^p \sum_{j=p+1}^{p+q} (h_i r_j - h_j r_i) e_i e_j$$

```

results = []
sigma_pq = torch.zeros(b, r, p, q)
for i in range(p):
    for j in range(q):
        sigma_pq[:, :, i, j] = hp[:, :, i] * rq[:, :, j] - hq[:, :, j] * rp[:, :, i]
print(sigma_pq.shape)

class dicee.DualE (args)
    Bases: dicee.models.base_model.BaseKGE

    Dual Quaternion Knowledge Graph Embeddings (https://ojs.aaai.org/index.php/AAAI/article/download/16850/16657)

    name = 'DualE'

    entity_embeddings

    relation_embeddings

    num_ent = None

    kvsall_score (e_1_h, e_2_h, e_3_h, e_4_h, e_5_h, e_6_h, e_7_h, e_8_h, e_1_t, e_2_t, e_3_t, e_4_t,
        e_5_t, e_6_t, e_7_t, e_8_t, r_1, r_2, r_3, r_4, r_5, r_6, r_7, r_8) → torch.tensor
        KvsAll scoring function

```

Input

x: torch.LongTensor with (n,) shape

Output

torch.FloatTensor with (n) shape

forward_triples (idx_triple: torch.tensor) → torch.tensor

Negative Sampling forward pass:

Input

x: torch.LongTensor with (n,) shape

Output

torch.FloatTensor with (n) shape

forward_k_vs_all(x)

KvsAll forward pass

Input

x: torch.LongTensor with (n,) shape

Output

torch.FloatTensor with (n) shape

T(x: torch.tensor) → torch.tensor

Transpose function

Input: Tensor with shape (nxm) Output: Tensor with shape (mxn)

class dicee.**Complex**(args)

Bases: *dicee.models.base_model.BaseKGE*

Base class for all neural network modules.

Your models should also subclass this class.

Modules can also contain other Modules, allowing them to be nested in a tree structure. You can assign the sub-modules as regular attributes:

```
import torch.nn as nn
import torch.nn.functional as F

class Model(nn.Module):
    def __init__(self) -> None:
        super().__init__()
        self.conv1 = nn.Conv2d(1, 20, 5)
        self.conv2 = nn.Conv2d(20, 20, 5)

    def forward(self, x):
        x = F.relu(self.conv1(x))
        return F.relu(self.conv2(x))
```

Submodules assigned in this way will be registered, and will also have their parameters converted when you call `to()`, etc.

Note

As per the example above, an `__init__()` call to the parent class must be made before assignment on the child.

Variables

training (bool) – Boolean represents whether this module is in training or evaluation mode.

```

name = 'Complex'

static score(head_ent_emb: torch.FloatTensor, rel_ent_emb: torch.FloatTensor,
            tail_ent_emb: torch.FloatTensor)

static k_vs_all_score(emb_h: torch.FloatTensor, emb_r: torch.FloatTensor,
                    emb_E: torch.FloatTensor)

    Parameters
        • emb_h
        • emb_r
        • emb_E

forward_k_vs_all(x: torch.LongTensor) → torch.FloatTensor

forward_k_vs_sample(x: torch.LongTensor, target_entity_idx: torch.LongTensor)

class dicee.AConEx(args)
    Bases: dicee.models.base_model.BaseKGE
    Additive Convolutional ComplEx Knowledge Graph Embeddings
    name = 'AConEx'

    conv2d

    fc_num_input

    fc1

    norm_fc1

    bn_conv2d

    feature_map_dropout

    residual_convolution(C_1: Tuple[torch.Tensor, torch.Tensor],
                        C_2: Tuple[torch.Tensor, torch.Tensor]) → torch.FloatTensor
        Compute residual score of two complex-valued embeddings. :param C_1: a tuple of two pytorch tensors
        that corresponds complex-valued embeddings :param C_2: a tuple of two pytorch tensors that corresponds
        complex-valued embeddings :return:

    forward_k_vs_all(x: torch.Tensor) → torch.FloatTensor

    forward_triples(x: torch.Tensor) → torch.FloatTensor

    Parameters
        x

    forward_k_vs_sample(x: torch.Tensor, target_entity_idx: torch.Tensor)

class dicee.AConvO(args: dict)
    Bases: dicee.models.base_model.BaseKGE
    Additive Convolutional Octonion Knowledge Graph Embeddings
    name = 'AConvO'

    conv2d

```

```

    fc_num_input

    fc1

    bn_conv2d

    norm_fc1

    feature_map_dropout

    static octonion_normalizer(emb_rel_e0, emb_rel_e1, emb_rel_e2, emb_rel_e3, emb_rel_e4,
                               emb_rel_e5, emb_rel_e6, emb_rel_e7)

    residual_convolution(O_1, O_2)

    forward_triples(x: torch.Tensor) → torch.Tensor

    Parameters
        x

    forward_k_vs_all(x: torch.Tensor)
        Given a head entity and a relation (h,r), we compute scores for all entities. [score(h,r,x)|x in Entities] =>
        [0.0,0.1,...,0.8], shape=> (1, Entities) Given a batch of head entities and relations => shape (size of batch,|
        Entities)
class dicee.AConvQ(args)
    Bases: dicee.models.base_model.BaseKGE
    Additive Convolutional Quaternion Knowledge Graph Embeddings
    name = 'AConvQ'
    entity_embeddings
    relation_embeddings
    conv2d
    fc_num_input
    fc1
    bn_conv1
    bn_conv2
    feature_map_dropout
    residual_convolution(Q_1, Q_2)
    forward_triples(indexed_triple: torch.Tensor) → torch.Tensor

    Parameters
        x

    forward_k_vs_all(x: torch.Tensor)
        Given a head entity and a relation (h,r), we compute scores for all entities. [score(h,r,x)|x in Entities] =>
        [0.0,0.1,...,0.8], shape=> (1, Entities) Given a batch of head entities and relations => shape (size of batch,|
        Entities)

```

```

class dicee.ConvQ(args)
    Bases: dicee.models.base_model.BaseKGE
    Convolutional Quaternion Knowledge Graph Embeddings
    name = 'ConvQ'
    entity_embeddings
    relation_embeddings
    conv2d
    fc_num_input
    fc1
    bn_conv1
    bn_conv2
    feature_map_dropout
    residual_convolution(Q_1, Q_2)
    forward_triples(indexed_triple: torch.Tensor) → torch.Tensor

```

Parameters

x

forward_k_vs_all (*x*: torch.Tensor)

Given a head entity and a relation (h,r), we compute scores for all entities. [score(h,r,x)|x in Entities] => [0.0,0.1,...,0.8], shape=> (1, **Entities**) Given a batch of head entities and relations => shape (size of batch, l Entities)

```

class dicee.ConvO(args: dict)

```

Bases: *dicee.models.base_model.BaseKGE*

Base class for all neural network modules.

Your models should also subclass this class.

Modules can also contain other Modules, allowing them to be nested in a tree structure. You can assign the sub-modules as regular attributes:

```

import torch.nn as nn
import torch.nn.functional as F

class Model(nn.Module):
    def __init__(self) -> None:
        super().__init__()
        self.conv1 = nn.Conv2d(1, 20, 5)
        self.conv2 = nn.Conv2d(20, 20, 5)

    def forward(self, x):
        x = F.relu(self.conv1(x))
        return F.relu(self.conv2(x))

```

Submodules assigned in this way will be registered, and will also have their parameters converted when you call `to()`, etc.

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 `dicce.ConEx` (*args*)

Bases: `dicce.models.base_model.BaseKGE`

Convolutional ComplEx Knowledge Graph Embeddings

name = 'ConEx'

conv2d

fc_num_input

fc1

norm_fc1

bn_conv2d

feature_map_dropout

```
residual_convolution (C_1: Tuple[torch.Tensor, torch.Tensor],
                       C_2: Tuple[torch.Tensor, torch.Tensor]) → torch.FloatTensor
```

Compute residual score of two complex-valued embeddings. :param C_1: a tuple of two pytorch tensors that corresponds complex-valued embeddings :param C_2: a tuple of two pytorch tensors that corresponds complex-valued embeddings :return:

```
forward_k_vs_all (x: torch.Tensor) → torch.FloatTensor
```

```
forward_triples (x: torch.Tensor) → torch.FloatTensor
```

Parameters

x

```
forward_k_vs_sample (x: torch.Tensor, target_entity_idx: torch.Tensor)
```

```
class dicee.QMult (args)
```

Bases: `dicee.models.base_model.BaseKGE`

Base class for all neural network modules.

Your models should also subclass this class.

Modules can also contain other Modules, allowing them to be nested in a tree structure. You can assign the sub-modules as regular attributes:

```
import torch.nn as nn
import torch.nn.functional as F

class Model (nn.Module):
    def __init__(self) -> None:
        super ().__init__()
        self.conv1 = nn.Conv2d(1, 20, 5)
        self.conv2 = nn.Conv2d(20, 20, 5)

    def forward(self, x):
        x = F.relu(self.conv1(x))
        return F.relu(self.conv2(x))
```

Submodules assigned in this way will be registered, and will also have their parameters converted when you call `to()`, etc.

Note

As per the example above, an `__init__()` call to the parent class must be made before assignment on the child.

Variables

training (*bool*) – Boolean represents whether this module is in training or evaluation mode.

```
name = 'QMult'
```

```
explicit = True
```

```
quaternion_multiplication_followed_by_inner_product (h, r, t)
```

Parameters

- **h** – shape: (**batch_dims*, dim) The head representations.
- **r** – shape: (**batch_dims*, dim) The head representations.
- **t** – shape: (**batch_dims*, dim) The tail representations.

Returns

Triple scores.

static quaternion_normalizer (*x*: torch.FloatTensor) → torch.FloatTensor

Normalize the length of relation vectors, if the forward constraint has not been applied yet.

Absolute value of a quaternion

$$|a + bi + cj + dk| = \sqrt{a^2 + b^2 + c^2 + d^2}$$

L2 norm of quaternion vector:

$$\|x\|^2 = \sum_{i=1}^d |x_i|^2 = \sum_{i=1}^d (x_i.re^2 + x_i.im_1^2 + x_i.im_2^2 + x_i.im_3^2)$$

Parameters

x – The vector.

Returns

The normalized vector.

score (*head_ent_emb*: torch.FloatTensor, *rel_ent_emb*: torch.FloatTensor, *tail_ent_emb*: torch.FloatTensor)

k_vs_all_score (*bpe_head_ent_emb*, *bpe_rel_ent_emb*, *E*)

Parameters

- **bpe_head_ent_emb**
- **bpe_rel_ent_emb**
- **E**

forward_k_vs_all (*x*)

Parameters

x

forward_k_vs_sample (*x*, *target_entity_idx*)

Completed. Given a head entity and a relation (h,r), we compute scores for all possible triples,i.e., [score(h,r,x)|x in Entities] => [0.0,0.1,...,0.8], shape=> (1, **Entities**) Given a batch of head entities and relations => shape (size of batch,| Entities|)

class dicee.OMult (*args*)

Bases: *dicee.models.base_model.BaseKGE*

Base class for all neural network modules.

Your models should also subclass this class.

Modules can also contain other Modules, allowing them to be nested in a tree structure. You can assign the sub-modules as regular attributes:

```

import torch.nn as nn
import torch.nn.functional as F

class Model(nn.Module):
    def __init__(self) -> None:
        super().__init__()
        self.conv1 = nn.Conv2d(1, 20, 5)
        self.conv2 = nn.Conv2d(20, 20, 5)

    def forward(self, x):
        x = F.relu(self.conv1(x))
        return F.relu(self.conv2(x))

```

Submodules assigned in this way will be registered, and will also have their parameters converted when you call `to()`, etc.

Note

As per the example above, an `__init__()` call to the parent class must be made before assignment on the child.

Variables

training (*bool*) – Boolean represents whether this module is in training or evaluation mode.

name = 'OMult'

static octonion_normalizer (*emb_rel_e0, emb_rel_e1, emb_rel_e2, emb_rel_e3, emb_rel_e4, emb_rel_e5, emb_rel_e6, emb_rel_e7*)

score (*head_ent_emb: torch.FloatTensor, rel_ent_emb: torch.FloatTensor, tail_ent_emb: torch.FloatTensor*)

k_vs_all_score (*bpe_head_ent_emb, bpe_rel_ent_emb, E*)

forward_k_vs_all (*x*)

Completed. Given a head entity and a relation (h,r), we compute scores for all possible triples, i.e., $[score(h,r,x) | x \text{ in Entities}] \Rightarrow [0.0, 0.1, \dots, 0.8]$, shape $\Rightarrow (1, |\text{Entities}|)$ Given a batch of head entities and relations \Rightarrow shape (size of batch, |Entities|)

class `dicee.Shallom` (*args*)

Bases: `dicee.models.base_model.BaseKGE`

A shallow neural model for relation prediction (<https://arxiv.org/abs/2101.09090>)

name = 'Shallom'

shallom

get_embeddings () \rightarrow Tuple[numpy.ndarray, None]

forward_k_vs_all (*x*) \rightarrow torch.FloatTensor

forward_triples (*x*) \rightarrow torch.FloatTensor

Parameters

x

Returns

class `dictee.LFMult` (*args*)

Bases: `dictee.models.base_model.BaseKGE`

Embedding with polynomial functions. We represent all entities and relations in the polynomial space as: $f(x) = \sum_{i=0}^{d-1} a_i x^i$ and use the three differents scoring function as in the paper to evaluate the score. We also consider combining with Neural Networks.

name = 'LFMult'

entity_embeddings

relation_embeddings

degree

m

x_values

forward_triples (*idx_triple*)

Parameters

x

construct_multi_coeff (*x*)

poly_NN (*x, coefh, coefr, coeft*)

Constructing a 2 layers NN to represent the embeddings. $h = \sigma(wh^T x + bh)$, $r = \sigma(wr^T x + br)$, $t = \sigma(wt^T x + bt)$

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:

$\text{score}(h,r,t) = \int_0^1 h(x)r(x)t(x) dx = \sum_{i,j,k=0}^{d-1} \text{dfrac}\{a_i*b_j*c_k\} \{1+(i+j+k)\%d\}$

1. generate the range for i,j and k from [0 d-1]
2. perform $\text{dfrac}\{a_i*b_j*c_k\} \{1+(i+j+k)\%d\}$ in parallel for every batch
3. take the sum over each batch

vtp_score (*h, r, t*)

this part implement the vector triple product scoring techniques:

$\text{score}(h,r,t) = \int_0^1 h(x)r(x)t(x) dx = \sum_{i,j,k=0}^{d-1} \text{dfrac}\{a_i*c_j*b_k - b_i*c_j*a_k\} \{(1+(i+j)\%d)(1+k)\}$

1. generate the range for i,j and k from [0 d-1]
2. Compute the first and second terms of the sum
3. Multiply with then denominator and take the sum
4. take the sum over each batch

comp_func (*h, r, t*)

this part implement the function composition scoring techniques: i.e. $\text{score} = \langle \text{hor}, \text{t} \rangle$

polynomial (*coeff, x, degree*)

This function takes a matrix tensor of coefficients (*coeff*), a tensor vector of points *x* and range of integer $[0, 1, \dots, d]$ and return a vector tensor ($\text{coeff}[0][0] + \text{coeff}[0][1]x + \dots + \text{coeff}[0][d]x^d$,

$\text{coeff}[1][0] + \text{coeff}[1][1]x + \dots + \text{coeff}[1][d]x^d$)

pop (*coeff, x, degree*)

This function allow us to evaluate the composition of two polynomes without for loops :) it takes a matrix tensor of coefficients (*coeff*), a matrix tensor of points *x* and range of integer $[0, 1, \dots, d]$

and return a tensor ($\text{coeff}[0][0] + \text{coeff}[0][1]x + \dots + \text{coeff}[0][d]x^d$,

$\text{coeff}[1][0] + \text{coeff}[1][1]x + \dots + \text{coeff}[1][d]x^d$)

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.ByteE(*args, **kwargs)

```

Bases: `dicee.models.base_model.BaseKGE`

Base class for all neural network modules.

Your models should also subclass this class.

Modules can also contain other Modules, allowing them to be nested in a tree structure. You can assign the sub-modules as regular attributes:

```

import torch.nn as nn
import torch.nn.functional as F

class Model(nn.Module):
    def __init__(self) -> None:
        super() .__init__()
        self.conv1 = nn.Conv2d(1, 20, 5)
        self.conv2 = nn.Conv2d(20, 20, 5)

    def forward(self, x):
        x = F.relu(self.conv1(x))
        return F.relu(self.conv2(x))

```

Submodules assigned in this way will be registered, and will also have their parameters converted when you call `to()`, etc.

Note

As per the example above, an `__init__()` call to the parent class must be made before assignment on the child.

Variables

training (*bool*) – Boolean represents whether this module is in training or evaluation mode.

name = 'ByteE'

config

temperature = 0.5

topk = 2

transformer

lm_head

loss_function(*yhat_batch*, *y_batch*)

Parameters

- **yhat_batch**
- **y_batch**

forward(*x*: *torch.LongTensor*)

Parameters

x (*B by T tensor*)

generate(*idx*, *max_new_tokens*, *temperature=1.0*, *top_k=None*)

Take a conditioning sequence of indices *idx* (LongTensor of shape (b,t)) and complete the sequence *max_new_tokens* times, feeding the predictions back into the model each time. Most likely you'll want to make sure to be in `model.eval()` mode of operation for this.

training_step(*batch*, *batch_idx=None*)

Here you compute and return the training loss and some additional metrics for e.g. the progress bar or logger.

Parameters

- **batch** – The output of your data iterable, normally a `DataLoader`.
- **batch_idx** – The index of this batch.
- **dataloader_idx** – The index of the dataloader that produced this batch. (only if multiple dataloaders used)

Returns

- **Tensor** - The loss tensor
- **dict** - A dictionary which can include any keys, but must include the key 'loss' in the case of automatic optimization.
- **None** - In automatic optimization, this will skip to the next batch (but is not supported for multi-GPU, TPU, or DeepSpeed). For manual optimization, this has no special meaning, as returning the loss is not required.

In this step you'd normally do the forward pass and calculate the loss for a batch. You can also do fancier things like multiple forward passes or something model specific.

Example:

```
def training_step(self, batch, batch_idx):
    x, y, z = batch
    out = self.encoder(x)
    loss = self.loss(out, x)
    return loss
```

To use multiple optimizers, you can switch to 'manual optimization' and control their stepping:

```
def __init__(self):
    super().__init__()
    self.automatic_optimization = False
```

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```
# Multiple optimizers (e.g.: GANs)
def training_step(self, batch, batch_idx):
    opt1, opt2 = self.optimizers()

    # do training_step with encoder
    ...
    opt1.step()
    # do training_step with decoder
    ...
    opt2.step()
```

Note

When `accumulate_grad_batches > 1`, the loss returned here will be automatically normalized by `accumulate_grad_batches` internally.

```
class dicee.BaseKGE (args: dict)
```

Bases: 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:

```
import torch.nn as nn
import torch.nn.functional as F

class Model(nn.Module):
    def __init__(self) -> None:
        super().__init__()
        self.conv1 = nn.Conv2d(1, 20, 5)
        self.conv2 = nn.Conv2d(20, 20, 5)

    def forward(self, x):
        x = F.relu(self.conv1(x))
        return F.relu(self.conv2(x))
```

Submodules assigned in this way will be registered, and will also have their parameters converted when you call `to()`, etc.

Note

As per the example above, an `__init__()` call to the parent class must be made before assignment on the child.

Variables

training (*bool*) – Boolean represents whether this module is in training or evaluation mode.

args

```

embedding_dim = None

num_entities = None

num_relations = None

num_tokens = None

learning_rate = None

apply_unit_norm = None

input_dropout_rate = None

hidden_dropout_rate = None

optimizer_name = None

feature_map_dropout_rate = None

kernel_size = None

num_of_output_channels = None

weight_decay = None

loss

selected_optimizer = None

normalizer_class = None

normalize_head_entity_embeddings

normalize_relation_embeddings

normalize_tail_entity_embeddings

hidden_normalizer

param_init

input_dp_ent_real

input_dp_rel_real

hidden_dropout

loss_history = []

byte_pair_encoding

max_length_subword_tokens

block_size

forward_byte_pair_encoded_k_vs_all (x: torch.LongTensor)

```

Parameters

$\mathbf{x} (B \times 2 \times T)$


```

forward_byte_pair_encoded_triple (x: Tuple[torch.LongTensor, torch.LongTensor])
    byte pair encoded neural link predictors

    Parameters
    -----

init_params_with_sanity_checking()

forward (x: torch.LongTensor | Tuple[torch.LongTensor, torch.LongTensor],
         y_idx: torch.LongTensor = None)

    Parameters
    • x
    • y_idx
    • ordered_bpe_entities

forward_triples (x: torch.LongTensor) → torch.Tensor

    Parameters
    • x

forward_k_vs_all (*args, **kwargs)

forward_k_vs_sample (*args, **kwargs)

get_triple_representation (idx_hrt)

get_head_relation_representation (indexed_triple)

get_sentence_representation (x: torch.LongTensor)

    Parameters
    • (b (x shape)
    • 3
    • t)

get_bpe_head_and_relation_representation (x: torch.LongTensor)
    → Tuple[torch.FloatTensor, torch.FloatTensor]

    Parameters
    • x (B x 2 x T)

get_embeddings () → Tuple[numpy.ndarray, numpy.ndarray]

class dicee.EnsembleKGE (seed_model=None, pretrained_models: List = None)

    name

    train_mode = True

    named_children()

    property example_input_array

    parameters()

    modules()

```

```

__iter__()
__len__()
eval()
to(device)
mem_of_model()
__call__(x_batch)
step()
get_embeddings()
__str__()

dicee.create_recipriocal_triples(x)
    Add inverse triples into dask dataframe :param x: :return:
dicee.get_er_vocab(data, file_path: str = None)
dicee.get_re_vocab(data, file_path: str = None)
dicee.get_ee_vocab(data, file_path: str = None)
dicee.timeit(func)
dicee.save_pickle(*, data: object = None, file_path=str)
dicee.load_pickle(file_path=str)
dicee.load_term_mapping(file_path=str)
dicee.select_model(args: dict, is_continual_training: bool = None, storage_path: str = None)
dicee.load_model(path_of_experiment_folder: str, model_name='model.pt', verbose=0)
    → Tuple[object, Tuple[dict, dict]]
    Load weights and initialize pytorch module from namespace arguments
dicee.load_model_ensemble(path_of_experiment_folder: str)
    → Tuple[dicee.models.base_model.BaseKGE, Tuple[pandas.DataFrame, pandas.DataFrame]]
    Construct Ensemble Of weights and initialize pytorch module from namespace arguments
    (1) Detect models under given path
    (2) Accumulate parameters of detected models
    (3) Normalize parameters
    (4) Insert (3) into model.
dicee.save_numpy_ndarray(*, data: numpy.ndarray, file_path: str)
dicee.numpy_data_type_changer(train_set: numpy.ndarray, num: int) → numpy.ndarray
    Detect most efficient data type for a given triples :param train_set: :param num: :return:
dicee.save_checkpoint_model(model, path: str) → None
    Store Pytorch model into disk

```

```

dicee.store(trained_model, model_name: str = 'model', full_storage_path: str = None,
            save_embeddings_as_csv=False) → None

dicee.add_noisy_triples(train_set: pandas.DataFrame, add_noise_rate: float) → pandas.DataFrame
    Add randomly constructed triples :param train_set: :param add_noise_rate: :return:

dicee.read_or_load_kg(args, cls)

dicee.intialize_model(args: dict, verbose=0) → Tuple[object, str]

dicee.load_json(p: str) → dict

dicee.save_embeddings(embeddings: numpy.ndarray, indexes, path: str) → None
    Save it as CSV if memory allows. :param embeddings: :param indexes: :param path: :return:

dicee.random_prediction(pre_trained_kge)

dicee.deploy_triple_prediction(pre_trained_kge, str_subject, str_predicate, str_object)

dicee.deploy_tail_entity_prediction(pre_trained_kge, str_subject, str_predicate, top_k)

dicee.deploy_head_entity_prediction(pre_trained_kge, str_object, str_predicate, top_k)

dicee.deploy_relation_prediction(pre_trained_kge, str_subject, str_object, top_k)

dicee.vocab_to_parquet(vocab_to_idx, name, path_for_serialization, print_into)

dicee.create_experiment_folder(folder_name='Experiments')

dicee.continual_training_setup_executor(executor) → None

dicee.exponential_function(x: numpy.ndarray, lam: float, ascending_order=True) → torch.FloatTensor

dicee.load_numpy(path) → numpy.ndarray

dicee.evaluate(entity_to_idx, scores, easy_answers, hard_answers)
    # @TODO: CD: Renamed this function Evaluate multi hop query answering on different query types

dicee.download_file(url, destination_folder='.')

dicee.download_files_from_url(base_url: str, destination_folder='.') → None

```

Parameters

- **base_url** (e.g. ["https://files.dice-research.org/projects/DiceEmbeddings/KINSHIP-Keci-dim128-epoch256-KvsAll"](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.trainer.cpu_trainer.CPUTrainer](#)

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.

$\text{argmax}_{\{r \in R\}} f(h,r,t)$, where $h, t \in E$.

Parameter

head_entity: List[str]

String representation of selected entities.

tail_entity: List[str]

String representation of selected entities.

k: int

Highest ranked k entities.

Returns: Tuple

Highest K scores and entities

predict_missing_tail_entity (*head_entity: List[str] | str, relation: List[str] | str, within: List[str] = None, batch_size=2, topk=1, return_indices=False*) → torch.FloatTensor

Given a head entity and a relation, return top k ranked entities

$\text{argmax}_{\{e \in E\}} f(h,r,e)$, where $h \in E$ and $r \in R$.

Parameter

head_entity: List[str]

String representation of selected entities.

tail_entity: List[str]

String representation of selected entities.

Returns: Tuple

scores

predict (*, *h: List[str] | str = None, r: List[str] | str = None, t: List[str] | str = None, within=None, logits=True*) → torch.FloatTensor

Parameters

- **logits**
- **h**
- **r**
- **t**
- **within**

predict_topk (*, h: str | List[str] = None, r: str | List[str] = None, t: str | List[str] = None, topk: int = 10, within: List[str] = None, batch_size: int = 1024)

Predict missing item in a given triple.

Returns

- If you query a single (h, r, ?) or (?, r, t) or (h, ?, t), returns List[(item, score)]
- If you query a batch of B, returns List of B such lists.

triple_score (h: List[str] | str = None, r: List[str] | str = None, t: List[str] | str = None, logits=False)
→ torch.FloatTensor

Predict triple score

Parameter

head_entity: List[str]

String representation of selected entities.

relation: List[str]

String representation of selected relations.

tail_entity: List[str]

String representation of selected entities.

logits: bool

If logits is True, unnormalized score returned

Returns: Tuple

pytorch tensor of triple score

return_multi_hop_query_results (aggregated_query_for_all_entities, k: int, only_scores)

single_hop_query_answering (query: tuple, only_scores: bool = True, k: int = None)

answer_multi_hop_query (query_type: str = None, query: Tuple[str | Tuple[str, str], Ellipsis] = None, queries: List[Tuple[str | Tuple[str, str], Ellipsis]] = None, tnorm: str = 'prod', neg_norm: str = 'standard', lambda_: float = 0.0, k: int = 10, only_scores=False)
→ List[Tuple[str, torch.Tensor]]

@TODO: Refactoring is needed # @TODO: Score computation for each query type should be done in a static function

Find an answer set for EPFO queries including negation and disjunction

Parameter

query_type: str The type of the query, e.g., “2p”.

query: Union[str, Tuple[str, Tuple[str, str]]] The query itself, either a string or a nested tuple.

queries: List of Tuple[Union[str, Tuple[str, str]], ...]

tnorm: str The t-norm operator.

neg_norm: str The negation norm.

lambda_: float lambda parameter for sugeno and yager negation norms

k: int The top-k substitutions for intermediate variables.

returns

- *List[Tuple[str, torch.Tensor]]*
- *Entities and corresponding scores sorted in the descening order of scores*

find_missing_triples (*confidence: float, entities: List[str] = None, relations: List[str] = None, topk: int = 10, at_most: int = sys.maxsize*) → Set

Find missing triples

Iterative over a set of entities E and a set of relation R :

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

class dicee.**Execute** (*args, continuous_training=False*)

A class for Training, Retraining and Evaluation a model.

- (1) Loading & Preprocessing & Serializing input data.
- (2) Training & Validation & Testing
- (3) Storing all necessary info

args

is_continual_training = False

trainer = None

trained_model = None

knowledge_graph = None

report

evaluator = None

start_time = None

setup_executor() → None

save_trained_model() → None

Save a knowledge graph embedding model

- (1) Send model to eval mode and cpu.
- (2) Store the memory footprint of the model.
- (3) Save the model into disk.
- (4) Update the stats of KG again ?

Parameter

rtype

None

end(*form_of_labelling: str*) → dict

End training

- (1) Store trained model.
- (2) Report runtimes.
- (3) Eval model if required.

Parameter

rtype

A dict containing information about the training and/or evaluation

write_report() → None

Report training related information in a report.json file

start() → dict

Start training

(1) Loading the Data # (2) Create an evaluator object. # (3) Create a trainer object. # (4) Start the training

Parameter

rtype

A dict containing information about the training and/or evaluation

```

dicee.mapping_from_first_two_cols_to_third(train_set_idx)

dicee.timeit(func)

dicee.load_term_mapping(file_path=str)

dicee.reload_dataset(path: str, form_of_labelling, scoring_technique, neg_ratio, label_smoothing_rate)
    Reload the files from disk to construct the Pytorch dataset

dicee.construct_dataset(*, train_set: numpy.ndarray | list, valid_set=None, test_set=None,
    ordered_bpe_entities=None, train_target_indices=None, target_dim: int = None, entity_to_idx: dict,
    relation_to_idx: dict, form_of_labelling: str, scoring_technique: str, neg_ratio: int,
    label_smoothing_rate: float, byte_pair_encoding=None, block_size: int = None)
    → torch.utils.data.Dataset

```

```

class dicee.BPE_NegativeSamplingDataset(train_set: torch.LongTensor,
    ordered_shaped_bpe_entities: torch.LongTensor, neg_ratio: int)

```

Bases: torch.utils.data.Dataset

An abstract class representing a Dataset.

All datasets that represent a map from keys to data samples should subclass it. All subclasses should overwrite `__getitem__()`, supporting fetching a data sample for a given key. Subclasses could also optionally overwrite `__len__()`, which is expected to return the size of the dataset by many `Sampler` implementations and the default options of `DataLoader`. Subclasses could also optionally implement `__getitems__()`, for speedup batched samples loading. This method accepts list of indices of samples of batch and returns list of samples.

Note

`DataLoader` by default constructs an index sampler that yields integral indices. To make it work with a map-style dataset with non-integral indices/keys, a custom sampler must be provided.

```

train_set

ordered_bpe_entities

num_bpe_entities

neg_ratio

num_datapoints

__len__()

__getitem__(idx)

collate_fn(batch_shaped_bpe_triples: List[Tuple[torch.Tensor, torch.Tensor]])

```

```

class dicee.MultiLabelDataset(train_set: torch.LongTensor, train_indices_target: torch.LongTensor,
    target_dim: int, torch_ordered_shaped_bpe_entities: torch.LongTensor)

```

Bases: torch.utils.data.Dataset

An abstract class representing a Dataset.

All datasets that represent a map from keys to data samples should subclass it. All subclasses should overwrite `__getitem__()`, supporting fetching a data sample for a given key. Subclasses could also optionally overwrite `__len__()`, which is expected to return the size of the dataset by many `Sampler` implementations and the default

options of `DataLoader`. Subclasses could also optionally implement `__getitem__()`, for speedup batched samples loading. This method accepts list of indices of samples of batch and returns list of samples.

Note

`DataLoader` by default constructs an index sampler that yields integral indices. To make it work with a map-style dataset with non-integral indices/keys, a custom sampler must be provided.

```
train_set
train_indices_target
target_dim
num_datapoints
torch_ordered_shaped_bpe_entities
collate_fn = None
__len__()
__getitem__(idx)
```

```
class dicee.MultiClassClassificationDataset (subword_units: numpy.ndarray, block_size: int = 8)
```

Bases: `torch.utils.data.Dataset`

Dataset for the 1vsALL training strategy

Parameters

- **train_set_idx** – Indexed triples for the training.
- **entity_idxs** – mapping.
- **relation_idxs** – mapping.
- **form** – ?
- **num_workers** – int for <https://pytorch.org/docs/stable/data.html#torch.utils.data.DataLoader>

Return type

`torch.utils.data.Dataset`

```
train_data
block_size = 8
num_of_data_points
collate_fn = None
__len__()
__getitem__(idx)
```

```
class dicee.OnevsAllDataset (train_set_idx: numpy.ndarray, entity_idx)
```

Bases: torch.utils.data.Dataset

Dataset for the 1vsALL training strategy

Parameters

- **train_set_idx** – Indexed triples for the training.
- **entity_idx** – mapping.
- **relation_idx** – mapping.
- **form** – ?
- **num_workers** – int for <https://pytorch.org/docs/stable/data.html#torch.utils.data.DataLoader>

Return type

torch.utils.data.Dataset

train_data

target_dim

collate_fn = None

__len__()

__getitem__(idx)

```
class dicee.KvsAll (train_set_idx: numpy.ndarray, entity_idx, relation_idx, form, store=None,
label_smoothing_rate: float = 0.0)
```

Bases: torch.utils.data.Dataset

Creates a dataset for KvsAll training by inheriting from torch.utils.data.Dataset.

Let D denote a dataset for KvsAll training and be defined as $D := \{(x, y)_i\}_i^N$, where $x: (h, r)$ is a unique tuple of an entity h in E and a relation r in R that has been seed in the input graph. y : denotes a multi-label vector in $[0, 1]^{|E|}$ is a binary label.

orall $y_i = 1$ s.t. $(h \ r \ E_i)$ in KG

Note

TODO

train_set_idx

[numpy.ndarray] n by 3 array representing n triples

entity_idx

[dictionary] string representation of an entity to its integer id

relation_idx

[dictionary] string representation of a relation to its integer id

self : torch.utils.data.Dataset

```
>>> a = KvsAll()
>>> a
? array([0, 1, 2, 3, 4, 5, 6, 7, 8, 9])
```

```

train_data = None

train_target = None

label_smoothing_rate

collate_fn = None

__len__()

__getitem__(idx)

```

```

class dicee.AllvsAll (train_set_idx: numpy.ndarray, entity_idx, relation_idx, label_smoothing_rate=0.0)

```

Bases: torch.utils.data.Dataset

Creates a dataset for AllvsAll training by inheriting from torch.utils.data.Dataset.

Let D denote a dataset for AllvsAll training and be defined as $D := \{(x, y)_i\}_i^N$, where $x: (h, r)$ is a possible unique tuple of an entity h in E and a relation r in R . Hence $N = |E| \times |R|$ y_i denotes a multi-label vector in $[0, 1]^{|E|}$ is a binary label.

orall $y_i = 1$ s.t. $(h, r) \in KG$

Note

AllvsAll extends KvsAll via none existing (h,r). Hence, it adds data points that are labelled without 1s, only with 0s.

```

train_set_idx
    [numpy.ndarray] n by 3 array representing n triples

entity_idx
    [dictionary] string representation of an entity to its integer id

relation_idx
    [dictionary] string representation of a relation to its integer id

self : torch.utils.data.Dataset

```

```

>>> a = AllvsAll()
>>> a
? array([0, 1, 2, 3, 4, 5, 6, 7, 8, 9])

```

```

train_data = None

train_target = None

label_smoothing_rate

collate_fn = None

target_dim

__len__()

__getitem__(idx)

```

```
class dicee.OnevsSample(train_set: numpy.ndarray, num_entities, num_relations,  
                      neg_sample_ratio: int = None, label_smoothing_rate: float = 0.0)
```

Bases: torch.utils.data.Dataset

A custom PyTorch Dataset class for knowledge graph embeddings, which includes both positive and negative sampling for a given dataset for multi-class classification problem..

Parameters

- **train_set** (*np.ndarray*) – A numpy array containing triples of knowledge graph data. Each triple consists of (head_entity, relation, tail_entity).
- **num_entities** (*int*) – The number of unique entities in the knowledge graph.
- **num_relations** (*int*) – The number of unique relations in the knowledge graph.
- **neg_sample_ratio** (*int, optional*) – The number of negative samples to be generated per positive sample. Must be a positive integer and less than num_entities.
- **label_smoothing_rate** (*float, optional*) – A label smoothing rate to apply to the positive and negative labels. Defaults to 0.0.

train_data

The input data converted into a PyTorch tensor.

Type

torch.Tensor

num_entities

Number of entities in the dataset.

Type

int

num_relations

Number of relations in the dataset.

Type

int

neg_sample_ratio

Ratio of negative samples to be drawn for each positive sample.

Type

int

label_smoothing_rate

The smoothing factor applied to the labels.

Type

torch.Tensor

collate_fn

A function that can be used to collate data samples into batches (set to None by default).

Type

function, optional

train_data

num_entities

`num_relations`

`neg_sample_ratio = None`

`label_smoothing_rate`

`collate_fn = None`

`__len__()`

Returns the number of samples in the dataset.

`__getitem__(idx)`

Retrieves a single data sample from the dataset at the given index.

Parameters

`idx` (*int*) – The index of the sample to retrieve.

Returns

A tuple consisting of:

- `x` (`torch.Tensor`): The head and relation part of the triple.
- `y_idx` (`torch.Tensor`): The concatenated indices of the true object (tail entity) and the indices of the negative samples.
- `y_vec` (`torch.Tensor`): A vector containing the labels for the positive and negative samples, with label smoothing applied.

Return type

tuple

```
class dicee.KvsSampleDataset (train_set_idx: numpy.ndarray, entity_idxxs, relation_idxxs, form,
                             store=None, neg_ratio=None, label_smoothing_rate: float = 0.0)
```

Bases: `torch.utils.data.Dataset`

KvsSample a Dataset:

$D := \{(x, y)_i\}_i^N$, where

. $x: (h, r)$ is a unique h in E and a relation r in R and . y in $[0, 1]^{|E|}$ is a binary label.

forall $y_i = 1$ s.t. $(h \ r \ E_i)$ in KG

At each mini-batch construction, we subsample(y), hence n

$|new_y| \ll |E|$ new_y contains all 1's if $\sum(y) < neg_sample\ ratio$ new_y contains

`train_set_idx`

Indexed triples for the training.

`entity_idxxs`

mapping.

`relation_idxxs`

mapping.

`form`

?

`store`

?

`label_smoothing_rate`

?

`torch.utils.data.Dataset`

```
train_data = None

train_target = None

neg_ratio = None

num_entities

label_smoothing_rate

collate_fn = None

max_num_of_classes

__len__()

__getitem__(idx)
```

```
class dicee.NegSampleDataset (train_set: numpy.ndarray, num_entities: int, num_relations: int,
                             neg_sample_ratio: int = 1)
```

Bases: `torch.utils.data.Dataset`

An abstract class representing a `Dataset`.

All datasets that represent a map from keys to data samples should subclass it. All subclasses should overwrite `__getitem__()`, supporting fetching a data sample for a given key. Subclasses could also optionally overwrite `__len__()`, which is expected to return the size of the dataset by many `Sampler` implementations and the default options of `DataLoader`. Subclasses could also optionally implement `__getitems__()`, for speedup batched samples loading. This method accepts list of indices of samples of batch and returns list of samples.

Note

`DataLoader` by default constructs an index sampler that yields integral indices. To make it work with a map-style dataset with non-integral indices/keys, a custom sampler must be provided.

```
neg_sample_ratio

train_set

length

num_entities

num_relations

__len__()

__getitem__(idx)
```

```
class dicee.TriplePredictionDataset (train_set: numpy.ndarray, num_entities: int, num_relations: int,
                                     neg_sample_ratio: int = 1, label_smoothing_rate: float = 0.0)
```

Bases: `torch.utils.data.Dataset`

Triple Dataset

D:= {(x)_i}_i ^N, where

. x:(h,r, t) in KG is a unique h in E and a relation r in R and . collect_fn => Generates negative triples

collect_fn:

orall (h,r,t) in G obtain, create negative triples{(h,r,x),(r,t),(h,m,t)}

y:labels are represented in torch.float16

train_set_idx

Indexed triples for the training.

entity_idxxs

mapping.

relation_idxxs

mapping.

form

?

store

?

label_smoothing_rate

collate_fn: batch:List[torch.IntTensor] Returns —— torch.utils.data.Dataset

label_smoothing_rate

neg_sample_ratio

train_set

length

num_entities

num_relations

__len__()

__getitem__(idx)

collate_fn(batch: List[torch.Tensor])

class dicee.CVDDataModule (train_set_idx: numpy.ndarray, num_entities, num_relations, neg_sample_ratio, batch_size, num_workers)

Bases: pytorch_lightning.LightningDataModule

Create a Dataset for cross validation

Parameters

- **train_set_idx** – Indexed triples for the training.
- **num_entities** – entity to index mapping.
- **num_relations** – relation to index mapping.
- **batch_size** – int
- **form** – ?

- `num_workers` – int for <https://pytorch.org/docs/stable/data.html#torch.utils.data.DataLoader>

Return type

?

`train_set_idx`

`num_entities`

`num_relations`

`neg_sample_ratio`

`batch_size`

`num_workers`

`train_dataloader()` → `torch.utils.data.DataLoader`

An iterable or collection of iterables specifying training samples.

For more information about multiple dataloaders, see this section.

The dataloader you return will not be reloaded unless you set **:param-ref:~pytorch_lightning.trainer.trainer.Trainer.reload_dataloaders_every_n_epochs** to a positive integer.

For data processing use the following pattern:

- download in `prepare_data()`
- process and split in `setup()`

However, the above are only necessary for distributed processing.

Warning

do not assign state in `prepare_data`

- `fit()`
- `prepare_data()`
- `setup()`

Note

Lightning tries to add the correct sampler for distributed and arbitrary hardware. There is no need to set it yourself.

`setup(*args, **kwargs)`

Called at the beginning of fit (train + validate), validate, test, or predict. This is a good hook when you need to build models dynamically or adjust something about them. This hook is called on every process when using DDP.

Parameters

stage – either 'fit', 'validate', 'test', or 'predict'

Example:

```
class LitModel(...):
    def __init__(self):
        self.l1 = None

    def prepare_data(self):
        download_data()
        tokenize()

        # don't do this
        self.something = else

    def setup(self, stage):
        data = load_data(...)
        self.l1 = nn.Linear(28, data.num_classes)
```

transfer_batch_to_device(*args, **kwargs)

Override this hook if your `DataLoader` returns tensors wrapped in a custom data structure.

The data types listed below (and any arbitrary nesting of them) are supported out of the box:

- `torch.Tensor` or anything that implements `.to(...)`
- `list`
- `dict`
- `tuple`

For anything else, you need to define how the data is moved to the target device (CPU, GPU, TPU, ...).

Note

This hook should only transfer the data and not modify it, nor should it move the data to any other device than the one passed in as argument (unless you know what you are doing). To check the current state of execution of this hook you can use `self.trainer.training/testing/validating/predicting` so that you can add different logic as per your requirement.

Parameters

- **batch** – A batch of data that needs to be transferred to a new device.
- **device** – The target device as defined in PyTorch.
- **dataloader_idx** – The index of the dataloader to which the batch belongs.

Returns

A reference to the data on the new device.

Example:

```
def transfer_batch_to_device(self, batch, device, dataloader_idx):
    if isinstance(batch, CustomBatch):
        # move all tensors in your custom data structure to the device
        batch.samples = batch.samples.to(device)
        batch.targets = batch.targets.to(device)
```

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```
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
```

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```
# call on GLOBAL_RANK=0 (great for shared file systems)
class LitDataModule(LightningDataModule):
    def __init__(self):
        super().__init__()
        self.prepare_data_per_node = False
```

This is called before requesting the dataloaders:

```
model.prepare_data()
initialize_distributed()
model.setup(stage)
model.train_dataloader()
model.val_dataloader()
model.test_dataloader()
model.predict_dataloader()
```

```
class dicee.LiteralDataset (file_path: str, ent_idx: dict = None, normalization_type: str = 'z-norm',
                           sampling_ratio: float = None, loader_backend: str = 'pandas')
```

Bases: torch.utils.data.Dataset

Dataset for loading and processing literal data for training Literal Embedding model. This dataset handles the loading, normalization, and preparation of triples for training a literal embedding model.

Extends torch.utils.data.Dataset for supporting PyTorch dataloaders.

train_file_path

Path to the training data file.

Type

str

normalization

Type of normalization to apply ('z-norm', 'min-max', or None).

Type

str

normalization_params

Parameters used for normalization.

Type

dict

sampling_ratio

Fraction of the training set to use for ablations.

Type

float

entity_to_idx

Mapping of entities to their indices.

Type

dict

num_entities

Total number of entities.

Type
int

data_property_to_idx
Mapping of data properties to their indices.

Type
dict

num_data_properties
Total number of data properties.

Type
int

loader_backend
Backend to use for loading data ('pandas' or 'rdflib').

Type
str

train_file_path

loader_backend = 'pandas'

normalization_type = 'z-norm'

normalization_params

sampling_ratio = None

entity_to_idx = None

num_entities

__getitem__ (*index*)

__len__ ()

static load_and_validate_literal_data (*file_path: str = None, loader_backend: str = 'pandas'*)
→ pandas.DataFrame

Loads and validates the literal data file. :param file_path: Path to the literal data file. :type file_path: str

Returns
DataFrame containing the loaded and validated data.

Return type
pd.DataFrame

static denormalize (*preds_norm, attributes, normalization_params*) → numpy.ndarray

Denormalizes the predictions based on the normalization type.

Args: preds_norm (np.ndarray): Normalized predictions to be denormalized. attributes (list): List of attributes corresponding to the predictions. normalization_params (dict): Dictionary containing normalization parameters for each attribute.

Returns
Denormalized predictions.

Return type
np.ndarray

```

class dicee.QueryGenerator (train_path: str, val_path: str, test_path: str, ent2id: Dict = None,
                             rel2id: Dict = None, seed: int = 1, gen_valid: bool = False, gen_test: bool = True)

    train_path

    val_path

    test_path

    gen_valid = False

    gen_test = True

    seed = 1

    max_ans_num = 1000000.0

    mode

    ent2id = None

    rel2id: Dict = None

    ent_in: Dict

    ent_out: Dict

    query_name_to_struct

    list2tuple (list_data)

    tuple2list (x: List | Tuple) → List | Tuple
        Convert a nested tuple to a nested list.

    set_global_seed (seed: int)
        Set seed

    construct_graph (paths: List[str]) → Tuple[Dict, Dict]
        Construct graph from triples Returns dicts with incoming and outgoing edges

    fill_query (query_structure: List[str | List], ent_in: Dict, ent_out: Dict, answer: int) → bool
        Private method for fill_query logic.

    achieve_answer (query: List[str | List], ent_in: Dict, ent_out: Dict) → set
        Private method for achieve_answer logic. @TODO: Document the code

    write_links (ent_out, small_ent_out)

    ground_queries (query_structure: List[str | List], ent_in: Dict, ent_out: Dict, small_ent_in: Dict,
                    small_ent_out: Dict, gen_num: int, query_name: str)
        Generating queries and achieving answers

    unmap (query_type, queries, tp_answers, fp_answers, fn_answers)

    unmap_query (query_structure, query, id2ent, id2rel)

    generate_queries (query_struct: List, gen_num: int, query_type: str)
        Passing incoming and outgoing edges to ground queries depending on mode [train valid or text] and getting
        queries and answers in return @ TODO: create a class for each single query struct

```

```

save_queries (query_type: str, gen_num: int, save_path: str)

abstract load_queries (path)

get_queries (query_type: str, gen_num: int)

static save_queries_and_answers (path: str, data: List[Tuple[str, Tuple[collections.defaultdict]]])
    → None
    Save Queries into Disk

static load_queries_and_answers (path: str) → List[Tuple[str, Tuple[collections.defaultdict]]]
    Load Queries from Disk to Memory

dicee.__version__ = '0.1.5'

```


Python Module Index

d

- `dicee`, 12
- `dicee.__main__`, 12
- `dicee.abstracts`, 12
- `dicee.analyse_experiments`, 19
- `dicee.callbacks`, 20
- `dicee.config`, 28
- `dicee.dataset_classes`, 31
- `dicee.eval_static_funcs`, 45
- `dicee.evaluator`, 47
- `dicee.executer`, 48
- `dicee.knowledge_graph`, 50
- `dicee.knowledge_graph_embeddings`, 51
- `dicee.models`, 55
 - `adopt`, 55
 - `base_model`, 56
 - `clifford`, 65
 - `complex`, 72
 - `dualE`, 75
 - `ensemble`, 76
 - `function_space`, 77
 - `literal`, 80
 - `octonion`, 82
 - `pykeen_models`, 85
 - `quaternion`, 86
 - `real`, 89
 - `static_funcs`, 90
 - `transformers`, 91
- `dicee.query_generator`, 144
- `dicee.read_preprocess_save_load_kg`, 146
 - `read_preprocess_save_load_kg.preprocess`, 146
 - `read_preprocess_save_load_kg.read_from_disk`, 147
 - `read_preprocess_save_load_kg.save_load_disk`, 147
 - `read_preprocess_save_load_kg.util`, 148
- `dicee.sanity_checkers`, 152
- `dicee.scripts`, 153
 - `index_serve`, 153
 - `run`, 156
- `dicee.static_funcs`, 156
- `dicee.static_funcs_training`, 159
- `dicee.static_preprocess_funcs`, 160
- `dicee.trainer`, 161
 - `dice_trainer`, 161
 - `model_parallelism`, 163
 - `torch_trainer`, 163
 - `torch_trainer_ddp`, 165

Index

Non-alphabetical

`__call__()` (*dicee.EnsembleKGE method*), 194
`__call__()` (*dicee.models.base_model.IdentityClass method*), 65
`__call__()` (*dicee.models.ensemble.EnsembleKGE method*), 76
`__call__()` (*dicee.models.IdentityClass method*), 108, 119, 125
`__class_vars__` (*dicee.scripts.index_serve.StringListRequest attribute*), 154
`__getitem__()` (*dicee.AllvsAll method*), 205
`__getitem__()` (*dicee.BPE_NegativeSamplingDataset method*), 202
`__getitem__()` (*dicee.dataset_classes.AllvsAll method*), 36
`__getitem__()` (*dicee.dataset_classes.BPE_NegativeSamplingDataset method*), 32
`__getitem__()` (*dicee.dataset_classes.KvsAll method*), 35
`__getitem__()` (*dicee.dataset_classes.KvsSampleDataset method*), 38
`__getitem__()` (*dicee.dataset_classes.LiteralDataset method*), 44
`__getitem__()` (*dicee.dataset_classes.MultiClassClassificationDataset method*), 34
`__getitem__()` (*dicee.dataset_classes.MultiLabelDataset method*), 33
`__getitem__()` (*dicee.dataset_classes.NegSampleDataset method*), 39
`__getitem__()` (*dicee.dataset_classes.OnevsAllDataset method*), 34
`__getitem__()` (*dicee.dataset_classes.OnevsSample method*), 37
`__getitem__()` (*dicee.dataset_classes.TriplePredictionDataset method*), 39
`__getitem__()` (*dicee.KvsAll method*), 205
`__getitem__()` (*dicee.KvsSampleDataset method*), 208
`__getitem__()` (*dicee.LiteralDataset method*), 214
`__getitem__()` (*dicee.MultiClassClassificationDataset method*), 203
`__getitem__()` (*dicee.MultiLabelDataset method*), 203
`__getitem__()` (*dicee.NegSampleDataset method*), 208
`__getitem__()` (*dicee.OnevsAllDataset method*), 204
`__getitem__()` (*dicee.OnevsSample method*), 207
`__getitem__()` (*dicee.TriplePredictionDataset method*), 209
`__iter__()` (*dicee.config.Namespace method*), 31
`__iter__()` (*dicee.EnsembleKGE method*), 193
`__iter__()` (*dicee.knowledge_graph.KG method*), 51
`__iter__()` (*dicee.models.ensemble.EnsembleKGE method*), 76
`__len__()` (*dicee.AllvsAll method*), 205
`__len__()` (*dicee.BPE_NegativeSamplingDataset method*), 202
`__len__()` (*dicee.dataset_classes.AllvsAll method*), 36
`__len__()` (*dicee.dataset_classes.BPE_NegativeSamplingDataset method*), 32
`__len__()` (*dicee.dataset_classes.KvsAll method*), 35
`__len__()` (*dicee.dataset_classes.KvsSampleDataset method*), 38
`__len__()` (*dicee.dataset_classes.LiteralDataset method*), 44
`__len__()` (*dicee.dataset_classes.MultiClassClassificationDataset method*), 34
`__len__()` (*dicee.dataset_classes.MultiLabelDataset method*), 33
`__len__()` (*dicee.dataset_classes.NegSampleDataset method*), 38
`__len__()` (*dicee.dataset_classes.OnevsAllDataset method*), 34
`__len__()` (*dicee.dataset_classes.OnevsSample method*), 37
`__len__()` (*dicee.dataset_classes.TriplePredictionDataset method*), 39
`__len__()` (*dicee.EnsembleKGE method*), 194
`__len__()` (*dicee.knowledge_graph.KG method*), 51
`__len__()` (*dicee.KvsAll method*), 205
`__len__()` (*dicee.KvsSampleDataset method*), 208
`__len__()` (*dicee.LiteralDataset method*), 214
`__len__()` (*dicee.models.ensemble.EnsembleKGE method*), 76
`__len__()` (*dicee.MultiClassClassificationDataset method*), 203
`__len__()` (*dicee.MultiLabelDataset method*), 203
`__len__()` (*dicee.NegSampleDataset method*), 208
`__len__()` (*dicee.OnevsAllDataset method*), 204
`__len__()` (*dicee.OnevsSample method*), 207
`__len__()` (*dicee.TriplePredictionDataset method*), 209
`__private_attributes__` (*dicee.scripts.index_serve.StringListRequest attribute*), 155
`__pydantic_complete__` (*dicee.scripts.index_serve.StringListRequest attribute*), 155
`__pydantic_computed_fields__` (*dicee.scripts.index_serve.StringListRequest attribute*), 155
`__pydantic_core_schema__` (*dicee.scripts.index_serve.StringListRequest attribute*), 155
`__pydantic_custom_init__` (*dicee.scripts.index_serve.StringListRequest attribute*), 155
`__pydantic_decorators__` (*dicee.scripts.index_serve.StringListRequest attribute*), 155
`__pydantic_extra__` (*dicee.scripts.index_serve.StringListRequest attribute*), 155
`__pydantic_fields__` (*dicee.scripts.index_serve.StringListRequest attribute*), 155

- `__pydantic_fields_set__` (*dicee.scripts.index_serve.StringListRequest attribute*), 155
- `__pydantic_generic_metadata__` (*dicee.scripts.index_serve.StringListRequest attribute*), 155
- `__pydantic_parent_namespace__` (*dicee.scripts.index_serve.StringListRequest attribute*), 155
- `__pydantic_post_init__` (*dicee.scripts.index_serve.StringListRequest attribute*), 155
- `__pydantic_private__` (*dicee.scripts.index_serve.StringListRequest attribute*), 155
- `__pydantic_root_model__` (*dicee.scripts.index_serve.StringListRequest attribute*), 155
- `__pydantic_serializer__` (*dicee.scripts.index_serve.StringListRequest attribute*), 155
- `__pydantic_validator__` (*dicee.scripts.index_serve.StringListRequest attribute*), 155
- `__setstate__` () (*dicee.models.ADOPT method*), 99
- `__setstate__` () (*dicee.models.adopt.ADOPT method*), 56
- `__signature__` (*dicee.scripts.index_serve.StringListRequest attribute*), 155
- `__str__` () (*dicee.EnsembleKGE method*), 194
- `__str__` () (*dicee.KGE method*), 197
- `__str__` () (*dicee.knowledge_graph_embeddings.KGE method*), 52
- `__str__` () (*dicee.models.ensemble.EnsembleKGE method*), 76
- `__version__` (*in module dicee*), 216

A

- `AbstractCallback` (*class in dicee.abstracts*), 16
- `AbstractPPECallback` (*class in dicee.abstracts*), 17
- `AbstractTrainer` (*class in dicee.abstracts*), 12
- `AccumulateEpochLossCallback` (*class in dicee.callbacks*), 21
- `achieve_answer` () (*dicee.query_generator.QueryGenerator method*), 145
- `achieve_answer` () (*dicee.QueryGenerator method*), 215
- `AConEx` (*class in dicee*), 180
- `AConEx` (*class in dicee.models*), 114
- `AConEx` (*class in dicee.models.complex*), 73
- `AConvO` (*class in dicee*), 180
- `AConvO` (*class in dicee.models*), 127
- `AConvO` (*class in dicee.models.octonion*), 84
- `AConvQ` (*class in dicee*), 181
- `AConvQ` (*class in dicee.models*), 121
- `AConvQ` (*class in dicee.models.quaternion*), 88
- `adaptive_lr` (*dicee.config.Namespace attribute*), 31
- `adaptive_swa` (*dicee.config.Namespace attribute*), 30
- `add_new_entity_embeddings` () (*dicee.abstracts.BaseInteractiveKGE method*), 15
- `add_noise_rate` (*dicee.config.Namespace attribute*), 29
- `add_noise_rate` (*dicee.knowledge_graph.KG attribute*), 50
- `add_noisy_triples` () (*in module dicee*), 195
- `add_noisy_triples` () (*in module dicee.static_funcs*), 158
- `add_noisy_triples_into_training` () (*dicee.read_preprocess_save_load_kg.read_from_disk.ReadFromDisk method*), 147
- `add_noisy_triples_into_training` () (*dicee.read_preprocess_save_load_kg.ReadFromDisk method*), 152
- `add_reciprocal` (*dicee.knowledge_graph.KG attribute*), 50
- `ADOPT` (*class in dicee.models*), 98
- `ADOPT` (*class in dicee.models.adopt*), 55
- `adopt` () (*in module dicee.models.adopt*), 56
- `AllvsAll` (*class in dicee*), 205
- `AllvsAll` (*class in dicee.dataset_classes*), 35
- `alphas` (*dicee.abstracts.AbstractPPECallback attribute*), 17
- `alphas` (*dicee.callbacks.ASWA attribute*), 24
- `analyse` () (*in module dicee.analyse_experiments*), 20
- `answer_multi_hop_query` () (*dicee.KGE method*), 199
- `answer_multi_hop_query` () (*dicee.knowledge_graph_embeddings.KGE method*), 54
- `app` (*in module dicee.scripts.index_serve*), 154
- `apply_coefficients` () (*dicee.DeCaL method*), 176
- `apply_coefficients` () (*dicee.Keci method*), 173
- `apply_coefficients` () (*dicee.models.clifford.DeCaL method*), 70
- `apply_coefficients` () (*dicee.models.clifford.Keci method*), 67
- `apply_coefficients` () (*dicee.models.DeCaL method*), 133
- `apply_coefficients` () (*dicee.models.Keci method*), 129
- `apply_reciprical_or_noise` () (*in module dicee.read_preprocess_save_load_kg.util*), 150
- `apply_semantic_constraint` (*dicee.abstracts.BaseInteractiveKGE attribute*), 14
- `apply_unit_norm` (*dicee.BaseKGE attribute*), 192
- `apply_unit_norm` (*dicee.models.base_model.BaseKGE attribute*), 63
- `apply_unit_norm` (*dicee.models.BaseKGE attribute*), 105, 109, 112, 117, 123, 135, 139
- `args` (*dicee.BaseKGE attribute*), 191
- `args` (*dicee.DICE_Trainer attribute*), 196

- args (*dicee.evaluator.Evaluator* attribute), 47
- args (*dicee.Execute* attribute), 200
- args (*dicee.executer.Execute* attribute), 48
- args (*dicee.models.base_model.BaseKGE* attribute), 63
- args (*dicee.models.base_model.IdentityClass* attribute), 65
- args (*dicee.models.BaseKGE* attribute), 105, 108, 112, 116, 122, 135, 138
- args (*dicee.models.IdentityClass* attribute), 108, 119, 125
- args (*dicee.models.pykeen_models.PykeenKGE* attribute), 85
- args (*dicee.models.PykeenKGE* attribute), 137
- args (*dicee.PykeenKGE* attribute), 188
- args (*dicee.trainer.DICE_Trainer* attribute), 166
- args (*dicee.trainer.dice_trainer.DICE_Trainer* attribute), 161
- ASWA (*class in dicee.callbacks*), 23
- aswa (*dicee.analyse_experiments.Experiment* attribute), 19
- attn (*dicee.models.transformers.Block* attribute), 96
- attn_dropout (*dicee.models.transformers.CausalSelfAttention* attribute), 94
- attributes (*dicee.abstracts.AbstractTrainer* attribute), 13
- auto_batch_finding (*dicee.config.Namespace* attribute), 31

B

- backend (*dicee.config.Namespace* attribute), 29
- backend (*dicee.knowledge_graph.KG* attribute), 51
- BaseInteractiveKGE (*class in dicee.abstracts*), 14
- BaseInteractiveTrainKGE (*class in dicee.abstracts*), 18
- BaseKGE (*class in dicee*), 191
- BaseKGE (*class in dicee.models*), 104, 108, 111, 116, 122, 134, 138
- BaseKGE (*class in dicee.models.base_model*), 62
- BaseKGELightning (*class in dicee.models*), 99
- BaseKGELightning (*class in dicee.models.base_model*), 56
- batch_kronecker_product () (*dicee.callbacks.KronE* static method), 26
- batch_size (*dicee.analyse_experiments.Experiment* attribute), 19
- batch_size (*dicee.callbacks.PseudoLabellingCallback* attribute), 23
- batch_size (*dicee.config.Namespace* attribute), 29
- batch_size (*dicee.CVDataModule* attribute), 210
- batch_size (*dicee.dataset_classes.CVDataModule* attribute), 40
- batches_per_epoch (*dicee.callbacks.LRScheduler* attribute), 27
- bias (*dicee.models.transformers.GPTConfig* attribute), 96
- bias (*dicee.models.transformers.LayerNorm* attribute), 93
- Block (*class in dicee.models.transformers*), 95
- block_size (*dicee.BaseKGE* attribute), 192
- block_size (*dicee.config.Namespace* attribute), 31
- block_size (*dicee.dataset_classes.MultiClassClassificationDataset* attribute), 33
- block_size (*dicee.models.base_model.BaseKGE* attribute), 63
- block_size (*dicee.models.BaseKGE* attribute), 106, 109, 113, 117, 123, 136, 139
- block_size (*dicee.models.transformers.GPTConfig* attribute), 96
- block_size (*dicee.MultiClassClassificationDataset* attribute), 203
- bn_conv1 (*dicee.AConvQ* attribute), 181
- bn_conv1 (*dicee.ConvQ* attribute), 182
- bn_conv1 (*dicee.models.AConvQ* attribute), 121
- bn_conv1 (*dicee.models.ConvQ* attribute), 121
- bn_conv1 (*dicee.models.quaternion.AConvQ* attribute), 88
- bn_conv1 (*dicee.models.quaternion.ConvQ* attribute), 88
- bn_conv2 (*dicee.AConvQ* attribute), 181
- bn_conv2 (*dicee.ConvQ* attribute), 182
- bn_conv2 (*dicee.models.AConvQ* attribute), 122
- bn_conv2 (*dicee.models.ConvQ* attribute), 121
- bn_conv2 (*dicee.models.quaternion.AConvQ* attribute), 88
- bn_conv2 (*dicee.models.quaternion.ConvQ* attribute), 88
- bn_conv2d (*dicee.AConEx* attribute), 180
- bn_conv2d (*dicee.AConvO* attribute), 181
- bn_conv2d (*dicee.ConEx* attribute), 183
- bn_conv2d (*dicee.ConvO* attribute), 183
- bn_conv2d (*dicee.models.AConEx* attribute), 115
- bn_conv2d (*dicee.models.AConvO* attribute), 127
- bn_conv2d (*dicee.models.complex.AConEx* attribute), 73
- bn_conv2d (*dicee.models.complex.ConEx* attribute), 73
- bn_conv2d (*dicee.models.ConEx* attribute), 114

bn_conv2d (*dicee.models.ConvO attribute*), 127
 bn_conv2d (*dicee.models.octonion.AConvO attribute*), 84
 bn_conv2d (*dicee.models.octonion.ConvO attribute*), 84
 BPE_NegativeSamplingDataset (*class in dicee*), 202
 BPE_NegativeSamplingDataset (*class in dicee.dataset_classes*), 32
 build_chain_funcs () (*dicee.models.FMult2 method*), 142
 build_chain_funcs () (*dicee.models.function_space.FMult2 method*), 78
 build_func () (*dicee.models.FMult2 method*), 142
 build_func () (*dicee.models.function_space.FMult2 method*), 78
 Byte (*class in dicee*), 189
 Byte (*class in dicee.models.transformers*), 91
 byte_pair_encoding (*dicee.analyse_experiments.Experiment attribute*), 19
 byte_pair_encoding (*dicee.BaseKGE attribute*), 192
 byte_pair_encoding (*dicee.config.Namespace attribute*), 30
 byte_pair_encoding (*dicee.knowledge_graph.KG attribute*), 50
 byte_pair_encoding (*dicee.models.base_model.BaseKGE attribute*), 63
 byte_pair_encoding (*dicee.models.BaseKGE attribute*), 106, 109, 113, 117, 123, 136, 139

C

c_attn (*dicee.models.transformers.CausalSelfAttention attribute*), 94
 c_fc (*dicee.models.transformers.MLP attribute*), 95
 c_proj (*dicee.models.transformers.CausalSelfAttention attribute*), 94
 c_proj (*dicee.models.transformers.MLP attribute*), 95
 callbacks (*dicee.abstracts.AbstractTrainer attribute*), 13
 callbacks (*dicee.analyse_experiments.Experiment attribute*), 19
 callbacks (*dicee.config.Namespace attribute*), 29
 callbacks (*dicee.trainer.torch_trainer_ddp.NodeTrainer attribute*), 166
 CausalSelfAttention (*class in dicee.models.transformers*), 93
 chain_func () (*dicee.models.FMult method*), 141
 chain_func () (*dicee.models.function_space.FMult method*), 77
 chain_func () (*dicee.models.function_space.GFMult method*), 78
 chain_func () (*dicee.models.GFMult method*), 141
 CKeci (*class in dicee*), 171
 CKeci (*class in dicee.models*), 131
 CKeci (*class in dicee.models.clifford*), 68
 cl_pqr () (*dicee.DeCaL method*), 175
 cl_pqr () (*dicee.models.clifford.DeCaL method*), 70
 cl_pqr () (*dicee.models.DeCaL method*), 132
 clifford_multiplication () (*dicee.Keci method*), 173
 clifford_multiplication () (*dicee.models.clifford.Keci method*), 67
 clifford_multiplication () (*dicee.models.Keci method*), 129
 clip_lambda (*dicee.models.ADOPT attribute*), 99
 clip_lambda (*dicee.models.adopt.ADOPT attribute*), 56
 collate_fn (*dicee.AllvsAll attribute*), 205
 collate_fn (*dicee.dataset_classes.AllvsAll attribute*), 35
 collate_fn (*dicee.dataset_classes.KvsAll attribute*), 35
 collate_fn (*dicee.dataset_classes.KvsSampleDataset attribute*), 38
 collate_fn (*dicee.dataset_classes.MultiClassClassificationDataset attribute*), 33
 collate_fn (*dicee.dataset_classes.MultiLabelDataset attribute*), 33
 collate_fn (*dicee.dataset_classes.OnevsAllDataset attribute*), 34
 collate_fn (*dicee.dataset_classes.OnevsSample attribute*), 36, 37
 collate_fn (*dicee.KvsAll attribute*), 205
 collate_fn (*dicee.KvsSampleDataset attribute*), 208
 collate_fn (*dicee.MultiClassClassificationDataset attribute*), 203
 collate_fn (*dicee.MultiLabelDataset attribute*), 203
 collate_fn (*dicee.OnevsAllDataset attribute*), 204
 collate_fn (*dicee.OnevsSample attribute*), 206, 207
 collate_fn () (*dicee.BPE_NegativeSamplingDataset method*), 202
 collate_fn () (*dicee.dataset_classes.BPE_NegativeSamplingDataset method*), 32
 collate_fn () (*dicee.dataset_classes.TriplePredictionDataset method*), 39
 collate_fn () (*dicee.TriplePredictionDataset method*), 209
 collection_name (*dicee.scripts.index_serve.NeuralSearcher attribute*), 154
 comp_func () (*dicee.LFMult method*), 187
 comp_func () (*dicee.models.function_space.LFMult method*), 80
 comp_func () (*dicee.models.LFMult method*), 143
 ComplEx (*class in dicee*), 179
 ComplEx (*class in dicee.models*), 115

ComplEx (class in *dicee.models.complex*), 73
 compute_convergence () (in module *dicee.callbacks*), 23
 compute_func () (*dicee.models.FMult* method), 141
 compute_func () (*dicee.models.FMult2* method), 142
 compute_func () (*dicee.models.function_space.FMult* method), 77
 compute_func () (*dicee.models.function_space.FMult2* method), 78
 compute_func () (*dicee.models.function_space.GFMult* method), 78
 compute_func () (*dicee.models.GFMult* method), 141
 compute_mrr () (*dicee.callbacks.ASWA* static method), 24
 compute_sigma_pp () (*dicee.DeCaL* method), 176
 compute_sigma_pp () (*dicee.Keci* method), 172
 compute_sigma_pp () (*dicee.models.clifford.DeCaL* method), 71
 compute_sigma_pp () (*dicee.models.clifford.Keci* method), 66
 compute_sigma_pp () (*dicee.models.DeCaL* method), 133
 compute_sigma_pp () (*dicee.models.Keci* method), 128
 compute_sigma_pq () (*dicee.DeCaL* method), 177
 compute_sigma_pq () (*dicee.Keci* method), 172
 compute_sigma_pq () (*dicee.models.clifford.DeCaL* method), 72
 compute_sigma_pq () (*dicee.models.clifford.Keci* method), 67
 compute_sigma_pq () (*dicee.models.DeCaL* method), 134
 compute_sigma_pq () (*dicee.models.Keci* method), 129
 compute_sigma_pr () (*dicee.DeCaL* method), 178
 compute_sigma_pr () (*dicee.models.clifford.DeCaL* method), 72
 compute_sigma_pr () (*dicee.models.DeCaL* method), 134
 compute_sigma_qq () (*dicee.DeCaL* method), 177
 compute_sigma_qq () (*dicee.Keci* method), 172
 compute_sigma_qq () (*dicee.models.clifford.DeCaL* method), 71
 compute_sigma_qq () (*dicee.models.clifford.Keci* method), 66
 compute_sigma_qq () (*dicee.models.DeCaL* method), 133
 compute_sigma_qq () (*dicee.models.Keci* method), 129
 compute_sigma_qr () (*dicee.DeCaL* method), 178
 compute_sigma_qr () (*dicee.models.clifford.DeCaL* method), 72
 compute_sigma_qr () (*dicee.models.DeCaL* method), 134
 compute_sigma_rr () (*dicee.DeCaL* method), 177
 compute_sigma_rr () (*dicee.models.clifford.DeCaL* method), 71
 compute_sigma_rr () (*dicee.models.DeCaL* method), 134
 compute_sigmas_multivect () (*dicee.DeCaL* method), 176
 compute_sigmas_multivect () (*dicee.models.clifford.DeCaL* method), 70
 compute_sigmas_multivect () (*dicee.models.DeCaL* method), 132
 compute_sigmas_single () (*dicee.DeCaL* method), 175
 compute_sigmas_single () (*dicee.models.clifford.DeCaL* method), 70
 compute_sigmas_single () (*dicee.models.DeCaL* method), 132
 ConEx (class in *dicee*), 183
 ConEx (class in *dicee.models*), 114
 ConEx (class in *dicee.models.complex*), 72
 config (*dicee.BytE* attribute), 189
 config (*dicee.models.transformers.BytE* attribute), 92
 config (*dicee.models.transformers.GPT* attribute), 97
 configs (*dicee.abstracts.BaseInteractiveKGE* attribute), 14
 configure_optimizers () (*dicee.models.base_model.BaseKGELightning* method), 61
 configure_optimizers () (*dicee.models.BaseKGELightning* method), 103
 configure_optimizers () (*dicee.models.transformers.GPT* method), 97
 construct_batch_selected_cl_multivector () (*dicee.Keci* method), 173
 construct_batch_selected_cl_multivector () (*dicee.models.clifford.Keci* method), 68
 construct_batch_selected_cl_multivector () (*dicee.models.Keci* method), 130
 construct_cl_multivector () (*dicee.DeCaL* method), 176
 construct_cl_multivector () (*dicee.Keci* method), 173
 construct_cl_multivector () (*dicee.models.clifford.DeCaL* method), 70
 construct_cl_multivector () (*dicee.models.clifford.Keci* method), 67
 construct_cl_multivector () (*dicee.models.DeCaL* method), 133
 construct_cl_multivector () (*dicee.models.Keci* method), 130
 construct_dataset () (in module *dicee*), 202
 construct_dataset () (in module *dicee.dataset_classes*), 32
 construct_ensemble (*dicee.abstracts.BaseInteractiveKGE* attribute), 14
 construct_graph () (*dicee.query_generator.QueryGenerator* method), 145
 construct_graph () (*dicee.QueryGenerator* method), 215
 construct_input_and_output () (*dicee.abstracts.BaseInteractiveKGE* method), 15
 construct_multi_coeff () (*dicee.LFMult* method), 187

`construct_multi_coeff()` (*dicee.models.function_space.LFMMult method*), 79
`construct_multi_coeff()` (*dicee.models.LFMMult method*), 143
`continual_learning` (*dicee.config.Namespace attribute*), 31
`continual_start()` (*dicee.DICE_Trainer method*), 196
`continual_start()` (*dicee.executor.ContinuousExecute method*), 49
`continual_start()` (*dicee.trainer.DICE_Trainer method*), 166
`continual_start()` (*dicee.trainer.dice_trainer.DICE_Trainer method*), 162
`continual_training_setup_executor()` (*in module dicee*), 195
`continual_training_setup_executor()` (*in module dicee.static_funcs*), 159
`ContinuousExecute` (*class in dicee.executor*), 49
`conv2d` (*dicee.AConEx attribute*), 180
`conv2d` (*dicee.AConvO attribute*), 180
`conv2d` (*dicee.AConvQ attribute*), 181
`conv2d` (*dicee.ConEx attribute*), 183
`conv2d` (*dicee.ConvO attribute*), 183
`conv2d` (*dicee.ConvQ attribute*), 182
`conv2d` (*dicee.models.AConEx attribute*), 114
`conv2d` (*dicee.models.AConvO attribute*), 127
`conv2d` (*dicee.models.AConvQ attribute*), 121
`conv2d` (*dicee.models.complex.AConEx attribute*), 73
`conv2d` (*dicee.models.complex.ConEx attribute*), 72
`conv2d` (*dicee.models.ConEx attribute*), 114
`conv2d` (*dicee.models.ConvO attribute*), 127
`conv2d` (*dicee.models.ConvQ attribute*), 121
`conv2d` (*dicee.models.octonion.AConvO attribute*), 84
`conv2d` (*dicee.models.octonion.ConvO attribute*), 83
`conv2d` (*dicee.models.quaternion.AConvQ attribute*), 88
`conv2d` (*dicee.models.quaternion.ConvQ attribute*), 88
`ConvO` (*class in dicee*), 182
`ConvO` (*class in dicee.models*), 126
`ConvO` (*class in dicee.models.octonion*), 83
`ConvQ` (*class in dicee*), 181
`ConvQ` (*class in dicee.models*), 121
`ConvQ` (*class in dicee.models.quaternion*), 88
`create_constraints()` (*in module dicee.read_preprocess_save_load_kg.util*), 150
`create_constraints()` (*in module dicee.static_preprocess_funcs*), 160
`create_experiment_folder()` (*in module dicee*), 195
`create_experiment_folder()` (*in module dicee.static_funcs*), 159
`create_random_data()` (*dicee.callbacks.PseudoLabellingCallback method*), 23
`create_recipriocal_triples()` (*in module dicee*), 194
`create_recipriocal_triples()` (*in module dicee.read_preprocess_save_load_kg.util*), 151
`create_recipriocal_triples()` (*in module dicee.static_funcs*), 157
`create_vector_database()` (*dicee.KGE method*), 197
`create_vector_database()` (*dicee.knowledge_graph_embeddings.KGE method*), 52
`crop_block_size()` (*dicee.models.transformers.GPT method*), 97
`ctx` (*dicee.trainer.torch_trainer_ddp.NodeTrainer attribute*), 166
`CVDDataModule` (*class in dicee*), 209
`CVDDataModule` (*class in dicee.dataset_classes*), 39
`cycle_length` (*dicee.callbacks.LRScheduler attribute*), 27

D

`data_module` (*dicee.callbacks.PseudoLabellingCallback attribute*), 23
`data_property_embeddings` (*dicee.models.literal.LiteralEmbeddings attribute*), 81
`data_property_to_idx` (*dicee.dataset_classes.LiteralDataset attribute*), 44
`data_property_to_idx` (*dicee.LiteralDataset attribute*), 214
`dataset_dir` (*dicee.config.Namespace attribute*), 28
`dataset_dir` (*dicee.knowledge_graph.KG attribute*), 50
`dataset_sanity_checking()` (*in module dicee.read_preprocess_save_load_kg.util*), 151
`DeCaL` (*class in dicee*), 174
`DeCaL` (*class in dicee.models*), 131
`DeCaL` (*class in dicee.models.clifford*), 69
`decide()` (*dicee.callbacks.ASWA method*), 24
`default_eval_model` (*dicee.callbacks.PeriodicEvalCallback attribute*), 27
`degree` (*dicee.LFMMult attribute*), 187
`degree` (*dicee.models.function_space.LFMMult attribute*), 79
`degree` (*dicee.models.LFMMult attribute*), 142
`denormalize()` (*dicee.dataset_classes.LiteralDataset static method*), 44

- denormalize() (*dicee.LiteralDataset static method*), 214
- deploy() (*dicee.KGE method*), 200
- deploy() (*dicee.knowledge_graph_embeddings.KGE method*), 55
- deploy_head_entity_prediction() (*in module dicee*), 195
- deploy_head_entity_prediction() (*in module dicee.static_funcs*), 158
- deploy_relation_prediction() (*in module dicee*), 195
- deploy_relation_prediction() (*in module dicee.static_funcs*), 159
- deploy_tail_entity_prediction() (*in module dicee*), 195
- deploy_tail_entity_prediction() (*in module dicee.static_funcs*), 158
- deploy_triple_prediction() (*in module dicee*), 195
- deploy_triple_prediction() (*in module dicee.static_funcs*), 158
- describe() (*dicee.knowledge_graph.KG method*), 51
- description_of_input (*dicee.knowledge_graph.KG attribute*), 51
- device (*dicee.models.literal.LiteralEmbeddings property*), 81
- DICE_Trainer (*class in dicee*), 195
- DICE_Trainer (*class in dicee.trainer*), 166
- DICE_Trainer (*class in dicee.trainer.dice_trainer*), 161
- dicee
 - module, 12
- dicee.__main__
 - module, 12
- dicee.abstracts
 - module, 12
- dicee.analyse_experiments
 - module, 19
- dicee.callbacks
 - module, 20
- dicee.config
 - module, 28
- dicee.dataset_classes
 - module, 31
- dicee.eval_static_funcs
 - module, 45
- dicee.evaluator
 - module, 47
- dicee.executer
 - module, 48
- dicee.knowledge_graph
 - module, 50
- dicee.knowledge_graph_embeddings
 - module, 51
- dicee.models
 - module, 55
- dicee.models.adopt
 - module, 55
- dicee.models.base_model
 - module, 56
- dicee.models.clifford
 - module, 65
- dicee.models.complex
 - module, 72
- dicee.models.dualE
 - module, 75
- dicee.models.ensemble
 - module, 76
- dicee.models.function_space
 - module, 77
- dicee.models.literal
 - module, 80
- dicee.models.octonion
 - module, 82
- dicee.models.pykeen_models
 - module, 85
- dicee.models.quaternion
 - module, 86
- dicee.models.real
 - module, 89
- dicee.models.static_funcs

- module, 90
- dicee.models.transformers
 - module, 91
- dicee.query_generator
 - module, 144
- dicee.read_preprocess_save_load_kg
 - module, 146
- dicee.read_preprocess_save_load_kg.preprocess
 - module, 146
- dicee.read_preprocess_save_load_kg.read_from_disk
 - module, 147
- dicee.read_preprocess_save_load_kg.save_load_disk
 - module, 147
- dicee.read_preprocess_save_load_kg.util
 - module, 148
- dicee.sanity_checkers
 - module, 152
- dicee.scripts
 - module, 153
- dicee.scripts.index_serve
 - module, 153
- dicee.scripts.run
 - module, 156
- dicee.static_funcs
 - module, 156
- dicee.static_funcs_training
 - module, 159
- dicee.static_preprocess_funcs
 - module, 160
- dicee.trainer
 - module, 161
- dicee.trainer.dice_trainer
 - module, 161
- dicee.trainer.model_parallelism
 - module, 163
- dicee.trainer.torch_trainer
 - module, 163
- dicee.trainer.torch_trainer_ddp
 - module, 165
- discrete_points (*dicee.models.FMult2 attribute*), 141
- discrete_points (*dicee.models.function_space.FMult2 attribute*), 78
- dist_func (*dicee.models.Pyke attribute*), 111
- dist_func (*dicee.models.real.Pyke attribute*), 90
- dist_func (*dicee.Pyke attribute*), 170
- DistMult (*class in dicee*), 170
- DistMult (*class in dicee.models*), 110
- DistMult (*class in dicee.models.real*), 89
- download_file() (*in module dicee*), 195
- download_file() (*in module dicee.static_funcs*), 159
- download_files_from_url() (*in module dicee*), 195
- download_files_from_url() (*in module dicee.static_funcs*), 159
- download_pretrained_model() (*in module dicee*), 195
- download_pretrained_model() (*in module dicee.static_funcs*), 159
- dropout (*dicee.models.literal.LiteralEmbeddings attribute*), 80, 81
- dropout (*dicee.models.transformers.CausalSelfAttention attribute*), 94
- dropout (*dicee.models.transformers.GPTConfig attribute*), 96
- dropout (*dicee.models.transformers.MLP attribute*), 95
- DualE (*class in dicee*), 178
- DualE (*class in dicee.models*), 143
- DualE (*class in dicee.models.dualE*), 75
- dummy_eval() (*dicee.evaluator.Evaluator method*), 48
- dummy_id (*dicee.knowledge_graph.KG attribute*), 51
- during_training (*dicee.evaluator.Evaluator attribute*), 47

E

- ee_vocab (*dicee.evaluator.Evaluator attribute*), 47
- efficient_zero_grad() (*in module dicee.static_funcs_training*), 160

embedding_dim (*dicee.analyse_experiments.Experiment* attribute), 19
 embedding_dim (*dicee.BaseKGE* attribute), 191
 embedding_dim (*dicee.config.Namespace* attribute), 29
 embedding_dim (*dicee.models.base_model.BaseKGE* attribute), 63
 embedding_dim (*dicee.models.BaseKGE* attribute), 105, 108, 112, 117, 122, 135, 138
 embedding_dim (*dicee.models.literal.LiteralEmbeddings* attribute), 81
 embedding_dims (*dicee.models.literal.LiteralEmbeddings* attribute), 80
 enable_log (in module *dicee.static_preprocess_funcs*), 160
 enc (*dicee.knowledge_graph.KG* attribute), 51
 end () (*dicee.Execute* method), 201
 end () (*dicee.executer.Execute* method), 49
 EnsembleKGE (class in *dicee*), 193
 EnsembleKGE (class in *dicee.models.ensemble*), 76
 ent2id (*dicee.query_generator.QueryGenerator* attribute), 145
 ent2id (*dicee.QueryGenerator* attribute), 215
 ent_in (*dicee.query_generator.QueryGenerator* attribute), 145
 ent_in (*dicee.QueryGenerator* attribute), 215
 ent_out (*dicee.query_generator.QueryGenerator* attribute), 145
 ent_out (*dicee.QueryGenerator* attribute), 215
 entities_str (*dicee.knowledge_graph.KG* property), 51
 entity_embeddings (*dicee.AConvQ* attribute), 181
 entity_embeddings (*dicee.ConvQ* attribute), 182
 entity_embeddings (*dicee.DeCaL* attribute), 175
 entity_embeddings (*dicee.DualE* attribute), 178
 entity_embeddings (*dicee.LFMult* attribute), 187
 entity_embeddings (*dicee.models.AConvQ* attribute), 121
 entity_embeddings (*dicee.models.clifford.DeCaL* attribute), 69
 entity_embeddings (*dicee.models.ConvQ* attribute), 121
 entity_embeddings (*dicee.models.DeCaL* attribute), 132
 entity_embeddings (*dicee.models.DualE* attribute), 144
 entity_embeddings (*dicee.models.dualE.DualE* attribute), 75
 entity_embeddings (*dicee.models.FMult* attribute), 140
 entity_embeddings (*dicee.models.FMult2* attribute), 141
 entity_embeddings (*dicee.models.function_space.FMult* attribute), 77
 entity_embeddings (*dicee.models.function_space.FMult2* attribute), 78
 entity_embeddings (*dicee.models.function_space.GFMult* attribute), 77
 entity_embeddings (*dicee.models.function_space.LFMult* attribute), 79
 entity_embeddings (*dicee.models.function_space.LFMult1* attribute), 78
 entity_embeddings (*dicee.models.GFMult* attribute), 141
 entity_embeddings (*dicee.models.LFMult* attribute), 142
 entity_embeddings (*dicee.models.LFMult1* attribute), 142
 entity_embeddings (*dicee.models.literal.LiteralEmbeddings* attribute), 80, 81
 entity_embeddings (*dicee.models.pykeen_models.PykeenKGE* attribute), 85
 entity_embeddings (*dicee.models.PykeenKGE* attribute), 137
 entity_embeddings (*dicee.models.quaternion.AConvQ* attribute), 88
 entity_embeddings (*dicee.models.quaternion.ConvQ* attribute), 88
 entity_embeddings (*dicee.PykeenKGE* attribute), 188
 entity_to_idx (*dicee.dataset_classes.LiteralDataset* attribute), 43, 44
 entity_to_idx (*dicee.knowledge_graph.KG* attribute), 50
 entity_to_idx (*dicee.LiteralDataset* attribute), 213, 214
 entity_to_idx (*dicee.scripts.index_serve.NeuralSearcher* attribute), 154
 epoch_count (*dicee.abstracts.AbstractPPECallback* attribute), 17
 epoch_count (*dicee.callbacks.ASWA* attribute), 24
 epoch_counter (*dicee.callbacks.Eval* attribute), 25
 epoch_counter (*dicee.callbacks.KGESaveCallback* attribute), 22
 epoch_counter (*dicee.callbacks.PeriodicEvalCallback* attribute), 27
 epoch_ratio (*dicee.callbacks.Eval* attribute), 25
 er_vocab (*dicee.evaluator.Evaluator* attribute), 47
 estimate_mfu () (*dicee.models.transformers.GPT* method), 97
 estimate_q () (in module *dicee.callbacks*), 23
 Eval (class in *dicee.callbacks*), 24
 eval () (*dicee.EnsembleKGE* method), 194
 eval () (*dicee.evaluator.Evaluator* method), 47
 eval () (*dicee.models.ensemble.EnsembleKGE* method), 76
 eval_at_epochs (*dicee.config.Namespace* attribute), 31
 eval_epochs (*dicee.callbacks.PeriodicEvalCallback* attribute), 27
 eval_every_n_epochs (*dicee.config.Namespace* attribute), 31
 eval_lp_performance () (*dicee.KGE* method), 197

eval_lp_performance() (*dicee.knowledge_graph_embeddings.KGE method*), 52
 eval_model (*dicee.config.Namespace attribute*), 30
 eval_model (*dicee.knowledge_graph.KG attribute*), 50
 eval_rank_of_head_and_tail_byte_pair_encoded_entity() (*dicee.evaluator.Evaluator method*), 47
 eval_rank_of_head_and_tail_entity() (*dicee.evaluator.Evaluator method*), 47
 eval_with_bpe_vs_all() (*dicee.evaluator.Evaluator method*), 47
 eval_with_byte() (*dicee.evaluator.Evaluator method*), 47
 eval_with_data() (*dicee.evaluator.Evaluator method*), 48
 eval_with_vs_all() (*dicee.evaluator.Evaluator method*), 47
 evaluate() (*in module dicee*), 195
 evaluate() (*in module dicee.static_funcs*), 159
 evaluate_bpe_lp() (*in module dicee.static_funcs_training*), 160
 evaluate_ensemble_link_prediction_performance() (*in module dicee.eval_static_funcs*), 46
 evaluate_link_prediction_performance() (*in module dicee.eval_static_funcs*), 45
 evaluate_link_prediction_performance_with_bpe() (*in module dicee.eval_static_funcs*), 45
 evaluate_link_prediction_performance_with_bpe_reciprocals() (*in module dicee.eval_static_funcs*), 45
 evaluate_link_prediction_performance_with_reciprocals() (*in module dicee.eval_static_funcs*), 45
 evaluate_literal_prediction() (*in module dicee.eval_static_funcs*), 46
 evaluate_lp() (*dicee.evaluator.Evaluator method*), 48
 evaluate_lp() (*in module dicee.static_funcs_training*), 159
 evaluate_lp_bpe_k_vs_all() (*dicee.evaluator.Evaluator method*), 48
 evaluate_lp_bpe_k_vs_all() (*in module dicee.eval_static_funcs*), 46
 evaluate_lp_k_vs_all() (*dicee.evaluator.Evaluator method*), 48
 evaluate_lp_with_byte() (*dicee.evaluator.Evaluator method*), 48
 Evaluator (*class in dicee.evaluator*), 47
 evaluator (*dicee.DICE_Trainer attribute*), 196
 evaluator (*dicee.Execute attribute*), 201
 evaluator (*dicee.executor.Execute attribute*), 48
 evaluator (*dicee.trainer.DICE_Trainer attribute*), 166
 evaluator (*dicee.trainer.dice_trainer.DICE_Trainer attribute*), 162
 every_x_epoch (*dicee.callbacks.KGESaveCallback attribute*), 22
 example_input_array (*dicee.EnsembleKGE property*), 193
 example_input_array (*dicee.models.ensemble.EnsembleKGE property*), 76
 Execute (*class in dicee*), 200
 Execute (*class in dicee.executor*), 48
 exists() (*dicee.knowledge_graph.KG method*), 51
 Experiment (*class in dicee.analyse_experiments*), 19
 experiment_dir (*dicee.callbacks.LRScheduler attribute*), 27
 experiment_dir (*dicee.callbacks.PeriodicEvalCallback attribute*), 27
 explicit (*dicee.models.QMult attribute*), 120
 explicit (*dicee.models.quaternion.QMult attribute*), 87
 explicit (*dicee.QMult attribute*), 184
 exponential_function() (*in module dicee*), 195
 exponential_function() (*in module dicee.static_funcs*), 159
 extract_input_outputs() (*dicee.trainer.torch_trainer_ddp.NodeTrainer method*), 166
 extract_input_outputs() (*in module dicee.trainer.model_parallelism*), 163
 extract_input_outputs_set_device() (*dicee.trainer.torch_trainer.TorchTrainer method*), 164

F

f (*dicee.callbacks.KronE attribute*), 26
 fc (*dicee.models.literal.LiteralEmbeddings attribute*), 81
 fc1 (*dicee.AConEx attribute*), 180
 fc1 (*dicee.AConvO attribute*), 181
 fc1 (*dicee.AConvQ attribute*), 181
 fc1 (*dicee.ConEx attribute*), 183
 fc1 (*dicee.ConvO attribute*), 183
 fc1 (*dicee.ConvQ attribute*), 182
 fc1 (*dicee.models.AConEx attribute*), 114
 fc1 (*dicee.models.AConvO attribute*), 127
 fc1 (*dicee.models.AConvQ attribute*), 121
 fc1 (*dicee.models.complex.AConEx attribute*), 73
 fc1 (*dicee.models.complex.ConEx attribute*), 73
 fc1 (*dicee.models.ConEx attribute*), 114
 fc1 (*dicee.models.ConvO attribute*), 127
 fc1 (*dicee.models.ConvQ attribute*), 121
 fc1 (*dicee.models.octonion.AConvO attribute*), 84
 fc1 (*dicee.models.octonion.ConvO attribute*), 84

`fc1` (*dicee.models.quaternion.AConvQ attribute*), 88
`fc1` (*dicee.models.quaternion.ConvQ attribute*), 88
`fc_num_input` (*dicee.AConEx attribute*), 180
`fc_num_input` (*dicee.AConvO attribute*), 180
`fc_num_input` (*dicee.AConvQ attribute*), 181
`fc_num_input` (*dicee.ConEx attribute*), 183
`fc_num_input` (*dicee.ConvO attribute*), 183
`fc_num_input` (*dicee.ConvQ attribute*), 182
`fc_num_input` (*dicee.models.AConEx attribute*), 114
`fc_num_input` (*dicee.models.AConvO attribute*), 127
`fc_num_input` (*dicee.models.AConvQ attribute*), 121
`fc_num_input` (*dicee.models.complex.AConEx attribute*), 73
`fc_num_input` (*dicee.models.complex.ConEx attribute*), 73
`fc_num_input` (*dicee.models.ConEx attribute*), 114
`fc_num_input` (*dicee.models.ConvO attribute*), 127
`fc_num_input` (*dicee.models.ConvQ attribute*), 121
`fc_num_input` (*dicee.models.octonion.AConvO attribute*), 84
`fc_num_input` (*dicee.models.octonion.ConvO attribute*), 83
`fc_num_input` (*dicee.models.quaternion.AConvQ attribute*), 88
`fc_num_input` (*dicee.models.quaternion.ConvQ attribute*), 88
`fc_out` (*dicee.models.literal.LiteralEmbeddings attribute*), 81
`feature_map_dropout` (*dicee.AConEx attribute*), 180
`feature_map_dropout` (*dicee.AConvO attribute*), 181
`feature_map_dropout` (*dicee.AConvQ attribute*), 181
`feature_map_dropout` (*dicee.ConEx attribute*), 183
`feature_map_dropout` (*dicee.ConvO attribute*), 183
`feature_map_dropout` (*dicee.ConvQ attribute*), 182
`feature_map_dropout` (*dicee.models.AConEx attribute*), 115
`feature_map_dropout` (*dicee.models.AConvO attribute*), 127
`feature_map_dropout` (*dicee.models.AConvQ attribute*), 122
`feature_map_dropout` (*dicee.models.complex.AConEx attribute*), 73
`feature_map_dropout` (*dicee.models.complex.ConEx attribute*), 73
`feature_map_dropout` (*dicee.models.ConEx attribute*), 114
`feature_map_dropout` (*dicee.models.ConvO attribute*), 127
`feature_map_dropout` (*dicee.models.ConvQ attribute*), 121
`feature_map_dropout` (*dicee.models.octonion.AConvO attribute*), 84
`feature_map_dropout` (*dicee.models.octonion.ConvO attribute*), 84
`feature_map_dropout` (*dicee.models.quaternion.AConvQ attribute*), 88
`feature_map_dropout` (*dicee.models.quaternion.ConvQ attribute*), 88
`feature_map_dropout_rate` (*dicee.BaseKGE attribute*), 192
`feature_map_dropout_rate` (*dicee.config.Namespace attribute*), 30
`feature_map_dropout_rate` (*dicee.models.base_model.BaseKGE attribute*), 63
`feature_map_dropout_rate` (*dicee.models.BaseKGE attribute*), 105, 109, 112, 117, 123, 135, 139
`fill_query()` (*dicee.query_generator.QueryGenerator method*), 145
`fill_query()` (*dicee.QueryGenerator method*), 215
`find_good_batch_size()` (in module *dicee.trainer.model_parallelism*), 163
`find_missing_triples()` (*dicee.KGE method*), 200
`find_missing_triples()` (*dicee.knowledge_graph_embeddings.KGE method*), 54
`fit()` (*dicee.trainer.model_parallelism.TensorParallel method*), 163
`fit()` (*dicee.trainer.torch_trainer_ddp.TorchDDPTrainer method*), 165
`fit()` (*dicee.trainer.torch_trainer.TorchTrainer method*), 164
`flash` (*dicee.models.transformers.CausalSelfAttention attribute*), 94
`FMult` (class in *dicee.models*), 140
`FMult` (class in *dicee.models.function_space*), 77
`FMult2` (class in *dicee.models*), 141
`FMult2` (class in *dicee.models.function_space*), 78
`form_of_labelling` (*dicee.DICE_Trainer attribute*), 196
`form_of_labelling` (*dicee.trainer.DICE_Trainer attribute*), 166
`form_of_labelling` (*dicee.trainer.dice_trainer.DICE_Trainer attribute*), 162
`forward()` (*dicee.BaseKGE method*), 193
`forward()` (*dicee.BytE method*), 190
`forward()` (*dicee.models.base_model.BaseKGE method*), 64
`forward()` (*dicee.models.base_model.IdentityClass static method*), 65
`forward()` (*dicee.models.BaseKGE method*), 106, 110, 113, 118, 124, 136, 140
`forward()` (*dicee.models.IdentityClass static method*), 108, 119, 125
`forward()` (*dicee.models.literal.LiteralEmbeddings method*), 81
`forward()` (*dicee.models.transformers.Block method*), 96
`forward()` (*dicee.models.transformers.BytE method*), 92

`forward()` (*dicee.models.transformers.CausalSelfAttention method*), 94
`forward()` (*dicee.models.transformers.GPT method*), 97
`forward()` (*dicee.models.transformers.LayerNorm method*), 93
`forward()` (*dicee.models.transformers.MLP method*), 95
`forward_backward_update()` (*dicee.trainer.torch_trainer.TorchTrainer method*), 164
`forward_backward_update_loss()` (in module *dicee.trainer.model_parallelism*), 163
`forward_byte_pair_encoded_k_vs_all()` (*dicee.BaseKGE method*), 192
`forward_byte_pair_encoded_k_vs_all()` (*dicee.models.base_model.BaseKGE method*), 63
`forward_byte_pair_encoded_k_vs_all()` (*dicee.models.BaseKGE method*), 106, 109, 113, 117, 123, 136, 139
`forward_byte_pair_encoded_triple()` (*dicee.BaseKGE method*), 192
`forward_byte_pair_encoded_triple()` (*dicee.models.base_model.BaseKGE method*), 64
`forward_byte_pair_encoded_triple()` (*dicee.models.BaseKGE method*), 106, 109, 113, 117, 123, 136, 139
`forward_k_vs_all()` (*dicee.AConEx method*), 180
`forward_k_vs_all()` (*dicee.AConvO method*), 181
`forward_k_vs_all()` (*dicee.AConvQ method*), 181
`forward_k_vs_all()` (*dicee.BaseKGE method*), 193
`forward_k_vs_all()` (*dicee.ComplEx method*), 180
`forward_k_vs_all()` (*dicee.ConEx method*), 184
`forward_k_vs_all()` (*dicee.ConvO method*), 183
`forward_k_vs_all()` (*dicee.ConvQ method*), 182
`forward_k_vs_all()` (*dicee.DeCaL method*), 176
`forward_k_vs_all()` (*dicee.DistMult method*), 171
`forward_k_vs_all()` (*dicee.DualE method*), 179
`forward_k_vs_all()` (*dicee.Keci method*), 173
`forward_k_vs_all()` (*dicee.models.AConEx method*), 115
`forward_k_vs_all()` (*dicee.models.AConvO method*), 128
`forward_k_vs_all()` (*dicee.models.AConvQ method*), 122
`forward_k_vs_all()` (*dicee.models.base_model.BaseKGE method*), 64
`forward_k_vs_all()` (*dicee.models.BaseKGE method*), 107, 110, 113, 118, 124, 137, 140
`forward_k_vs_all()` (*dicee.models.clifford.DeCaL method*), 70
`forward_k_vs_all()` (*dicee.models.clifford.Keci method*), 68
`forward_k_vs_all()` (*dicee.models.ComplEx method*), 116
`forward_k_vs_all()` (*dicee.models.complex.AConEx method*), 73
`forward_k_vs_all()` (*dicee.models.complex.ComplEx method*), 74
`forward_k_vs_all()` (*dicee.models.complex.ConEx method*), 73
`forward_k_vs_all()` (*dicee.models.ConEx method*), 114
`forward_k_vs_all()` (*dicee.models.ConvO method*), 127
`forward_k_vs_all()` (*dicee.models.ConvQ method*), 121
`forward_k_vs_all()` (*dicee.models.DeCaL method*), 132
`forward_k_vs_all()` (*dicee.models.DistMult method*), 110
`forward_k_vs_all()` (*dicee.models.DualE method*), 144
`forward_k_vs_all()` (*dicee.models.dualE.DualE method*), 75
`forward_k_vs_all()` (*dicee.models.Keci method*), 130
`forward_k_vs_all()` (*dicee.models.octonion.AConvO method*), 84
`forward_k_vs_all()` (*dicee.models.octonion.ConvO method*), 84
`forward_k_vs_all()` (*dicee.models.octonion.OMult method*), 83
`forward_k_vs_all()` (*dicee.models.OMult method*), 126
`forward_k_vs_all()` (*dicee.models.pykeen_models.PykeenKGE method*), 85
`forward_k_vs_all()` (*dicee.models.PykeenKGE method*), 137
`forward_k_vs_all()` (*dicee.models.QMult method*), 120
`forward_k_vs_all()` (*dicee.models.quaternion.AConvQ method*), 89
`forward_k_vs_all()` (*dicee.models.quaternion.ConvQ method*), 88
`forward_k_vs_all()` (*dicee.models.quaternion.QMult method*), 87
`forward_k_vs_all()` (*dicee.models.real.DistMult method*), 89
`forward_k_vs_all()` (*dicee.models.real.Shallom method*), 90
`forward_k_vs_all()` (*dicee.models.real.TransE method*), 90
`forward_k_vs_all()` (*dicee.models.Shallom method*), 111
`forward_k_vs_all()` (*dicee.models.TransE method*), 111
`forward_k_vs_all()` (*dicee.OMult method*), 186
`forward_k_vs_all()` (*dicee.PykeenKGE method*), 188
`forward_k_vs_all()` (*dicee.QMult method*), 185
`forward_k_vs_all()` (*dicee.Shallom method*), 186
`forward_k_vs_all()` (*dicee.TransE method*), 174
`forward_k_vs_sample()` (*dicee.AConEx method*), 180
`forward_k_vs_sample()` (*dicee.BaseKGE method*), 193
`forward_k_vs_sample()` (*dicee.ComplEx method*), 180
`forward_k_vs_sample()` (*dicee.ConEx method*), 184
`forward_k_vs_sample()` (*dicee.DistMult method*), 171

`forward_k_vs_sample()` (*dicee.Keci method*), 174
`forward_k_vs_sample()` (*dicee.models.AConEx method*), 115
`forward_k_vs_sample()` (*dicee.models.base_model.BaseKGE method*), 64
`forward_k_vs_sample()` (*dicee.models.BaseKGE method*), 107, 110, 113, 118, 124, 137, 140
`forward_k_vs_sample()` (*dicee.models.clifford.Keci method*), 68
`forward_k_vs_sample()` (*dicee.models.ComplEx method*), 116
`forward_k_vs_sample()` (*dicee.models.complex.AConEx method*), 73
`forward_k_vs_sample()` (*dicee.models.complex.ComplEx method*), 74
`forward_k_vs_sample()` (*dicee.models.complex.ConEx method*), 73
`forward_k_vs_sample()` (*dicee.models.ConEx method*), 114
`forward_k_vs_sample()` (*dicee.models.DistMult method*), 110
`forward_k_vs_sample()` (*dicee.models.Keci method*), 130
`forward_k_vs_sample()` (*dicee.models.pykeen_models.PykeenKGE method*), 86
`forward_k_vs_sample()` (*dicee.models.PykeenKGE method*), 138
`forward_k_vs_sample()` (*dicee.models.QMult method*), 121
`forward_k_vs_sample()` (*dicee.models.quaternion.QMult method*), 87
`forward_k_vs_sample()` (*dicee.models.real.DistMult method*), 89
`forward_k_vs_sample()` (*dicee.PykeenKGE method*), 189
`forward_k_vs_sample()` (*dicee.QMult method*), 185
`forward_k_vs_with_explicit()` (*dicee.Keci method*), 173
`forward_k_vs_with_explicit()` (*dicee.models.clifford.Keci method*), 67
`forward_k_vs_with_explicit()` (*dicee.models.Keci method*), 130
`forward_triples()` (*dicee.AConEx method*), 180
`forward_triples()` (*dicee.AConvO method*), 181
`forward_triples()` (*dicee.AConvQ method*), 181
`forward_triples()` (*dicee.BaseKGE method*), 193
`forward_triples()` (*dicee.ConEx method*), 184
`forward_triples()` (*dicee.ConvO method*), 183
`forward_triples()` (*dicee.ConvQ method*), 182
`forward_triples()` (*dicee.DeCaL method*), 175
`forward_triples()` (*dicee.DualE method*), 178
`forward_triples()` (*dicee.Keci method*), 174
`forward_triples()` (*dicee.LFMult method*), 187
`forward_triples()` (*dicee.models.AConEx method*), 115
`forward_triples()` (*dicee.models.AConvO method*), 128
`forward_triples()` (*dicee.models.AConvQ method*), 122
`forward_triples()` (*dicee.models.base_model.BaseKGE method*), 64
`forward_triples()` (*dicee.models.BaseKGE method*), 106, 110, 113, 118, 124, 136, 140
`forward_triples()` (*dicee.models.clifford.DeCaL method*), 69
`forward_triples()` (*dicee.models.clifford.Keci method*), 68
`forward_triples()` (*dicee.models.complex.AConEx method*), 73
`forward_triples()` (*dicee.models.complex.ConEx method*), 73
`forward_triples()` (*dicee.models.ConEx method*), 114
`forward_triples()` (*dicee.models.ConvO method*), 127
`forward_triples()` (*dicee.models.ConvQ method*), 121
`forward_triples()` (*dicee.models.DeCaL method*), 132
`forward_triples()` (*dicee.models.DualE method*), 144
`forward_triples()` (*dicee.models.dualE.DualE method*), 75
`forward_triples()` (*dicee.models.FMult method*), 141
`forward_triples()` (*dicee.models.FMult2 method*), 142
`forward_triples()` (*dicee.models.function_space.FMult method*), 77
`forward_triples()` (*dicee.models.function_space.FMult2 method*), 78
`forward_triples()` (*dicee.models.function_space.GFMult method*), 78
`forward_triples()` (*dicee.models.function_space.LFMult method*), 79
`forward_triples()` (*dicee.models.function_space.LFMult1 method*), 78
`forward_triples()` (*dicee.models.GFMult method*), 141
`forward_triples()` (*dicee.models.Keci method*), 131
`forward_triples()` (*dicee.models.LFMult method*), 142
`forward_triples()` (*dicee.models.LFMult1 method*), 142
`forward_triples()` (*dicee.models.octonion.AConvO method*), 84
`forward_triples()` (*dicee.models.octonion.ConvO method*), 84
`forward_triples()` (*dicee.models.Pyke method*), 111
`forward_triples()` (*dicee.models.pykeen_models.PykeenKGE method*), 85
`forward_triples()` (*dicee.models.PykeenKGE method*), 138
`forward_triples()` (*dicee.models.quaternion.AConvQ method*), 89
`forward_triples()` (*dicee.models.quaternion.ConvQ method*), 88
`forward_triples()` (*dicee.models.real.Pyke method*), 90
`forward_triples()` (*dicee.models.real.Shallom method*), 90

`forward_triples()` (*dicee.models.Shallom method*), 111
`forward_triples()` (*dicee.Pyke method*), 170
`forward_triples()` (*dicee.PykeenKGE method*), 188
`forward_triples()` (*dicee.Shallom method*), 186
`freeze_entity_embeddings` (*dicee.models.literal.LiteralEmbeddings attribute*), 81
`frequency` (*dicee.callbacks.Perturb attribute*), 26
`from_pretrained()` (*dicee.models.transformers.GPT class method*), 97
`from_pretrained_model_write_embeddings_into_csv()` (*in module dicee*), 195
`from_pretrained_model_write_embeddings_into_csv()` (*in module dicee.static_funcs*), 159
`full_storage_path` (*dicee.analyse_experiments.Experiment attribute*), 19
`func_triple_to_bpe_representation` (*dicee.evaluator.Evaluator attribute*), 47
`func_triple_to_bpe_representation()` (*dicee.knowledge_graph.KG method*), 51
`function()` (*dicee.models.FMult2 method*), 142
`function()` (*dicee.models.function_space.FMult2 method*), 78

G

`gamma` (*dicee.models.FMult attribute*), 141
`gamma` (*dicee.models.function_space.FMult attribute*), 77
`gate_residual` (*dicee.models.literal.LiteralEmbeddings attribute*), 81
`gated_residual_proj` (*dicee.models.literal.LiteralEmbeddings attribute*), 81
`gelu` (*dicee.models.transformers.MLP attribute*), 95
`gen_test` (*dicee.query_generator.QueryGenerator attribute*), 145
`gen_test` (*dicee.QueryGenerator attribute*), 215
`gen_valid` (*dicee.query_generator.QueryGenerator attribute*), 145
`gen_valid` (*dicee.QueryGenerator attribute*), 215
`generate()` (*dicee.BytE method*), 190
`generate()` (*dicee.KGE method*), 197
`generate()` (*dicee.knowledge_graph_embeddings.KGE method*), 52
`generate()` (*dicee.models.transformers.BytE method*), 92
`generate_queries()` (*dicee.query_generator.QueryGenerator method*), 145
`generate_queries()` (*dicee.QueryGenerator method*), 215
`get_aswa_state_dict()` (*dicee.callbacks.ASWA method*), 24
`get_bpe_head_and_relation_representation()` (*dicee.BaseKGE method*), 193
`get_bpe_head_and_relation_representation()` (*dicee.models.base_model.BaseKGE method*), 64
`get_bpe_head_and_relation_representation()` (*dicee.models.BaseKGE method*), 107, 110, 114, 118, 124, 137, 140
`get_bpe_token_representation()` (*dicee.abstracts.BaseInteractiveKGE method*), 14
`get_callbacks()` (*in module dicee.trainer.dice_trainer*), 161
`get_default_arguments()` (*in module dicee.analyse_experiments*), 19
`get_default_arguments()` (*in module dicee.scripts.index_serve*), 154
`get_default_arguments()` (*in module dicee.scripts.run*), 156
`get_ee_vocab()` (*in module dicee*), 194
`get_ee_vocab()` (*in module dicee.read_preprocess_save_load_kg.util*), 150
`get_ee_vocab()` (*in module dicee.static_funcs*), 157
`get_ee_vocab()` (*in module dicee.static_preprocess_funcs*), 160
`get_embeddings()` (*dicee.BaseKGE method*), 193
`get_embeddings()` (*dicee.EnsembleKGE method*), 194
`get_embeddings()` (*dicee.models.base_model.BaseKGE method*), 64
`get_embeddings()` (*dicee.models.BaseKGE method*), 107, 110, 114, 118, 124, 137, 140
`get_embeddings()` (*dicee.models.ensemble.EnsembleKGE method*), 76
`get_embeddings()` (*dicee.models.real.Shallom method*), 90
`get_embeddings()` (*dicee.models.Shallom method*), 111
`get_embeddings()` (*dicee.Shallom method*), 186
`get_entity_embeddings()` (*dicee.abstracts.BaseInteractiveKGE method*), 15
`get_entity_index()` (*dicee.abstracts.BaseInteractiveKGE method*), 15
`get_er_vocab()` (*in module dicee*), 194
`get_er_vocab()` (*in module dicee.read_preprocess_save_load_kg.util*), 150
`get_er_vocab()` (*in module dicee.static_funcs*), 157
`get_er_vocab()` (*in module dicee.static_preprocess_funcs*), 160
`get_eval_report()` (*dicee.abstracts.BaseInteractiveKGE method*), 14
`get_head_relation_representation()` (*dicee.BaseKGE method*), 193
`get_head_relation_representation()` (*dicee.models.base_model.BaseKGE method*), 64
`get_head_relation_representation()` (*dicee.models.BaseKGE method*), 107, 110, 113, 118, 124, 137, 140
`get_kronecker_triple_representation()` (*dicee.callbacks.KronE method*), 26
`get_num_params()` (*dicee.models.transformers.GPT method*), 97
`get_padded_bpe_triple_representation()` (*dicee.abstracts.BaseInteractiveKGE method*), 14
`get_queries()` (*dicee.query_generator.QueryGenerator method*), 146
`get_queries()` (*dicee.QueryGenerator method*), 216

`get_re_vocab()` (in module *dicee*), 194
`get_re_vocab()` (in module *dicee.read_preprocess_save_load_kg.util*), 150
`get_re_vocab()` (in module *dicee.static_funcs*), 157
`get_re_vocab()` (in module *dicee.static_preprocess_funcs*), 160
`get_relation_embeddings()` (*dicee.abstracts.BaseInteractiveKGE* method), 15
`get_relation_index()` (*dicee.abstracts.BaseInteractiveKGE* method), 15
`get_sentence_representation()` (*dicee.BaseKGE* method), 193
`get_sentence_representation()` (*dicee.models.base_model.BaseKGE* method), 64
`get_sentence_representation()` (*dicee.models.BaseKGE* method), 107, 110, 113, 118, 124, 137, 140
`get_transductive_entity_embeddings()` (*dicee.KGE* method), 197
`get_transductive_entity_embeddings()` (*dicee.knowledge_graph_embeddings.KGE* method), 52
`get_triple_representation()` (*dicee.BaseKGE* method), 193
`get_triple_representation()` (*dicee.models.base_model.BaseKGE* method), 64
`get_triple_representation()` (*dicee.models.BaseKGE* method), 107, 110, 113, 118, 124, 137, 140
`GFMult` (class in *dicee.models*), 141
`GFMult` (class in *dicee.models.function_space*), 77
`global_rank` (*dicee.abstracts.AbstractTrainer* attribute), 13
`global_rank` (*dicee.trainer.torch_trainer_ddp.NodeTrainer* attribute), 165
`GPT` (class in *dicee.models.transformers*), 96
`GPTConfig` (class in *dicee.models.transformers*), 96
`gpus` (*dicee.config.Namespace* attribute), 29
`gradient_accumulation_steps` (*dicee.config.Namespace* attribute), 29
`ground_queries()` (*dicee.query_generator.QueryGenerator* method), 145
`ground_queries()` (*dicee.QueryGenerator* method), 215

H

`hidden_dim` (*dicee.models.literal.LiteralEmbeddings* attribute), 81
`hidden_dropout` (*dicee.BaseKGE* attribute), 192
`hidden_dropout` (*dicee.models.base_model.BaseKGE* attribute), 63
`hidden_dropout` (*dicee.models.BaseKGE* attribute), 106, 109, 113, 117, 123, 136, 139
`hidden_dropout_rate` (*dicee.BaseKGE* attribute), 192
`hidden_dropout_rate` (*dicee.config.Namespace* attribute), 30
`hidden_dropout_rate` (*dicee.models.base_model.BaseKGE* attribute), 63
`hidden_dropout_rate` (*dicee.models.BaseKGE* attribute), 105, 109, 112, 117, 123, 135, 139
`hidden_normalizer` (*dicee.BaseKGE* attribute), 192
`hidden_normalizer` (*dicee.models.base_model.BaseKGE* attribute), 63
`hidden_normalizer` (*dicee.models.BaseKGE* attribute), 106, 109, 113, 117, 123, 136, 139

I

`IdentityClass` (class in *dicee.models*), 107, 118, 124
`IdentityClass` (class in *dicee.models.base_model*), 64
`idx_entity_to_bpe_shaped` (*dicee.knowledge_graph.KG* attribute), 51
`index()` (in module *dicee.scripts.index_serve*), 154
`index_triple()` (*dicee.abstracts.BaseInteractiveKGE* method), 15
`init_dataloader()` (*dicee.DICE_Trainer* method), 196
`init_dataloader()` (*dicee.trainer.DICE_Trainer* method), 167
`init_dataloader()` (*dicee.trainer.dice_trainer.DICE_Trainer* method), 162
`init_dataset()` (*dicee.DICE_Trainer* method), 196
`init_dataset()` (*dicee.trainer.DICE_Trainer* method), 167
`init_dataset()` (*dicee.trainer.dice_trainer.DICE_Trainer* method), 162
`init_param` (*dicee.config.Namespace* attribute), 29
`init_params_with_sanity_checking()` (*dicee.BaseKGE* method), 193
`init_params_with_sanity_checking()` (*dicee.models.base_model.BaseKGE* method), 64
`init_params_with_sanity_checking()` (*dicee.models.BaseKGE* method), 106, 109, 113, 118, 124, 136, 140
`initial_eval_setting` (*dicee.callbacks.ASWA* attribute), 24
`initialize_or_load_model()` (*dicee.DICE_Trainer* method), 196
`initialize_or_load_model()` (*dicee.trainer.DICE_Trainer* method), 167
`initialize_or_load_model()` (*dicee.trainer.dice_trainer.DICE_Trainer* method), 162
`initialize_trainer()` (*dicee.DICE_Trainer* method), 196
`initialize_trainer()` (*dicee.trainer.DICE_Trainer* method), 167
`initialize_trainer()` (*dicee.trainer.dice_trainer.DICE_Trainer* method), 162
`initialize_trainer()` (in module *dicee.trainer.dice_trainer*), 161
`input_dp_ent_real` (*dicee.BaseKGE* attribute), 192
`input_dp_ent_real` (*dicee.models.base_model.BaseKGE* attribute), 63
`input_dp_ent_real` (*dicee.models.BaseKGE* attribute), 106, 109, 113, 117, 123, 136, 139
`input_dp_rel_real` (*dicee.BaseKGE* attribute), 192
`input_dp_rel_real` (*dicee.models.base_model.BaseKGE* attribute), 63

dicee.models.BaseKGE attribute), 106, 109, 113, 117, 123, 136, 139
dicee.BaseKGE attribute), 192
dicee.config.Namespace attribute), 30
dicee.models.base_model.BaseKGE attribute), 63
dicee.models.BaseKGE attribute), 105, 109, 112, 117, 123, 135, 139
InteractiveQueryDecomposition (class in *dicee.abstracts*), 16
intialize_model() (in module *dicee*), 195
intialize_model() (in module *dicee.static_funcs*), 158
is_continual_training (*dicee.DICE_Trainer* attribute), 196
is_continual_training (*dicee.evaluator.Evaluator* attribute), 47
is_continual_training (*dicee.Execute* attribute), 200
is_continual_training (*dicee.executer.Execute* attribute), 48
is_continual_training (*dicee.trainer.DICE_Trainer* attribute), 166
is_continual_training (*dicee.trainer.dice_trainer.DICE_Trainer* attribute), 161
is_global_zero (*dicee.abstracts.AbstractTrainer* attribute), 13
is_seen() (*dicee.abstracts.BaseInteractiveKGE* method), 15
is_sparql_endpoint_alive() (in module *dicee.sanity_checkers*), 153

K

k (*dicee.models.FMult* attribute), 140
k (*dicee.models.FMult2* attribute), 141
k (*dicee.models.function_space.FMult* attribute), 77
k (*dicee.models.function_space.FMult2* attribute), 78
k (*dicee.models.function_space.GFMult* attribute), 77
k (*dicee.models.GFMult* attribute), 141
k_fold_cross_validation() (*dicee.DICE_Trainer* method), 197
k_fold_cross_validation() (*dicee.trainer.DICE_Trainer* method), 167
k_fold_cross_validation() (*dicee.trainer.dice_trainer.DICE_Trainer* method), 162
k_vs_all_score() (*dicee.ComplEx* static method), 180
k_vs_all_score() (*dicee.DistMult* method), 171
k_vs_all_score() (*dicee.Keci* method), 173
k_vs_all_score() (*dicee.models.clifford.Keci* method), 68
k_vs_all_score() (*dicee.models.ComplEx* static method), 116
k_vs_all_score() (*dicee.models.complex.ComplEx* static method), 74
k_vs_all_score() (*dicee.models.DistMult* method), 110
k_vs_all_score() (*dicee.models.Keci* method), 130
k_vs_all_score() (*dicee.models.octonion.OMult* method), 83
k_vs_all_score() (*dicee.models.OMult* method), 126
k_vs_all_score() (*dicee.models.QMult* method), 120
k_vs_all_score() (*dicee.models.quaternion.QMult* method), 87
k_vs_all_score() (*dicee.models.real.DistMult* method), 89
k_vs_all_score() (*dicee.OMult* method), 186
k_vs_all_score() (*dicee.QMult* method), 185
Keci (class in *dicee*), 171
Keci (class in *dicee.models*), 128
Keci (class in *dicee.models.clifford*), 65
kernel_size (*dicee.BaseKGE* attribute), 192
kernel_size (*dicee.config.Namespace* attribute), 30
kernel_size (*dicee.models.base_model.BaseKGE* attribute), 63
kernel_size (*dicee.models.BaseKGE* attribute), 105, 109, 112, 117, 123, 135, 139
KG (class in *dicee.knowledge_graph*), 50
kg (*dicee.callbacks.PseudoLabellingCallback* attribute), 23
kg (*dicee.read_preprocess_save_load_kg.LoadSaveToDisk* attribute), 152
kg (*dicee.read_preprocess_save_load_kg.PreprocessKG* attribute), 151
kg (*dicee.read_preprocess_save_load_kg.preprocess.PreprocessKG* attribute), 146
kg (*dicee.read_preprocess_save_load_kg.read_from_disk.ReadFromDisk* attribute), 147
kg (*dicee.read_preprocess_save_load_kg.ReadFromDisk* attribute), 152
kg (*dicee.read_preprocess_save_load_kg.save_load_disk.LoadSaveToDisk* attribute), 148
KGE (class in *dicee*), 197
KGE (class in *dicee.knowledge_graph_embeddings*), 52
KGESaveCallback (class in *dicee.callbacks*), 22
knowledge_graph (*dicee.Execute* attribute), 201
knowledge_graph (*dicee.executer.Execute* attribute), 48
KronE (class in *dicee.callbacks*), 25
KvsAll (class in *dicee*), 204
KvsAll (class in *dicee.dataset_classes*), 34
kvsall_score() (*dicee.DualE* method), 178

`kvsall_score()` (*dicee.models.DualE method*), 144
`kvsall_score()` (*dicee.models.dualE.DualE method*), 75
`KvsSampleDataset` (*class in dicee*), 207
`KvsSampleDataset` (*class in dicee.dataset_classes*), 37

L

`label_smoothing_rate` (*dicee.AllvsAll attribute*), 205
`label_smoothing_rate` (*dicee.config.Namespace attribute*), 30
`label_smoothing_rate` (*dicee.dataset_classes.AllvsAll attribute*), 35
`label_smoothing_rate` (*dicee.dataset_classes.KvsAll attribute*), 35
`label_smoothing_rate` (*dicee.dataset_classes.KvsSampleDataset attribute*), 38
`label_smoothing_rate` (*dicee.dataset_classes.OnevsSample attribute*), 36, 37
`label_smoothing_rate` (*dicee.dataset_classes.TriplePredictionDataset attribute*), 39
`label_smoothing_rate` (*dicee.KvsAll attribute*), 205
`label_smoothing_rate` (*dicee.KvsSampleDataset attribute*), 208
`label_smoothing_rate` (*dicee.OnevsSample attribute*), 206, 207
`label_smoothing_rate` (*dicee.TriplePredictionDataset attribute*), 209
`layer_norm` (*dicee.models.literal.LiteralEmbeddings attribute*), 81
`LayerNorm` (*class in dicee.models.transformers*), 93
`learning_rate` (*dicee.BaseKGE attribute*), 192
`learning_rate` (*dicee.models.base_model.BaseKGE attribute*), 63
`learning_rate` (*dicee.models.BaseKGE attribute*), 105, 109, 112, 117, 123, 135, 139
`length` (*dicee.dataset_classes.NegSampleDataset attribute*), 38
`length` (*dicee.dataset_classes.TriplePredictionDataset attribute*), 39
`length` (*dicee.NegSampleDataset attribute*), 208
`length` (*dicee.TriplePredictionDataset attribute*), 209
`level` (*dicee.callbacks.Perturb attribute*), 26
`LFMult` (*class in dicee*), 187
`LFMult` (*class in dicee.models*), 142
`LFMult` (*class in dicee.models.function_space*), 79
`LFMult1` (*class in dicee.models*), 142
`LFMult1` (*class in dicee.models.function_space*), 78
`linear()` (*dicee.LFMult method*), 187
`linear()` (*dicee.models.function_space.LFMult method*), 79
`linear()` (*dicee.models.LFMult method*), 143
`list2tuple()` (*dicee.query_generator.QueryGenerator method*), 145
`list2tuple()` (*dicee.QueryGenerator method*), 215
`LiteralDataset` (*class in dicee*), 213
`LiteralDataset` (*class in dicee.dataset_classes*), 43
`LiteralEmbeddings` (*class in dicee.models.literal*), 80
`lm_head` (*dicee.BytE attribute*), 189
`lm_head` (*dicee.models.transformers.BytE attribute*), 92
`lm_head` (*dicee.models.transformers.GPT attribute*), 97
`ln_1` (*dicee.models.transformers.Block attribute*), 96
`ln_2` (*dicee.models.transformers.Block attribute*), 96
`load()` (*dicee.read_preprocess_save_load_kg.LoadSaveToDisk method*), 152
`load()` (*dicee.read_preprocess_save_load_kg.save_load_disk.LoadSaveToDisk method*), 148
`load_and_validate_literal_data()` (*dicee.dataset_classes.LiteralDataset static method*), 44
`load_and_validate_literal_data()` (*dicee.LiteralDataset static method*), 214
`load_json()` (*in module dicee*), 195
`load_json()` (*in module dicee.static_funcs*), 158
`load_model()` (*in module dicee*), 194
`load_model()` (*in module dicee.static_funcs*), 158
`load_model_ensemble()` (*in module dicee*), 194
`load_model_ensemble()` (*in module dicee.static_funcs*), 158
`load_numpy()` (*in module dicee*), 195
`load_numpy()` (*in module dicee.static_funcs*), 159
`load_numpy_ndarray()` (*in module dicee.read_preprocess_save_load_kg.util*), 151
`load_pickle()` (*in module dicee*), 194
`load_pickle()` (*in module dicee.read_preprocess_save_load_kg.util*), 151
`load_pickle()` (*in module dicee.static_funcs*), 158
`load_queries()` (*dicee.query_generator.QueryGenerator method*), 146
`load_queries()` (*dicee.QueryGenerator method*), 216
`load_queries_and_answers()` (*dicee.query_generator.QueryGenerator static method*), 146
`load_queries_and_answers()` (*dicee.QueryGenerator static method*), 216
`load_term_mapping()` (*in module dicee*), 194, 202
`load_term_mapping()` (*in module dicee.static_funcs*), 158

- `load_term_mapping()` (in module `diccee.trainer.dice_trainer`), 161
- `load_with_pandas()` (in module `diccee.read_preprocess_save_load_kg.util`), 151
- `loader_backend` (`diccee.dataset_classes.LiteralDataset` attribute), 44
- `loader_backend` (`diccee.LiteralDataset` attribute), 214
- `LoadSaveToDisk` (class in `diccee.read_preprocess_save_load_kg`), 152
- `LoadSaveToDisk` (class in `diccee.read_preprocess_save_load_kg.save_load_disk`), 148
- `local_rank` (`diccee.abstracts.AbstractTrainer` attribute), 13
- `local_rank` (`diccee.trainer.torch_trainer_ddp.NodeTrainer` attribute), 165
- `loss` (`diccee.BaseKGE` attribute), 192
- `loss` (`diccee.models.base_model.BaseKGE` attribute), 63
- `loss` (`diccee.models.BaseKGE` attribute), 106, 109, 112, 117, 123, 136, 139
- `loss_func` (`diccee.trainer.torch_trainer_ddp.NodeTrainer` attribute), 166
- `loss_function` (`diccee.trainer.torch_trainer.TorchTrainer` attribute), 164
- `loss_function()` (`diccee.BytE` method), 190
- `loss_function()` (`diccee.models.base_model.BaseKGELightning` method), 58
- `loss_function()` (`diccee.models.BaseKGELightning` method), 101
- `loss_function()` (`diccee.models.transformers.BytE` method), 92
- `loss_history` (`diccee.BaseKGE` attribute), 192
- `loss_history` (`diccee.models.base_model.BaseKGE` attribute), 63
- `loss_history` (`diccee.models.BaseKGE` attribute), 106, 109, 113, 117, 123, 136, 139
- `loss_history` (`diccee.models.pykeen_models.PykeenKGE` attribute), 85
- `loss_history` (`diccee.models.PykeenKGE` attribute), 137
- `loss_history` (`diccee.PykeenKGE` attribute), 188
- `loss_history` (`diccee.trainer.torch_trainer_ddp.NodeTrainer` attribute), 166
- `lr` (`diccee.analyse_experiments.Experiment` attribute), 19
- `lr` (`diccee.config.Namespace` attribute), 29
- `lr_lambda` (`diccee.callbacks.LRScheduler` attribute), 27
- `LRScheduler` (class in `diccee.callbacks`), 27

M

- `m` (`diccee.LFMult` attribute), 187
- `m` (`diccee.models.function_space.LFMult` attribute), 79
- `m` (`diccee.models.LFMult` attribute), 142
- `main()` (in module `diccee.scripts.index_serve`), 156
- `main()` (in module `diccee.scripts.run`), 156
- `make_iterable_verbose()` (in module `diccee.static_funcs_training`), 159
- `make_iterable_verbose()` (in module `diccee.trainer.torch_trainer_ddp`), 165
- `mapping_from_first_two_cols_to_third()` (in module `diccee`), 201
- `mapping_from_first_two_cols_to_third()` (in module `diccee.static_preprocess_funcs`), 161
- `margin` (`diccee.models.Pyke` attribute), 111
- `margin` (`diccee.models.real.Pyke` attribute), 90
- `margin` (`diccee.models.real.TransE` attribute), 90
- `margin` (`diccee.models.TransE` attribute), 111
- `margin` (`diccee.Pyke` attribute), 170
- `margin` (`diccee.TransE` attribute), 174
- `max_ans_num` (`diccee.query_generator.QueryGenerator` attribute), 145
- `max_ans_num` (`diccee.QueryGenerator` attribute), 215
- `max_epochs` (`diccee.callbacks.KGESaveCallback` attribute), 22
- `max_epochs` (`diccee.callbacks.PeriodicEvalCallback` attribute), 27
- `max_length_subword_tokens` (`diccee.BaseKGE` attribute), 192
- `max_length_subword_tokens` (`diccee.knowledge_graph.KG` attribute), 51
- `max_length_subword_tokens` (`diccee.models.base_model.BaseKGE` attribute), 63
- `max_length_subword_tokens` (`diccee.models.BaseKGE` attribute), 106, 109, 113, 117, 123, 136, 139
- `max_num_of_classes` (`diccee.dataset_classes.KvsSampleDataset` attribute), 38
- `max_num_of_classes` (`diccee.KvsSampleDataset` attribute), 208
- `mem_of_model()` (`diccee.EnsembleKGE` method), 194
- `mem_of_model()` (`diccee.models.base_model.BaseKGELightning` method), 57
- `mem_of_model()` (`diccee.models.BaseKGELightning` method), 100
- `mem_of_model()` (`diccee.models.ensemble.EnsembleKGE` method), 76
- `method` (`diccee.callbacks.Perturb` attribute), 26
- `MLP` (class in `diccee.models.transformers`), 94
- `mlp` (`diccee.models.transformers.Block` attribute), 96
- `mode` (`diccee.query_generator.QueryGenerator` attribute), 145
- `mode` (`diccee.QueryGenerator` attribute), 215
- `model` (`diccee.config.Namespace` attribute), 28
- `model` (`diccee.models.pykeen_models.PykeenKGE` attribute), 85
- `model` (`diccee.models.PykeenKGE` attribute), 137

- model (*dicee.PykeenKGE attribute*), 188
- model (*dicee.trainer.torch_trainer_ddp.NodeTrainer attribute*), 166
- model (*dicee.trainer.torch_trainer.TorchTrainer attribute*), 164
- model_kwargs (*dicee.models.pykeen_models.PykeenKGE attribute*), 85
- model_kwargs (*dicee.models.PykeenKGE attribute*), 137
- model_kwargs (*dicee.PykeenKGE attribute*), 188
- model_name (*dicee.analyse_experiments.Experiment attribute*), 19
- module
 - dicee, 12
 - dicee.__main__, 12
 - dicee.abstracts, 12
 - dicee.analyse_experiments, 19
 - dicee.callbacks, 20
 - dicee.config, 28
 - dicee.dataset_classes, 31
 - dicee.eval_static_funcs, 45
 - dicee.evaluator, 47
 - dicee.executer, 48
 - dicee.knowledge_graph, 50
 - dicee.knowledge_graph_embeddings, 51
 - dicee.models, 55
 - dicee.models.adopt, 55
 - dicee.models.base_model, 56
 - dicee.models.clifford, 65
 - dicee.models.complex, 72
 - dicee.models.dualE, 75
 - dicee.models.ensemble, 76
 - dicee.models.function_space, 77
 - dicee.models.literal, 80
 - dicee.models.octonion, 82
 - dicee.models.pykeen_models, 85
 - dicee.models.quaternion, 86
 - dicee.models.real, 89
 - dicee.models.static_funcs, 90
 - dicee.models.transformers, 91
 - dicee.query_generator, 144
 - dicee.read_preprocess_save_load_kg, 146
 - dicee.read_preprocess_save_load_kg.preprocess, 146
 - dicee.read_preprocess_save_load_kg.read_from_disk, 147
 - dicee.read_preprocess_save_load_kg.save_load_disk, 147
 - dicee.read_preprocess_save_load_kg.util, 148
 - dicee.sanity_checkers, 152
 - dicee.scripts, 153
 - dicee.scripts.index_serve, 153
 - dicee.scripts.run, 156
 - dicee.static_funcs, 156
 - dicee.static_funcs_training, 159
 - dicee.static_preprocess_funcs, 160
 - dicee.trainer, 161
 - dicee.trainer.dice_trainer, 161
 - dicee.trainer.model_parallelism, 163
 - dicee.trainer.torch_trainer, 163
 - dicee.trainer.torch_trainer_ddp, 165
- modules () (*dicee.EnsembleKGE method*), 193
- modules () (*dicee.models.ensemble.EnsembleKGE method*), 76
- MultiClassClassificationDataset (*class in dicee*), 203
- MultiClassClassificationDataset (*class in dicee.dataset_classes*), 33
- MultiLabelDataset (*class in dicee*), 202
- MultiLabelDataset (*class in dicee.dataset_classes*), 32

N

- n (*dicee.models.FMult2 attribute*), 141
- n (*dicee.models.function_space.FMult2 attribute*), 78
- n_embd (*dicee.models.transformers.CausalSelfAttention attribute*), 94
- n_embd (*dicee.models.transformers.GPTConfig attribute*), 96
- n_epochs_eval_model (*dicee.callbacks.PeriodicEvalCallback attribute*), 27
- n_epochs_eval_model (*dicee.config.Namespace attribute*), 31

`n_head` (*dicee.models.transformers.CausalSelfAttention* attribute), 94
`n_head` (*dicee.models.transformers.GPTConfig* attribute), 96
`n_layer` (*dicee.models.transformers.GPTConfig* attribute), 96
`n_layers` (*dicee.models.FMult2* attribute), 141
`n_layers` (*dicee.models.function_space.FMult2* attribute), 78
`name` (*dicee.abstracts.BaseInteractiveKGE* property), 15
`name` (*dicee.AConEx* attribute), 180
`name` (*dicee.AConvO* attribute), 180
`name` (*dicee.AConvQ* attribute), 181
`name` (*dicee.BytE* attribute), 189
`name` (*dicee.CKeci* attribute), 171
`name` (*dicee.ComplEx* attribute), 180
`name` (*dicee.ConEx* attribute), 183
`name` (*dicee.ConvO* attribute), 183
`name` (*dicee.ConvQ* attribute), 182
`name` (*dicee.DeCaL* attribute), 175
`name` (*dicee.DistMult* attribute), 171
`name` (*dicee.DualE* attribute), 178
`name` (*dicee.EnsembleKGE* attribute), 193
`name` (*dicee.Keci* attribute), 172
`name` (*dicee.LFMult* attribute), 187
`name` (*dicee.models.AConEx* attribute), 114
`name` (*dicee.models.AConvO* attribute), 127
`name` (*dicee.models.AConvQ* attribute), 121
`name` (*dicee.models.CKeci* attribute), 131
`name` (*dicee.models.clifford.CKeci* attribute), 68
`name` (*dicee.models.clifford.DeCaL* attribute), 69
`name` (*dicee.models.clifford.Keci* attribute), 66
`name` (*dicee.models.ComplEx* attribute), 115
`name` (*dicee.models.complex.AConEx* attribute), 73
`name` (*dicee.models.complex.ComplEx* attribute), 74
`name` (*dicee.models.complex.ConEx* attribute), 72
`name` (*dicee.models.ConEx* attribute), 114
`name` (*dicee.models.ConvO* attribute), 127
`name` (*dicee.models.ConvQ* attribute), 121
`name` (*dicee.models.DeCaL* attribute), 132
`name` (*dicee.models.DistMult* attribute), 110
`name` (*dicee.models.DualE* attribute), 143
`name` (*dicee.models.dualE.DualE* attribute), 75
`name` (*dicee.models.ensemble.EnsembleKGE* attribute), 76
`name` (*dicee.models.FMult* attribute), 140
`name` (*dicee.models.FMult2* attribute), 141
`name` (*dicee.models.function_space.FMult* attribute), 77
`name` (*dicee.models.function_space.FMult2* attribute), 78
`name` (*dicee.models.function_space.GFMult* attribute), 77
`name` (*dicee.models.function_space.LFMult* attribute), 79
`name` (*dicee.models.function_space.LFMult1* attribute), 78
`name` (*dicee.models.GFMult* attribute), 141
`name` (*dicee.models.Keci* attribute), 128
`name` (*dicee.models.LFMult* attribute), 142
`name` (*dicee.models.LFMult1* attribute), 142
`name` (*dicee.models.octonion.AConvO* attribute), 84
`name` (*dicee.models.octonion.ConvO* attribute), 83
`name` (*dicee.models.octonion.OMult* attribute), 83
`name` (*dicee.models.OMult* attribute), 126
`name` (*dicee.models.Pyke* attribute), 111
`name` (*dicee.models.pykeen_models.PykeenKGE* attribute), 85
`name` (*dicee.models.PykeenKGE* attribute), 137
`name` (*dicee.models.QMult* attribute), 120
`name` (*dicee.models.quaternion.AConvQ* attribute), 88
`name` (*dicee.models.quaternion.ConvQ* attribute), 88
`name` (*dicee.models.quaternion.QMult* attribute), 87
`name` (*dicee.models.real.DistMult* attribute), 89
`name` (*dicee.models.real.Pyke* attribute), 90
`name` (*dicee.models.real.Shallom* attribute), 90
`name` (*dicee.models.real.TransE* attribute), 89
`name` (*dicee.models.Shallom* attribute), 111
`name` (*dicee.models.TransE* attribute), 111

name (*dicee.models.transformers.BytE* attribute), 92
 name (*dicee.OMult* attribute), 186
 name (*dicee.Pyke* attribute), 170
 name (*dicee.PykeenKGE* attribute), 188
 name (*dicee.QMult* attribute), 184
 name (*dicee.Shallom* attribute), 186
 name (*dicee.TransE* attribute), 174
 named_children() (*dicee.EnsembleKGE* method), 193
 named_children() (*dicee.models.ensemble.EnsembleKGE* method), 76
 Namespace (class in *dicee.config*), 28
 neg_ratio (*dicee.BPE_NegativeSamplingDataset* attribute), 202
 neg_ratio (*dicee.config.Namespace* attribute), 29
 neg_ratio (*dicee.dataset_classes.BPE_NegativeSamplingDataset* attribute), 32
 neg_ratio (*dicee.dataset_classes.KvsSampleDataset* attribute), 38
 neg_ratio (*dicee.KvsSampleDataset* attribute), 208
 neg_sample_ratio (*dicee.CVDataModule* attribute), 210
 neg_sample_ratio (*dicee.dataset_classes.CVDataModule* attribute), 40
 neg_sample_ratio (*dicee.dataset_classes.NegSampleDataset* attribute), 38
 neg_sample_ratio (*dicee.dataset_classes.OnevsSample* attribute), 36, 37
 neg_sample_ratio (*dicee.dataset_classes.TriplePredictionDataset* attribute), 39
 neg_sample_ratio (*dicee.NegSampleDataset* attribute), 208
 neg_sample_ratio (*dicee.OnevsSample* attribute), 206, 207
 neg_sample_ratio (*dicee.TriplePredictionDataset* attribute), 209
 negnorm() (*dicee.abstracts.InteractiveQueryDecomposition* method), 16
 NegSampleDataset (class in *dicee*), 208
 NegSampleDataset (class in *dicee.dataset_classes*), 38
 neural_searcher (in module *dicee.scripts.index_serve*), 154
 NeuralSearcher (class in *dicee.scripts.index_serve*), 154
 NodeTrainer (class in *dicee.trainer.torch_trainer_ddp*), 165
 norm_fc1 (*dicee.AConEx* attribute), 180
 norm_fc1 (*dicee.AConvO* attribute), 181
 norm_fc1 (*dicee.ConEx* attribute), 183
 norm_fc1 (*dicee.ConvO* attribute), 183
 norm_fc1 (*dicee.models.AConEx* attribute), 115
 norm_fc1 (*dicee.models.AConvO* attribute), 127
 norm_fc1 (*dicee.models.complex.AConEx* attribute), 73
 norm_fc1 (*dicee.models.complex.ConEx* attribute), 73
 norm_fc1 (*dicee.models.ConEx* attribute), 114
 norm_fc1 (*dicee.models.ConvO* attribute), 127
 norm_fc1 (*dicee.models.octonion.AConvO* attribute), 84
 norm_fc1 (*dicee.models.octonion.ConvO* attribute), 84
 normalization (*dicee.analyse_experiments.Experiment* attribute), 20
 normalization (*dicee.config.Namespace* attribute), 29
 normalization (*dicee.dataset_classes.LiteralDataset* attribute), 43
 normalization (*dicee.LiteralDataset* attribute), 213
 normalization_params (*dicee.dataset_classes.LiteralDataset* attribute), 43, 44
 normalization_params (*dicee.LiteralDataset* attribute), 213, 214
 normalization_type (*dicee.dataset_classes.LiteralDataset* attribute), 44
 normalization_type (*dicee.LiteralDataset* attribute), 214
 normalize_head_entity_embeddings (*dicee.BaseKGE* attribute), 192
 normalize_head_entity_embeddings (*dicee.models.base_model.BaseKGE* attribute), 63
 normalize_head_entity_embeddings (*dicee.models.BaseKGE* attribute), 106, 109, 113, 117, 123, 136, 139
 normalize_relation_embeddings (*dicee.BaseKGE* attribute), 192
 normalize_relation_embeddings (*dicee.models.base_model.BaseKGE* attribute), 63
 normalize_relation_embeddings (*dicee.models.BaseKGE* attribute), 106, 109, 113, 117, 123, 136, 139
 normalize_tail_entity_embeddings (*dicee.BaseKGE* attribute), 192
 normalize_tail_entity_embeddings (*dicee.models.base_model.BaseKGE* attribute), 63
 normalize_tail_entity_embeddings (*dicee.models.BaseKGE* attribute), 106, 109, 113, 117, 123, 136, 139
 normalizer_class (*dicee.BaseKGE* attribute), 192
 normalizer_class (*dicee.models.base_model.BaseKGE* attribute), 63
 normalizer_class (*dicee.models.BaseKGE* attribute), 106, 109, 112, 117, 123, 136, 139
 num_bpe_entities (*dicee.BPE_NegativeSamplingDataset* attribute), 202
 num_bpe_entities (*dicee.dataset_classes.BPE_NegativeSamplingDataset* attribute), 32
 num_bpe_entities (*dicee.knowledge_graph.KG* attribute), 51
 num_core (*dicee.config.Namespace* attribute), 30
 num_data_properties (*dicee.dataset_classes.LiteralDataset* attribute), 44
 num_data_properties (*dicee.LiteralDataset* attribute), 214
 num_datapoints (*dicee.BPE_NegativeSamplingDataset* attribute), 202

num_datapoints (*dicee.dataset_classes.BPE_NegativeSamplingDataset* attribute), 32
 num_datapoints (*dicee.dataset_classes.MultiLabelDataset* attribute), 33
 num_datapoints (*dicee.MultiLabelDataset* attribute), 203
 num_ent (*dicee.DualE* attribute), 178
 num_ent (*dicee.models.DualE* attribute), 144
 num_ent (*dicee.models.dualE.DualE* attribute), 75
 num_entities (*dicee.BaseKGE* attribute), 192
 num_entities (*dicee.CVDDataModule* attribute), 210
 num_entities (*dicee.dataset_classes.CVDDataModule* attribute), 40
 num_entities (*dicee.dataset_classes.KvsSampleDataset* attribute), 38
 num_entities (*dicee.dataset_classes.LiteralDataset* attribute), 44
 num_entities (*dicee.dataset_classes.NegSampleDataset* attribute), 38
 num_entities (*dicee.dataset_classes.OnevsSample* attribute), 36, 37
 num_entities (*dicee.dataset_classes.TriplePredictionDataset* attribute), 39
 num_entities (*dicee.evaluator.Evaluator* attribute), 47
 num_entities (*dicee.knowledge_graph.KG* attribute), 50
 num_entities (*dicee.KvsSampleDataset* attribute), 208
 num_entities (*dicee.LiteralDataset* attribute), 213, 214
 num_entities (*dicee.models.base_model.BaseKGE* attribute), 63
 num_entities (*dicee.models.BaseKGE* attribute), 105, 108, 112, 117, 122, 135, 139
 num_entities (*dicee.NegSampleDataset* attribute), 208
 num_entities (*dicee.OnevsSample* attribute), 206
 num_entities (*dicee.TriplePredictionDataset* attribute), 209
 num_epochs (*dicee.abstracts.AbstractPPECallback* attribute), 17
 num_epochs (*dicee.analyse_experiments.Experiment* attribute), 19
 num_epochs (*dicee.callbacks.ASWA* attribute), 23
 num_epochs (*dicee.config.Namespace* attribute), 29
 num_epochs (*dicee.trainer.torch_trainer_ddp.NodeTrainer* attribute), 166
 num_folds_for_cv (*dicee.config.Namespace* attribute), 29
 num_of_data_points (*dicee.dataset_classes.MultiClassClassificationDataset* attribute), 33
 num_of_data_points (*dicee.MultiClassClassificationDataset* attribute), 203
 num_of_data_properties (*dicee.models.literal.LiteralEmbeddings* attribute), 80, 81
 num_of_epochs (*dicee.callbacks.PseudoLabellingCallback* attribute), 23
 num_of_output_channels (*dicee.BaseKGE* attribute), 192
 num_of_output_channels (*dicee.config.Namespace* attribute), 30
 num_of_output_channels (*dicee.models.base_model.BaseKGE* attribute), 63
 num_of_output_channels (*dicee.models.BaseKGE* attribute), 106, 109, 112, 117, 123, 136, 139
 num_params (*dicee.analyse_experiments.Experiment* attribute), 19
 num_relations (*dicee.BaseKGE* attribute), 192
 num_relations (*dicee.CVDDataModule* attribute), 210
 num_relations (*dicee.dataset_classes.CVDDataModule* attribute), 40
 num_relations (*dicee.dataset_classes.NegSampleDataset* attribute), 38
 num_relations (*dicee.dataset_classes.OnevsSample* attribute), 36, 37
 num_relations (*dicee.dataset_classes.TriplePredictionDataset* attribute), 39
 num_relations (*dicee.evaluator.Evaluator* attribute), 47
 num_relations (*dicee.knowledge_graph.KG* attribute), 50
 num_relations (*dicee.models.base_model.BaseKGE* attribute), 63
 num_relations (*dicee.models.BaseKGE* attribute), 105, 108, 112, 117, 123, 135, 139
 num_relations (*dicee.NegSampleDataset* attribute), 208
 num_relations (*dicee.OnevsSample* attribute), 206
 num_relations (*dicee.TriplePredictionDataset* attribute), 209
 num_sample (*dicee.models.FMult* attribute), 140
 num_sample (*dicee.models.function_space.FMult* attribute), 77
 num_sample (*dicee.models.function_space.GFMult* attribute), 77
 num_sample (*dicee.models.GFMult* attribute), 141
 num_tokens (*dicee.BaseKGE* attribute), 192
 num_tokens (*dicee.knowledge_graph.KG* attribute), 51
 num_tokens (*dicee.models.base_model.BaseKGE* attribute), 63
 num_tokens (*dicee.models.BaseKGE* attribute), 105, 109, 112, 117, 123, 135, 139
 num_workers (*dicee.CVDDataModule* attribute), 210
 num_workers (*dicee.dataset_classes.CVDDataModule* attribute), 40
 numpy_data_type_changer () (in module *dicee*), 194
 numpy_data_type_changer () (in module *dicee.static_funcs*), 158

O

octonion_mul () (in module *dicee.models*), 125
 octonion_mul () (in module *dicee.models.octonion*), 82

octonion_mul_norm() (in module *dicee.models*), 125
 octonion_mul_norm() (in module *dicee.models.octonion*), 82
 octonion_normalizer() (*dicee.AConvO* static method), 181
 octonion_normalizer() (*dicee.ConvO* static method), 183
 octonion_normalizer() (*dicee.models.AConvO* static method), 127
 octonion_normalizer() (*dicee.models.ConvO* static method), 127
 octonion_normalizer() (*dicee.models.octonion.AConvO* static method), 84
 octonion_normalizer() (*dicee.models.octonion.ConvO* static method), 84
 octonion_normalizer() (*dicee.models.octonion.OMult* static method), 83
 octonion_normalizer() (*dicee.models.OMult* static method), 126
 octonion_normalizer() (*dicee.OMult* static method), 186
 OMult (class in *dicee*), 185
 OMult (class in *dicee.models*), 125
 OMult (class in *dicee.models.octonion*), 82
 on_epoch_end() (*dicee.callbacks.KGESaveCallback* method), 23
 on_epoch_end() (*dicee.callbacks.PseudoLabellingCallback* method), 23
 on_fit_end() (*dicee.abstracts.AbstractCallback* method), 17
 on_fit_end() (*dicee.abstracts.AbstractPPECallback* method), 18
 on_fit_end() (*dicee.abstracts.AbstractTrainer* method), 13
 on_fit_end() (*dicee.callbacks.AccumulateEpochLossCallback* method), 21
 on_fit_end() (*dicee.callbacks.ASWA* method), 24
 on_fit_end() (*dicee.callbacks.Eval* method), 25
 on_fit_end() (*dicee.callbacks.KGESaveCallback* method), 23
 on_fit_end() (*dicee.callbacks.LRScheduler* method), 28
 on_fit_end() (*dicee.callbacks.PeriodicEvalCallback* method), 27
 on_fit_end() (*dicee.callbacks.PrintCallback* method), 21
 on_fit_start() (*dicee.abstracts.AbstractCallback* method), 16
 on_fit_start() (*dicee.abstracts.AbstractPPECallback* method), 17
 on_fit_start() (*dicee.abstracts.AbstractTrainer* method), 13
 on_fit_start() (*dicee.callbacks.Eval* method), 25
 on_fit_start() (*dicee.callbacks.KGESaveCallback* method), 22
 on_fit_start() (*dicee.callbacks.KronE* method), 26
 on_fit_start() (*dicee.callbacks.PrintCallback* method), 21
 on_init_end() (*dicee.abstracts.AbstractCallback* method), 16
 on_init_start() (*dicee.abstracts.AbstractCallback* method), 16
 on_train_batch_end() (*dicee.abstracts.AbstractCallback* method), 17
 on_train_batch_end() (*dicee.abstracts.AbstractTrainer* method), 13
 on_train_batch_end() (*dicee.callbacks.Eval* method), 25
 on_train_batch_end() (*dicee.callbacks.KGESaveCallback* method), 22
 on_train_batch_end() (*dicee.callbacks.LRScheduler* method), 28
 on_train_batch_end() (*dicee.callbacks.PrintCallback* method), 21
 on_train_batch_start() (*dicee.callbacks.Perturb* method), 26
 on_train_epoch_end() (*dicee.abstracts.AbstractCallback* method), 16
 on_train_epoch_end() (*dicee.abstracts.AbstractTrainer* method), 13
 on_train_epoch_end() (*dicee.callbacks.ASWA* method), 24
 on_train_epoch_end() (*dicee.callbacks.Eval* method), 25
 on_train_epoch_end() (*dicee.callbacks.KGESaveCallback* method), 22
 on_train_epoch_end() (*dicee.callbacks.PeriodicEvalCallback* method), 27
 on_train_epoch_end() (*dicee.callbacks.PrintCallback* method), 22
 on_train_epoch_end() (*dicee.models.base_model.BaseKGELightning* method), 58
 on_train_epoch_end() (*dicee.models.BaseKGELightning* method), 101
 on_train_start() (*dicee.callbacks.LRScheduler* method), 28
 OnevsAllDataset (class in *dicee*), 203
 OnevsAllDataset (class in *dicee.dataset_classes*), 34
 OnevsSample (class in *dicee*), 205
 OnevsSample (class in *dicee.dataset_classes*), 36
 optim (*dicee.config.Namespace* attribute), 29
 optimizer (*dicee.trainer.torch_trainer_ddp.NodeTrainer* attribute), 165
 optimizer (*dicee.trainer.torch_trainer.TorchTrainer* attribute), 164
 optimizer_name (*dicee.BaseKGE* attribute), 192
 optimizer_name (*dicee.models.base_model.BaseKGE* attribute), 63
 optimizer_name (*dicee.models.BaseKGE* attribute), 105, 109, 112, 117, 123, 135, 139
 ordered_bpe_entities (*dicee.BPE_NegativeSamplingDataset* attribute), 202
 ordered_bpe_entities (*dicee.dataset_classes.BPE_NegativeSamplingDataset* attribute), 32
 ordered_bpe_entities (*dicee.knowledge_graph.KG* attribute), 51
 ordered_shaped_bpe_tokens (*dicee.knowledge_graph.KG* attribute), 50

P

- `p` (*dicee.config.Namespace* attribute), 30
- `p` (*dicee.DeCaL* attribute), 175
- `p` (*dicee.Keci* attribute), 172
- `p` (*dicee.models.clifford.DeCaL* attribute), 69
- `p` (*dicee.models.clifford.Keci* attribute), 66
- `p` (*dicee.models.DeCaL* attribute), 132
- `p` (*dicee.models.Keci* attribute), 128
- `padding` (*dicee.knowledge_graph.KG* attribute), 51
- `pandas_dataframe_indexer()` (in module *dicee.read_preprocess_save_load_kg.util*), 150
- `param_init` (*dicee.BaseKGE* attribute), 192
- `param_init` (*dicee.models.base_model.BaseKGE* attribute), 63
- `param_init` (*dicee.models.BaseKGE* attribute), 106, 109, 113, 117, 123, 136, 139
- `parameters()` (*dicee.abstracts.BaseInteractiveKGE* method), 15
- `parameters()` (*dicee.EnsembleKGE* method), 193
- `parameters()` (*dicee.models.ensemble.EnsembleKGE* method), 76
- `path` (*dicee.abstracts.AbstractPPECallback* attribute), 17
- `path` (*dicee.callbacks.AccumulateEpochLossCallback* attribute), 21
- `path` (*dicee.callbacks.ASWA* attribute), 23
- `path` (*dicee.callbacks.Eval* attribute), 25
- `path` (*dicee.callbacks.KGESaveCallback* attribute), 22
- `path_dataset_folder` (*dicee.analyse_experiments.Experiment* attribute), 19
- `path_for_deserialization` (*dicee.knowledge_graph.KG* attribute), 50
- `path_for_serialization` (*dicee.knowledge_graph.KG* attribute), 50
- `path_single_kg` (*dicee.config.Namespace* attribute), 28
- `path_single_kg` (*dicee.knowledge_graph.KG* attribute), 50
- `path_to_store_single_run` (*dicee.config.Namespace* attribute), 28
- PeriodicEvalCallback* (class in *dicee.callbacks*), 26
- Perturb* (class in *dicee.callbacks*), 26
- `polars_dataframe_indexer()` (in module *dicee.read_preprocess_save_load_kg.util*), 149
- `poly_NN()` (*dicee.LFMult* method), 187
- `poly_NN()` (*dicee.models.function_space.LFMult* method), 79
- `poly_NN()` (*dicee.models.LFMult* method), 143
- `polynomial()` (*dicee.LFMult* method), 188
- `polynomial()` (*dicee.models.function_space.LFMult* method), 80
- `polynomial()` (*dicee.models.LFMult* method), 143
- `pop()` (*dicee.LFMult* method), 188
- `pop()` (*dicee.models.function_space.LFMult* method), 80
- `pop()` (*dicee.models.LFMult* method), 143
- `pq` (*dicee.analyse_experiments.Experiment* attribute), 19
- `predict()` (*dicee.KGE* method), 198
- `predict()` (*dicee.knowledge_graph_embeddings.KGE* method), 53
- `predict_data_loader()` (*dicee.models.base_model.BaseKGELightning* method), 60
- `predict_data_loader()` (*dicee.models.BaseKGELightning* method), 102
- `predict_literals()` (*dicee.KGE* method), 200
- `predict_literals()` (*dicee.knowledge_graph_embeddings.KGE* method), 55
- `predict_missing_head_entity()` (*dicee.KGE* method), 197
- `predict_missing_head_entity()` (*dicee.knowledge_graph_embeddings.KGE* method), 52
- `predict_missing_relations()` (*dicee.KGE* method), 198
- `predict_missing_relations()` (*dicee.knowledge_graph_embeddings.KGE* method), 52
- `predict_missing_tail_entity()` (*dicee.KGE* method), 198
- `predict_missing_tail_entity()` (*dicee.knowledge_graph_embeddings.KGE* method), 53
- `predict_topk()` (*dicee.KGE* method), 198
- `predict_topk()` (*dicee.knowledge_graph_embeddings.KGE* method), 53
- `prepare_data()` (*dicee.CVDataModule* method), 212
- `prepare_data()` (*dicee.dataset_classes.CVDataModule* method), 42
- `preprocess_with_byte_pair_encoding()` (*dicee.read_preprocess_save_load_kg.PreprocessKG* method), 151
- `preprocess_with_byte_pair_encoding()` (*dicee.read_preprocess_save_load_kg.preprocess.PreprocessKG* method), 146
- `preprocess_with_byte_pair_encoding_with_padding()` (*dicee.read_preprocess_save_load_kg.PreprocessKG* method), 151
- `preprocess_with_byte_pair_encoding_with_padding()` (*dicee.read_preprocess_save_load_kg.preprocess.PreprocessKG* method), 146
- `preprocess_with_pandas()` (*dicee.read_preprocess_save_load_kg.PreprocessKG* method), 151
- `preprocess_with_pandas()` (*dicee.read_preprocess_save_load_kg.preprocess.PreprocessKG* method), 146
- `preprocess_with_polars()` (*dicee.read_preprocess_save_load_kg.PreprocessKG* method), 152
- `preprocess_with_polars()` (*dicee.read_preprocess_save_load_kg.preprocess.PreprocessKG* method), 147
- `preprocesses_input_args()` (in module *dicee.static_preprocess_funcs*), 160
- PreprocessKG* (class in *dicee.read_preprocess_save_load_kg*), 151
- PreprocessKG* (class in *dicee.read_preprocess_save_load_kg.preprocess*), 146
- PrintCallback* (class in *dicee.callbacks*), 21

process (*dicee.trainer.torch_trainer.TorchTrainer* attribute), 164
PseudoLabellingCallback (class in *dicee.callbacks*), 23
Pyke (class in *dicee*), 170
Pyke (class in *dicee.models*), 111
Pyke (class in *dicee.models.real*), 90
pykeen_model_kwargs (*dicee.config.Namespace* attribute), 30
PykeenKGE (class in *dicee*), 188
PykeenKGE (class in *dicee.models*), 137
PykeenKGE (class in *dicee.models.pykeen_models*), 85

Q

q (*dicee.config.Namespace* attribute), 30
q (*dicee.DeCaL* attribute), 175
q (*dicee.Keci* attribute), 172
q (*dicee.models.clifford.DeCaL* attribute), 69
q (*dicee.models.clifford.Keci* attribute), 66
q (*dicee.models.DeCaL* attribute), 132
q (*dicee.models.Keci* attribute), 128
qdrant_client (*dicee.scripts.index_serve.NeuralSearcher* attribute), 154
QMult (class in *dicee*), 184
QMult (class in *dicee.models*), 119
QMult (class in *dicee.models.quaternion*), 86
quaternion_mul () (in module *dicee.models*), 116
quaternion_mul () (in module *dicee.models.static_funcs*), 90
quaternion_mul_with_unit_norm () (in module *dicee.models*), 119
quaternion_mul_with_unit_norm () (in module *dicee.models.quaternion*), 86
quaternion_multiplication_followed_by_inner_product () (*dicee.models.QMult* method), 120
quaternion_multiplication_followed_by_inner_product () (*dicee.models.quaternion.QMult* method), 87
quaternion_multiplication_followed_by_inner_product () (*dicee.QMult* method), 184
quaternion_normalizer () (*dicee.models.QMult* static method), 120
quaternion_normalizer () (*dicee.models.quaternion.QMult* static method), 87
quaternion_normalizer () (*dicee.QMult* static method), 185
queries (*dicee.scripts.index_serve.StringListRequest* attribute), 155
query_name_to_struct (*dicee.query_generator.QueryGenerator* attribute), 145
query_name_to_struct (*dicee.QueryGenerator* attribute), 215
QueryGenerator (class in *dicee*), 214
QueryGenerator (class in *dicee.query_generator*), 145

R

r (*dicee.DeCaL* attribute), 175
r (*dicee.Keci* attribute), 172
r (*dicee.models.clifford.DeCaL* attribute), 69
r (*dicee.models.clifford.Keci* attribute), 66
r (*dicee.models.DeCaL* attribute), 132
r (*dicee.models.Keci* attribute), 128
random_prediction () (in module *dicee*), 195
random_prediction () (in module *dicee.static_funcs*), 158
random_seed (*dicee.config.Namespace* attribute), 30
ratio (*dicee.callbacks.Perturb* attribute), 26
re (*dicee.DeCaL* attribute), 175
re (*dicee.models.clifford.DeCaL* attribute), 69
re (*dicee.models.DeCaL* attribute), 132
re_vocab (*dicee.evaluator.Evaluator* attribute), 47
read_from_disk () (in module *dicee.read_preprocess_save_load_kg.util*), 150
read_from_triple_store () (in module *dicee.read_preprocess_save_load_kg.util*), 150
read_only_few (*dicee.config.Namespace* attribute), 30
read_only_few (*dicee.knowledge_graph.KG* attribute), 50
read_or_load_kg () (in module *dicee*), 195
read_or_load_kg () (in module *dicee.static_funcs*), 158
read_with_pandas () (in module *dicee.read_preprocess_save_load_kg.util*), 150
read_with_polars () (in module *dicee.read_preprocess_save_load_kg.util*), 150
ReadFromDisk (class in *dicee.read_preprocess_save_load_kg*), 152
ReadFromDisk (class in *dicee.read_preprocess_save_load_kg.read_from_disk*), 147
reducer (*dicee.scripts.index_serve.StringListRequest* attribute), 155
rel2id (*dicee.query_generator.QueryGenerator* attribute), 145
rel2id (*dicee.QueryGenerator* attribute), 215
relation_embeddings (*dicee.AConvQ* attribute), 181

- relation_embeddings (*dicee.ConvQ* attribute), 182
- relation_embeddings (*dicee.DeCaL* attribute), 175
- relation_embeddings (*dicee.DualE* attribute), 178
- relation_embeddings (*dicee.LFMult* attribute), 187
- relation_embeddings (*dicee.models.AConvQ* attribute), 121
- relation_embeddings (*dicee.models.clifford.DeCaL* attribute), 69
- relation_embeddings (*dicee.models.ConvQ* attribute), 121
- relation_embeddings (*dicee.models.DeCaL* attribute), 132
- relation_embeddings (*dicee.models.DualE* attribute), 144
- relation_embeddings (*dicee.models.dualE.DualE* attribute), 75
- relation_embeddings (*dicee.models.FMult* attribute), 140
- relation_embeddings (*dicee.models.FMult2* attribute), 142
- relation_embeddings (*dicee.models.function_space.FMult* attribute), 77
- relation_embeddings (*dicee.models.function_space.FMult2* attribute), 78
- relation_embeddings (*dicee.models.function_space.GFMult* attribute), 77
- relation_embeddings (*dicee.models.function_space.LFMult* attribute), 79
- relation_embeddings (*dicee.models.function_space.LFMult1* attribute), 78
- relation_embeddings (*dicee.models.GFMult* attribute), 141
- relation_embeddings (*dicee.models.LFMult* attribute), 142
- relation_embeddings (*dicee.models.LFMult1* attribute), 142
- relation_embeddings (*dicee.models.pykeen_models.PykeenKGE* attribute), 85
- relation_embeddings (*dicee.models.PykeenKGE* attribute), 137
- relation_embeddings (*dicee.models.quaternion.AConvQ* attribute), 88
- relation_embeddings (*dicee.models.quaternion.ConvQ* attribute), 88
- relation_embeddings (*dicee.PykeenKGE* attribute), 188
- relation_to_idx (*dicee.knowledge_graph.KG* attribute), 51
- relations_str (*dicee.knowledge_graph.KG* property), 51
- reload_dataset () (in module *dicee*), 202
- reload_dataset () (in module *dicee.dataset_classes*), 32
- report (*dicee.DICE_Trainer* attribute), 196
- report (*dicee.evaluator.Evaluator* attribute), 47
- report (*dicee.Execute* attribute), 201
- report (*dicee.executer.Execute* attribute), 48
- report (*dicee.trainer.DICE_Trainer* attribute), 166
- report (*dicee.trainer.dice_trainer.DICE_Trainer* attribute), 161
- reports (*dicee.callbacks.Eval* attribute), 25
- reports (*dicee.callbacks.PeriodicEvalCallback* attribute), 27
- requires_grad_for_interactions (*dicee.CKeci* attribute), 171
- requires_grad_for_interactions (*dicee.Keci* attribute), 172
- requires_grad_for_interactions (*dicee.models.CKeci* attribute), 131
- requires_grad_for_interactions (*dicee.models.clifford.CKeci* attribute), 68
- requires_grad_for_interactions (*dicee.models.clifford.Keci* attribute), 66
- requires_grad_for_interactions (*dicee.models.Keci* attribute), 128
- resid_dropout (*dicee.models.transformers.CausalSelfAttention* attribute), 94
- residual_convolution () (*dicee.AConEx* method), 180
- residual_convolution () (*dicee.AConvO* method), 181
- residual_convolution () (*dicee.AConvQ* method), 181
- residual_convolution () (*dicee.ConEx* method), 183
- residual_convolution () (*dicee.ConvO* method), 183
- residual_convolution () (*dicee.ConvQ* method), 182
- residual_convolution () (*dicee.models.AConEx* method), 115
- residual_convolution () (*dicee.models.AConvO* method), 127
- residual_convolution () (*dicee.models.AConvQ* method), 122
- residual_convolution () (*dicee.models.complex.AConEx* method), 73
- residual_convolution () (*dicee.models.complex.ConEx* method), 73
- residual_convolution () (*dicee.models.ConEx* method), 114
- residual_convolution () (*dicee.models.ConvO* method), 127
- residual_convolution () (*dicee.models.ConvQ* method), 121
- residual_convolution () (*dicee.models.octonion.AConvO* method), 84
- residual_convolution () (*dicee.models.octonion.ConvO* method), 84
- residual_convolution () (*dicee.models.quaternion.AConvQ* method), 89
- residual_convolution () (*dicee.models.quaternion.ConvQ* method), 88
- retrieve_embedding () (*dicee.scripts.index_serve.NeuralSearcher* method), 154
- retrieve_embeddings () (in module *dicee.scripts.index_serve*), 154
- return_multi_hop_query_results () (*dicee.KGE* method), 199
- return_multi_hop_query_results () (*dicee.knowledge_graph_embeddings.KGE* method), 54
- root () (in module *dicee.scripts.index_serve*), 154
- roots (*dicee.models.FMult* attribute), 141

roots (*dicее.models.function_space.FMult* attribute), 77
 roots (*dicее.models.function_space.GFMult* attribute), 77
 roots (*dicее.models.GFMult* attribute), 141
 runtime (*dicее.analyse_experiments.Experiment* attribute), 20

S

sample_counter (*dicее.abstracts.AbstractPPECallback* attribute), 17
 sample_entity() (*dicее.abstracts.BaseInteractiveKGE* method), 15
 sample_relation() (*dicее.abstracts.BaseInteractiveKGE* method), 15
 sample_triples_ratio (*dicее.config.Namespace* attribute), 30
 sample_triples_ratio (*dicее.knowledge_graph.KG* attribute), 50
 sampling_ratio (*dicее.dataset_classes.LiteralDataset* attribute), 43, 44
 sampling_ratio (*dicее.LiteralDataset* attribute), 213, 214
 sanity_checking_with_arguments() (in module *dicее.sanity_checkers*), 153
 save() (*dicее.abstracts.BaseInteractiveKGE* method), 15
 save() (*dicее.read_preprocess_save_load_kg.LoadSaveToDisk* method), 152
 save() (*dicее.read_preprocess_save_load_kg.save_load_disk.LoadSaveToDisk* method), 148
 save_checkpoint() (*dicее.abstracts.AbstractTrainer* static method), 13
 save_checkpoint_model() (in module *dicее*), 194
 save_checkpoint_model() (in module *dicее.static_funcs*), 158
 save_embeddings() (in module *dicее*), 195
 save_embeddings() (in module *dicее.static_funcs*), 158
 save_embeddings_as_csv (*dicее.config.Namespace* attribute), 28
 save_every_n_epochs (*dicее.config.Namespace* attribute), 31
 save_experiment() (*dicее.analyse_experiments.Experiment* method), 20
 save_model_at_every_epoch (*dicее.config.Namespace* attribute), 30
 save_model_every_n_epoch (*dicее.callbacks.PeriodicEvalCallback* attribute), 27
 save_numpy_ndarray() (in module *dicее*), 194
 save_numpy_ndarray() (in module *dicее.read_preprocess_save_load_kg.util*), 151
 save_numpy_ndarray() (in module *dicее.static_funcs*), 158
 save_pickle() (in module *dicее*), 194
 save_pickle() (in module *dicее.read_preprocess_save_load_kg.util*), 151
 save_pickle() (in module *dicее.static_funcs*), 158
 save_queries() (*dicее.query_generator.QueryGenerator* method), 146
 save_queries() (*dicее.QueryGenerator* method), 215
 save_queries_and_answers() (*dicее.query_generator.QueryGenerator* static method), 146
 save_queries_and_answers() (*dicее.QueryGenerator* static method), 216
 save_trained_model() (*dicее.Execute* method), 201
 save_trained_model() (*dicее.executer.Execute* method), 49
 scalar_batch_NN() (*dicее.LFMult* method), 187
 scalar_batch_NN() (*dicее.models.function_space.LFMult* method), 79
 scalar_batch_NN() (*dicее.models.LFMult* method), 143
 scaler (*dicее.callbacks.Perturb* attribute), 26
 scaler (*dicее.trainer.torch_trainer_ddp.NodeTrainer* attribute), 166
 scheduler (*dicее.callbacks.LRScheduler* attribute), 27
 score() (*dicее.ComplEx* static method), 180
 score() (*dicее.DistMult* method), 171
 score() (*dicее.Keci* method), 174
 score() (*dicее.models.clifford.Keci* method), 68
 score() (*dicее.models.ComplEx* static method), 116
 score() (*dicее.models.complex.ComplEx* static method), 74
 score() (*dicее.models.DistMult* method), 111
 score() (*dicее.models.Keci* method), 131
 score() (*dicее.models.octonion.OMult* method), 83
 score() (*dicее.models.OMult* method), 126
 score() (*dicее.models.QMult* method), 120
 score() (*dicее.models.quaternion.QMult* method), 87
 score() (*dicее.models.real.DistMult* method), 89
 score() (*dicее.models.real.TransE* method), 90
 score() (*dicее.models.TransE* method), 111
 score() (*dicее.OMult* method), 186
 score() (*dicее.QMult* method), 185
 score() (*dicее.TransE* method), 174
 score_func (*dicее.models.FMult2* attribute), 141
 score_func (*dicее.models.function_space.FMult2* attribute), 78
 scoring_technique (*dicее.analyse_experiments.Experiment* attribute), 20
 scoring_technique (*dicее.config.Namespace* attribute), 29

`search()` (*dicee.scripts.index_serve.NeuralSearcher method*), 154
`search_embeddings()` (*in module dicee.scripts.index_serve*), 154
`search_embeddings_batch()` (*in module dicee.scripts.index_serve*), 156
`seed` (*dicee.query_generator.QueryGenerator attribute*), 145
`seed` (*dicee.QueryGenerator attribute*), 215
`select_model()` (*in module dicee*), 194
`select_model()` (*in module dicee.static_funcs*), 158
`selected_optimizer` (*dicee.BaseKGE attribute*), 192
`selected_optimizer` (*dicee.models.base_model.BaseKGE attribute*), 63
`selected_optimizer` (*dicee.models.BaseKGE attribute*), 106, 109, 112, 117, 123, 136, 139
`separator` (*dicee.config.Namespace attribute*), 29
`separator` (*dicee.knowledge_graph.KG attribute*), 51
`sequential_vocabulary_construction()` (*dicee.read_preprocess_save_load_kg.PreprocessKG method*), 152
`sequential_vocabulary_construction()` (*dicee.read_preprocess_save_load_kg.preprocess.PreprocessKG method*), 147
`serve()` (*in module dicee.scripts.index_serve*), 156
`set_global_seed()` (*dicee.query_generator.QueryGenerator method*), 145
`set_global_seed()` (*dicee.QueryGenerator method*), 215
`set_model_eval_mode()` (*dicee.abstracts.BaseInteractiveKGE method*), 14
`set_model_train_mode()` (*dicee.abstracts.BaseInteractiveKGE method*), 14
`setup()` (*dicee.CVDataModule method*), 210
`setup()` (*dicee.dataset_classes.CVDataModule method*), 41
`setup_executor()` (*dicee.Execute method*), 201
`setup_executor()` (*dicee.executer.Execute method*), 49
`Shallom` (*class in dicee*), 186
`Shallom` (*class in dicee.models*), 111
`Shallom` (*class in dicee.models.real*), 90
`shallom` (*dicee.models.real.Shallom attribute*), 90
`shallom` (*dicee.models.Shallom attribute*), 111
`shallom` (*dicee.Shallom attribute*), 186
`single_hop_query_answering()` (*dicee.KGE method*), 199
`single_hop_query_answering()` (*dicee.knowledge_graph_embeddings.KGE method*), 54
`snapshot_dir` (*dicee.callbacks.LRScheduler attribute*), 27
`snapshot_loss` (*dicee.callbacks.LRScheduler attribute*), 28
`sparql_endpoint` (*dicee.config.Namespace attribute*), 28
`sparql_endpoint` (*dicee.knowledge_graph.KG attribute*), 50
`start()` (*dicee.DICE_Trainer method*), 196
`start()` (*dicee.Execute method*), 201
`start()` (*dicee.executer.Execute method*), 49
`start()` (*dicee.read_preprocess_save_load_kg.PreprocessKG method*), 151
`start()` (*dicee.read_preprocess_save_load_kg.preprocess.PreprocessKG method*), 146
`start()` (*dicee.read_preprocess_save_load_kg.read_from_disk.ReadFromDisk method*), 147
`start()` (*dicee.read_preprocess_save_load_kg.ReadFromDisk method*), 152
`start()` (*dicee.trainer.DICE_Trainer method*), 167
`start()` (*dicee.trainer.dice_trainer.DICE_Trainer method*), 162
`start_time` (*dicee.callbacks.PrintCallback attribute*), 21
`start_time` (*dicee.Execute attribute*), 201
`start_time` (*dicee.executer.Execute attribute*), 48
`step()` (*dicee.EnsembleKGE method*), 194
`step()` (*dicee.models.ADOPT method*), 99
`step()` (*dicee.models.adopt.ADOPT method*), 56
`step()` (*dicee.models.ensemble.EnsembleKGE method*), 76
`step_count` (*dicee.callbacks.LRScheduler attribute*), 28
`storage_path` (*dicee.config.Namespace attribute*), 28
`storage_path` (*dicee.DICE_Trainer attribute*), 196
`storage_path` (*dicee.trainer.DICE_Trainer attribute*), 166
`storage_path` (*dicee.trainer.dice_trainer.DICE_Trainer attribute*), 162
`store()` (*in module dicee*), 194
`store()` (*in module dicee.static_funcs*), 158
`store_ensemble()` (*dicee.abstracts.AbstractPPECallback method*), 18
`strategy` (*dicee.abstracts.AbstractTrainer attribute*), 13
`StringListRequest` (*class in dicee.scripts.index_serve*), 154
`swa` (*dicee.config.Namespace attribute*), 30
`swa_start_epoch` (*dicee.config.Namespace attribute*), 31

T

`T()` (*dicee.DualE method*), 179
`T()` (*dicee.models.DualE method*), 144

`T()` (*dicее.models.dualE.DualE method*), 76
`t_conorm()` (*dicее.abstracts.InteractiveQueryDecomposition method*), 16
`t_norm()` (*dicее.abstracts.InteractiveQueryDecomposition method*), 16
`target_dim` (*dicее.AllvsAll attribute*), 205
`target_dim` (*dicее.dataset_classes.AllvsAll attribute*), 36
`target_dim` (*dicее.dataset_classes.MultiLabelDataset attribute*), 33
`target_dim` (*dicее.dataset_classes.OnevsAllDataset attribute*), 34
`target_dim` (*dicее.knowledge_graph.KG attribute*), 51
`target_dim` (*dicее.MultiLabelDataset attribute*), 203
`target_dim` (*dicее.OnevsAllDataset attribute*), 204
`temperature` (*dicее.BytE attribute*), 189
`temperature` (*dicее.models.transformers.BytE attribute*), 92
`tensor_t_norm()` (*dicее.abstracts.InteractiveQueryDecomposition method*), 16
`TensorParallel` (class in *dicее.trainer.model_parallelism*), 163
`test_data_loader()` (*dicее.models.base_model.BaseKGELightning method*), 59
`test_data_loader()` (*dicее.models.BaseKGELightning method*), 101
`test_epoch_end()` (*dicее.models.base_model.BaseKGELightning method*), 59
`test_epoch_end()` (*dicее.models.BaseKGELightning method*), 101
`test_h1` (*dicее.analyse_experiments.Experiment attribute*), 20
`test_h3` (*dicее.analyse_experiments.Experiment attribute*), 20
`test_h10` (*dicее.analyse_experiments.Experiment attribute*), 20
`test_mrr` (*dicее.analyse_experiments.Experiment attribute*), 20
`test_path` (*dicее.query_generator.QueryGenerator attribute*), 145
`test_path` (*dicее.QueryGenerator attribute*), 215
`timeit()` (in module *dicее*), 194, 202
`timeit()` (in module *dicее.read_preprocess_save_load_kg.util*), 150
`timeit()` (in module *dicее.static_funcs*), 158
`timeit()` (in module *dicее.static_preprocess_funcs*), 160
`to()` (*dicее.EnsembleKGE method*), 194
`to()` (*dicее.KGE method*), 197
`to()` (*dicее.knowledge_graph_embeddings.KGE method*), 52
`to()` (*dicее.models.ensemble.EnsembleKGE method*), 76
`to_df()` (*dicее.analyse_experiments.Experiment method*), 20
`topk` (*dicее.BytE attribute*), 189
`topk` (*dicее.models.transformers.BytE attribute*), 92
`topk` (*dicее.scripts.index_serve.NeuralSearcher attribute*), 154
`torch_ordered_shaped_bpe_entities` (*dicее.dataset_classes.MultiLabelDataset attribute*), 33
`torch_ordered_shaped_bpe_entities` (*dicее.MultiLabelDataset attribute*), 203
`TorchDDPTrainer` (class in *dicее.trainer.torch_trainer_ddp*), 165
`TorchTrainer` (class in *dicее.trainer.torch_trainer*), 164
`total_epochs` (*dicее.callbacks.LRScheduler attribute*), 27
`total_steps` (*dicее.callbacks.LRScheduler attribute*), 27
`train()` (*dicее.abstracts.BaseInteractiveTrainKGE method*), 18
`train()` (*dicее.trainer.torch_trainer_ddp.NodeTrainer method*), 166
`train_data` (*dicее.AllvsAll attribute*), 205
`train_data` (*dicее.dataset_classes.AllvsAll attribute*), 35
`train_data` (*dicее.dataset_classes.KvsAll attribute*), 35
`train_data` (*dicее.dataset_classes.KvsSampleDataset attribute*), 38
`train_data` (*dicее.dataset_classes.MultiClassClassificationDataset attribute*), 33
`train_data` (*dicее.dataset_classes.OnevsAllDataset attribute*), 34
`train_data` (*dicее.dataset_classes.OnevsSample attribute*), 36, 37
`train_data` (*dicее.KvsAll attribute*), 204
`train_data` (*dicее.KvsSampleDataset attribute*), 208
`train_data` (*dicее.MultiClassClassificationDataset attribute*), 203
`train_data` (*dicее.OnevsAllDataset attribute*), 204
`train_data` (*dicее.OnevsSample attribute*), 206
`train_data_loader()` (*dicее.CVDDataModule method*), 210
`train_data_loader()` (*dicее.dataset_classes.CVDDataModule method*), 40
`train_data_loader()` (*dicее.models.base_model.BaseKGELightning method*), 60
`train_data_loader()` (*dicее.models.BaseKGELightning method*), 103
`train_data_loaders` (*dicее.trainer.torch_trainer.TorchTrainer attribute*), 164
`train_dataset_loader` (*dicее.trainer.torch_trainer_ddp.NodeTrainer attribute*), 166
`train_file_path` (*dicее.dataset_classes.LiteralDataset attribute*), 43, 44
`train_file_path` (*dicее.LiteralDataset attribute*), 213, 214
`train_h1` (*dicее.analyse_experiments.Experiment attribute*), 19
`train_h3` (*dicее.analyse_experiments.Experiment attribute*), 19
`train_h10` (*dicее.analyse_experiments.Experiment attribute*), 19
`train_indices_target` (*dicее.dataset_classes.MultiLabelDataset attribute*), 33

train_indices_target (*dicee.MultiLabelDataset* attribute), 203
 train_k_vs_all () (*dicee.abstracts.BaseInteractiveTrainKGE* method), 18
 train_literals () (*dicee.abstracts.BaseInteractiveTrainKGE* method), 18
 train_mode (*dicee.EnsembleKGE* attribute), 193
 train_mode (*dicee.models.ensemble.EnsembleKGE* attribute), 76
 train_mrr (*dicee.analyse_experiments.Experiment* attribute), 19
 train_path (*dicee.query_generator.QueryGenerator* attribute), 145
 train_path (*dicee.QueryGenerator* attribute), 215
 train_set (*dicee.BPE_NegativeSamplingDataset* attribute), 202
 train_set (*dicee.dataset_classes.BPE_NegativeSamplingDataset* attribute), 32
 train_set (*dicee.dataset_classes.MultiLabelDataset* attribute), 33
 train_set (*dicee.dataset_classes.NegSampleDataset* attribute), 38
 train_set (*dicee.dataset_classes.TriplePredictionDataset* attribute), 39
 train_set (*dicee.MultiLabelDataset* attribute), 203
 train_set (*dicee.NegSampleDataset* attribute), 208
 train_set (*dicee.TriplePredictionDataset* attribute), 209
 train_set_idx (*dicee.CVDataModule* attribute), 210
 train_set_idx (*dicee.dataset_classes.CVDataModule* attribute), 40
 train_set_target (*dicee.knowledge_graph.KG* attribute), 51
 train_target (*dicee.AllvsAll* attribute), 205
 train_target (*dicee.dataset_classes.AllvsAll* attribute), 35
 train_target (*dicee.dataset_classes.KvsAll* attribute), 35
 train_target (*dicee.dataset_classes.KvsSampleDataset* attribute), 38
 train_target (*dicee.KvsAll* attribute), 205
 train_target (*dicee.KvsSampleDataset* attribute), 208
 train_target_indices (*dicee.knowledge_graph.KG* attribute), 51
 train_triples () (*dicee.abstracts.BaseInteractiveTrainKGE* method), 18
 trained_model (*dicee.Execute* attribute), 201
 trained_model (*dicee.executer.Execute* attribute), 48
 trainer (*dicee.config.Namespace* attribute), 29
 trainer (*dicee.DICE_Trainer* attribute), 196
 trainer (*dicee.Execute* attribute), 201
 trainer (*dicee.executer.Execute* attribute), 48
 trainer (*dicee.trainer.DICE_Trainer* attribute), 166
 trainer (*dicee.trainer.dice_trainer.DICE_Trainer* attribute), 161
 trainer (*dicee.trainer.torch_trainer_ddp.NodeTrainer* attribute), 165
 training_step (*dicee.trainer.torch_trainer.TorchTrainer* attribute), 164
 training_step () (*dicee.BytE* method), 190
 training_step () (*dicee.models.base_model.BaseKGELightning* method), 57
 training_step () (*dicee.models.BaseKGELightning* method), 100
 training_step () (*dicee.models.transformers.BytE* method), 92
 training_step_outputs (*dicee.models.base_model.BaseKGELightning* attribute), 57
 training_step_outputs (*dicee.models.BaseKGELightning* attribute), 100
 training_technique (*dicee.knowledge_graph.KG* attribute), 51
 TransE (*class in dicee*), 174
 TransE (*class in dicee.models*), 111
 TransE (*class in dicee.models.real*), 89
 transfer_batch_to_device () (*dicee.CVDataModule* method), 211
 transfer_batch_to_device () (*dicee.dataset_classes.CVDataModule* method), 41
 transformer (*dicee.BytE* attribute), 189
 transformer (*dicee.models.transformers.BytE* attribute), 92
 transformer (*dicee.models.transformers.GPT* attribute), 97
 trapezoid () (*dicee.models.FMult2* method), 142
 trapezoid () (*dicee.models.function_space.FMult2* method), 78
 tri_score () (*dicee.LFMult* method), 187
 tri_score () (*dicee.models.function_space.LFMult* method), 79
 tri_score () (*dicee.models.function_space.LFMult1* method), 79
 tri_score () (*dicee.models.LFMult* method), 143
 tri_score () (*dicee.models.LFMult1* method), 142
 triple_score () (*dicee.KGE* method), 199
 triple_score () (*dicee.knowledge_graph_embeddings.KGE* method), 53
 TriplePredictionDataset (*class in dicee*), 208
 TriplePredictionDataset (*class in dicee.dataset_classes*), 39
 tuple2list () (*dicee.query_generator.QueryGenerator* method), 145
 tuple2list () (*dicee.QueryGenerator* method), 215

U

`unlabelled_size` (*dicee.callbacks.PseudoLabellingCallback attribute*), 23
`unmap()` (*dicee.query_generator.QueryGenerator method*), 145
`unmap()` (*dicee.QueryGenerator method*), 215
`unmap_query()` (*dicee.query_generator.QueryGenerator method*), 145
`unmap_query()` (*dicee.QueryGenerator method*), 215

V

`val_aswa` (*dicee.callbacks.ASWA attribute*), 24
`val_dataloader()` (*dicee.models.base_model.BaseKGELighting method*), 59
`val_dataloader()` (*dicee.models.BaseKGELighting method*), 102
`val_h1` (*dicee.analyse_experiments.Experiment attribute*), 20
`val_h3` (*dicee.analyse_experiments.Experiment attribute*), 20
`val_h10` (*dicee.analyse_experiments.Experiment attribute*), 20
`val_mrr` (*dicee.analyse_experiments.Experiment attribute*), 19
`val_path` (*dicee.query_generator.QueryGenerator attribute*), 145
`val_path` (*dicee.QueryGenerator attribute*), 215
`validate_knowledge_graph()` (in module *dicee.sanity_checkers*), 153
`vocab_preparation()` (*dicee.evaluator.Evaluator method*), 47
`vocab_size` (*dicee.models.transformers.GPTConfig attribute*), 96
`vocab_to_parquet()` (in module *dicee*), 195
`vocab_to_parquet()` (in module *dicee.static_funcs*), 159
`vtp_score()` (*dicee.LFMulti method*), 187
`vtp_score()` (*dicee.models.function_space.LFMulti method*), 79
`vtp_score()` (*dicee.models.function_space.LFMulti1 method*), 79
`vtp_score()` (*dicee.models.LFMulti method*), 143
`vtp_score()` (*dicee.models.LFMulti1 method*), 142

W

`warmup_steps` (*dicee.callbacks.LRScheduler attribute*), 27
`weight` (*dicee.models.transformers.LayerNorm attribute*), 93
`weight_decay` (*dicee.BaseKGE attribute*), 192
`weight_decay` (*dicee.config.Namespace attribute*), 29
`weight_decay` (*dicee.models.base_model.BaseKGE attribute*), 63
`weight_decay` (*dicee.models.BaseKGE attribute*), 106, 109, 112, 117, 123, 136, 139
`weights` (*dicee.models.FMulti attribute*), 141
`weights` (*dicee.models.function_space.FMulti attribute*), 77
`weights` (*dicee.models.function_space.GFMulti attribute*), 78
`weights` (*dicee.models.GFMulti attribute*), 141
`write_csv_from_model_parallel()` (in module *dicee*), 195
`write_csv_from_model_parallel()` (in module *dicee.static_funcs*), 159
`write_links()` (*dicee.query_generator.QueryGenerator method*), 145
`write_links()` (*dicee.QueryGenerator method*), 215
`write_report()` (*dicee.Execute method*), 201
`write_report()` (*dicee.executer.Execute method*), 49

X

`x_values` (*dicee.LFMulti attribute*), 187
`x_values` (*dicee.models.function_space.LFMulti attribute*), 79
`x_values` (*dicee.models.LFMulti attribute*), 142