
DICE Embeddings

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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	160
14.3	Classes	160
14.4	Functions	161
14.5	Package Contents	163
	Python Module Index	208

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

1 Dicee Manual

Version: dicee 0.1.3.2

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

Publisher and maintainer: Caglar Demir²

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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	201	82	59%	104-105, 107-108, 110-111, 113-114, 116-117, 119-120, 122-123, 125-126, 128-129, 131-132, 134-135, 137-138, 140-141, 143-144, 146-147, 149-150, 152-153, 155-156, 158-159, 161-162, 164-165, 167-168, 170-171, 173-174, 176-177, 179-180, 182-183, 185-186, 188-189, 191-192, 194-195, 197-198, 200-201, 203-204, 206-207, 209-210, 212-213, 215-216, 218-219, 221-222, 224-225, 227-228, 230-231, 233-234, 236-237, 239-240, 242-243, 245-246, 248-249, 251-252, 254-255, 257-258, 260-261, 263-264, 266-267, 269-270, 272-273, 275-276, 278-279, 281-282, 284-285, 287-288, 290-291, 293-294, 296-297, 299-300, 302-303, 305-306, 308-309, 311-312, 314-315, 317-318, 320-321, 323-324, 326-327, 329-330, 332-333, 335-336, 338-339, 341-342, 344-345, 347-348, 350-351, 353-354, 356-357, 359-360, 362-363, 365-366, 368-369, 371-372, 374-375, 377-378, 380-381, 383-384, 386-387, 389-390, 392-393, 395-396, 398-399, 401-402, 404-405, 407-408, 410-411, 413-414, 416-417, 419-420, 422-423, 425-426, 428-429, 431-432, 434-435, 437-438, 440-441, 443-444, 446-447, 449-450, 452-453, 455-456, 458-459, 461-462, 464-465, 467-468, 470-471, 473-474, 476-477, 479-480, 482-483, 485-486, 488-489, 491-492, 494-495, 497-498, 500-501, 503-504, 506-507, 509-510, 512-513, 515-516, 518-519, 521-522, 524-525, 527-528, 530-531, 533-534, 536-537, 539-540, 542-543, 545-546, 548-549, 551-552, 554-555, 557-558, 560-561, 563-564, 566-567, 569-570, 572-573, 575-576, 578-579, 581-582, 584-585, 587-588, 590-591, 593-594, 596-597, 599-600, 602-603, 605-606, 608-609, 611-612, 614-615, 617-618, 620-621, 623-624, 626-627, 629-630, 632-633, 635-636, 638-639, 641-642, 644-645, 647-648, 650-651, 653-654, 656-657, 659-660, 662-663, 665-666, 668-669, 671-672, 674-675, 677-678, 680-681, 683-684, 686-687, 689-690, 692-693, 695-696, 698-699, 701-702, 704-705, 707-708, 710-711, 713-714, 716-717, 719-720, 722-723, 725-726, 728-729, 731-732, 734-735, 737-738, 740-741, 743-744, 746-747, 749-750, 752-753, 755-756, 758-759, 761-762, 764-765, 767-768, 770-771, 773-774, 776-777, 779-780, 782-783, 785-786, 788-789, 791-792, 794-795, 797-798, 800-801, 803-804, 806-807, 809-810, 812-813, 815-816, 818-819, 821-822, 824-825, 827-828, 830-831, 833-834, 836-837, 839-840, 842-843, 845-846, 848-849, 851-852, 854-855, 857-858, 860-861, 863-864, 866-867, 869-870, 872-873, 875-876, 878-879, 881-882, 884-885, 887-888, 890-891, 893-894, 896-897, 899-900, 902-903, 905-906, 908-909, 911-912, 914-915, 917-918, 920-921, 923-924, 926-927, 929-930, 932-933, 935-936, 938-939, 941-942, 944-945, 947-948, 950-951, 953-954, 956-957, 959-960, 962-963, 965-966, 968-969, 971-972, 974-975, 977-978, 980-981, 983-984, 986-987, 989-990, 992-993, 995-996, 998-999

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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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```
→123, 146-147, 152, 165, 197, 240-254, 257-260, 263-266, 301, 314-317, 320-324, 364-  
→375, 390-398, 413, 424-428, 555-575, 581-585, 589-591  
dicee/callbacks.py 245 102 58% 50-55,   
→67-73, 76, 88-93, 98-103, 106-109, 116-133, 138-142, 146-147, 276-280, 286-287, 305-  
→311, 314, 319-320, 332-338, 344-353, 358-360, 405, 416-429, 433-468, 480-486  
dicee/config.py 93 2 98% 141-142  
dicee/dataset_classes.py 299 74 75% 41, 54,   
→87, 93, 99-106, 109, 112, 115-139, 195-201, 204, 207-209, 314, 325-328, 344, 410-  
→411, 429, 528-536, 539, 543-557, 700-707, 710-714  
dicee/eval_static_funcs.py 227 95 58% 101, 106,  
→ 111, 258-353, 360-411  
dicee/evaluator.py 262 51 81% 46, 51,   
→56, 84, 89-90, 93, 109, 126, 137, 141, 146, 177-188, 195-206, 314, 344-367, 455,   
→465, 482-487  
dicee/executer.py 113 4 96% 116, 258-  
→259, 291  
dicee/knowledge_graph.py 65 3 95% 79, 110,   
→114  
dicee/knowledge_graph_embeddings.py 636 443 30% 27, 30-  
→31, 39-52, 57-90, 93-127, 131-139, 170-184, 215-228, 254-274, 324-327, 330-333, 346,  
→ 381-426, 484-486, 502-503, 509-517, 522-525, 528-533, 538, 547, 592-598, 630, 688-  
→1053, 1084-1145, 1149-1177, 1200, 1227-1265  
dicee/models/__init__.py 9 0 100%  
dicee/models/base_model.py 234 31 87% 54, 56,   
→82, 88-103, 157, 190, 230, 236, 245, 248, 252, 259, 263, 265, 280, 288-289, 296-297,  
→ 351, 354, 427, 439  
dicee/models/clifford.py 556 357 36% 31-42,   
→68-117, 122-133, 156-168, 190-220, 235, 237, 241, 248-249, 276-280, 303-311, 325-  
→327, 332-333, 364-384, 406, 413, 417-478, 495-499, 511, 514, 519, 524, 571-607, 625-  
→631, 644, 647, 652, 657, 686-692, 705, 708, 713, 718, 728-737, 753-754, 774-845,   
→856-859, 884-909, 933-966, 1002-1006, 1019, 1029, 1032, 1037, 1042, 1047, 1051,   
→1055, 1064-1065, 1095, 1102, 1107, 1135-1139, 1167-1176, 1186-1194, 1212-1214, 1232-  
→1234, 1250-1252  
dicee/models/complex.py 151 15 90% 86-109  
dicee/models/dualE.py 59 10 83% 93-102,   
→142-156  
dicee/models/function_space.py 262 221 16% 10-24,   
→28-37, 40-49, 53-70, 77-86, 89-98, 101-110, 114-126, 134-156, 159-165, 168-185, 188-  
→194, 197-205, 208, 213-234, 243-246, 250-254, 258-267, 271-292, 301-307, 311-328,   
→332-335, 344-352, 355, 366-372, 392-406, 424-438, 443-453, 461-465, 474-478  
dicee/models/octonion.py 227 83 63% 21-44,   
→320-329, 334-345, 348-370, 374-416, 426-474  
dicee/models/pykeen_models.py 50 5 90% 60-63,   
→118  
dicee/models/quaternion.py 192 69 64% 7-21, 30-  
→55, 68-72, 107, 185, 328-342, 345-364, 368-389, 399-426  
dicee/models/real.py 61 12 80% 36-39,   
→66-69, 87, 103-106  
dicee/models/static_funcs.py 10 0 100%  
dicee/models/transformers.py 236 189 20% 24-43,   
→46, 60-75, 84-102, 105-116, 123-125, 128, 134-151, 155-180, 186-190, 193-197, 203-  
→207, 210-212, 229-256, 265-268, 271-276, 279-304, 310-315, 319-372, 376-398, 404-414
```

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(continued from previous page)

dicee/query_generator.py	374	346	7%	18-52, ↪
↪56, 62-65, 69-70, 78-92, 100-147, 155-188, 192-206, 212-269, 274-303, 307-443, 453-↪472, 480-501, 508-512, 517, 522-528				
dicee/read_preprocess_save_load_kg/___init___py	3	0	100%	
dicee/read_preprocess_save_load_kg/preprocess.py	256	41	84%	34, 40, ↪
↪78, 102-127, 133, 138-151, 184, 214, 388-389, 444				
dicee/read_preprocess_save_load_kg/read_from_disk.py	36	11	69%	33, 38-↪40, 47, 55, 58-72
dicee/read_preprocess_save_load_kg/save_load_disk.py	45	18	60%	39-60
dicee/read_preprocess_save_load_kg/util.py	219	126	42%	65-67, ↪
↪72-73, 91-97, 100-102, 107-109, 121, 134, 140-143, 148-156, 161-167, 172-177, 182-↪187, 199-220, 226-282, 286-290, 294-295, 299, 303-304, 334, 351, 356, 363-364				
dicee/sanity_checkers.py	54	23	57%	8-12, 21-↪31, 46, 51, 58, 64-79, 85, 89, 96
dicee/static_funcs.py	418	163	61%	40, 50, ↪
↪56-61, 83, 105-106, 115, 138, 152, 157-159, 163-165, 167, 194-198, 246, 254, 263-↪268, 290-304, 316-336, 340-357, 362, 386-387, 392-393, 410-411, 413-414, 416-417, ↪				
↪419-420, 428, 446-450, 467-470, 474-479, 483-487, 491-492, 498-500, 526-527, 539-↪542, 547-550, 559-610, 615-627, 644-658, 661-669				
dicee/static_funcs_training.py	123	63	49%	118-215, ↪
↪223-224				
dicee/static_preprocess_funcs.py	100	44	56%	17-25, ↪
↪52, 56, 64, 67, 78, 91-115, 120-123, 128-131, 136-139				
dicee/trainer/___init___py	1	0	100%	
dicee/trainer/dice_trainer.py	126	13	90%	27-32, ↪
↪91, 98, 103-108, 147				
dicee/trainer/torch_trainer.py	79	4	95%	31, 196, ↪
↪207-208				
dicee/trainer/torch_trainer_ddp.py	152	128	16%	13-14, ↪
↪43, 47-72, 83-112, 131-137, 140-149, 164-194, 204-217, 226-246, 251-260, 263-272, ↪				
↪275-299, 302-309				

TOTAL	6181	2828	54%	

13 How to cite

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

```
# Keci
@inproceedings{demir2023clifford,
  title={Clifford Embeddings--A Generalized Approach for Embedding in Normed Algebras}
  ↪,
  author={Demir, Caglar and Ngonga Ngomo, Axel-Cyrille},
  booktitle={Joint European Conference on Machine Learning and Knowledge Discovery in ↪
  ↪Databases},
  pages={567--582},
  year={2023},
  organization={Springer}
}
# LitCQD
```

(continues on next page)

```

@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}}
# Shallow
@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>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

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

apply_semantic_constraint

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.**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

dicee.analyse_experiments

This script should be moved to dicee/scripts

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

Functions

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

Module Contents

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

Bases: *dicee.abstracts.AbstractCallback*

Abstract class for Callback class for knowledge graph embedding models

Parameter

path

on_fit_end (*trainer, model*) → None

Store epoch loss

Parameter

trainer:

model:

rtype

None

class dicee.callbacks.**PrintCallback**

Bases: *dicee.abstracts.AbstractCallback*

Abstract class for Callback class for knowledge graph embedding models

Parameter

start_time

on_fit_start (*trainer, pl_module*)

Call at the beginning of the training.

Parameter

trainer:

model:

rtype

None

on_fit_end (*trainer, pl_module*)

Call at the end of the training.

Parameter

trainer:

model:

rtype

None

on_train_batch_end (**args, **kwargs*)

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

Parameter

trainer:

model:

rtype
None

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

Parameter

trainer:

model:

rtype
None

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

Bases: *dicee.abstracts.AbstractCallback*

Abstract class for Callback class for knowledge graph embedding models

Parameter

every_x_epoch

max_epochs

epoch_counter = 0

path

on_train_batch_end (*args, **kwargs)
Call at the end of each mini-batch during the training.

Parameter

trainer:

model:

rtype
None

on_fit_start (trainer, pl_module)
Call at the beginning of the training.

Parameter

trainer:

model:

rtype
None

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

Parameter

trainer:

model:

rtype

None

on_fit_end (*args, **kwargs)

Call at the end of the training.

Parameter

trainer:

model:

rtype

None

on_epoch_end (model, trainer, **kwargs)

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

Bases: *dicee.abstracts.AbstractCallback*

Abstract class for Callback class for knowledge graph embedding models

Parameter

data_module

kg

num_of_epochs = 0

unlabelled_size

batch_size

create_random_data ()

on_epoch_end (trainer, model)

`dicee.callbacks.estimate_q` (eps)

estimate rate of convergence q from sequence esp

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

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

Bases: *dicee.abstracts.AbstractCallback*

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

path

num_epochs

initial_eval_setting = None

```
epoch_count = 0

alphas = []

val_aswa

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

```
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 match :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

ratio

method

scaler

frequency

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

Called when the train batch begins.

dicee.config

Classes

Namespace

Simple object for storing attributes.

Module Contents

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

Bases: argparse.Namespace

Simple object for storing attributes.

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

```
dataset_dir: str = None
```

The path of a folder containing train.txt, and/or valid.txt and/or test.txt

```
save_embeddings_as_csv: bool = False
```

Embeddings of entities and relations are stored into CSV files to facilitate easy usage.

```
storage_path: str = 'Experiments'
```

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

```
path_to_store_single_run: str = None
```

A single directory created that contains related data about embeddings.

```
path_single_kg = None
```

Path of a file corresponding to the input knowledge graph

```
sparql_endpoint = None
```

An endpoint of a triple store.

```
model: str = 'Keci'
```

KGE model

```
optim: str = 'Adam'
```

Optimizer

```
embedding_dim: int = 64
```

Size of continuous vector representation of an entity/relation

```
num_epochs: int = 150
```

Number of pass over the training data

```
batch_size: int = 1024
```

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

```
lr: float = 0.1
```

Learning rate

```
add_noise_rate: float = None
```

The ratio of added random triples into training dataset

```
gpus = None
```

Number GPUs to be used during training

```
callbacks
```

```
10}}
```

Type

Callbacks, e.g., {“PPE”

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

__iter__()

```

dicee.dataset_classes

Classes

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

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

num_of_data_points

collate_fn = None

__len__()

__getitem__(idx)

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

Bases: torch.utils.data.Dataset

Dataset for the 1vsALL training strategy

Parameters

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

Return type

torch.utils.data.Dataset

train_data

target_dim

collate_fn = None

__len__()

__getitem__(idx)

class dicee.dataset_classes.**KvsAll** (train_set_idx: numpy.ndarray, entity_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 $[0, 1]^{|IE|}$ 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.dataset_classes.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 : denotes a multi-label vector in $[0, 1]^{|E|}$ is a binary label.

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

Note

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

train_set_idx

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

entity_idx

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

relation_idx

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

self : torch.utils.data.Dataset

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

train_data = None

train_target = None

label_smoothing_rate

collate_fn = None

target_dim

__len__()

__getitem__(idx)

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

Bases: torch.utils.data.Dataset

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

Parameters

- **train_set** (*np.ndarray*) – A numpy array containing triples of knowledge graph data. Each triple consists of (head_entity, relation, tail_entity).
- **num_entities** (*int*) – The number of unique entities in the knowledge graph.
- **num_relations** (*int*) – The number of unique relations in the knowledge graph.
- **neg_sample_ratio** (*int, optional*) – The number of negative samples to be generated per positive sample. Must be a positive integer and less than num_entities.
- **label_smoothing_rate** (*float, optional*) – A label smoothing rate to apply to the positive and negative labels. Defaults to 0.0.

train_data

The input data converted into a PyTorch tensor.

Type

torch.Tensor

num_entities

Number of entities in the dataset.

Type

int

num_relations

Number of relations in the dataset.

Type

int

neg_sample_ratio

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

Type

int

label_smoothing_rate

The smoothing factor applied to the labels.

Type

torch.Tensor

collate_fn

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

Type

function, optional

train_data

num_entities

num_relations

neg_sample_ratio

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.

or all $y_i = 1$ 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 $\sum(y) < \text{neg_sample_ratio}$ new_y contains

train_set_idx

Indexed triples for the training.

entity_idxes

mapping.

relation_idxes

mapping.

form

?

store

?

label_smoothing_rate

?

torch.utils.data.Dataset

train_data = None

train_target = None

neg_ratio

num_entities

label_smoothing_rate

collate_fn = None

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:
    or all (h,r,t) in G obtain, create negative triples{(h,r,x),(r,t),(h,m,t)}
    y:labels are represented in torch.float16

    train_set_idx
        Indexed triples for the training.

    entity_idx
        mapping.

    relation_idx
        mapping.

    form
        ?

    store
        ?

    label_smoothing_rate

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

label_smoothing_rate

neg_sample_ratio

train_set

length

num_entities

num_relations

__len__()

```

`__getitem__(idx)`

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

```
class dicee.dataset_classes.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()
```

dicee.eval_static_funcs

Functions

```
evaluate_link_prediction_performance(→
Dict)
evaluate_link_prediction_performance_with_
evaluate_link_prediction_performance_with_
evaluate_link_prediction_performance_with_
...)
evaluate_lp_bpe_k_vs_all(model, triples[,
er_vocab, ...])
```

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.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
```

```
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

trainer = None

trained_model = None

knowledge_graph = None

report

evaluator = None

start_time = None

setup_executor() → None

dept_read_preprocess_index_serialize_data() → None

Read & Preprocess & Index & Serialize Input Data

- (1) Read or load the data from disk into memory.
- (2) Store the statistics of the data.

Parameter

rtype

None

save_trained_model() → None

Save a knowledge graph embedding model

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

Parameter

rtype

None

end (*form_of_labelling: str*) → dict

End training

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

Parameter

rtype

A dict containing information about the training and/or evaluation

write_report () → None

Report training related information in a report.json file

start () → dict

Start training

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

Parameter

rtype

A dict containing information about the training and/or evaluation

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

Bases: *Execute*

A subclass of Execute Class for retraining

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

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

continual_start () → dict

Start Continual Training

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

Parameter

rtype

A dict containing information about the training and/or evaluation

dicee.knowledge_graph

Classes

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

Module Contents

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

Knowledge Graph

dataset_dir

sparql_endpoint

path_single_kg

byte_pair_encoding

ordered_shaped_bpe_tokens = None

add_noise_rate

num_entities = None

num_relations = None

path_for_deserialization

add_reciprocal

eval_model

read_only_few

sample_triples_ratio

path_for_serialization

entity_to_idx

relation_to_idx

backend

training_technique

```

idx_entity_to_bpe_shaped
enc
num_tokens
num_bpe_entities = None
padding
dummy_id
max_length_subword_tokens = None
train_set_target = None
target_dim = None
train_target_indices = None
ordered_bpe_entities = None
separator
description_of_input = None
describe() → None
property entities_str: List
property relations_str: List
exists(h: str, r: str, t: str)
__iter__()
__len__()
func_triple_to_bpe_representation(triple: List[str])

```

dicee.knowledge_graph_embeddings

Classes

<i>KGE</i>	Knowledge Graph Embedding Class for interactive usage of pre-trained models
------------	---

Module Contents

```

class dicee.knowledge_graph_embeddings.KGE(path=None, url=None, construct_ensemble=False,
    model_name=None)
    Bases: dicee.abstracts.BaseInteractiveKGE
    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*) → 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*) → 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*) → 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)

Predict missing item in a given triple.

Parameter

head_entity: Union[str, List[str]]

String representation of selected entities.

relation: Union[str, List[str]]

String representation of selected relations.

tail_entity: Union[str, List[str]]

String representation of selected entities.

k: int

Highest ranked k item.

Returns: Tuple

Highest K scores and items

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

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

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*)

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

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

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

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

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

dicee.models

Submodules

dicee.models.adopt

Classes

ADOPT

Base class for all optimizers.

Functions

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

Module Contents

```
class dicee.models.adapt.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.adapt.adapt (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 to nest them in a tree structure. You can assign the submodules as regular attributes:

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

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

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

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

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__()
```

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```
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 to monitor for schedulers like `ReduceLROnPlateau`
    "monitor": "val_loss",
```

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

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

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

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

Submodules assigned in this way will be registered, and will have their parameters converted too 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

         $\mathbf{x}$ 

forward_k_vs_all (*args, **kwargs)

forward_k_vs_sample (*args, **kwargs)

get_triple_representation (idx_hrt)

get_head_relation_representation (indexed_triple)

get_sentence_representation (x: torch.LongTensor)

    Parameters

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

        • 3

        •  $\mathbf{t}$ )

```

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

Parameters

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

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

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

Bases: torch.nn.Module

Base class for all neural network modules.

Your models should also subclass this class.

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

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

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

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

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

Note

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

Variables

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

`args`

`__call__(x)`

`static forward(x)`

`dicee.models.clifford`

Classes

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

Module Contents

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

Bases: *dicee.models.base_model.BaseKGE*

Base class for all neural network modules.

Your models should also subclass this class.

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

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

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

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

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

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 $p \in \{e_1, e_2, e_3\}$, we compute interactions between $e_1 e_2, e_1 e_3$, and $e_2 e_3$ This can be implemented with a nested two for loops

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

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

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

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

Yet, this computation would be quite inefficient. Instead, we compute interactions along all p , e.g., 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_qq (hq, rq)

Compute $\sigma_{qq} = \sum_{j=1}^{p+q-1} \sum_{k=j+1}^{p+q} (h_{j,r_k} - h_{k,r_j}) e_j e_k$ captures the interactions between along q bases For instance, let $q = e_1, e_2, e_3$, we compute interactions between e_1e_2 , e_1e_3 , and e_2e_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($hq[:, :, j] * rq[:, :, k] - hq[:, :, k] * rq[:, :, j]$)

$\sigma_{qq} = \text{torch.stack}(\text{results}, \text{dim}=2)$ assert $\sigma_{qq}.\text{shape} == (b, r, \text{int}((q * (q - 1)) / 2))$

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 = [] $\sigma_{pq} = \text{torch.zeros}(b, r, p, q)$ for i in range(p):

for j in range(q):

$\sigma_{pq}[:, :, i, j] = hp[:, :, i] * rq[:, :, j] - hq[:, :, j] * rp[:, :, i]$

print($\sigma_{pq}.\text{shape}$)

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

$e_q j$

$h r = \sigma_0 + \sigma_p + \sigma_q + \sigma_{pp} + \sigma_{q} + \sigma_{pq}$ 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 ($x: \text{torch.FloatTensor}, r: \text{int}, p: \text{int}, q: \text{int}$)

→ 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.KeciBase(args)
```

Bases: *Keci*

Without learning dimension scaling

```
name = 'KeciBase'
```

```
requires_grad_for_interactions = False
```

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

Bases: *dicee.models.base_model.BaseKGE*

Base class for all neural network modules.

Your models should also subclass this class.

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

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

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

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

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

Note

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

Variables

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

```
name = 'DeCaL'
```

```
entity_embeddings
```

```
relation_embeddings
```

```
p
```


q

r

re

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

Parameter

x: torch.LongTensor with (n,) shape

rtype

torch.FloatTensor with (n) shape

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

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

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

compute_sigmas_single (*list_h_emb, list_r_emb, list_t_emb*)

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

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

and return:

$$\sigma_{pqr} t = \sigma_0 \cdot t_0 = s0 + s1 - s2s3, s4 \text{ and } s5$$

compute_sigmas_multivect (*list_h_emb, list_r_emb*)

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

For same bases vectors interaction we have

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

For different base vector interactions, we have

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

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 $\text{Cl}_{\{p,q,r\}}(\mathbb{R}^d)$.
- (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 e_1, e_2, e_3, we compute interactions between e_1 e_2, e_1 e_3 , and e_2 e_3 This can be implemented with a nested two for loops

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

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

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

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

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

e2e1, e2e2, e2e3, e3e1, e3e2, e3e3

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

compute_sigma_qq (hq, rq)

Compute

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

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

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

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

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

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

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

e2e1, e2e2, e2e3, e3e1, e3e2, e3e3

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

`compute_sigma_rr(hk, rk)`

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

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

Compute

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

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

for j in range(q):

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

print(sigma_pq.shape)

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

Compute

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

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

for j in range(q):

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

print(sigma_pq.shape)

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

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

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

for j in range(q):

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

print(sigma_pq.shape)

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

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

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

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

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

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)

dicее.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 dicее.models.dualE.**DualE** (*args*)

Bases: *dicее.models.base_model.BaseKGE*

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

name = 'DualE'

entity_embeddings

relation_embeddings

num_ent

kvsall_score (*e_1_h, e_2_h, e_3_h, e_4_h, e_5_h, e_6_h, e_7_h, e_8_h, e_1_t, e_2_t, e_3_t, e_4_t, e_5_t, e_6_t, e_7_t, e_8_t, r_1, r_2, r_3, r_4, r_5, r_6, r_7, r_8*) → 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)

dicee.models.ensemble

Classes

EnsembleKGE

Module Contents

```
class dicee.models.ensemble.EnsembleKGE(seed_model)
```

```
models = []
```

```
optimizers = []
```

```
loss_history = []
```

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

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

pop (*coeff, x, degree*)

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

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

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

dicee.models.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 Em-beddings

Functions

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

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

```

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

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

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

```

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

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

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

Bases: `dicee.models.base_model.BaseKGE`

Base class for all neural network modules.

Your models should also subclass this class.

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

```

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

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

```

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```
self.conv1 = nn.Conv2d(1, 20, 5)
self.conv2 = nn.Conv2d(20, 20, 5)

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

Submodules assigned in this way will be registered, and will have their parameters converted too 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

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

Module Contents

```

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

    model_kwargs

    name

    model

    loss_history = []

    args

    entity_embeddings = None

    relation_embeddings = None

```

```

forward_k_vs_all (x: torch.LongTensor)
    # => Explicit version by this we can apply bn and dropout

    # (1) Retrieve embeddings of heads and relations + apply Dropout & Normalization if given. h, r =
    self.get_head_relation_representation(x) # (2) Reshape (1). if self.last_dim > 0:

        h = h.reshape(len(x), self.embedding_dim, self.last_dim) r = r.reshape(len(x), self.embedding_dim,
        self.last_dim)

    # (3) Reshape all entities. if self.last_dim > 0:

        t = self.entity_embeddings.weight.reshape(self.num_entities, self.embedding_dim, self.last_dim)

    else:
        t = self.entity_embeddings.weight

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

forward_triples (x: torch.LongTensor) → torch.FloatTensor
    # => Explicit version by this we can apply bn and dropout

    # (1) Retrieve embeddings of heads, relations and tails and apply Dropout & Normalization if given. h, r, t =
    self.get_triple_representation(x) # (2) Reshape (1). if self.last_dim > 0:

        h = h.reshape(len(x), self.embedding_dim, self.last_dim) r = r.reshape(len(x), self.embedding_dim,
        self.last_dim) t = t.reshape(len(x), self.embedding_dim, self.last_dim)

    # (3) Compute the triple score return self.interaction.score(h=h, r=r, t=t, slice_size=None, slice_dim=0)

abstract forward_k_vs_sample (x: torch.LongTensor, target_entity_idx)

```

dicee.models.quaternion

Classes

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

Functions

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

Module Contents

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

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

Bases: `dicee.models.base_model.BaseKGE`

Base class for all neural network modules.

Your models should also subclass this class.

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

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

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

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

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

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*) \rightarrow torch.FloatTensor

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

Absolute value of a quaternion

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

L2 norm of quaternion vector:

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

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

dicee.models.transformers

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

Classes

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

Module Contents

```
class dicee.models.transformers.Byte(*args, **kwargs)
```

Bases: *dicee.models.base_model.BaseKGE*

Base class for all neural network modules.

Your models should also subclass this class.

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

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

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

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

Submodules assigned in this way will be registered, and will have their parameters converted too 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 to nest them in a tree structure. You can assign the submodules as regular attributes:

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

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

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

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

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`

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

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

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

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

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

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

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

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

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

Submodules assigned in this way will be registered, and will have their parameters converted too 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 to nest them in a tree structure. You can assign the submodules as regular attributes:

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

class Model(nn.Module):
```

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

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

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

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

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Table 1 – continued from previous page

<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.
<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>KeciBase</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.BaseKGLightning(*args, **kwargs)
```

Bases: `lightning.LightningModule`

Base class for all neural network modules.

Your models should also subclass this class.

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

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

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

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)
```

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```
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 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 `dicce.models.BaseKGE` (*args: dict*)

Bases: `BaseKGELightning`

Base class for all neural network modules.

Your models should also subclass this class.

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

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

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

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

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

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 ($B \times 2 \times T$)

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

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

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

Submodules assigned in this way will be registered, and will have their parameters converted too 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

__call__(*x*)

static forward(*x*)

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

Bases: `BaseKGELightning`

Base class for all neural network modules.

Your models should also subclass this class.

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

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

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

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

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

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
         $\mathbf{x}$ 

forward_k_vs_all (*args, **kwargs)

forward_k_vs_sample (*args, **kwargs)

get_triple_representation (idx_hrt)

get_head_relation_representation (indexed_triple)

get_sentence_representation (x: torch.LongTensor)

    Parameters

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

        • 3

        •  $\mathbf{t}$ )

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

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

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

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

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

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

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

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

Note

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

Variables

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

args

embedding_dim = None

num_entities = None

num_relations = None

num_tokens = None

learning_rate = None

apply_unit_norm = None

input_dropout_rate = None

hidden_dropout_rate = None

```

optimizer_name = None

feature_map_dropout_rate = None

kernel_size = None

num_of_output_channels = None

weight_decay = None

loss

selected_optimizer = None

normalizer_class = None

normalize_head_entity_embeddings

normalize_relation_embeddings

normalize_tail_entity_embeddings

hidden_normalizer

param_init

input_dp_ent_real

input_dp_rel_real

hidden_dropout

loss_history = []

byte_pair_encoding

max_length_subword_tokens

block_size

forward_byte_pair_encoded_k_vs_all (x: torch.LongTensor)

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

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

    Parameters
    -----

init_params_with_sanity_checking()

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

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

```

```

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

    Parameters
    x

forward_k_vs_all (*args, **kwargs)

forward_k_vs_sample (*args, **kwargs)

get_triple_representation (idx_hrt)

get_head_relation_representation (indexed_triple)

get_sentence_representation (x: torch.LongTensor)

    Parameters
    • (b (x shape)
    • 3
    • t)

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

    Parameters
    x (B × 2 × T)

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

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

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

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

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

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

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

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

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

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

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

Note

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

Variables

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

`args`

`embedding_dim = None`

`num_entities = None`

`num_relations = None`

`num_tokens = None`

`learning_rate = None`

`apply_unit_norm = None`

`input_dropout_rate = None`

`hidden_dropout_rate = None`

`optimizer_name = None`

`feature_map_dropout_rate = None`

`kernel_size = None`

`num_of_output_channels = None`

`weight_decay = None`

`loss`

`selected_optimizer = None`

`normalizer_class = None`

`normalize_head_entity_embeddings`

`normalize_relation_embeddings`

`normalize_tail_entity_embeddings`

`hidden_normalizer`

`param_init`

`input_dp_ent_real`

`input_dp_rel_real`

```

hidden_dropout

loss_history = []

byte_pair_encoding

max_length_subword_tokens

block_size

forward_byte_pair_encoded_k_vs_all (x: torch.LongTensor)

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

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

    Parameters
    -----

init_params_with_sanity_checking()

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

    Parameters

        •  $\mathbf{x}$ 

        •  $\mathbf{y\_idx}$ 

        • ordered_bpe_entities

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

    Parameters
         $\mathbf{x}$ 

forward_k_vs_all (*args, **kwargs)

forward_k_vs_sample (*args, **kwargs)

get_triple_representation (idx_hrt)

get_head_relation_representation (indexed_triple)

get_sentence_representation (x: torch.LongTensor)

    Parameters

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

        • 3

        •  $\mathbf{t}$ )

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

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

```

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

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

Bases: `torch.nn.Module`

Base class for all neural network modules.

Your models should also subclass this class.

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

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

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

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

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

Note

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

Variables

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

`args`

`__call__(x)`

`static forward(x)`

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

`class dicee.models.QMult (args)`

Bases: `dicee.models.base_model.BaseKGE`

Base class for all neural network modules.

Your models should also subclass this class.

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

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

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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 have their parameters converted too 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 to nest them in a tree structure. You can assign the submodules as regular attributes:

```

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

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

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

```

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

Note

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

Variables

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

`args`

`embedding_dim = None`

`num_entities = None`

`num_relations = None`

`num_tokens = None`

`learning_rate = None`

`apply_unit_norm = None`

`input_dropout_rate = None`

`hidden_dropout_rate = None`

`optimizer_name = None`

`feature_map_dropout_rate = None`

`kernel_size = None`

`num_of_output_channels = None`

`weight_decay = None`

`loss`

`selected_optimizer = None`

`normalizer_class = None`

`normalize_head_entity_embeddings`

`normalize_relation_embeddings`

`normalize_tail_entity_embeddings`

`hidden_normalizer`

`param_init`

`input_dp_ent_real`

`input_dp_rel_real`

`hidden_dropout`

```

loss_history = []

byte_pair_encoding

max_length_subword_tokens

block_size

forward_byte_pair_encoded_k_vs_all (x: torch.LongTensor)

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

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

    Parameters
    -----

init_params_with_sanity_checking ()

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

    Parameters

        •  $\mathbf{x}$ 

        •  $\mathbf{y\_idx}$ 

        • ordered_bpe_entities

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

    Parameters

         $\mathbf{x}$ 

forward_k_vs_all (*args, **kwargs)

forward_k_vs_sample (*args, **kwargs)

get_triple_representation (idx_hrt)

get_head_relation_representation (indexed_triple)

get_sentence_representation (x: torch.LongTensor)

    Parameters

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

        • 3

        •  $\mathbf{t}$ )

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

    Parameters

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

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

```

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

Bases: torch.nn.Module

Base class for all neural network modules.

Your models should also subclass this class.

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

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

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

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

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

Note

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

Variables

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

args

__call__ (*x*)

static forward (*x*)

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

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

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

Bases: *dicee.models.base_model.BaseKGE*

Base class for all neural network modules.

Your models should also subclass this class.

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

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

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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 have their parameters converted too 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 to nest them in a tree structure. You can assign the submodules as regular attributes:

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

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

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

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

Submodules assigned in this way will be registered, and will have their parameters converted too 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 to nest them in a tree structure. You can assign the submodules as regular attributes:

```

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

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

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

```

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

Note

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

Variables

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

```

name = 'Keci'

p

q

r

requires_grad_for_interactions = True

compute_sigma_pp(hp, rp)
    Compute  $\sigma_{pp} = \sum_{i=1}^{p-1} \sum_{k=i+1}^p (h_i r_k - h_k r_i) e_i e_k$ 
     $\sigma_{pp}$  captures the interactions between along p bases For instance, let p e_1, e_2, e_3, we compute
    interactions between e_1 e_2, e_1 e_3, and e_2 e_3 This can be implemented with a nested two for loops

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

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

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

    e2e1, e2e2, e2e3, e3e1, e3e2, e3e3

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

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

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

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

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

    e2e1, e2e2, e2e3, e3e1, e3e2, e3e3

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

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

    print(sigma_pq.shape)

apply_coefficients(hp, hq, rp, rq)
    Multiplying a base vector with its scalar coefficient

```

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

Compute our CL multiplication

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

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

e_j

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

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

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

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

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

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

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

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.KeciBase (args)
```

Bases: *Keci*

Without learning dimension scaling

name = 'KeciBase'

requires_grad_for_interactions = False

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

Bases: *dicee.models.base_model.BaseKGE*

Base class for all neural network modules.

Your models should also subclass this class.

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

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

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

(continues on next page)

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

Submodules assigned in this way will be registered, and will have their parameters converted too 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

$$\sigma_{pp} = \sum_{i=1}^{p-1} \sum_{i'=i+1}^p (h_i r_{i'} - h_{i'} r_i) (\text{modelstheinteractionsbetweene}_i \text{and} e'_{i'} \text{for } 1 \leq i, i' \leq p) \sigma_{qq} = \sum_{j=p+1}^{p+q-1} \sum_{j'=j+1}^{p+q} (h_j r_{j'} - h_{j'} r_j)$$

For different base vector interactions, we have

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

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

Kvsall training

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

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

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

Multiplying a base vector with its scalar coefficient

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

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

Parameter

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

returns

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

compute_sigma_pp (*hp, rp*)

Compute .. math:

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

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

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

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

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

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

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

e2e1, e2e2, e2e3, e3e1, e3e2, e3e3

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

compute_sigma_qq(hq, rq)

Compute

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

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

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

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

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

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

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

e2e1, e2e2, e2e3, e3e1, e3e2, e3e3

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

compute_sigma_rr(hk, rk)

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

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

Compute

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

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

for j in range(q):

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

print(sigma_pq.shape)

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

Compute

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

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

```

    for j in range(q):
        sigma_pq[:, :, i, j] = hp[:, :, i] * rq[:, :, j] - hq[:, :, j] * rp[:, :, i]
    print(sigma_pq.shape)
compute_sigma_qr(*, hq, hk, rq, rk)

```

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

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

```

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

```

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

Bases: *BaseKGELightning*

Base class for all neural network modules.

Your models should also subclass this class.

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

```

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

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

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

```

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

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 ($B \times 2 \times T$)

```
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:

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

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

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

Note

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

Variables

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

`args`

`embedding_dim = None`

`num_entities = None`

`num_relations = None`

`num_tokens = None`

`learning_rate = None`

`apply_unit_norm = None`

`input_dropout_rate = None`

`hidden_dropout_rate = None`

`optimizer_name = None`

`feature_map_dropout_rate = None`

`kernel_size = None`

`num_of_output_channels = None`

`weight_decay = None`

`loss`

`selected_optimizer = None`

`normalizer_class = None`

`normalize_head_entity_embeddings`

`normalize_relation_embeddings`

`normalize_tail_entity_embeddings`

`hidden_normalizer`

`param_init`

`input_dp_ent_real`

`input_dp_rel_real`

`hidden_dropout`

`loss_history = []`

```

byte_pair_encoding

max_length_subword_tokens

block_size

forward_byte_pair_encoded_k_vs_all (x: torch.LongTensor)

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

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

    Parameters
    -----

init_params_with_sanity_checking()

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

    Parameters

    •  $\mathbf{x}$ 

    •  $\mathbf{y\_idx}$ 

    • ordered_bpe_entities

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

    Parameters
         $\mathbf{x}$ 

forward_k_vs_all (*args, **kwargs)

forward_k_vs_sample (*args, **kwargs)

get_triple_representation (idx_hrt)

get_head_relation_representation (indexed_triple)

get_sentence_representation (x: torch.LongTensor)

    Parameters

    • ( $\mathbf{b}$  ( $x$  shape))

    • 3

    •  $\mathbf{t}$ )

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

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

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

```

```

class dicee.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:
 $f(x) = \sum_{i=0}^{d-1} a_i x^{i\%d}$  and use the three differents scoring function as in the paper to evaluate the score.
We also consider combining with Neural Networks.

name = 'LFMult'

```

entity_embeddings

relation_embeddings

degree

m

x_values

forward_triples (*idx_triple*)

Parameters

x

construct_multi_coeff (*x*)

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

Constructing a 2 layers NN to represent the embeddings. $h = \text{sigma}(w_h^T x + b_h)$, $r = \text{sigma}(w_r^T x + b_r)$, $t = \text{sigma}(w_t^T x + b_t)$

linear (*x, w, b*)

scalar_batch_NN (*a, b, c*)

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

tri_score (*coeff_h, coeff_r, coeff_t*)

this part implement the trilinear scoring techniques:

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

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

vtp_score (*h, r, t*)

this part implement the vector triple product scoring techniques:

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

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

comp_func (*h, r, t*)

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

polynomial (*coeff, x, degree*)

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

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

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

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

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

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

Bases: `dicee.models.base_model.BaseKGE`

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

name = 'DualE'

entity_embeddings

relation_embeddings

num_ent

kvsall_score (*e_1_h*, *e_2_h*, *e_3_h*, *e_4_h*, *e_5_h*, *e_6_h*, *e_7_h*, *e_8_h*, *e_1_t*, *e_2_t*, *e_3_t*, *e_4_t*,
e_5_t, *e_6_t*, *e_7_t*, *e_8_t*, *r_1*, *r_2*, *r_3*, *r_4*, *r_5*, *r_6*, *r_7*, *r_8*) → 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  
  
    gen_test  
  
    seed  
  
    max_ans_num = 1000000.0  
  
    mode  
  
    ent2id  
  
    rel2id: Dict  
  
    ent_in: Dict  
  
    ent_out: Dict  
  
    query_name_to_struct  
  
    list2tuple (list_data)  
  
    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

<i>PreprocessKG</i>	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(→ polars.DataFrame)</code>	Replaces 'subject', 'relation', and 'object' columns in the input Polars DataFrame with their corresponding index values
<code>pandas_dataframe_indexer(→ pandas.DataFrame)</code>	Replaces 'subject', 'relation', and 'object' columns in the input Pandas DataFrame with their corresponding index values
<code>apply_reciprical_or_noise(add_reciprical, eval_model)</code> <code>timeit(func)</code>	
<code>read_with_polars(→ polars.DataFrame)</code>	Load and Preprocess via Polars
<code>read_with_pandas(data_path[, read_only_few, ...])</code>	
<code>read_from_disk(→ Tuple[polars.DataFrame, pandas.DataFrame])</code>	
<code>read_from_triple_store([endpoint])</code>	Read triples from triple store into pandas 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>create_constraints(triples[, file_path])</code>	
<code>load_with_pandas(→ None)</code>	Deserialize data
<code>save_numpy_ndarray(*, data, file_path)</code>	
<code>load_numpy_ndarray(*, file_path)</code>	
<code>save_pickle(*, data[, file_path])</code>	
<code>load_pickle(*[, file_path])</code>	
<code>create_reciprical_triples(x)</code>	Add inverse triples into dask dataframe
<code>dataset_sanity_checking(→ 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

```
is_sparql_endpoint_alive([sparql_endpoint])
```

```
validate_knowledge_graph(args)
```

Validating the source of knowledge graph

```
sanity_checking_with_arguments(args)
```

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

Functions

`get_default_arguments()`

`main()`

Module Contents

`dicee.scripts.index.get_default_arguments ()`

`dicee.scripts.index.main ()`

dicee.scripts.run

Functions

`get_default_arguments([description])`

Extends pytorch_lightning Trainer's arguments with ours

`main()`

Module Contents

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

Extends pytorch_lightning Trainer's arguments with ours

`dicee.scripts.run.main ()`

dicee.scripts.serve

Attributes

`app`

`neural_searcher`

Classes

NeuralSearcher

Functions

get_default_arguments()

root()

search_embeddings(q)

retrieve_embeddings(q)

main()

Module Contents

```
dicee.scripts.serve.app
dicee.scripts.serve.neural_searcher = None
dicee.scripts.serve.get_default_arguments()
async dicee.scripts.serve.root()
async dicee.scripts.serve.search_embeddings(q: str)
async dicee.scripts.serve.retrieve_embeddings(q: str)
class dicee.scripts.serve.NeuralSearcher(args)
    collection_name
    model
    qdrant_client
    get(entity: str)
    search(entity: str)
dicee.scripts.serve.main()
```

dicee.static_funcs

Functions

create_recipriocal_triples(x)

Add inverse triples into dask dataframe

continues on next page

Table 2 – continued from previous page

<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
<code>save_checkpoint_model(→ None)</code>	Store Pytorch model into disk
<code>store(→ None)</code>	Store trained_model model and save embeddings into csv file.
<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>	

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Table 2 – continued from previous page

<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(trainer, trained_model, model_name: str = 'model',
full_storage_path: str = None, save_embeddings_as_csv=False) → None`

Store trained_model model and save embeddings into csv file. :param trainer: an instance of trainer class :param full_storage_path: path to save parameters. :param model_name: string representation of the name of the model. :param trained_model: an instance of BaseKGE see core.models.base_model . :param save_embeddings_as_csv: for easy access of embeddings. :return:

`dicee.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.initialize_model(args: dict, verbose=0) → Tuple[object, str]`

`dicee.static_funcs.load_json(p: str) → dict`

`dicee.static_funcs.save_embeddings(embeddings: numpy.ndarray, indexes, path: str) → None`

Save it as CSV if memory allows. :param embeddings: :param indexes: :param path: :return:

`dicee.static_funcs.random_prediction(pre_trained_kge)`

`dicee.static_funcs.deploy_triple_prediction(pre_trained_kge, str_subject, str_predicate,
str_object)`

`dicee.static_funcs.deploy_tail_entity_prediction(pre_trained_kge, str_subject, str_predicate,
top_k)`

`dicee.static_funcs.deploy_head_entity_prediction(pre_trained_kge, str_object, str_predicate,
top_k)`

`dicee.static_funcs.deploy_relation_prediction(pre_trained_kge, str_subject, str_object, top_k)`

`dicee.static_funcs.vocab_to_parquet(vocab_to_idx, name, path_for_serialization, print_into)`

`dicee.static_funcs.create_experiment_folder(folder_name='Experiments')`

`dicee.static_funcs.continual_training_setup_executor(executor) → None`

`dicee.static_funcs.exponential_function(x: numpy.ndarray, lam: float, ascending_order=True)
→ torch.FloatTensor`

`dicee.static_funcs.load_numpy(path) → numpy.ndarray`

`dicee.static_funcs.evaluate(entity_to_idx, scores, easy_answers, hard_answers)`

@TODO: CD: Renamed this function Evaluate multi hop query answering on different query types

`dicee.static_funcs.download_file(url, destination_folder='.')`

`dicee.static_funcs.download_files_from_url(base_url: str, destination_folder='.') → None`

Parameters

- **base_url** (e.g. <https://files.dice-research.org/projects/DiceEmbeddings/KINSHIP-Keci-dim128-epoch256-KvsAll>)
- **destination_folder** (e.g. "KINSHIP-Keci-dim128-epoch256-KvsAll")

`dicee.static_funcs.download_pretrained_model(url: str) → str`

`dicee.static_funcs.write_csv_from_model_parallel(path: str)`

Create

`dicee.static_funcs.from_pretrained_model_write_embeddings_into_csv(path: str) → None`

dicee.static_funcs_training

Functions

`make_iterable_verbose(→ Iterable)`

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

`evaluate_bpe_lp(model, triple_idx, ..., info)`

`efficient_zero_grad(model)`

Module Contents

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

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

Evaluate model in a standard link prediction task

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

`dicee.static_funcs_training.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

<code>timeit(func)</code>	
<code>preprocesses_input_args(args)</code>	Sanity Checking in input arguments
<code>create_constraints(→ Tuple[dict, dict, dict, dict])</code>	
<code>get_er_vocab(data)</code>	
<code>get_re_vocab(data)</code>	
<code>get_ee_vocab(data)</code>	
<code>mapping_from_first_two_cols_to_third(train_se</code>	

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

<code>DICE_Trainer</code>	DICE_Trainer implement
---------------------------	------------------------

Functions

```
load_term_mapping([file_path])
```

```
initialize_trainer(...)
```

```
get_callbacks(args)
```

Module Contents

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

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

```
dicee.trainer.dice_trainer.get_callbacks(args)
```

```
class dicee.trainer.dice_trainer.DICE_Trainer(args, is_continual_training, storage_path,  
evaluator=None)
```

DICE_Trainer implement

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

args

is_continual_training:bool

storage_path:str

evaluator:

report:dict

report

args

trainer = None

is_continual_training

storage_path

evaluator

form_of_labelling = None

continual_start (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` | `diccee.trainer.model_parallelism.TensorParallel` | `diccee.trainer.torch_trainer.TorchTrainer` | `diccee.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: diccee.knowledge_graph.KG* | *numpy.memmap*)

→ `Tuple[diccee.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[diccee.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

diccee.trainer.model_parallelism

Classes

TensorParallel

Abstract class for Trainer class for knowledge graph embedding models

Functions

<code>extract_input_outputs(z[, device])</code>	
<code>find_good_batch_size(train_loader, ensemble_model[, ...])</code>	ensem-
<code>forward_backward_update_loss(z, ensemble_model)</code>	ensem-

Module Contents

`dicee.trainer.model_parallelism.extract_input_outputs` (*z: list, device=None*)

`dicee.trainer.model_parallelism.find_good_batch_size` (*train_loader, ensemble_model, max_available_gpu_memory: float = 0.1*)

`dicee.trainer.model_parallelism.forward_backward_update_loss` (*z: Tuple, ensemble_model*)

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

?

models = []

get_ensemble()

fit (**args, **kwargs*)

Train model

`dicee.trainer.torch_trainer`

Classes

<code>TorchTrainer</code>	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

TorchDDPTrainer

A Trainer based on torch.nn.parallel.DistributedDataParallel

NodeTrainer

Functions

make_iterable_verbose(→ Iterable)

Module Contents

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

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

Bases: `dicee.abstracts.AbstractTrainer`

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

Arguments

entity_idx

mapping.

relation_idx

mapping.

form

?

store

?

label_smoothing_rate

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

Return type

`torch.utils.data.Dataset`

fit (*args, **kwargs)

Train model

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

trainer

local_rank

global_rank

optimizer

train_dataset_loader

loss_func

callbacks

model

num_epochs

loss_history = []

ctx

scaler

extract_input_outputs (*z: list*)

train()

Training loop for DDP

Classes

DICE_Trainer

DICE_Trainer implement

Package Contents

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

DICE_Trainer implement

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

args

is_continual_training:bool

storage_path:str

evaluator:

report:dict

report

args

trainer = None

is_continual_training

storage_path

evaluator

form_of_labelling = None

continual_start (*knowledge_graph*)

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

Parameter

returns

- *model*
- **form_of_labelling** (*str*)

```

initialize_trainer (callbacks: List)
    → lightning.Trainer | dicee.trainer.model_parallelism.TensorParallel | dicee.trainer.torch_trainer.TorchTrainer | dicee.
    Initialize Trainer from input arguments

initialize_or_load_model ()

init_dataloader (dataset: torch.utils.data.Dataset) → torch.utils.data.DataLoader

init_dataset () → torch.utils.data.Dataset

start (knowledge_graph: dicee.knowledge_graph.KG | numpy.memmap)
    → Tuple[dicee.models.base_model.BaseKGE, str]
    Start the training
    (1) Initialize Trainer
    (2) Initialize or load a pretrained KGE model
    in DDP setup, we need to load the memory map of already read/index KG.

k_fold_cross_validation (dataset) → Tuple[dicee.models.base_model.BaseKGE, str]
    Perform K-fold Cross-Validation
    1. Obtain K train and test splits.
    2. For each split,
        2.1 initialize trainer and model
        2.2. Train model with configuration provided in args.
        2.3. Compute the mean reciprocal rank (MRR) score of the model on the test respective split.
    3. Report the mean and average MRR .

Parameters
    • self
    • dataset

Returns
    model

```

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>KeciBase</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.

continues on next page

Table 3 – continued from previous page

<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
<i>CVDataModule</i>	Create a Dataset for cross validation
<i>QueryGenerator</i>	

14.4 Functions

<i>create_recipriocal triples(x)</i>	Add inverse triples into dask dataframe
--------------------------------------	---

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Table 4 – continued from previous page

<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
<code>save_checkpoint_model(→ None)</code>	Store Pytorch model into disk
<code>store(→ None)</code>	Store trained_model model and save embeddings into csv file.
<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>	

continues on next page

Table 4 – continued from previous page

<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_into 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.KeciBase(args)
```

Bases: *Keci*

Without learning dimension scaling

```
name = 'KeciBase'
```

```
requires_grad_for_interactions = False
```

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

Bases: *dicee.models.base_model.BaseKGE*

Base class for all neural network modules.

Your models should also subclass this class.

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

for j in range(q):

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

print(sigma_pq.shape)

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

Multiplying a base vector with its scalar coefficient

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

Compute our CL multiplication

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

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

$e_i e_j$

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

- (1) $\sigma_0 = h_{0r_0} + \sum_{i=1}^p (h_{0r_i} e_i - \sum_{j=p+1}^{p+q} (h_{jr_j} e_j$
- (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*)
→ 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 to nest them in a tree structure. You can assign the submodules as regular attributes:

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

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

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

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

Note

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

Variables

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

name = 'DeCaL'

entity_embeddings

relation_embeddings

p

q

r

re

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

Parameter

x: torch.LongTensor with (n,) shape

rtype

torch.FloatTensor with (n) shape

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

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

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

compute_sigmas_single (*list_h_emb, list_r_emb, list_t_emb*)

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

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

and return:

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

compute_sigmas_multivect (*list_h_emb, list_r_emb*)

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

For same bases vectors interaction we have

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

For different base vector interactions, we have

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

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

Kvsall training

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

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

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

Multiplying a base vector with its scalar coefficient

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

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

Parameter

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

returns

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

compute_sigma_pp (*hp, rp*)

Compute .. math:

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

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

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

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

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

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

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

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

compute_sigma_qq (*hq, rq*)

Compute

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

$\text{sigma}_{\{q\}}$ 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_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
    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 to nest them in a tree structure. You can assign the submodules as regular attributes:

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

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

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

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

Note

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

Variables

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

```
name = 'ComplEx'
```

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

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

Parameters

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

```
forward_k_vs_all(x: torch.LongTensor) -> torch.FloatTensor
```

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

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

Bases: *dicee.models.base_model.BaseKGE*

Additive Convolutional ComplEx Knowledge Graph Embeddings

```

name = 'AConEx'

conv2d

fc_num_input

fc1

norm_fc1

bn_conv2d

feature_map_dropout

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

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

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

    Parameters
    x

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

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

    conv2d

    fc_num_input

    fc1

    bn_conv2d

    norm_fc1

    feature_map_dropout

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

    residual_convolution (O_1, O_2)

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

    Parameters
    x

```

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

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

class *dicee.AConvQ* (*args*)

Bases: *dicee.models.base_model.BaseKGE*

Additive Convolutional Quaternion Knowledge Graph Embeddings

name = 'AConvQ'

entity_embeddings

relation_embeddings

conv2d

fc_num_input

fc1

bn_conv1

bn_conv2

feature_map_dropout

residual_convolution (*Q_1*, *Q_2*)

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

Parameters

x

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

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

class *dicee.ConvQ* (*args*)

Bases: *dicee.models.base_model.BaseKGE*

Convolutional Quaternion Knowledge Graph Embeddings

name = 'ConvQ'

entity_embeddings

relation_embeddings

conv2d

fc_num_input

fc1

bn_conv1

bn_conv2

`feature_map_dropout`

`residual_convolution(Q_1, Q_2)`

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

Parameters

x

`forward_k_vs_all(x: torch.Tensor)`

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

`class dicee.ConvO(args: dict)`

Bases: `dicee.models.base_model.BaseKGE`

Base class for all neural network modules.

Your models should also subclass this class.

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

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

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

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

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

Note

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

Variables

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

`name = 'ConvO'`

`conv2d`

`fc_num_input`

`fc1`

```

bn_conv2d

norm_fc1

feature_map_dropout

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

residual_convolution(O_1, O_2)

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

    Parameters
    x

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

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

    conv2d

    fc_num_input

    fc1

    norm_fc1

    bn_conv2d

    feature_map_dropout

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

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

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

    Parameters
    x

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

class dicee.QMult(args)
    Bases: dicee.models.base_model.BaseKGE
    Base class for all neural network modules.
    Your models should also subclass this class.

```


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

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

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

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

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

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

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

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

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

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

Note

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

Variables

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

```

name = 'OMult'

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

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

k_vs_all_score(bpe_head_ent_emb, bpe_rel_ent_emb, E)

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

class dicee.Shallom(args)
    Bases: dicee.models.base_model.BaseKGE
    A shallow neural model for relation prediction (https://arxiv.org/abs/2101.09090)
    name = 'Shallom'
    shallom
    get_embeddings() → Tuple[numpy.ndarray, None]
    forward_k_vs_all(x) → torch.FloatTensor
    forward_triples(x) → torch.FloatTensor

    Parameters
    x

    Returns

class dicee.LFMult(args)
    Bases: dicee.models.base_model.BaseKGE
    Embedding with polynomial functions. We represent all entities and relations in the polynomial space as:  $f(x) = \sum_{i=0}^{d-1} a_k x^{i \bmod d}$  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. $h = \text{sigma}(wh^T x + bh)$, $r = \text{sigma}(wr^T x + br)$,
 $t = \text{sigma}(wt^T x + bt)$

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:

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

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

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

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

comp_func (*h, r, t*)

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

polynomial (*coeff, x, degree*)

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

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

pop (*coeff, x, degree*)

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

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

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

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

Bases: *dicee.models.base_model.BaseKGE*

A class for using knowledge graph embedding models implemented in Pykeen

Notes: Pykeen_DistMult: C Pykeen_ComplEx: Pykeen_QuatE: Pykeen_MuRE: Pykeen_CP: Pykeen_HolE: Py-keen_HolE:

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

```

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

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

```

(continues on next page)

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

Submodules assigned in this way will be registered, and will have their parameters converted too 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.BaseKGE(args: dict)
```

Bases: `BaseKGE Lightning`

Base class for all neural network modules.

Your models should also subclass this class.

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

```

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

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

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

```

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

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

- $(b \times shape)$
- 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.EnsembleKGE(seed_model)`

`models = []`

`optimizers = []`

`loss_history = []`

`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(trainer, trained_model, model_name: str = 'model', full_storage_path: str = None,
    save_embeddings_as_csv=False) → None
    Store trained_model model and save embeddings into csv file. :param trainer: an instance of trainer class :param
    full_storage_path: path to save parameters. :param model_name: string representation of the name of the model.
    :param trained_model: an instance of BaseKGE see core.models.base_model . :param save_embeddings_as_csv:
    for easy access of embeddings. :return:

dicee.add_noisy_triples(train_set: pandas.DataFrame, add_noise_rate: float) → 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, storage_path, evaluator=None)

```

DICE_Trainer implement

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

args

is_continual_training:bool

storage_path:str

evaluator:

report:dict

report

args

trainer = None

is_continual_training

storage_path

evaluator

form_of_labelling = None

continual_start (*knowledge_graph*)

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

Parameter

returns

- *model*
- **form_of_labelling** (*str*)

initialize_trainer (*callbacks: List*)

→ `lightning.Trainer` | `dicee.trainer.model_parallelism.TensorParallel` | `dicee.trainer.torch_trainer.TorchTrainer` | `dicee.`

Initialize Trainer from input arguments

initialize_or_load_model ()

init_dataloader (*dataset: torch.utils.data.Dataset*) → `torch.utils.data.DataLoader`

init_dataset () → `torch.utils.data.Dataset`

start (*knowledge_graph: dicee.knowledge_graph.KG* | *numpy.memmap*)

→ `Tuple[dicee.models.base_model.BaseKGE, str]`

Start the training

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

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

k_fold_cross_validation (*dataset*) → `Tuple[dicee.models.base_model.BaseKGE, str]`

Perform K-fold Cross-Validation

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

Parameters

- **self**
- **dataset**

Returns

model

```

class dicee.KGE (path=None, url=None, construct_ensemble=False, model_name=None)
    Bases: dicee.abstracts.BaseInteractiveKGE

    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)
        → Tuple

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

         $\operatorname{argmax}_{\{e \in E\}} f(e, r, t)$ , 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)
    → Tuple

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

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

```

Parameter

head_entity: List[str]
 String representation of selected entities.

tail_entity: List[str]
 String representation of selected entities.

k: int
 Highest ranked k entities.

Returns: Tuple

Highest K scores and entities

predict_missing_tail_entity (*head_entity: List[str] | str, relation: List[str] | str, within: List[str] = None*) → 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*)

Predict missing item in a given triple.

Parameter

head_entity: Union[str, List[str]]

String representation of selected entities.

relation: Union[str, List[str]]

String representation of selected relations.

tail_entity: Union[str, List[str]]

String representation of selected entities.

k: int

Highest ranked k item.

Returns: Tuple

Highest K scores and items

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

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

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*)

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.

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

trainer = None

trained_model = None

knowledge_graph = None

report

evaluator = None

start_time = None

setup_executor() → None

dept_read_preprocess_index_serialize_data() → None

Read & Preprocess & Index & Serialize Input Data

- (1) Read or load the data from disk into memory.
- (2) Store the statistics of the data.

Parameter

rtype

None

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: str, scoring_technique: str, neg_ratio: int, label_smoothing_rate)
```

Reload the files from disk to construct the Pytorch dataset

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

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

Bases: torch.utils.data.Dataset

An abstract class representing a Dataset.

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

Note

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

train_set

ordered_bpe_entities

num_bpe_entities

neg_ratio

num_datapoints

__len__()

__getitem__(idx)

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

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

Bases: torch.utils.data.Dataset

An abstract class representing a Dataset.

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

Note

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

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

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

Bases: `torch.utils.data.Dataset`

Dataset for the 1vsALL training strategy

Parameters

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

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

Note

TODO

train_set_idx

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

entity_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_idxxs, relation_idxxs, label_smoothing_rate=0.0)

```

Bases: torch.utils.data.Dataset

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

Let D denote a dataset for AllvsAll training and be defined as $D := \{(x, y)_i\}_i^N$, where $x: (h, r)$ is a possible unique tuple of an entity h in E and a relation r in R . Hence $N = |E| \times |R|$ y_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_idxxs
[dictionary] string representation of an entity to its integer id

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

self : torch.utils.data.Dataset

```

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

```

```

train_data = None

train_target = None

label_smoothing_rate

collate_fn = None

target_dim

__len__()

__getitem__(idx)

```

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

Bases: torch.utils.data.Dataset

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

Parameters

- **train_set** (*np.ndarray*) – A numpy array containing triples of knowledge graph data. Each triple consists of (head_entity, relation, tail_entity).
- **num_entities** (*int*) – The number of unique entities in the knowledge graph.
- **num_relations** (*int*) – The number of unique relations in the knowledge graph.
- **neg_sample_ratio** (*int, optional*) – The number of negative samples to be generated per positive sample. Must be a positive integer and less than num_entities.
- **label_smoothing_rate** (*float, optional*) – A label smoothing rate to apply to the positive and negative labels. Defaults to 0.0.

train_data

The input data converted into a PyTorch tensor.

Type

torch.Tensor

num_entities

Number of entities in the dataset.

Type

int

num_relations

Number of relations in the dataset.

Type

int

neg_sample_ratio

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

Type

int

label_smoothing_rate

The smoothing factor applied to the labels.

Type

torch.Tensor

collate_fn

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

Type

function, optional

train_data

num_entities

`num_relations`

`neg_sample_ratio`

`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_idx, relation_idx, form,
                              store=None, neg_ratio=None, label_smoothing_rate: float = 0.0)
```

Bases: `torch.utils.data.Dataset`

KvsSample a Dataset:

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

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

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

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

$|new_y| \ll |E|$ new_y contains all 1's if $\sum(y) < neg_sample_ratio$ new_y contains

`train_set_idx`

Indexed triples for the training.

`entity_idx`

mapping.

`relation_idx`

mapping.

`form`

?

`store`

?

`label_smoothing_rate`

?


```

        torch.utils.data.Dataset

    train_data = None

    train_target = None

    neg_ratio

    num_entities

    label_smoothing_rate

    collate_fn = None

    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 __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.

```

    neg_sample_ratio

    train_set

    length

    num_entities

    num_relations

    __len__()

    __getitem__(idx)

class dicee.TriplePredictionDataset (train_set: numpy.ndarray, num_entities: int, num_relations: int,
                                      neg_sample_ratio: int = 1, label_smoothing_rate: float = 0.0)
    Bases: torch.utils.data.Dataset
        Triple Dataset

```

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

. x:(h,r, t) in KG is a unique h in E and a relation r in R and . collect_fn => Generates negative triples

collect_fn:

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

y:labels are represented in torch.float16

train_set_idx

Indexed triples for the training.

entity_idx

mapping.

relation_idx

mapping.

form

?

store

?

label_smoothing_rate

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

label_smoothing_rate

neg_sample_ratio

train_set

length

num_entities

num_relations

__len__()

__getitem__(idx)

collate_fn(batch: List[torch.Tensor])

class dicee.CVDDataModule (train_set_idx: numpy.ndarray, num_entities, num_relations, neg_sample_ratio, batch_size, num_workers)

Bases: pytorch_lightning.LightningDataModule

Create a Dataset for cross validation

Parameters

- **train_set_idx** – Indexed triples for the training.
- **num_entities** – entity to index mapping.
- **num_relations** – relation to index mapping.
- **batch_size** – int
- **form** – ?

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

Return type

?

`train_set_idx`

`num_entities`

`num_relations`

`neg_sample_ratio`

`batch_size`

`num_workers`

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

An iterable or collection of iterables specifying training samples.

For more information about multiple dataloaders, see this section.

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

For data processing use the following pattern:

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

However, the above are only necessary for distributed processing.

Warning

do not assign state in `prepare_data`

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

Note

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

`setup(*args, **kwargs)`

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

Parameters

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

Example:

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

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

        # don't do this
        self.something = else

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

transfer_batch_to_device(*args, **kwargs)

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

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

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

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

Note

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

Parameters

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

Returns

A reference to the data on the new device.

Example:

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

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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.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

gen_test

seed

max_ans_num = 1000000.0

mode

ent2id

rel2id: Dict

ent_in: Dict

ent_out: Dict

query_name_to_struct

list2tuple(list_data)

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`, 17
- `dicee.callbacks`, 19
- `dicee.config`, 25
- `dicee.dataset_classes`, 28
- `dicee.eval_static_funcs`, 40
- `dicee.evaluator`, 41
- `dicee.executer`, 43
- `dicee.knowledge_graph`, 45
- `dicee.knowledge_graph_embeddings`, 46
- `dicee.models`, 50
 - `adopt`, 50
 - `base_model`, 51
 - `clifford`, 60
 - `complex`, 67
 - `dualE`, 70
 - `ensemble`, 71
 - `function_space`, 72
 - `octonion`, 75
 - `pykeen_models`, 78
 - `quaternion`, 79
 - `real`, 82
 - `static_funcs`, 84
 - `transformers`, 84
- `dicee.query_generator`, 138
- `dicee.read_preprocess_save_load_kg`, 139
 - `read_preprocess_save_load_kg.preprocess`, 139
 - `read_preprocess_save_load_kg.read_from_disk`, 140
 - `read_preprocess_save_load_kg.save_load_disk`, 141
 - `read_preprocess_save_load_kg.util`, 141
- `dicee.sanity_checkers`, 146
- `dicee.scripts`, 147
 - `index`, 147
 - `run`, 147
 - `serve`, 147
- `dicee.static_funcs`, 148
- `dicee.static_funcs_training`, 152
- `dicee.static_preprocess_funcs`, 152
- `dicee.trainer`, 153
 - `dice_trainer`, 153
 - `model_parallelism`, 155
 - `torch_trainer`, 156
 - `torch_trainer_ddp`, 157

Index

Non-alphabetical

`__call__` () (*dicee.EnsembleKGE method*), 186
`__call__` () (*dicee.models.base_model.IdentityClass method*), 60
`__call__` () (*dicee.models.ensemble.EnsembleKGE method*), 71
`__call__` () (*dicee.models.IdentityClass method*), 101, 112, 118
`__getitem__` () (*dicee.AllvsAll method*), 198
`__getitem__` () (*dicee.BPE_NegativeSamplingDataset method*), 195
`__getitem__` () (*dicee.dataset_classes.AllvsAll method*), 33
`__getitem__` () (*dicee.dataset_classes.BPE_NegativeSamplingDataset method*), 30
`__getitem__` () (*dicee.dataset_classes.KvsAll method*), 32
`__getitem__` () (*dicee.dataset_classes.KvsSampleDataset method*), 35
`__getitem__` () (*dicee.dataset_classes.MultiClassClassificationDataset method*), 31
`__getitem__` () (*dicee.dataset_classes.MultiLabelDataset method*), 30
`__getitem__` () (*dicee.dataset_classes.NegSampleDataset method*), 36
`__getitem__` () (*dicee.dataset_classes.OnevsAllDataset method*), 31
`__getitem__` () (*dicee.dataset_classes.OnevsSample method*), 34
`__getitem__` () (*dicee.dataset_classes.TriplePredictionDataset method*), 36
`__getitem__` () (*dicee.KvsAll method*), 198
`__getitem__` () (*dicee.KvsSampleDataset method*), 201
`__getitem__` () (*dicee.MultiClassClassificationDataset method*), 196
`__getitem__` () (*dicee.MultiLabelDataset method*), 196
`__getitem__` () (*dicee.NegSampleDataset method*), 201
`__getitem__` () (*dicee.OnevsAllDataset method*), 197
`__getitem__` () (*dicee.OnevsSample method*), 200
`__getitem__` () (*dicee.TriplePredictionDataset method*), 202
`__iter__` () (*dicee.config.Namespace method*), 28
`__iter__` () (*dicee.EnsembleKGE method*), 186
`__iter__` () (*dicee.knowledge_graph.KG method*), 46
`__iter__` () (*dicee.models.ensemble.EnsembleKGE method*), 71
`__len__` () (*dicee.AllvsAll method*), 198
`__len__` () (*dicee.BPE_NegativeSamplingDataset method*), 195
`__len__` () (*dicee.dataset_classes.AllvsAll method*), 33
`__len__` () (*dicee.dataset_classes.BPE_NegativeSamplingDataset method*), 30
`__len__` () (*dicee.dataset_classes.KvsAll method*), 32
`__len__` () (*dicee.dataset_classes.KvsSampleDataset method*), 35
`__len__` () (*dicee.dataset_classes.MultiClassClassificationDataset method*), 31
`__len__` () (*dicee.dataset_classes.MultiLabelDataset method*), 30
`__len__` () (*dicee.dataset_classes.NegSampleDataset method*), 36
`__len__` () (*dicee.dataset_classes.OnevsAllDataset method*), 31
`__len__` () (*dicee.dataset_classes.OnevsSample method*), 34
`__len__` () (*dicee.dataset_classes.TriplePredictionDataset method*), 36
`__len__` () (*dicee.EnsembleKGE method*), 186
`__len__` () (*dicee.knowledge_graph.KG method*), 46
`__len__` () (*dicee.KvsAll method*), 198
`__len__` () (*dicee.KvsSampleDataset method*), 201
`__len__` () (*dicee.models.ensemble.EnsembleKGE method*), 71
`__len__` () (*dicee.MultiClassClassificationDataset method*), 196
`__len__` () (*dicee.MultiLabelDataset method*), 196
`__len__` () (*dicee.NegSampleDataset method*), 201
`__len__` () (*dicee.OnevsAllDataset method*), 197
`__len__` () (*dicee.OnevsSample method*), 200
`__len__` () (*dicee.TriplePredictionDataset method*), 202
`__setstate__` () (*dicee.models.ADOPT method*), 92
`__setstate__` () (*dicee.models.adopt.ADOPT method*), 51
`__str__` () (*dicee.EnsembleKGE method*), 186
`__str__` () (*dicee.KGE method*), 190
`__str__` () (*dicee.knowledge_graph_embeddings.KGE method*), 46
`__str__` () (*dicee.models.ensemble.EnsembleKGE method*), 71
`__version__` (*in module dicee*), 207

A

`AbstractCallback` (*class in dicee.abstracts*), 15
`AbstractPPECallback` (*class in dicee.abstracts*), 17
`AbstractTrainer` (*class in dicee.abstracts*), 12
`AccumulateEpochLossCallback` (*class in dicee.callbacks*), 19

achieve_answer() (*dicee.query_generator.QueryGenerator method*), 138
 achieve_answer() (*dicee.QueryGenerator method*), 207
 AConEx (*class in dicee*), 172
 AConEx (*class in dicee.models*), 108
 AConEx (*class in dicee.models.complex*), 68
 AConvO (*class in dicee*), 173
 AConvO (*class in dicee.models*), 120
 AConvO (*class in dicee.models.octonion*), 77
 AConvQ (*class in dicee*), 174
 AConvQ (*class in dicee.models*), 114
 AConvQ (*class in dicee.models.quaternion*), 81
 adaptive_swa (*dicee.config.Namespace attribute*), 28
 add_new_entity_embeddings() (*dicee.abstracts.BaseInteractiveKGE method*), 15
 add_noise_rate (*dicee.config.Namespace attribute*), 26
 add_noise_rate (*dicee.knowledge_graph.KG attribute*), 45
 add_noisy_triples() (*in module dicee*), 187
 add_noisy_triples() (*in module dicee.static_funcs*), 151
 add_noisy_triples_into_training() (*dicee.read_preprocess_save_load_kg.read_from_disk.ReadFromDisk method*), 140
 add_noisy_triples_into_training() (*dicee.read_preprocess_save_load_kg.ReadFromDisk method*), 146
 add_reciprocal (*dicee.knowledge_graph.KG attribute*), 45
 ADOPT (*class in dicee.models*), 92
 ADOPT (*class in dicee.models.adopt*), 51
 adopt() (*in module dicee.models.adopt*), 51
 AllvsAll (*class in dicee*), 198
 AllvsAll (*class in dicee.dataset_classes*), 32
 alphas (*dicee.abstracts.AbstractPPECallback attribute*), 17
 alphas (*dicee.callbacks.ASWA attribute*), 23
 analyse() (*in module dicee.analyse_experiments*), 19
 answer_multi_hop_query() (*dicee.KGE method*), 192
 answer_multi_hop_query() (*dicee.knowledge_graph_embeddings.KGE method*), 49
 app (*in module dicee.scripts.serve*), 148
 apply_coefficients() (*dicee.DeCaL method*), 169
 apply_coefficients() (*dicee.Keci method*), 165
 apply_coefficients() (*dicee.models.clifford.DeCaL method*), 66
 apply_coefficients() (*dicee.models.clifford.Keci method*), 62
 apply_coefficients() (*dicee.models.DeCaL method*), 126
 apply_coefficients() (*dicee.models.Keci method*), 122
 apply_reciprocal_or_noise() (*in module dicee.read_preprocess_save_load_kg.util*), 144
 apply_semantic_constraint (*dicee.abstracts.BaseInteractiveKGE attribute*), 14
 apply_unit_norm (*dicee.BaseKGE attribute*), 184
 apply_unit_norm (*dicee.models.base_model.BaseKGE attribute*), 58
 apply_unit_norm (*dicee.models.BaseKGE attribute*), 99, 102, 105, 110, 116, 129, 132
 args (*dicee.BaseKGE attribute*), 184
 args (*dicee.DICE_Trainer attribute*), 188
 args (*dicee.evaluator.Evaluator attribute*), 42
 args (*dicee.Execute attribute*), 193
 args (*dicee.executer.Execute attribute*), 43
 args (*dicee.models.base_model.BaseKGE attribute*), 58
 args (*dicee.models.base_model.IdentityClass attribute*), 60
 args (*dicee.models.BaseKGE attribute*), 98, 102, 105, 110, 116, 128, 132
 args (*dicee.models.IdentityClass attribute*), 101, 112, 118
 args (*dicee.models.pykeen_models.PykeenKGE attribute*), 78
 args (*dicee.models.PykeenKGE attribute*), 130
 args (*dicee.PykeenKGE attribute*), 181
 args (*dicee.trainer.DICE_Trainer attribute*), 159
 args (*dicee.trainer.dice_trainer.DICE_Trainer attribute*), 154
 ASWA (*class in dicee.callbacks*), 22
 aswa (*dicee.analyse_experiments.Experiment attribute*), 18
 attn (*dicee.models.transformers.Block attribute*), 89
 attn_dropout (*dicee.models.transformers.CausalSelfAttention attribute*), 87
 attributes (*dicee.abstracts.AbstractTrainer attribute*), 12
 auto_batch_finding (*dicee.config.Namespace attribute*), 28

B

backend (*dicee.config.Namespace attribute*), 26
 backend (*dicee.knowledge_graph.KG attribute*), 45
 BaseInteractiveKGE (*class in dicee.abstracts*), 13

BaseKGE (*class in dicee*), 183
 BaseKGE (*class in dicee.models*), 98, 101, 105, 109, 115, 128, 131
 BaseKGE (*class in dicee.models.base_model*), 57
 BaseKGELightning (*class in dicee.models*), 92
 BaseKGELightning (*class in dicee.models.base_model*), 52
 batch_kronecker_product () (*dicee.callbacks.KronE static method*), 25
 batch_size (*dicee.analyse_experiments.Experiment attribute*), 18
 batch_size (*dicee.callbacks.PseudoLabellingCallback attribute*), 22
 batch_size (*dicee.config.Namespace attribute*), 26
 batch_size (*dicee.CVDataModule attribute*), 203
 batch_size (*dicee.dataset_classes.CVDataModule attribute*), 37
 bias (*dicee.models.transformers.GPTConfig attribute*), 89
 bias (*dicee.models.transformers.LayerNorm attribute*), 86
 Block (*class in dicee.models.transformers*), 88
 block_size (*dicee.BaseKGE attribute*), 185
 block_size (*dicee.config.Namespace attribute*), 28
 block_size (*dicee.dataset_classes.MultiClassClassificationDataset attribute*), 31
 block_size (*dicee.models.base_model.BaseKGE attribute*), 59
 block_size (*dicee.models.BaseKGE attribute*), 99, 102, 106, 111, 117, 129, 133
 block_size (*dicee.models.transformers.GPTConfig attribute*), 89
 block_size (*dicee.MultiClassClassificationDataset attribute*), 196
 bn_conv1 (*dicee.AConvQ attribute*), 174
 bn_conv1 (*dicee.ConvQ attribute*), 174
 bn_conv1 (*dicee.models.AConvQ attribute*), 115
 bn_conv1 (*dicee.models.ConvQ attribute*), 114
 bn_conv1 (*dicee.models.quaternion.AConvQ attribute*), 82
 bn_conv1 (*dicee.models.quaternion.ConvQ attribute*), 81
 bn_conv2 (*dicee.AConvQ attribute*), 174
 bn_conv2 (*dicee.ConvQ attribute*), 174
 bn_conv2 (*dicee.models.AConvQ attribute*), 115
 bn_conv2 (*dicee.models.ConvQ attribute*), 114
 bn_conv2 (*dicee.models.quaternion.AConvQ attribute*), 82
 bn_conv2 (*dicee.models.quaternion.ConvQ attribute*), 81
 bn_conv2d (*dicee.AConEx attribute*), 173
 bn_conv2d (*dicee.AConvO attribute*), 173
 bn_conv2d (*dicee.ConEx attribute*), 176
 bn_conv2d (*dicee.ConvO attribute*), 175
 bn_conv2d (*dicee.models.AConEx attribute*), 108
 bn_conv2d (*dicee.models.AConvO attribute*), 121
 bn_conv2d (*dicee.models.complex.AConEx attribute*), 68
 bn_conv2d (*dicee.models.complex.ConEx attribute*), 68
 bn_conv2d (*dicee.models.ConEx attribute*), 107
 bn_conv2d (*dicee.models.ConvO attribute*), 120
 bn_conv2d (*dicee.models.octonion.AConvO attribute*), 78
 bn_conv2d (*dicee.models.octonion.ConvO attribute*), 77
 BPE_NegativeSamplingDataset (*class in dicee*), 195
 BPE_NegativeSamplingDataset (*class in dicee.dataset_classes*), 29
 build_chain_funcs () (*dicee.models.FMult2 method*), 135
 build_chain_funcs () (*dicee.models.function_space.FMult2 method*), 73
 build_func () (*dicee.models.FMult2 method*), 135
 build_func () (*dicee.models.function_space.FMult2 method*), 73
 Byte (*class in dicee*), 181
 Byte (*class in dicee.models.transformers*), 84
 byte_pair_encoding (*dicee.analyse_experiments.Experiment attribute*), 18
 byte_pair_encoding (*dicee.BaseKGE attribute*), 185
 byte_pair_encoding (*dicee.config.Namespace attribute*), 28
 byte_pair_encoding (*dicee.knowledge_graph.KG attribute*), 45
 byte_pair_encoding (*dicee.models.base_model.BaseKGE attribute*), 59
 byte_pair_encoding (*dicee.models.BaseKGE attribute*), 99, 102, 106, 111, 117, 129, 132

C

c_attn (*dicee.models.transformers.CausalSelfAttention attribute*), 87
 c_fc (*dicee.models.transformers.MLP attribute*), 88
 c_proj (*dicee.models.transformers.CausalSelfAttention attribute*), 87
 c_proj (*dicee.models.transformers.MLP attribute*), 88
 callbacks (*dicee.abstracts.AbstractTrainer attribute*), 12
 callbacks (*dicee.analyse_experiments.Experiment attribute*), 18

callbacks (*dicee.config.Namespace* attribute), 26
 callbacks (*dicee.trainer.torch_trainer_ddp.NodeTrainer* attribute), 158
 CausalSelfAttention (class in *dicee.models.transformers*), 86
 chain_func() (*dicee.models.FMult* method), 134
 chain_func() (*dicee.models.function_space.FMult* method), 72
 chain_func() (*dicee.models.function_space.GFMult* method), 73
 chain_func() (*dicee.models.GFMult* method), 134
 cl_pqr() (*dicee.DeCaL* method), 168
 cl_pqr() (*dicee.models.clifford.DeCaL* method), 65
 cl_pqr() (*dicee.models.DeCaL* method), 125
 clifford_multiplication() (*dicee.Keci* method), 165
 clifford_multiplication() (*dicee.models.clifford.Keci* method), 62
 clifford_multiplication() (*dicee.models.Keci* method), 122
 clip_lambda (*dicee.models.ADOPT* attribute), 92
 clip_lambda (*dicee.models.adopt.ADOPT* attribute), 51
 collate_fn (*dicee.AllvsAll* attribute), 198
 collate_fn (*dicee.dataset_classes.AllvsAll* attribute), 33
 collate_fn (*dicee.dataset_classes.KvsAll* attribute), 32
 collate_fn (*dicee.dataset_classes.KvsSampleDataset* attribute), 35
 collate_fn (*dicee.dataset_classes.MultiClassClassificationDataset* attribute), 31
 collate_fn (*dicee.dataset_classes.MultiLabelDataset* attribute), 30
 collate_fn (*dicee.dataset_classes.OnevsAllDataset* attribute), 31
 collate_fn (*dicee.dataset_classes.OnevsSample* attribute), 34
 collate_fn (*dicee.KvsAll* attribute), 198
 collate_fn (*dicee.KvsSampleDataset* attribute), 201
 collate_fn (*dicee.MultiClassClassificationDataset* attribute), 196
 collate_fn (*dicee.MultiLabelDataset* attribute), 196
 collate_fn (*dicee.OnevsAllDataset* attribute), 197
 collate_fn (*dicee.OnevsSample* attribute), 199, 200
 collate_fn() (*dicee.BPE_NegativeSamplingDataset* method), 195
 collate_fn() (*dicee.dataset_classes.BPE_NegativeSamplingDataset* method), 30
 collate_fn() (*dicee.dataset_classes.TriplePredictionDataset* method), 37
 collate_fn() (*dicee.TriplePredictionDataset* method), 202
 collection_name (*dicee.scripts.serve.NeuralSearcher* attribute), 148
 comp_func() (*dicee.LFMult* method), 180
 comp_func() (*dicee.models.function_space.LFMult* method), 75
 comp_func() (*dicee.models.LFMult* method), 136
 ComplEx (class in *dicee*), 171
 ComplEx (class in *dicee.models*), 108
 ComplEx (class in *dicee.models.complex*), 69
 compute_convergence() (in module *dicee.callbacks*), 22
 compute_func() (*dicee.models.FMult* method), 134
 compute_func() (*dicee.models.FMult2* method), 135
 compute_func() (*dicee.models.function_space.FMult* method), 72
 compute_func() (*dicee.models.function_space.FMult2* method), 73
 compute_func() (*dicee.models.function_space.GFMult* method), 73
 compute_func() (*dicee.models.GFMult* method), 134
 compute_mrr() (*dicee.callbacks.ASWA* static method), 23
 compute_sigma_pp() (*dicee.DeCaL* method), 169
 compute_sigma_pp() (*dicee.Keci* method), 165
 compute_sigma_pp() (*dicee.models.clifford.DeCaL* method), 66
 compute_sigma_pp() (*dicee.models.clifford.Keci* method), 61
 compute_sigma_pp() (*dicee.models.DeCaL* method), 126
 compute_sigma_pp() (*dicee.models.Keci* method), 122
 compute_sigma_pq() (*dicee.DeCaL* method), 170
 compute_sigma_pq() (*dicee.Keci* method), 165
 compute_sigma_pq() (*dicee.models.clifford.DeCaL* method), 67
 compute_sigma_pq() (*dicee.models.clifford.Keci* method), 62
 compute_sigma_pq() (*dicee.models.DeCaL* method), 127
 compute_sigma_pq() (*dicee.models.Keci* method), 122
 compute_sigma_pr() (*dicee.DeCaL* method), 170
 compute_sigma_pr() (*dicee.models.clifford.DeCaL* method), 67
 compute_sigma_pr() (*dicee.models.DeCaL* method), 127
 compute_sigma_qq() (*dicee.DeCaL* method), 169
 compute_sigma_qq() (*dicee.Keci* method), 165
 compute_sigma_qq() (*dicee.models.clifford.DeCaL* method), 66
 compute_sigma_qq() (*dicee.models.clifford.Keci* method), 62
 compute_sigma_qq() (*dicee.models.DeCaL* method), 127

`compute_sigma_qq()` (*dicee.models.Keci method*), 122
`compute_sigma_qr()` (*dicee.DeCaL method*), 170
`compute_sigma_qr()` (*dicee.models.clifford.DeCaL method*), 67
`compute_sigma_qr()` (*dicee.models.DeCaL method*), 128
`compute_sigma_rr()` (*dicee.DeCaL method*), 170
`compute_sigma_rr()` (*dicee.models.clifford.DeCaL method*), 67
`compute_sigma_rr()` (*dicee.models.DeCaL method*), 127
`compute_sigmas_multivect()` (*dicee.DeCaL method*), 168
`compute_sigmas_multivect()` (*dicee.models.clifford.DeCaL method*), 65
`compute_sigmas_multivect()` (*dicee.models.DeCaL method*), 126
`compute_sigmas_single()` (*dicee.DeCaL method*), 168
`compute_sigmas_single()` (*dicee.models.clifford.DeCaL method*), 65
`compute_sigmas_single()` (*dicee.models.DeCaL method*), 125
`ConEx` (*class in dicee*), 176
`ConEx` (*class in dicee.models*), 107
`ConEx` (*class in dicee.models.complex*), 68
`config` (*dicee.BytE attribute*), 182
`config` (*dicee.models.transformers.BytE attribute*), 85
`config` (*dicee.models.transformers.GPT attribute*), 90
`configs` (*dicee.abstracts.BaseInteractiveKGE attribute*), 14
`configure_optimizers()` (*dicee.models.base_model.BaseKGELightning method*), 56
`configure_optimizers()` (*dicee.models.BaseKGELightning method*), 96
`configure_optimizers()` (*dicee.models.transformers.GPT method*), 90
`construct_batch_selected_cl_multivector()` (*dicee.Keci method*), 166
`construct_batch_selected_cl_multivector()` (*dicee.models.clifford.Keci method*), 63
`construct_batch_selected_cl_multivector()` (*dicee.models.Keci method*), 123
`construct_cl_multivector()` (*dicee.DeCaL method*), 169
`construct_cl_multivector()` (*dicee.Keci method*), 166
`construct_cl_multivector()` (*dicee.models.clifford.DeCaL method*), 66
`construct_cl_multivector()` (*dicee.models.clifford.Keci method*), 62
`construct_cl_multivector()` (*dicee.models.DeCaL method*), 126
`construct_cl_multivector()` (*dicee.models.Keci method*), 123
`construct_dataset()` (*in module dicee*), 195
`construct_dataset()` (*in module dicee.dataset_classes*), 29
`construct_ensemble` (*dicee.abstracts.BaseInteractiveKGE attribute*), 14
`construct_graph()` (*dicee.query_generator.QueryGenerator method*), 138
`construct_graph()` (*dicee.QueryGenerator method*), 206
`construct_input_and_output()` (*dicee.abstracts.BaseInteractiveKGE method*), 15
`construct_multi_coeff()` (*dicee.LFMult method*), 179
`construct_multi_coeff()` (*dicee.models.function_space.LFMult method*), 74
`construct_multi_coeff()` (*dicee.models.LFMult method*), 136
`continual_learning` (*dicee.config.Namespace attribute*), 28
`continual_start()` (*dicee.DICE_Trainer method*), 189
`continual_start()` (*dicee.executer.ContinuousExecute method*), 44
`continual_start()` (*dicee.trainer.DICE_Trainer method*), 159
`continual_start()` (*dicee.trainer.dice_trainer.DICE_Trainer method*), 154
`continual_training_setup_executor()` (*in module dicee*), 188
`continual_training_setup_executor()` (*in module dicee.static_funcs*), 151
`ContinuousExecute` (*class in dicee.executer*), 44
`conv2d` (*dicee.AConEx attribute*), 173
`conv2d` (*dicee.AConvO attribute*), 173
`conv2d` (*dicee.AConvQ attribute*), 174
`conv2d` (*dicee.ConEx attribute*), 176
`conv2d` (*dicee.ConvO attribute*), 175
`conv2d` (*dicee.ConvQ attribute*), 174
`conv2d` (*dicee.models.AConEx attribute*), 108
`conv2d` (*dicee.models.AConvO attribute*), 120
`conv2d` (*dicee.models.AConvQ attribute*), 115
`conv2d` (*dicee.models.complex.AConEx attribute*), 68
`conv2d` (*dicee.models.complex.ConEx attribute*), 68
`conv2d` (*dicee.models.ConEx attribute*), 107
`conv2d` (*dicee.models.ConvO attribute*), 120
`conv2d` (*dicee.models.ConvQ attribute*), 114
`conv2d` (*dicee.models.octonion.AConvO attribute*), 77
`conv2d` (*dicee.models.octonion.ConvO attribute*), 77
`conv2d` (*dicee.models.quaternion.AConvQ attribute*), 82
`conv2d` (*dicee.models.quaternion.ConvQ attribute*), 81
`ConvO` (*class in dicee*), 175

- ConvO (class in *dicee.models*), 119
- ConvO (class in *dicee.models.octonion*), 76
- ConvQ (class in *dicee*), 174
- ConvQ (class in *dicee.models*), 114
- ConvQ (class in *dicee.models.quaternion*), 81
- create_constraints() (in module *dicee.read_preprocess_save_load_kg.util*), 144
- create_constraints() (in module *dicee.static_preprocess_funcs*), 153
- create_experiment_folder() (in module *dicee*), 188
- create_experiment_folder() (in module *dicee.static_funcs*), 151
- create_random_data() (*dicee.callbacks.PseudoLabellingCallback* method), 22
- create_recipriocal_triples() (in module *dicee*), 186
- create_recipriocal_triples() (in module *dicee.read_preprocess_save_load_kg.util*), 145
- create_recipriocal_triples() (in module *dicee.static_funcs*), 150
- create_vector_database() (*dicee.KGE* method), 190
- create_vector_database() (*dicee.knowledge_graph_embeddings.KGE* method), 47
- crop_block_size() (*dicee.models.transformers.GPT* method), 90
- ctx (*dicee.trainer.torch_trainer_ddp.NodeTrainer* attribute), 158
- CVDDataModule (class in *dicee*), 202
- CVDDataModule (class in *dicee.dataset_classes*), 37

D

- data_module (*dicee.callbacks.PseudoLabellingCallback* attribute), 22
- dataset_dir (*dicee.config.Namespace* attribute), 26
- dataset_dir (*dicee.knowledge_graph.KG* attribute), 45
- dataset_sanity_checking() (in module *dicee.read_preprocess_save_load_kg.util*), 145
- DeCaL (class in *dicee*), 167
- DeCaL (class in *dicee.models*), 124
- DeCaL (class in *dicee.models.clifford*), 64
- decide() (*dicee.callbacks.ASWA* method), 23
- degree (*dicee.LFMult* attribute), 179
- degree (*dicee.models.function_space.LFMult* attribute), 74
- degree (*dicee.models.LFMult* attribute), 136
- deploy() (*dicee.KGE* method), 193
- deploy() (*dicee.knowledge_graph_embeddings.KGE* method), 50
- deploy_head_entity_prediction() (in module *dicee*), 187
- deploy_head_entity_prediction() (in module *dicee.static_funcs*), 151
- deploy_relation_prediction() (in module *dicee*), 188
- deploy_relation_prediction() (in module *dicee.static_funcs*), 151
- deploy_tail_entity_prediction() (in module *dicee*), 187
- deploy_tail_entity_prediction() (in module *dicee.static_funcs*), 151
- deploy_triple_prediction() (in module *dicee*), 187
- deploy_triple_prediction() (in module *dicee.static_funcs*), 151
- dept_read_preprocess_index_serialize_data() (*dicee.Execute* method), 194
- dept_read_preprocess_index_serialize_data() (*dicee.executer.Execute* method), 43
- describe() (*dicee.knowledge_graph.KG* method), 46
- description_of_input (*dicee.knowledge_graph.KG* attribute), 46
- DICE_Trainer (class in *dicee*), 188
- DICE_Trainer (class in *dicee.trainer*), 159
- DICE_Trainer (class in *dicee.trainer.dice_trainer*), 154
- dicee
 - module, 12
- dicee.__main__
 - module, 12
- dicee.abstracts
 - module, 12
- dicee.analyse_experiments
 - module, 17
- dicee.callbacks
 - module, 19
- dicee.config
 - module, 25
- dicee.dataset_classes
 - module, 28
- dicee.eval_static_funcs
 - module, 40
- dicee.evaluator
 - module, 41

- dicee.executer
 - module, 43
- dicee.knowledge_graph
 - module, 45
- dicee.knowledge_graph_embeddings
 - module, 46
- dicee.models
 - module, 50
- dicee.models.adopt
 - module, 50
- dicee.models.base_model
 - module, 51
- dicee.models.clifford
 - module, 60
- dicee.models.complex
 - module, 67
- dicee.models.dualE
 - module, 70
- dicee.models.ensemble
 - module, 71
- dicee.models.function_space
 - module, 72
- dicee.models.octonion
 - module, 75
- dicee.models.pykeen_models
 - module, 78
- dicee.models.quaternion
 - module, 79
- dicee.models.real
 - module, 82
- dicee.models.static_funcs
 - module, 84
- dicee.models.transformers
 - module, 84
- dicee.query_generator
 - module, 138
- dicee.read_preprocess_save_load_kg
 - module, 139
- dicee.read_preprocess_save_load_kg.preprocess
 - module, 139
- dicee.read_preprocess_save_load_kg.read_from_disk
 - module, 140
- dicee.read_preprocess_save_load_kg.save_load_disk
 - module, 141
- dicee.read_preprocess_save_load_kg.util
 - module, 141
- dicee.sanity_checkers
 - module, 146
- dicee.scripts
 - module, 147
- dicee.scripts.index
 - module, 147
- dicee.scripts.run
 - module, 147
- dicee.scripts.serve
 - module, 147
- dicee.static_funcs
 - module, 148
- dicee.static_funcs_training
 - module, 152
- dicee.static_preprocess_funcs
 - module, 152
- dicee.trainer
 - module, 153
- dicee.trainer.dice_trainer
 - module, 153
- dicee.trainer.model_parallelism
 - module, 155

- `dicee.trainer.torch_trainer`
 - module, 156
- `dicee.trainer.torch_trainer_ddp`
 - module, 157
- `discrete_points (dicee.models.FMult2 attribute)`, 135
- `discrete_points (dicee.models.function_space.FMult2 attribute)`, 73
- `dist_func (dicee.models.Pyke attribute)`, 104
- `dist_func (dicee.models.real.Pyke attribute)`, 83
- `dist_func (dicee.Pyke attribute)`, 163
- `DistMult (class in dicee)`, 163
- `DistMult (class in dicee.models)`, 103
- `DistMult (class in dicee.models.real)`, 82
- `download_file()` (in module `dicee`), 188
- `download_file()` (in module `dicee.static_funcs`), 151
- `download_files_from_url()` (in module `dicee`), 188
- `download_files_from_url()` (in module `dicee.static_funcs`), 151
- `download_pretrained_model()` (in module `dicee`), 188
- `download_pretrained_model()` (in module `dicee.static_funcs`), 151
- `dropout (dicee.models.transformers.CausalSelfAttention attribute)`, 87
- `dropout (dicee.models.transformers.GPTConfig attribute)`, 89
- `dropout (dicee.models.transformers.MLP attribute)`, 88
- `DualE (class in dicee)`, 171
- `DualE (class in dicee.models)`, 137
- `DualE (class in dicee.models.dualE)`, 70
- `dummy_eval()` (`dicee.evaluator.Evaluator` method), 42
- `dummy_id (dicee.knowledge_graph.KG attribute)`, 46
- `during_training (dicee.evaluator.Evaluator attribute)`, 42

E

- `ee_vocab (dicee.evaluator.Evaluator attribute)`, 41
- `efficient_zero_grad()` (in module `dicee.static_funcs_training`), 152
- `embedding_dim (dicee.analyse_experiments.Experiment attribute)`, 18
- `embedding_dim (dicee.BaseKGE attribute)`, 184
- `embedding_dim (dicee.config.Namespace attribute)`, 26
- `embedding_dim (dicee.models.base_model.BaseKGE attribute)`, 58
- `embedding_dim (dicee.models.BaseKGE attribute)`, 98, 102, 105, 110, 116, 128, 132
- `enable_log` (in module `dicee.static_preprocess_funcs`), 153
- `enc (dicee.knowledge_graph.KG attribute)`, 46
- `end()` (`dicee.Execute` method), 194
- `end()` (`dicee.executor.Execute` method), 44
- `EnsembleKGE (class in dicee)`, 186
- `EnsembleKGE (class in dicee.models.ensemble)`, 71
- `ent2id (dicee.query_generator.QueryGenerator attribute)`, 138
- `ent2id (dicee.QueryGenerator attribute)`, 206
- `ent_in (dicee.query_generator.QueryGenerator attribute)`, 138
- `ent_in (dicee.QueryGenerator attribute)`, 206
- `ent_out (dicee.query_generator.QueryGenerator attribute)`, 138
- `ent_out (dicee.QueryGenerator attribute)`, 206
- `entities_str (dicee.knowledge_graph.KG property)`, 46
- `entity_embeddings (dicee.AConvQ attribute)`, 174
- `entity_embeddings (dicee.ConvQ attribute)`, 174
- `entity_embeddings (dicee.DeCaL attribute)`, 168
- `entity_embeddings (dicee.DualE attribute)`, 171
- `entity_embeddings (dicee.LFMult attribute)`, 179
- `entity_embeddings (dicee.models.AConvQ attribute)`, 115
- `entity_embeddings (dicee.models.clifford.DeCaL attribute)`, 64
- `entity_embeddings (dicee.models.ConvQ attribute)`, 114
- `entity_embeddings (dicee.models.DeCaL attribute)`, 125
- `entity_embeddings (dicee.models.DualE attribute)`, 137
- `entity_embeddings (dicee.models.dualE.DualE attribute)`, 70
- `entity_embeddings (dicee.models.FMult attribute)`, 134
- `entity_embeddings (dicee.models.FMult2 attribute)`, 135
- `entity_embeddings (dicee.models.function_space.FMult attribute)`, 72
- `entity_embeddings (dicee.models.function_space.FMult2 attribute)`, 73
- `entity_embeddings (dicee.models.function_space.GFMult attribute)`, 72
- `entity_embeddings (dicee.models.function_space.LFMult attribute)`, 74
- `entity_embeddings (dicee.models.function_space.LFMult1 attribute)`, 73

entity_embeddings (*dicee.models.GFMult attribute*), 134
 entity_embeddings (*dicee.models.LFMult attribute*), 135
 entity_embeddings (*dicee.models.LFMult1 attribute*), 135
 entity_embeddings (*dicee.models.pykeen_models.PykeenKGE attribute*), 78
 entity_embeddings (*dicee.models.PykeenKGE attribute*), 130
 entity_embeddings (*dicee.models.quaternion.AConvQ attribute*), 82
 entity_embeddings (*dicee.models.quaternion.ConvQ attribute*), 81
 entity_embeddings (*dicee.PykeenKGE attribute*), 181
 entity_to_idx (*dicee.knowledge_graph.KG attribute*), 45
 epoch_count (*dicee.abstracts.AbstractPPECallback attribute*), 17
 epoch_count (*dicee.callbacks.ASWA attribute*), 22
 epoch_counter (*dicee.callbacks.Eval attribute*), 23
 epoch_counter (*dicee.callbacks.KGESaveCallback attribute*), 21
 epoch_ratio (*dicee.callbacks.Eval attribute*), 23
 er_vocab (*dicee.evaluator.Evaluator attribute*), 41
 estimate_mfu () (*dicee.models.transformers.GPT method*), 90
 estimate_q () (*in module dicee.callbacks*), 22
 Eval (*class in dicee.callbacks*), 23
 eval () (*dicee.EnsembleKGE method*), 186
 eval () (*dicee.evaluator.Evaluator method*), 42
 eval () (*dicee.models.ensemble.EnsembleKGE method*), 71
 eval_lp_performance () (*dicee.KGE method*), 190
 eval_lp_performance () (*dicee.knowledge_graph_embeddings.KGE method*), 47
 eval_model (*dicee.config.Namespace attribute*), 27
 eval_model (*dicee.knowledge_graph.KG attribute*), 45
 eval_rank_of_head_and_tail_byte_pair_encoded_entity () (*dicee.evaluator.Evaluator method*), 42
 eval_rank_of_head_and_tail_entity () (*dicee.evaluator.Evaluator method*), 42
 eval_with_bpe_vs_all () (*dicee.evaluator.Evaluator method*), 42
 eval_with_byte () (*dicee.evaluator.Evaluator method*), 42
 eval_with_data () (*dicee.evaluator.Evaluator method*), 42
 eval_with_vs_all () (*dicee.evaluator.Evaluator method*), 42
 evaluate () (*in module dicee*), 188
 evaluate () (*in module dicee.static_funcs*), 151
 evaluate_bpe_lp () (*in module dicee.static_funcs_training*), 152
 evaluate_link_prediction_performance () (*in module dicee.eval_static_funcs*), 40
 evaluate_link_prediction_performance_with_bpe () (*in module dicee.eval_static_funcs*), 41
 evaluate_link_prediction_performance_with_bpe_reciprocals () (*in module dicee.eval_static_funcs*), 41
 evaluate_link_prediction_performance_with_reciprocals () (*in module dicee.eval_static_funcs*), 41
 evaluate_lp () (*dicee.evaluator.Evaluator method*), 42
 evaluate_lp () (*in module dicee.static_funcs_training*), 152
 evaluate_lp_bpe_k_vs_all () (*dicee.evaluator.Evaluator method*), 42
 evaluate_lp_bpe_k_vs_all () (*in module dicee.eval_static_funcs*), 41
 evaluate_lp_k_vs_all () (*dicee.evaluator.Evaluator method*), 42
 evaluate_lp_with_byte () (*dicee.evaluator.Evaluator method*), 42
 Evaluator (*class in dicee.evaluator*), 41
 evaluator (*dicee.DICE_Trainer attribute*), 188
 evaluator (*dicee.Execute attribute*), 194
 evaluator (*dicee.executer.Execute attribute*), 43
 evaluator (*dicee.trainer.DICE_Trainer attribute*), 159
 evaluator (*dicee.trainer.dice_trainer.DICE_Trainer attribute*), 154
 every_x_epoch (*dicee.callbacks.KGESaveCallback attribute*), 21
 example_input_array (*dicee.EnsembleKGE property*), 186
 example_input_array (*dicee.models.ensemble.EnsembleKGE property*), 71
 Execute (*class in dicee*), 193
 Execute (*class in dicee.executer*), 43
 exists () (*dicee.knowledge_graph.KG method*), 46
 Experiment (*class in dicee.analyse_experiments*), 18
 explicit (*dicee.models.QMult attribute*), 113
 explicit (*dicee.models.quaternion.QMult attribute*), 80
 explicit (*dicee.QMult attribute*), 177
 exponential_function () (*in module dicee*), 188
 exponential_function () (*in module dicee.static_funcs*), 151
 extract_input_outputs () (*dicee.trainer.torch_trainer_ddp.NodeTrainer method*), 158
 extract_input_outputs () (*in module dicee.trainer.model_parallelism*), 156
 extract_input_outputs_set_device () (*dicee.trainer.torch_trainer.TorchTrainer method*), 157

F

f (*dicee.callbacks.KronE attribute*), 25

`fc1` (*dicee.AConEx* attribute), 173
`fc1` (*dicee.AConvO* attribute), 173
`fc1` (*dicee.AConvQ* attribute), 174
`fc1` (*dicee.ConEx* attribute), 176
`fc1` (*dicee.ConvO* attribute), 175
`fc1` (*dicee.ConvQ* attribute), 174
`fc1` (*dicee.models.AConEx* attribute), 108
`fc1` (*dicee.models.AConvO* attribute), 120
`fc1` (*dicee.models.AConvQ* attribute), 115
`fc1` (*dicee.models.complex.AConEx* attribute), 68
`fc1` (*dicee.models.complex.ConEx* attribute), 68
`fc1` (*dicee.models.ConEx* attribute), 107
`fc1` (*dicee.models.ConvO* attribute), 120
`fc1` (*dicee.models.ConvQ* attribute), 114
`fc1` (*dicee.models.octonion.AConvO* attribute), 78
`fc1` (*dicee.models.octonion.ConvO* attribute), 77
`fc1` (*dicee.models.quaternion.AConvQ* attribute), 82
`fc1` (*dicee.models.quaternion.ConvQ* attribute), 81
`fc_num_input` (*dicee.AConEx* attribute), 173
`fc_num_input` (*dicee.AConvO* attribute), 173
`fc_num_input` (*dicee.AConvQ* attribute), 174
`fc_num_input` (*dicee.ConEx* attribute), 176
`fc_num_input` (*dicee.ConvO* attribute), 175
`fc_num_input` (*dicee.ConvQ* attribute), 174
`fc_num_input` (*dicee.models.AConEx* attribute), 108
`fc_num_input` (*dicee.models.AConvO* attribute), 120
`fc_num_input` (*dicee.models.AConvQ* attribute), 115
`fc_num_input` (*dicee.models.complex.AConEx* attribute), 68
`fc_num_input` (*dicee.models.complex.ConEx* attribute), 68
`fc_num_input` (*dicee.models.ConEx* attribute), 107
`fc_num_input` (*dicee.models.ConvO* attribute), 120
`fc_num_input` (*dicee.models.ConvQ* attribute), 114
`fc_num_input` (*dicee.models.octonion.AConvO* attribute), 77
`fc_num_input` (*dicee.models.octonion.ConvO* attribute), 77
`fc_num_input` (*dicee.models.quaternion.AConvQ* attribute), 82
`fc_num_input` (*dicee.models.quaternion.ConvQ* attribute), 81
`feature_map_dropout` (*dicee.AConEx* attribute), 173
`feature_map_dropout` (*dicee.AConvO* attribute), 173
`feature_map_dropout` (*dicee.AConvQ* attribute), 174
`feature_map_dropout` (*dicee.ConEx* attribute), 176
`feature_map_dropout` (*dicee.ConvO* attribute), 176
`feature_map_dropout` (*dicee.ConvQ* attribute), 174
`feature_map_dropout` (*dicee.models.AConEx* attribute), 108
`feature_map_dropout` (*dicee.models.AConvO* attribute), 121
`feature_map_dropout` (*dicee.models.AConvQ* attribute), 115
`feature_map_dropout` (*dicee.models.complex.AConEx* attribute), 68
`feature_map_dropout` (*dicee.models.complex.ConEx* attribute), 68
`feature_map_dropout` (*dicee.models.ConEx* attribute), 107
`feature_map_dropout` (*dicee.models.ConvO* attribute), 120
`feature_map_dropout` (*dicee.models.ConvQ* attribute), 114
`feature_map_dropout` (*dicee.models.octonion.AConvO* attribute), 78
`feature_map_dropout` (*dicee.models.octonion.ConvO* attribute), 77
`feature_map_dropout` (*dicee.models.quaternion.AConvQ* attribute), 82
`feature_map_dropout` (*dicee.models.quaternion.ConvQ* attribute), 81
`feature_map_dropout_rate` (*dicee.BaseKGE* attribute), 184
`feature_map_dropout_rate` (*dicee.config.Namespace* attribute), 28
`feature_map_dropout_rate` (*dicee.models.base_model.BaseKGE* attribute), 58
`feature_map_dropout_rate` (*dicee.models.BaseKGE* attribute), 99, 102, 106, 110, 116, 129, 132
`fill_query` () (*dicee.query_generator.QueryGenerator* method), 138
`fill_query` () (*dicee.QueryGenerator* method), 206
`find_good_batch_size` () (*in module dicee.trainer.model_parallelism*), 156
`find_missing_triples` () (*dicee.KGE* method), 193
`find_missing_triples` () (*dicee.knowledge_graph_embeddings.KGE* method), 50
`fit` () (*dicee.trainer.model_parallelism.TensorParallel* method), 156
`fit` () (*dicee.trainer.torch_trainer_ddp.TorchDDPTrainer* method), 158
`fit` () (*dicee.trainer.torch_trainer.TorchTrainer* method), 157
`flash` (*dicee.models.transformers.CausalSelfAttention* attribute), 87
`FMult` (*class in dicee.models*), 133

FMult (class in *dicее.models.function_space*), 72
 FMult2 (class in *dicее.models*), 134
 FMult2 (class in *dicее.models.function_space*), 73
 form_of_labelling (*dicее.DICE_Trainer* attribute), 189
 form_of_labelling (*dicее.trainer.DICE_Trainer* attribute), 159
 form_of_labelling (*dicее.trainer.dice_trainer.DICE_Trainer* attribute), 154
 forward() (*dicее.BaseKGE* method), 185
 forward() (*dicее.BytE* method), 182
 forward() (*dicее.models.base_model.BaseKGE* method), 59
 forward() (*dicее.models.base_model.IdentityClass* static method), 60
 forward() (*dicее.models.BaseKGE* method), 100, 103, 106, 111, 117, 130, 133
 forward() (*dicее.models.IdentityClass* static method), 101, 112, 118
 forward() (*dicее.models.transformers.Block* method), 89
 forward() (*dicее.models.transformers.BytE* method), 85
 forward() (*dicее.models.transformers.CausalSelfAttention* method), 87
 forward() (*dicее.models.transformers.GPT* method), 90
 forward() (*dicее.models.transformers.LayerNorm* method), 86
 forward() (*dicее.models.transformers.MLP* method), 88
 forward_backward_update() (*dicее.trainer.torch_trainer.TorchTrainer* method), 157
 forward_backward_update_loss() (in module *dicее.trainer.model_parallelism*), 156
 forward_byte_pair_encoded_k_vs_all() (*dicее.BaseKGE* method), 185
 forward_byte_pair_encoded_k_vs_all() (*dicее.models.base_model.BaseKGE* method), 59
 forward_byte_pair_encoded_k_vs_all() (*dicее.models.BaseKGE* method), 99, 102, 106, 111, 117, 129, 133
 forward_byte_pair_encoded_triple() (*dicее.BaseKGE* method), 185
 forward_byte_pair_encoded_triple() (*dicее.models.base_model.BaseKGE* method), 59
 forward_byte_pair_encoded_triple() (*dicее.models.BaseKGE* method), 99, 103, 106, 111, 117, 129, 133
 forward_k_vs_all() (*dicее.AConEx* method), 173
 forward_k_vs_all() (*dicее.AConvO* method), 173
 forward_k_vs_all() (*dicее.AConvQ* method), 174
 forward_k_vs_all() (*dicее.BaseKGE* method), 185
 forward_k_vs_all() (*dicее.ComplEx* method), 172
 forward_k_vs_all() (*dicее.ConEx* method), 176
 forward_k_vs_all() (*dicее.ConvO* method), 176
 forward_k_vs_all() (*dicее.ConvQ* method), 175
 forward_k_vs_all() (*dicее.DeCaL* method), 169
 forward_k_vs_all() (*dicее.DistMult* method), 164
 forward_k_vs_all() (*dicее.DualE* method), 171
 forward_k_vs_all() (*dicее.Keci* method), 166
 forward_k_vs_all() (*dicее.models.AConEx* method), 108
 forward_k_vs_all() (*dicее.models.AConvO* method), 121
 forward_k_vs_all() (*dicее.models.AConvQ* method), 115
 forward_k_vs_all() (*dicее.models.base_model.BaseKGE* method), 59
 forward_k_vs_all() (*dicее.models.BaseKGE* method), 100, 103, 107, 111, 117, 130, 133
 forward_k_vs_all() (*dicее.models.clifford.DeCaL* method), 65
 forward_k_vs_all() (*dicее.models.clifford.Keci* method), 63
 forward_k_vs_all() (*dicее.models.ComplEx* method), 109
 forward_k_vs_all() (*dicее.models.complex.AConEx* method), 68
 forward_k_vs_all() (*dicее.models.complex.ComplEx* method), 69
 forward_k_vs_all() (*dicее.models.complex.ConEx* method), 68
 forward_k_vs_all() (*dicее.models.ConEx* method), 107
 forward_k_vs_all() (*dicее.models.ConvO* method), 120
 forward_k_vs_all() (*dicее.models.ConvQ* method), 114
 forward_k_vs_all() (*dicее.models.DeCaL* method), 126
 forward_k_vs_all() (*dicее.models.DistMult* method), 104
 forward_k_vs_all() (*dicее.models.DualE* method), 137
 forward_k_vs_all() (*dicее.models.dualE.DualE* method), 70
 forward_k_vs_all() (*dicее.models.Keci* method), 123
 forward_k_vs_all() (*dicее.models.octonion.AConvO* method), 78
 forward_k_vs_all() (*dicее.models.octonion.ConvO* method), 77
 forward_k_vs_all() (*dicее.models.octonion.OMult* method), 76
 forward_k_vs_all() (*dicее.models.OMult* method), 119
 forward_k_vs_all() (*dicее.models.pykeen_models.PykeenKGE* method), 78
 forward_k_vs_all() (*dicее.models.PykeenKGE* method), 131
 forward_k_vs_all() (*dicее.models.QMult* method), 114
 forward_k_vs_all() (*dicее.models.quaternion.AConvQ* method), 82
 forward_k_vs_all() (*dicее.models.quaternion.ConvQ* method), 81
 forward_k_vs_all() (*dicее.models.quaternion.QMult* method), 81
 forward_k_vs_all() (*dicее.models.real.DistMult* method), 83

`forward_k_vs_all()` (*dicee.models.real.Shallom method*), 83
`forward_k_vs_all()` (*dicee.models.real.TransE method*), 83
`forward_k_vs_all()` (*dicee.models.Shallom method*), 104
`forward_k_vs_all()` (*dicee.models.TransE method*), 104
`forward_k_vs_all()` (*dicee.OMult method*), 179
`forward_k_vs_all()` (*dicee.PykeenKGE method*), 181
`forward_k_vs_all()` (*dicee.QMult method*), 178
`forward_k_vs_all()` (*dicee.Shallom method*), 179
`forward_k_vs_all()` (*dicee.TransE method*), 167
`forward_k_vs_sample()` (*dicee.AConEx method*), 173
`forward_k_vs_sample()` (*dicee.BaseKGE method*), 185
`forward_k_vs_sample()` (*dicee.ComplEx method*), 172
`forward_k_vs_sample()` (*dicee.ConEx method*), 176
`forward_k_vs_sample()` (*dicee.DistMult method*), 164
`forward_k_vs_sample()` (*dicee.Keci method*), 166
`forward_k_vs_sample()` (*dicee.models.AConEx method*), 108
`forward_k_vs_sample()` (*dicee.models.base_model.BaseKGE method*), 59
`forward_k_vs_sample()` (*dicee.models.BaseKGE method*), 100, 103, 107, 111, 117, 130, 133
`forward_k_vs_sample()` (*dicee.models.clifford.Keci method*), 63
`forward_k_vs_sample()` (*dicee.models.ComplEx method*), 109
`forward_k_vs_sample()` (*dicee.models.complex.AConEx method*), 69
`forward_k_vs_sample()` (*dicee.models.complex.ComplEx method*), 70
`forward_k_vs_sample()` (*dicee.models.complex.ConEx method*), 68
`forward_k_vs_sample()` (*dicee.models.ConEx method*), 107
`forward_k_vs_sample()` (*dicee.models.DistMult method*), 104
`forward_k_vs_sample()` (*dicee.models.Keci method*), 124
`forward_k_vs_sample()` (*dicee.models.pykeen_models.PykeenKGE method*), 79
`forward_k_vs_sample()` (*dicee.models.PykeenKGE method*), 131
`forward_k_vs_sample()` (*dicee.models.QMult method*), 114
`forward_k_vs_sample()` (*dicee.models.quaternion.QMult method*), 81
`forward_k_vs_sample()` (*dicee.models.real.DistMult method*), 83
`forward_k_vs_sample()` (*dicee.PykeenKGE method*), 181
`forward_k_vs_sample()` (*dicee.QMult method*), 178
`forward_k_vs_with_explicit()` (*dicee.Keci method*), 166
`forward_k_vs_with_explicit()` (*dicee.models.clifford.Keci method*), 63
`forward_k_vs_with_explicit()` (*dicee.models.Keci method*), 123
`forward_triples()` (*dicee.AConEx method*), 173
`forward_triples()` (*dicee.AConvO method*), 173
`forward_triples()` (*dicee.AConvQ method*), 174
`forward_triples()` (*dicee.BaseKGE method*), 185
`forward_triples()` (*dicee.ConEx method*), 176
`forward_triples()` (*dicee.ConvO method*), 176
`forward_triples()` (*dicee.ConvQ method*), 175
`forward_triples()` (*dicee.DeCaL method*), 168
`forward_triples()` (*dicee.DualE method*), 171
`forward_triples()` (*dicee.Keci method*), 167
`forward_triples()` (*dicee.LFMult method*), 179
`forward_triples()` (*dicee.models.AConEx method*), 108
`forward_triples()` (*dicee.models.AConvO method*), 121
`forward_triples()` (*dicee.models.AConvQ method*), 115
`forward_triples()` (*dicee.models.base_model.BaseKGE method*), 59
`forward_triples()` (*dicee.models.BaseKGE method*), 100, 103, 106, 111, 117, 130, 133
`forward_triples()` (*dicee.models.clifford.DeCaL method*), 65
`forward_triples()` (*dicee.models.clifford.Keci method*), 63
`forward_triples()` (*dicee.models.complex.AConEx method*), 69
`forward_triples()` (*dicee.models.complex.ConEx method*), 68
`forward_triples()` (*dicee.models.ConEx method*), 107
`forward_triples()` (*dicee.models.ConvO method*), 120
`forward_triples()` (*dicee.models.ConvQ method*), 114
`forward_triples()` (*dicee.models.DeCaL method*), 125
`forward_triples()` (*dicee.models.DualE method*), 137
`forward_triples()` (*dicee.models.dualE.DualE method*), 70
`forward_triples()` (*dicee.models.FMult method*), 134
`forward_triples()` (*dicee.models.FMult2 method*), 135
`forward_triples()` (*dicee.models.function_space.FMult method*), 72
`forward_triples()` (*dicee.models.function_space.FMult2 method*), 73
`forward_triples()` (*dicee.models.function_space.GFMult method*), 73
`forward_triples()` (*dicee.models.function_space.LFMult method*), 74

`forward_triples()` (*dicee.models.function_space.LFMult1 method*), 73
`forward_triples()` (*dicee.models.GFMult method*), 134
`forward_triples()` (*dicee.models.Keci method*), 124
`forward_triples()` (*dicee.models.LFMult method*), 136
`forward_triples()` (*dicee.models.LFMult1 method*), 135
`forward_triples()` (*dicee.models.octonion.AConvO method*), 78
`forward_triples()` (*dicee.models.octonion.ConvO method*), 77
`forward_triples()` (*dicee.models.Pyke method*), 104
`forward_triples()` (*dicee.models.pykeen_models.PykeenKGE method*), 79
`forward_triples()` (*dicee.models.PykeenKGE method*), 131
`forward_triples()` (*dicee.models.quaternion.AConvQ method*), 82
`forward_triples()` (*dicee.models.quaternion.ConvQ method*), 81
`forward_triples()` (*dicee.models.real.Pyke method*), 83
`forward_triples()` (*dicee.models.real.Shallom method*), 83
`forward_triples()` (*dicee.models.Shallom method*), 104
`forward_triples()` (*dicee.Pyke method*), 163
`forward_triples()` (*dicee.PykeenKGE method*), 181
`forward_triples()` (*dicee.Shallom method*), 179
`frequency` (*dicee.callbacks.Perturb attribute*), 25
`from_pretrained()` (*dicee.models.transformers.GPT class method*), 90
`from_pretrained_model_write_embeddings_into_csv()` (*in module dicee*), 188
`from_pretrained_model_write_embeddings_into_csv()` (*in module dicee.static_funcs*), 152
`full_storage_path` (*dicee.analyse_experiments.Experiment attribute*), 18
`func_triple_to_bpe_representation` (*dicee.evaluator.Evaluator attribute*), 41
`func_triple_to_bpe_representation()` (*dicee.knowledge_graph.KG method*), 46
`function()` (*dicee.models.FMult2 method*), 135
`function()` (*dicee.models.function_space.FMult2 method*), 73

G

`gamma` (*dicee.models.FMult attribute*), 134
`gamma` (*dicee.models.function_space.FMult attribute*), 72
`gelu` (*dicee.models.transformers.MLP attribute*), 88
`gen_test` (*dicee.query_generator.QueryGenerator attribute*), 138
`gen_test` (*dicee.QueryGenerator attribute*), 206
`gen_valid` (*dicee.query_generator.QueryGenerator attribute*), 138
`gen_valid` (*dicee.QueryGenerator attribute*), 206
`generate()` (*dicee.BytE method*), 182
`generate()` (*dicee.KGE method*), 190
`generate()` (*dicee.knowledge_graph_embeddings.KGE method*), 47
`generate()` (*dicee.models.transformers.BytE method*), 85
`generate_queries()` (*dicee.query_generator.QueryGenerator method*), 139
`generate_queries()` (*dicee.QueryGenerator method*), 207
`get()` (*dicee.scripts.serve.NeuralSearcher method*), 148
`get_aswa_state_dict()` (*dicee.callbacks.ASWA method*), 23
`get_bpe_head_and_relation_representation()` (*dicee.BaseKGE method*), 186
`get_bpe_head_and_relation_representation()` (*dicee.models.base_model.BaseKGE method*), 59
`get_bpe_head_and_relation_representation()` (*dicee.models.BaseKGE method*), 100, 103, 107, 111, 117, 130, 133
`get_bpe_token_representation()` (*dicee.abstracts.BaseInteractiveKGE method*), 14
`get_callbacks()` (*in module dicee.trainer.dice_trainer*), 154
`get_default_arguments()` (*in module dicee.analyse_experiments*), 18
`get_default_arguments()` (*in module dicee.scripts.index*), 147
`get_default_arguments()` (*in module dicee.scripts.run*), 147
`get_default_arguments()` (*in module dicee.scripts.serve*), 148
`get_ee_vocab()` (*in module dicee*), 186
`get_ee_vocab()` (*in module dicee.read_preprocess_save_load_kg.util*), 144
`get_ee_vocab()` (*in module dicee.static_funcs*), 150
`get_ee_vocab()` (*in module dicee.static_preprocess_funcs*), 153
`get_embeddings()` (*dicee.BaseKGE method*), 186
`get_embeddings()` (*dicee.EnsembleKGE method*), 186
`get_embeddings()` (*dicee.models.base_model.BaseKGE method*), 60
`get_embeddings()` (*dicee.models.BaseKGE method*), 100, 103, 107, 111, 117, 130, 133
`get_embeddings()` (*dicee.models.ensemble.EnsembleKGE method*), 71
`get_embeddings()` (*dicee.models.real.Shallom method*), 83
`get_embeddings()` (*dicee.models.Shallom method*), 104
`get_embeddings()` (*dicee.Shallom method*), 179
`get_ensemble()` (*dicee.trainer.model_parallelism.TensorParallel method*), 156
`get_entity_embeddings()` (*dicee.abstracts.BaseInteractiveKGE method*), 15

`get_entity_index()` (*dicee.abstracts.BaseInteractiveKGE method*), 14
`get_er_vocab()` (*in module dicee*), 186
`get_er_vocab()` (*in module dicee.read_preprocess_save_load_kg.util*), 144
`get_er_vocab()` (*in module dicee.static_funcs*), 150
`get_er_vocab()` (*in module dicee.static_preprocess_funcs*), 153
`get_eval_report()` (*dicee.abstracts.BaseInteractiveKGE method*), 14
`get_head_relation_representation()` (*dicee.BaseKGE method*), 185
`get_head_relation_representation()` (*dicee.models.base_model.BaseKGE method*), 59
`get_head_relation_representation()` (*dicee.models.BaseKGE method*), 100, 103, 107, 111, 117, 130, 133
`get_kronecker_triple_representation()` (*dicee.callbacks.KronE method*), 25
`get_num_params()` (*dicee.models.transformers.GPT method*), 90
`get_padded_bpe_triple_representation()` (*dicee.abstracts.BaseInteractiveKGE method*), 14
`get_queries()` (*dicee.query_generator.QueryGenerator method*), 139
`get_queries()` (*dicee.QueryGenerator method*), 207
`get_re_vocab()` (*in module dicee*), 186
`get_re_vocab()` (*in module dicee.read_preprocess_save_load_kg.util*), 144
`get_re_vocab()` (*in module dicee.static_funcs*), 150
`get_re_vocab()` (*in module dicee.static_preprocess_funcs*), 153
`get_relation_embeddings()` (*dicee.abstracts.BaseInteractiveKGE method*), 15
`get_relation_index()` (*dicee.abstracts.BaseInteractiveKGE method*), 14
`get_sentence_representation()` (*dicee.BaseKGE method*), 185
`get_sentence_representation()` (*dicee.models.base_model.BaseKGE method*), 59
`get_sentence_representation()` (*dicee.models.BaseKGE method*), 100, 103, 107, 111, 117, 130, 133
`get_transductive_entity_embeddings()` (*dicee.KGE method*), 190
`get_transductive_entity_embeddings()` (*dicee.knowledge_graph_embeddings.KGE method*), 46
`get_triple_representation()` (*dicee.BaseKGE method*), 185
`get_triple_representation()` (*dicee.models.base_model.BaseKGE method*), 59
`get_triple_representation()` (*dicee.models.BaseKGE method*), 100, 103, 107, 111, 117, 130, 133
`GFMult` (*class in dicee.models*), 134
`GFMult` (*class in dicee.models.function_space*), 72
`global_rank` (*dicee.abstracts.AbstractTrainer attribute*), 12
`global_rank` (*dicee.trainer.torch_trainer_ddp.NodeTrainer attribute*), 158
`GPT` (*class in dicee.models.transformers*), 89
`GPTConfig` (*class in dicee.models.transformers*), 89
`gpus` (*dicee.config.Namespace attribute*), 26
`gradient_accumulation_steps` (*dicee.config.Namespace attribute*), 27
`ground_queries()` (*dicee.query_generator.QueryGenerator method*), 139
`ground_queries()` (*dicee.QueryGenerator method*), 207

H

`hidden_dropout` (*dicee.BaseKGE attribute*), 185
`hidden_dropout` (*dicee.models.base_model.BaseKGE attribute*), 59
`hidden_dropout` (*dicee.models.BaseKGE attribute*), 99, 102, 106, 110, 116, 129, 132
`hidden_dropout_rate` (*dicee.BaseKGE attribute*), 184
`hidden_dropout_rate` (*dicee.config.Namespace attribute*), 28
`hidden_dropout_rate` (*dicee.models.base_model.BaseKGE attribute*), 58
`hidden_dropout_rate` (*dicee.models.BaseKGE attribute*), 99, 102, 105, 110, 116, 129, 132
`hidden_normalizer` (*dicee.BaseKGE attribute*), 185
`hidden_normalizer` (*dicee.models.base_model.BaseKGE attribute*), 58
`hidden_normalizer` (*dicee.models.BaseKGE attribute*), 99, 102, 106, 110, 116, 129, 132

I

`IdentityClass` (*class in dicee.models*), 100, 112, 117
`IdentityClass` (*class in dicee.models.base_model*), 60
`idx_entity_to_bpe_shaped` (*dicee.knowledge_graph.KG attribute*), 45
`index_triple()` (*dicee.abstracts.BaseInteractiveKGE method*), 15
`init_dataloader()` (*dicee.DICE_Trainer method*), 189
`init_dataloader()` (*dicee.trainer.DICE_Trainer method*), 160
`init_dataloader()` (*dicee.trainer.dice_trainer.DICE_Trainer method*), 155
`init_dataset()` (*dicee.DICE_Trainer method*), 189
`init_dataset()` (*dicee.trainer.DICE_Trainer method*), 160
`init_dataset()` (*dicee.trainer.dice_trainer.DICE_Trainer method*), 155
`init_param` (*dicee.config.Namespace attribute*), 27
`init_params_with_sanity_checking()` (*dicee.BaseKGE method*), 185
`init_params_with_sanity_checking()` (*dicee.models.base_model.BaseKGE method*), 59
`init_params_with_sanity_checking()` (*dicee.models.BaseKGE method*), 99, 103, 106, 111, 117, 129, 133
`initial_eval_setting` (*dicee.callbacks.ASWA attribute*), 22

`initialize_or_load_model()` (*dicee.DICE_Trainer* method), 189
`initialize_or_load_model()` (*dicee.trainer.DICE_Trainer* method), 160
`initialize_or_load_model()` (*dicee.trainer.dice_trainer.DICE_Trainer* method), 155
`initialize_trainer()` (*dicee.DICE_Trainer* method), 189
`initialize_trainer()` (*dicee.trainer.DICE_Trainer* method), 159
`initialize_trainer()` (*dicee.trainer.dice_trainer.DICE_Trainer* method), 155
`initialize_trainer()` (in module *dicee.trainer.dice_trainer*), 154
`input_dp_ent_real` (*dicee.BaseKGE* attribute), 185
`input_dp_ent_real` (*dicee.models.base_model.BaseKGE* attribute), 59
`input_dp_ent_real` (*dicee.models.BaseKGE* attribute), 99, 102, 106, 110, 116, 129, 132
`input_dp_rel_real` (*dicee.BaseKGE* attribute), 185
`input_dp_rel_real` (*dicee.models.base_model.BaseKGE* attribute), 59
`input_dp_rel_real` (*dicee.models.BaseKGE* attribute), 99, 102, 106, 110, 116, 129, 132
`input_dropout_rate` (*dicee.BaseKGE* attribute), 184
`input_dropout_rate` (*dicee.config.Namespace* attribute), 28
`input_dropout_rate` (*dicee.models.base_model.BaseKGE* attribute), 58
`input_dropout_rate` (*dicee.models.BaseKGE* attribute), 99, 102, 105, 110, 116, 129, 132
`intialize_model()` (in module *dicee*), 187
`intialize_model()` (in module *dicee.static_funcs*), 151
`is_continual_training` (*dicee.DICE_Trainer* attribute), 188
`is_continual_training` (*dicee.evaluator.Evaluator* attribute), 41
`is_continual_training` (*dicee.Execute* attribute), 193
`is_continual_training` (*dicee.executer.Execute* attribute), 43
`is_continual_training` (*dicee.trainer.DICE_Trainer* attribute), 159
`is_continual_training` (*dicee.trainer.dice_trainer.DICE_Trainer* attribute), 154
`is_global_zero` (*dicee.abstracts.AbstractTrainer* attribute), 12
`is_seen()` (*dicee.abstracts.BaseInteractiveKGE* method), 14
`is_sparql_endpoint_alive()` (in module *dicee.sanity_checkers*), 146

K

`k` (*dicee.models.FMult* attribute), 134
`k` (*dicee.models.FMult2* attribute), 135
`k` (*dicee.models.function_space.FMult* attribute), 72
`k` (*dicee.models.function_space.FMult2* attribute), 73
`k` (*dicee.models.function_space.GFMult* attribute), 72
`k` (*dicee.models.GFMult* attribute), 134
`k_fold_cross_validation()` (*dicee.DICE_Trainer* method), 189
`k_fold_cross_validation()` (*dicee.trainer.DICE_Trainer* method), 160
`k_fold_cross_validation()` (*dicee.trainer.dice_trainer.DICE_Trainer* method), 155
`k_vs_all_score()` (*dicee.ComplEx* static method), 172
`k_vs_all_score()` (*dicee.DistMult* method), 163
`k_vs_all_score()` (*dicee.Keci* method), 166
`k_vs_all_score()` (*dicee.models.clifford.Keci* method), 63
`k_vs_all_score()` (*dicee.models.ComplEx* static method), 109
`k_vs_all_score()` (*dicee.models.complex.ComplEx* static method), 69
`k_vs_all_score()` (*dicee.models.DistMult* method), 103
`k_vs_all_score()` (*dicee.models.Keci* method), 123
`k_vs_all_score()` (*dicee.models.octonion.OMult* method), 76
`k_vs_all_score()` (*dicee.models.OMult* method), 119
`k_vs_all_score()` (*dicee.models.QMult* method), 114
`k_vs_all_score()` (*dicee.models.quaternion.QMult* method), 81
`k_vs_all_score()` (*dicee.models.real.DistMult* method), 82
`k_vs_all_score()` (*dicee.OMult* method), 179
`k_vs_all_score()` (*dicee.QMult* method), 178
`Keci` (class in *dicee*), 164
`Keci` (class in *dicee.models*), 121
`Keci` (class in *dicee.models.clifford*), 61
`KeciBase` (class in *dicee*), 164
`KeciBase` (class in *dicee.models*), 124
`KeciBase` (class in *dicee.models.clifford*), 64
`kernel_size` (*dicee.BaseKGE* attribute), 184
`kernel_size` (*dicee.config.Namespace* attribute), 27
`kernel_size` (*dicee.models.base_model.BaseKGE* attribute), 58
`kernel_size` (*dicee.models.BaseKGE* attribute), 99, 102, 106, 110, 116, 129, 132
`KG` (class in *dicee.knowledge_graph*), 45
`kg` (*dicee.callbacks.PseudoLabellingCallback* attribute), 22
`kg` (*dicee.read_preprocess_save_load_kg.LoadSaveToDisk* attribute), 146

kg (*dicee.read_preprocess_save_load_kg.PreprocessKG attribute*), 145
 kg (*dicee.read_preprocess_save_load_kg.preprocess.PreprocessKG attribute*), 139
 kg (*dicee.read_preprocess_save_load_kg.read_from_disk.ReadFromDisk attribute*), 140
 kg (*dicee.read_preprocess_save_load_kg.ReadFromDisk attribute*), 146
 kg (*dicee.read_preprocess_save_load_kg.save_load_disk.LoadSaveToDisk attribute*), 141
 KGE (*class in dicee*), 189
 KGE (*class in dicee.knowledge_graph_embeddings*), 46
 KGESaveCallback (*class in dicee.callbacks*), 21
 knowledge_graph (*dicee.Execute attribute*), 194
 knowledge_graph (*dicee.executer.Execute attribute*), 43
 KronE (*class in dicee.callbacks*), 24
 KvsAll (*class in dicee*), 197
 KvsAll (*class in dicee.dataset_classes*), 31
 kvsall_score () (*dicee.DualE method*), 171
 kvsall_score () (*dicee.models.DualE method*), 137
 kvsall_score () (*dicee.models.dualE.DualE method*), 70
 KvsSampleDataset (*class in dicee*), 200
 KvsSampleDataset (*class in dicee.dataset_classes*), 34

L

label_smoothing_rate (*dicee.AllvsAll attribute*), 198
 label_smoothing_rate (*dicee.config.Namespace attribute*), 27
 label_smoothing_rate (*dicee.dataset_classes.AllvsAll attribute*), 33
 label_smoothing_rate (*dicee.dataset_classes.KvsAll attribute*), 32
 label_smoothing_rate (*dicee.dataset_classes.KvsSampleDataset attribute*), 35
 label_smoothing_rate (*dicee.dataset_classes.OnevsSample attribute*), 34
 label_smoothing_rate (*dicee.dataset_classes.TriplePredictionDataset attribute*), 36
 label_smoothing_rate (*dicee.KvsAll attribute*), 198
 label_smoothing_rate (*dicee.KvsSampleDataset attribute*), 201
 label_smoothing_rate (*dicee.OnevsSample attribute*), 199, 200
 label_smoothing_rate (*dicee.TriplePredictionDataset attribute*), 202
 LayerNorm (*class in dicee.models.transformers*), 86
 learning_rate (*dicee.BaseKGE attribute*), 184
 learning_rate (*dicee.models.base_model.BaseKGE attribute*), 58
 learning_rate (*dicee.models.BaseKGE attribute*), 99, 102, 105, 110, 116, 129, 132
 length (*dicee.dataset_classes.NegSampleDataset attribute*), 36
 length (*dicee.dataset_classes.TriplePredictionDataset attribute*), 36
 length (*dicee.NegSampleDataset attribute*), 201
 length (*dicee.TriplePredictionDataset attribute*), 202
 level (*dicee.callbacks.Perturb attribute*), 25
 LFMult (*class in dicee*), 179
 LFMult (*class in dicee.models*), 135
 LFMult (*class in dicee.models.function_space*), 74
 LFMult1 (*class in dicee.models*), 135
 LFMult1 (*class in dicee.models.function_space*), 73
 linear () (*dicee.LFMult method*), 180
 linear () (*dicee.models.function_space.LFMult method*), 74
 linear () (*dicee.models.LFMult method*), 136
 list2tuple () (*dicee.query_generator.QueryGenerator method*), 138
 list2tuple () (*dicee.QueryGenerator method*), 206
 lm_head (*dicee.BytE attribute*), 182
 lm_head (*dicee.models.transformers.BytE attribute*), 85
 lm_head (*dicee.models.transformers.GPT attribute*), 90
 ln_1 (*dicee.models.transformers.Block attribute*), 89
 ln_2 (*dicee.models.transformers.Block attribute*), 89
 load () (*dicee.read_preprocess_save_load_kg.LoadSaveToDisk method*), 146
 load () (*dicee.read_preprocess_save_load_kg.save_load_disk.LoadSaveToDisk method*), 141
 load_json () (*in module dicee*), 187
 load_json () (*in module dicee.static_funcs*), 151
 load_model () (*in module dicee*), 187
 load_model () (*in module dicee.static_funcs*), 150
 load_model_ensemble () (*in module dicee*), 187
 load_model_ensemble () (*in module dicee.static_funcs*), 150
 load_numpy () (*in module dicee*), 188
 load_numpy () (*in module dicee.static_funcs*), 151
 load_numpy_ndarray () (*in module dicee.read_preprocess_save_load_kg.util*), 144
 load_pickle () (*in module dicee*), 187

- `load_pickle()` (in module `dicee.read_preprocess_save_load_kg.util`), 145
- `load_pickle()` (in module `dicee.static_funcs`), 150
- `load_queries()` (`dicee.query_generator.QueryGenerator` method), 139
- `load_queries()` (`dicee.QueryGenerator` method), 207
- `load_queries_and_answers()` (`dicee.query_generator.QueryGenerator` static method), 139
- `load_queries_and_answers()` (`dicee.QueryGenerator` static method), 207
- `load_term_mapping()` (in module `dicee`), 187, 195
- `load_term_mapping()` (in module `dicee.static_funcs`), 150
- `load_term_mapping()` (in module `dicee.trainer.dice_trainer`), 154
- `load_with_pandas()` (in module `dicee.read_preprocess_save_load_kg.util`), 144
- `LoadSaveToDisk` (class in `dicee.read_preprocess_save_load_kg`), 146
- `LoadSaveToDisk` (class in `dicee.read_preprocess_save_load_kg.save_load_disk`), 141
- `local_rank` (`dicee.abstracts.AbstractTrainer` attribute), 12
- `local_rank` (`dicee.trainer.torch_trainer_ddp.NodeTrainer` attribute), 158
- `loss` (`dicee.BaseKGE` attribute), 184
- `loss` (`dicee.models.base_model.BaseKGE` attribute), 58
- `loss` (`dicee.models.BaseKGE` attribute), 99, 102, 106, 110, 116, 129, 132
- `loss_func` (`dicee.trainer.torch_trainer_ddp.NodeTrainer` attribute), 158
- `loss_function` (`dicee.trainer.torch_trainer.TorchTrainer` attribute), 157
- `loss_function()` (`dicee.BytE` method), 182
- `loss_function()` (`dicee.models.base_model.BaseKGELightning` method), 53
- `loss_function()` (`dicee.models.BaseKGELightning` method), 94
- `loss_function()` (`dicee.models.transformers.BytE` method), 85
- `loss_history` (`dicee.BaseKGE` attribute), 185
- `loss_history` (`dicee.EnsembleKGE` attribute), 186
- `loss_history` (`dicee.models.base_model.BaseKGE` attribute), 59
- `loss_history` (`dicee.models.BaseKGE` attribute), 99, 102, 106, 111, 116, 129, 132
- `loss_history` (`dicee.models.ensemble.EnsembleKGE` attribute), 71
- `loss_history` (`dicee.models.pykeen_models.PykeenKGE` attribute), 78
- `loss_history` (`dicee.models.PykeenKGE` attribute), 130
- `loss_history` (`dicee.PykeenKGE` attribute), 181
- `loss_history` (`dicee.trainer.torch_trainer_ddp.NodeTrainer` attribute), 158
- `lr` (`dicee.analyse_experiments.Experiment` attribute), 18
- `lr` (`dicee.config.Namespace` attribute), 26

M

- `m` (`dicee.LFMMult` attribute), 179
- `m` (`dicee.models.function_space.LFMMult` attribute), 74
- `m` (`dicee.models.LFMMult` attribute), 136
- `main()` (in module `dicee.scripts.index`), 147
- `main()` (in module `dicee.scripts.run`), 147
- `main()` (in module `dicee.scripts.serve`), 148
- `make_iterable_verbose()` (in module `dicee.static_funcs_training`), 152
- `make_iterable_verbose()` (in module `dicee.trainer.torch_trainer_ddp`), 158
- `mapping_from_first_two_cols_to_third()` (in module `dicee`), 195
- `mapping_from_first_two_cols_to_third()` (in module `dicee.static_preprocess_funcs`), 153
- `margin` (`dicee.models.Pyke` attribute), 104
- `margin` (`dicee.models.real.Pyke` attribute), 83
- `margin` (`dicee.models.real.TransE` attribute), 83
- `margin` (`dicee.models.TransE` attribute), 104
- `margin` (`dicee.Pyke` attribute), 163
- `margin` (`dicee.TransE` attribute), 167
- `max_ans_num` (`dicee.query_generator.QueryGenerator` attribute), 138
- `max_ans_num` (`dicee.QueryGenerator` attribute), 206
- `max_epochs` (`dicee.callbacks.KGESaveCallback` attribute), 21
- `max_length_subword_tokens` (`dicee.BaseKGE` attribute), 185
- `max_length_subword_tokens` (`dicee.knowledge_graph.KG` attribute), 46
- `max_length_subword_tokens` (`dicee.models.base_model.BaseKGE` attribute), 59
- `max_length_subword_tokens` (`dicee.models.BaseKGE` attribute), 99, 102, 106, 111, 117, 129, 133
- `max_num_of_classes` (`dicee.dataset_classes.KvsSampleDataset` attribute), 35
- `max_num_of_classes` (`dicee.KvsSampleDataset` attribute), 201
- `mem_of_model()` (`dicee.EnsembleKGE` method), 186
- `mem_of_model()` (`dicee.models.base_model.BaseKGELightning` method), 52
- `mem_of_model()` (`dicee.models.BaseKGELightning` method), 93
- `mem_of_model()` (`dicee.models.ensemble.EnsembleKGE` method), 71
- `method` (`dicee.callbacks.Perturb` attribute), 25
- `MLP` (class in `dicee.models.transformers`), 87

- mlp (*dicee.models.transformers.Block* attribute), 89
- mode (*dicee.query_generator.QueryGenerator* attribute), 138
- mode (*dicee.QueryGenerator* attribute), 206
- model (*dicee.config.Namespace* attribute), 26
- model (*dicee.models.pykeen_models.PykeenKGE* attribute), 78
- model (*dicee.models.PykeenKGE* attribute), 130
- model (*dicee.PykeenKGE* attribute), 180
- model (*dicee.scripts.serve.NeuralSearcher* attribute), 148
- model (*dicee.trainer.torch_trainer_ddp.NodeTrainer* attribute), 158
- model (*dicee.trainer.torch_trainer.TorchTrainer* attribute), 157
- model_kwargs (*dicee.models.pykeen_models.PykeenKGE* attribute), 78
- model_kwargs (*dicee.models.PykeenKGE* attribute), 130
- model_kwargs (*dicee.PykeenKGE* attribute), 180
- model_name (*dicee.analyse_experiments.Experiment* attribute), 18
- models (*dicee.EnsembleKGE* attribute), 186
- models (*dicee.models.ensemble.EnsembleKGE* attribute), 71
- models (*dicee.trainer.model_parallelism.TensorParallel* attribute), 156
- module
 - dicee, 12
 - dicee.__main__, 12
 - dicee.abstracts, 12
 - dicee.analyse_experiments, 17
 - dicee.callbacks, 19
 - dicee.config, 25
 - dicee.dataset_classes, 28
 - dicee.eval_static_funcs, 40
 - dicee.evaluator, 41
 - dicee.executer, 43
 - dicee.knowledge_graph, 45
 - dicee.knowledge_graph_embeddings, 46
 - dicee.models, 50
 - dicee.models.adopt, 50
 - dicee.models.base_model, 51
 - dicee.models.clifford, 60
 - dicee.models.complex, 67
 - dicee.models.dualE, 70
 - dicee.models.ensemble, 71
 - dicee.models.function_space, 72
 - dicee.models.octonion, 75
 - dicee.models.pykeen_models, 78
 - dicee.models.quaternion, 79
 - dicee.models.real, 82
 - dicee.models.static_funcs, 84
 - dicee.models.transformers, 84
 - dicee.query_generator, 138
 - dicee.read_preprocess_save_load_kg, 139
 - dicee.read_preprocess_save_load_kg.preprocess, 139
 - dicee.read_preprocess_save_load_kg.read_from_disk, 140
 - dicee.read_preprocess_save_load_kg.save_load_disk, 141
 - dicee.read_preprocess_save_load_kg.util, 141
 - dicee.sanity_checkers, 146
 - dicee.scripts, 147
 - dicee.scripts.index, 147
 - dicee.scripts.run, 147
 - dicee.scripts.serve, 147
 - dicee.static_funcs, 148
 - dicee.static_funcs_training, 152
 - dicee.static_preprocess_funcs, 152
 - dicee.trainer, 153
 - dicee.trainer.dice_trainer, 153
 - dicee.trainer.model_parallelism, 155
 - dicee.trainer.torch_trainer, 156
 - dicee.trainer.torch_trainer_ddp, 157
- modules() (*dicee.EnsembleKGE* method), 186
- modules() (*dicee.models.ensemble.EnsembleKGE* method), 71
- MultiClassClassificationDataset (class in *dicee*), 196
- MultiClassClassificationDataset (class in *dicee.dataset_classes*), 30
- MultiLabelDataset (class in *dicee*), 195

MultiLabelDataset (class in *dicее.dataset_classes*), 30

N

n (*dicее.models.FMult2* attribute), 135
n (*dicее.models.function_space.FMult2* attribute), 73
n_embd (*dicее.models.transformers.CausalSelfAttention* attribute), 87
n_embd (*dicее.models.transformers.GPTConfig* attribute), 89
n_head (*dicее.models.transformers.CausalSelfAttention* attribute), 87
n_head (*dicее.models.transformers.GPTConfig* attribute), 89
n_layer (*dicее.models.transformers.GPTConfig* attribute), 89
n_layers (*dicее.models.FMult2* attribute), 135
n_layers (*dicее.models.function_space.FMult2* attribute), 73
name (*dicее.abstracts.BaseInteractiveKGE* property), 14
name (*dicее.AConEx* attribute), 172
name (*dicее.AConvO* attribute), 173
name (*dicее.AConvQ* attribute), 174
name (*dicее.BytE* attribute), 182
name (*dicее.ComplEx* attribute), 172
name (*dicее.ConEx* attribute), 176
name (*dicее.ConvO* attribute), 175
name (*dicее.ConvQ* attribute), 174
name (*dicее.DeCaL* attribute), 168
name (*dicее.DistMult* attribute), 163
name (*dicее.DualE* attribute), 171
name (*dicее.EnsembleKGE* attribute), 186
name (*dicее.Keci* attribute), 164
name (*dicее.KeciBase* attribute), 164
name (*dicее.LFMult* attribute), 179
name (*dicее.models.AConEx* attribute), 108
name (*dicее.models.AConvO* attribute), 120
name (*dicее.models.AConvQ* attribute), 114
name (*dicее.models.clifford.DeCaL* attribute), 64
name (*dicее.models.clifford.Keci* attribute), 61
name (*dicее.models.clifford.KeciBase* attribute), 64
name (*dicее.models.ComplEx* attribute), 109
name (*dicее.models.complex.AConEx* attribute), 68
name (*dicее.models.complex.ComplEx* attribute), 69
name (*dicее.models.complex.ConEx* attribute), 68
name (*dicее.models.ConEx* attribute), 107
name (*dicее.models.ConvO* attribute), 120
name (*dicее.models.ConvQ* attribute), 114
name (*dicее.models.DeCaL* attribute), 125
name (*dicее.models.DistMult* attribute), 103
name (*dicее.models.DualE* attribute), 137
name (*dicее.models.dualE.DualE* attribute), 70
name (*dicее.models.ensemble.EnsembleKGE* attribute), 71
name (*dicее.models.FMult* attribute), 134
name (*dicее.models.FMult2* attribute), 134
name (*dicее.models.function_space.FMult* attribute), 72
name (*dicее.models.function_space.FMult2* attribute), 73
name (*dicее.models.function_space.GFMult* attribute), 72
name (*dicее.models.function_space.LFMult* attribute), 74
name (*dicее.models.function_space.LFMult1* attribute), 73
name (*dicее.models.GFMult* attribute), 134
name (*dicее.models.Keci* attribute), 121
name (*dicее.models.KeciBase* attribute), 124
name (*dicее.models.LFMult* attribute), 135
name (*dicее.models.LFMult1* attribute), 135
name (*dicее.models.octonion.AConvO* attribute), 77
name (*dicее.models.octonion.ConvO* attribute), 77
name (*dicее.models.octonion.OMult* attribute), 76
name (*dicее.models.OMult* attribute), 119
name (*dicее.models.Pyke* attribute), 104
name (*dicее.models.pykeen_models.PykeenKGE* attribute), 78
name (*dicее.models.PykeenKGE* attribute), 130
name (*dicее.models.QMult* attribute), 113
name (*dicее.models.quaternion.AConvQ* attribute), 82

name (*dicee.models.quaternion.ConvQ attribute*), 81
 name (*dicee.models.quaternion.QMult attribute*), 80
 name (*dicee.models.real.DistMult attribute*), 82
 name (*dicee.models.real.Pyke attribute*), 83
 name (*dicee.models.real.Shallom attribute*), 83
 name (*dicee.models.real.TransE attribute*), 83
 name (*dicee.models.Shallom attribute*), 104
 name (*dicee.models.TransE attribute*), 104
 name (*dicee.models.transformers.Byte attribute*), 85
 name (*dicee.OMult attribute*), 179
 name (*dicee.Pyke attribute*), 163
 name (*dicee.PykeenKGE attribute*), 180
 name (*dicee.QMult attribute*), 177
 name (*dicee.Shallom attribute*), 179
 name (*dicee.TransE attribute*), 167
 named_children() (*dicee.EnsembleKGE method*), 186
 named_children() (*dicee.models.ensemble.EnsembleKGE method*), 71
 Namespace (*class in dicee.config*), 26
 neg_ratio (*dicee.BPE_NegativeSamplingDataset attribute*), 195
 neg_ratio (*dicee.config.Namespace attribute*), 27
 neg_ratio (*dicee.dataset_classes.BPE_NegativeSamplingDataset attribute*), 30
 neg_ratio (*dicee.dataset_classes.KvsSampleDataset attribute*), 35
 neg_ratio (*dicee.KvsSampleDataset attribute*), 201
 neg_sample_ratio (*dicee.CVDataModule attribute*), 203
 neg_sample_ratio (*dicee.dataset_classes.CVDataModule attribute*), 37
 neg_sample_ratio (*dicee.dataset_classes.NegSampleDataset attribute*), 35
 neg_sample_ratio (*dicee.dataset_classes.OnevsSample attribute*), 33, 34
 neg_sample_ratio (*dicee.dataset_classes.TriplePredictionDataset attribute*), 36
 neg_sample_ratio (*dicee.NegSampleDataset attribute*), 201
 neg_sample_ratio (*dicee.OnevsSample attribute*), 199, 200
 neg_sample_ratio (*dicee.TriplePredictionDataset attribute*), 202
 negnorm() (*dicee.KGE method*), 192
 negnorm() (*dicee.knowledge_graph_embeddings.KGE method*), 49
 NegSampleDataset (*class in dicee*), 201
 NegSampleDataset (*class in dicee.dataset_classes*), 35
 neural_searcher (*in module dicee.scripts.serve*), 148
 NeuralSearcher (*class in dicee.scripts.serve*), 148
 NodeTrainer (*class in dicee.trainer.torch_trainer_ddp*), 158
 norm_fc1 (*dicee.AConEx attribute*), 173
 norm_fc1 (*dicee.AConvO attribute*), 173
 norm_fc1 (*dicee.ConEx attribute*), 176
 norm_fc1 (*dicee.ConvO attribute*), 176
 norm_fc1 (*dicee.models.AConEx attribute*), 108
 norm_fc1 (*dicee.models.AConvO attribute*), 121
 norm_fc1 (*dicee.models.complex.AConEx attribute*), 68
 norm_fc1 (*dicee.models.complex.ConEx attribute*), 68
 norm_fc1 (*dicee.models.ConEx attribute*), 107
 norm_fc1 (*dicee.models.ConvO attribute*), 120
 norm_fc1 (*dicee.models.octonion.AConvO attribute*), 78
 norm_fc1 (*dicee.models.octonion.ConvO attribute*), 77
 normalization (*dicee.analyse_experiments.Experiment attribute*), 19
 normalization (*dicee.config.Namespace attribute*), 27
 normalize_head_entity_embeddings (*dicee.BaseKGE attribute*), 185
 normalize_head_entity_embeddings (*dicee.models.base_model.BaseKGE attribute*), 58
 normalize_head_entity_embeddings (*dicee.models.BaseKGE attribute*), 99, 102, 106, 110, 116, 129, 132
 normalize_relation_embeddings (*dicee.BaseKGE attribute*), 185
 normalize_relation_embeddings (*dicee.models.base_model.BaseKGE attribute*), 58
 normalize_relation_embeddings (*dicee.models.BaseKGE attribute*), 99, 102, 106, 110, 116, 129, 132
 normalize_tail_entity_embeddings (*dicee.BaseKGE attribute*), 185
 normalize_tail_entity_embeddings (*dicee.models.base_model.BaseKGE attribute*), 58
 normalize_tail_entity_embeddings (*dicee.models.BaseKGE attribute*), 99, 102, 106, 110, 116, 129, 132
 normalizer_class (*dicee.BaseKGE attribute*), 184
 normalizer_class (*dicee.models.base_model.BaseKGE attribute*), 58
 normalizer_class (*dicee.models.BaseKGE attribute*), 99, 102, 106, 110, 116, 129, 132
 num_bpe_entities (*dicee.BPE_NegativeSamplingDataset attribute*), 195
 num_bpe_entities (*dicee.dataset_classes.BPE_NegativeSamplingDataset attribute*), 30
 num_bpe_entities (*dicee.knowledge_graph.KG attribute*), 46
 num_core (*dicee.config.Namespace attribute*), 27

num_datapoints (*dicee.BPE_NegativeSamplingDataset* attribute), 195
 num_datapoints (*dicee.dataset_classes.BPE_NegativeSamplingDataset* attribute), 30
 num_datapoints (*dicee.dataset_classes.MultiLabelDataset* attribute), 30
 num_datapoints (*dicee.MultiLabelDataset* attribute), 196
 num_ent (*dicee.DualE* attribute), 171
 num_ent (*dicee.models.DualE* attribute), 137
 num_ent (*dicee.models.dualE.DualE* attribute), 70
 num_entities (*dicee.BaseKGE* attribute), 184
 num_entities (*dicee.CVDataModule* attribute), 203
 num_entities (*dicee.dataset_classes.CVDataModule* attribute), 37
 num_entities (*dicee.dataset_classes.KvsSampleDataset* attribute), 35
 num_entities (*dicee.dataset_classes.NegSampleDataset* attribute), 36
 num_entities (*dicee.dataset_classes.OnevsSample* attribute), 33, 34
 num_entities (*dicee.dataset_classes.TriplePredictionDataset* attribute), 36
 num_entities (*dicee.evaluator.Evaluator* attribute), 41
 num_entities (*dicee.knowledge_graph.KG* attribute), 45
 num_entities (*dicee.KvsSampleDataset* attribute), 201
 num_entities (*dicee.models.base_model.BaseKGE* attribute), 58
 num_entities (*dicee.models.BaseKGE* attribute), 98, 102, 105, 110, 116, 128, 132
 num_entities (*dicee.NegSampleDataset* attribute), 201
 num_entities (*dicee.OnevsSample* attribute), 199
 num_entities (*dicee.TriplePredictionDataset* attribute), 202
 num_epochs (*dicee.abstracts.AbstractPPECallback* attribute), 17
 num_epochs (*dicee.analyse_experiments.Experiment* attribute), 18
 num_epochs (*dicee.callbacks.ASWA* attribute), 22
 num_epochs (*dicee.config.Namespace* attribute), 26
 num_epochs (*dicee.trainer.torch_trainer_ddp.NodeTrainer* attribute), 158
 num_folds_for_cv (*dicee.config.Namespace* attribute), 27
 num_of_data_points (*dicee.dataset_classes.MultiClassClassificationDataset* attribute), 31
 num_of_data_points (*dicee.MultiClassClassificationDataset* attribute), 196
 num_of_epochs (*dicee.callbacks.PseudoLabellingCallback* attribute), 22
 num_of_output_channels (*dicee.BaseKGE* attribute), 184
 num_of_output_channels (*dicee.config.Namespace* attribute), 27
 num_of_output_channels (*dicee.models.base_model.BaseKGE* attribute), 58
 num_of_output_channels (*dicee.models.BaseKGE* attribute), 99, 102, 106, 110, 116, 129, 132
 num_params (*dicee.analyse_experiments.Experiment* attribute), 18
 num_relations (*dicee.BaseKGE* attribute), 184
 num_relations (*dicee.CVDataModule* attribute), 203
 num_relations (*dicee.dataset_classes.CVDataModule* attribute), 37
 num_relations (*dicee.dataset_classes.NegSampleDataset* attribute), 36
 num_relations (*dicee.dataset_classes.OnevsSample* attribute), 33, 34
 num_relations (*dicee.dataset_classes.TriplePredictionDataset* attribute), 36
 num_relations (*dicee.evaluator.Evaluator* attribute), 41
 num_relations (*dicee.knowledge_graph.KG* attribute), 45
 num_relations (*dicee.models.base_model.BaseKGE* attribute), 58
 num_relations (*dicee.models.BaseKGE* attribute), 98, 102, 105, 110, 116, 128, 132
 num_relations (*dicee.NegSampleDataset* attribute), 201
 num_relations (*dicee.OnevsSample* attribute), 199
 num_relations (*dicee.TriplePredictionDataset* attribute), 202
 num_sample (*dicee.models.FMult* attribute), 134
 num_sample (*dicee.models.function_space.FMult* attribute), 72
 num_sample (*dicee.models.function_space.GFMult* attribute), 72
 num_sample (*dicee.models.GFMult* attribute), 134
 num_tokens (*dicee.BaseKGE* attribute), 184
 num_tokens (*dicee.knowledge_graph.KG* attribute), 46
 num_tokens (*dicee.models.base_model.BaseKGE* attribute), 58
 num_tokens (*dicee.models.BaseKGE* attribute), 98, 102, 105, 110, 116, 129, 132
 num_workers (*dicee.CVDataModule* attribute), 203
 num_workers (*dicee.dataset_classes.CVDataModule* attribute), 37
 numpy_data_type_changer () (in module *dicee*), 187
 numpy_data_type_changer () (in module *dicee.static_funcs*), 150

O

octonion_mul () (in module *dicee.models*), 118
 octonion_mul () (in module *dicee.models.octonion*), 75
 octonion_mul_norm () (in module *dicee.models*), 118
 octonion_mul_norm () (in module *dicee.models.octonion*), 75

- `octonion_normalizer()` (*dicee.AConvO static method*), 173
- `octonion_normalizer()` (*dicee.ConvO static method*), 176
- `octonion_normalizer()` (*dicee.models.AConvO static method*), 121
- `octonion_normalizer()` (*dicee.models.ConvO static method*), 120
- `octonion_normalizer()` (*dicee.models.octonion.AConvO static method*), 78
- `octonion_normalizer()` (*dicee.models.octonion.ConvO static method*), 77
- `octonion_normalizer()` (*dicee.models.octonion.OMult static method*), 76
- `octonion_normalizer()` (*dicee.models.OMult static method*), 119
- `octonion_normalizer()` (*dicee.OMult static method*), 179
- `OMult` (*class in dicee*), 178
- `OMult` (*class in dicee.models*), 118
- `OMult` (*class in dicee.models.octonion*), 75
- `on_epoch_end()` (*dicee.callbacks.KGESaveCallback method*), 22
- `on_epoch_end()` (*dicee.callbacks.PseudoLabellingCallback method*), 22
- `on_fit_end()` (*dicee.abstracts.AbstractCallback method*), 16
- `on_fit_end()` (*dicee.abstracts.AbstractPPECallback method*), 17
- `on_fit_end()` (*dicee.abstracts.AbstractTrainer method*), 13
- `on_fit_end()` (*dicee.callbacks.AccumulateEpochLossCallback method*), 20
- `on_fit_end()` (*dicee.callbacks.ASWA method*), 23
- `on_fit_end()` (*dicee.callbacks.Eval method*), 24
- `on_fit_end()` (*dicee.callbacks.KGESaveCallback method*), 22
- `on_fit_end()` (*dicee.callbacks.PrintCallback method*), 20
- `on_fit_start()` (*dicee.abstracts.AbstractCallback method*), 16
- `on_fit_start()` (*dicee.abstracts.AbstractPPECallback method*), 17
- `on_fit_start()` (*dicee.abstracts.AbstractTrainer method*), 12
- `on_fit_start()` (*dicee.callbacks.Eval method*), 24
- `on_fit_start()` (*dicee.callbacks.KGESaveCallback method*), 21
- `on_fit_start()` (*dicee.callbacks.KronE method*), 25
- `on_fit_start()` (*dicee.callbacks.PrintCallback method*), 20
- `on_init_end()` (*dicee.abstracts.AbstractCallback method*), 16
- `on_init_start()` (*dicee.abstracts.AbstractCallback method*), 15
- `on_train_batch_end()` (*dicee.abstracts.AbstractCallback method*), 16
- `on_train_batch_end()` (*dicee.abstracts.AbstractTrainer method*), 13
- `on_train_batch_end()` (*dicee.callbacks.Eval method*), 24
- `on_train_batch_end()` (*dicee.callbacks.KGESaveCallback method*), 21
- `on_train_batch_end()` (*dicee.callbacks.PrintCallback method*), 20
- `on_train_batch_start()` (*dicee.callbacks.Perturb method*), 25
- `on_train_epoch_end()` (*dicee.abstracts.AbstractCallback method*), 16
- `on_train_epoch_end()` (*dicee.abstracts.AbstractTrainer method*), 13
- `on_train_epoch_end()` (*dicee.callbacks.ASWA method*), 23
- `on_train_epoch_end()` (*dicee.callbacks.Eval method*), 24
- `on_train_epoch_end()` (*dicee.callbacks.KGESaveCallback method*), 21
- `on_train_epoch_end()` (*dicee.callbacks.PrintCallback method*), 21
- `on_train_epoch_end()` (*dicee.models.base_model.BaseKGELightning method*), 53
- `on_train_epoch_end()` (*dicee.models.BaseKGELightning method*), 94
- `OnevsAllDataset` (*class in dicee*), 196
- `OnevsAllDataset` (*class in dicee.dataset_classes*), 31
- `OnevsSample` (*class in dicee*), 198
- `OnevsSample` (*class in dicee.dataset_classes*), 33
- `optim` (*dicee.config.Namespace attribute*), 26
- `optimizer` (*dicee.trainer.torch_trainer.NodeTrainer attribute*), 158
- `optimizer` (*dicee.trainer.torch_trainer.TorchTrainer attribute*), 157
- `optimizer_name` (*dicee.BaseKGE attribute*), 184
- `optimizer_name` (*dicee.models.base_model.BaseKGE attribute*), 58
- `optimizer_name` (*dicee.models.BaseKGE attribute*), 99, 102, 105, 110, 116, 129, 132
- `optimizers` (*dicee.EnsembleKGE attribute*), 186
- `optimizers` (*dicee.models.ensemble.EnsembleKGE attribute*), 71
- `ordered_bpe_entities` (*dicee.BPE_NegativeSamplingDataset attribute*), 195
- `ordered_bpe_entities` (*dicee.dataset_classes.BPE_NegativeSamplingDataset attribute*), 30
- `ordered_bpe_entities` (*dicee.knowledge_graph.KG attribute*), 46
- `ordered_shaped_bpe_tokens` (*dicee.knowledge_graph.KG attribute*), 45

P

- `p` (*dicee.config.Namespace attribute*), 28
- `p` (*dicee.DeCaL attribute*), 168
- `p` (*dicee.Keci attribute*), 164
- `p` (*dicee.models.clifford.DeCaL attribute*), 64

`p` (*dicee.models.clifford.Keci* attribute), 61
`p` (*dicee.models.DeCaL* attribute), 125
`p` (*dicee.models.Keci* attribute), 122
`padding` (*dicee.knowledge_graph.KG* attribute), 46
`pandas_dataframe_indexer()` (in module *dicee.read_preprocess_save_load_kg.util*), 143
`param_init` (*dicee.BaseKGE* attribute), 185
`param_init` (*dicee.models.base_model.BaseKGE* attribute), 58
`param_init` (*dicee.models.BaseKGE* attribute), 99, 102, 106, 110, 116, 129, 132
`parameters()` (*dicee.abstracts.BaseInteractiveKGE* method), 15
`parameters()` (*dicee.EnsembleKGE* method), 186
`parameters()` (*dicee.models.ensemble.EnsembleKGE* method), 71
`path` (*dicee.abstracts.AbstractPPECallback* attribute), 17
`path` (*dicee.callbacks.AccumulateEpochLossCallback* attribute), 20
`path` (*dicee.callbacks.ASWA* attribute), 22
`path` (*dicee.callbacks.Eval* attribute), 23
`path` (*dicee.callbacks.KGESaveCallback* attribute), 21
`path_dataset_folder` (*dicee.analyse_experiments.Experiment* attribute), 18
`path_for_deserialization` (*dicee.knowledge_graph.KG* attribute), 45
`path_for_serialization` (*dicee.knowledge_graph.KG* attribute), 45
`path_single_kg` (*dicee.config.Namespace* attribute), 26
`path_single_kg` (*dicee.knowledge_graph.KG* attribute), 45
`path_to_store_single_run` (*dicee.config.Namespace* attribute), 26
`Perturb` (class in *dicee.callbacks*), 25
`polars_dataframe_indexer()` (in module *dicee.read_preprocess_save_load_kg.util*), 142
`poly_NN()` (*dicee.LFMulti* method), 179
`poly_NN()` (*dicee.models.function_space.LFMulti* method), 74
`poly_NN()` (*dicee.models.LFMulti* method), 136
`polynomial()` (*dicee.LFMulti* method), 180
`polynomial()` (*dicee.models.function_space.LFMulti* method), 75
`polynomial()` (*dicee.models.LFMulti* method), 136
`pop()` (*dicee.LFMulti* method), 180
`pop()` (*dicee.models.function_space.LFMulti* method), 75
`pop()` (*dicee.models.LFMulti* method), 136
`pq` (*dicee.analyse_experiments.Experiment* attribute), 18
`predict()` (*dicee.KGE* method), 191
`predict()` (*dicee.knowledge_graph_embeddings.KGE* method), 48
`predict_data_loader()` (*dicee.models.base_model.BaseKGELightning* method), 55
`predict_data_loader()` (*dicee.models.BaseKGELightning* method), 96
`predict_missing_head_entity()` (*dicee.KGE* method), 190
`predict_missing_head_entity()` (*dicee.knowledge_graph_embeddings.KGE* method), 47
`predict_missing_relations()` (*dicee.KGE* method), 190
`predict_missing_relations()` (*dicee.knowledge_graph_embeddings.KGE* method), 47
`predict_missing_tail_entity()` (*dicee.KGE* method), 191
`predict_missing_tail_entity()` (*dicee.knowledge_graph_embeddings.KGE* method), 47
`predict_topk()` (*dicee.KGE* method), 191
`predict_topk()` (*dicee.knowledge_graph_embeddings.KGE* method), 48
`prepare_data()` (*dicee.CVDataModule* method), 205
`prepare_data()` (*dicee.dataset_classes.CVDataModule* method), 39
`preprocess_with_byte_pair_encoding()` (*dicee.read_preprocess_save_load_kg.PreprocessKG* method), 145
`preprocess_with_byte_pair_encoding()` (*dicee.read_preprocess_save_load_kg.preprocess.PreprocessKG* method), 139
`preprocess_with_byte_pair_encoding_with_padding()` (*dicee.read_preprocess_save_load_kg.PreprocessKG* method), 145
`preprocess_with_byte_pair_encoding_with_padding()` (*dicee.read_preprocess_save_load_kg.preprocess.PreprocessKG* method), 140
`preprocess_with_pandas()` (*dicee.read_preprocess_save_load_kg.PreprocessKG* method), 145
`preprocess_with_pandas()` (*dicee.read_preprocess_save_load_kg.preprocess.PreprocessKG* method), 140
`preprocess_with_polars()` (*dicee.read_preprocess_save_load_kg.PreprocessKG* method), 146
`preprocess_with_polars()` (*dicee.read_preprocess_save_load_kg.preprocess.PreprocessKG* method), 140
`preprocesses_input_args()` (in module *dicee.static_preprocess_funcs*), 153
`PreprocessKG` (class in *dicee.read_preprocess_save_load_kg*), 145
`PreprocessKG` (class in *dicee.read_preprocess_save_load_kg.preprocess*), 139
`PrintCallback` (class in *dicee.callbacks*), 20
`process` (*dicee.trainer.torch_trainer.TorchTrainer* attribute), 157
`PseudoLabellingCallback` (class in *dicee.callbacks*), 22
`Pyke` (class in *dicee*), 163
`Pyke` (class in *dicee.models*), 104
`Pyke` (class in *dicee.models.real*), 83
`pykeen_model_kwargs` (*dicee.config.Namespace* attribute), 27
`PykeenKGE` (class in *dicee*), 180
`PykeenKGE` (class in *dicee.models*), 130

PykeenKGE (class in *dicее.models.pykeen_models*), 78

Q

q (*dicее.config.Namespace* attribute), 28
q (*dicее.DeCaL* attribute), 168
q (*dicее.Keci* attribute), 164
q (*dicее.models.clifford.DeCaL* attribute), 64
q (*dicее.models.clifford.Keci* attribute), 61
q (*dicее.models.DeCaL* attribute), 125
q (*dicее.models.Keci* attribute), 122
qdrant_client (*dicее.scripts.serve.NeuralSearcher* attribute), 148
QMult (class in *dicее*), 176
QMult (class in *dicее.models*), 112
QMult (class in *dicее.models.quaternion*), 79
quaternion_mul() (in module *dicее.models*), 109
quaternion_mul() (in module *dicее.models.static_funcs*), 84
quaternion_mul_with_unit_norm() (in module *dicее.models*), 112
quaternion_mul_with_unit_norm() (in module *dicее.models.quaternion*), 79
quaternion_multiplication_followed_by_inner_product() (*dicее.models.QMult* method), 113
quaternion_multiplication_followed_by_inner_product() (*dicее.models.quaternion.QMult* method), 80
quaternion_multiplication_followed_by_inner_product() (*dicее.QMult* method), 177
quaternion_normalizer() (*dicее.models.QMult* static method), 113
quaternion_normalizer() (*dicее.models.quaternion.QMult* static method), 80
quaternion_normalizer() (*dicее.QMult* static method), 177
query_name_to_struct (*dicее.query_generator.QueryGenerator* attribute), 138
query_name_to_struct (*dicее.QueryGenerator* attribute), 206
QueryGenerator (class in *dicее*), 206
QueryGenerator (class in *dicее.query_generator*), 138

R

r (*dicее.DeCaL* attribute), 168
r (*dicее.Keci* attribute), 164
r (*dicее.models.clifford.DeCaL* attribute), 65
r (*dicее.models.clifford.Keci* attribute), 61
r (*dicее.models.DeCaL* attribute), 125
r (*dicее.models.Keci* attribute), 122
random_prediction() (in module *dicее*), 187
random_prediction() (in module *dicее.static_funcs*), 151
random_seed (*dicее.config.Namespace* attribute), 27
ratio (*dicее.callbacks.Perturb* attribute), 25
re (*dicее.DeCaL* attribute), 168
re (*dicее.models.clifford.DeCaL* attribute), 65
re (*dicее.models.DeCaL* attribute), 125
re_vocab (*dicее.evaluator.Evaluator* attribute), 41
read_from_disk() (in module *dicее.read_preprocess_save_load_kg.util*), 144
read_from_triple_store() (in module *dicее.read_preprocess_save_load_kg.util*), 144
read_only_few (*dicее.config.Namespace* attribute), 27
read_only_few (*dicее.knowledge_graph.KG* attribute), 45
read_or_load_kg() (in module *dicее*), 187
read_or_load_kg() (in module *dicее.static_funcs*), 151
read_with_pandas() (in module *dicее.read_preprocess_save_load_kg.util*), 144
read_with_polars() (in module *dicее.read_preprocess_save_load_kg.util*), 144
ReadFromDisk (class in *dicее.read_preprocess_save_load_kg*), 146
ReadFromDisk (class in *dicее.read_preprocess_save_load_kg.read_from_disk*), 140
rel2id (*dicее.query_generator.QueryGenerator* attribute), 138
rel2id (*dicее.QueryGenerator* attribute), 206
relation_embeddings (*dicее.AConvQ* attribute), 174
relation_embeddings (*dicее.ConvQ* attribute), 174
relation_embeddings (*dicее.DeCaL* attribute), 168
relation_embeddings (*dicее.DualE* attribute), 171
relation_embeddings (*dicее.LFMult* attribute), 179
relation_embeddings (*dicее.models.AConvQ* attribute), 115
relation_embeddings (*dicее.models.clifford.DeCaL* attribute), 64
relation_embeddings (*dicее.models.ConvQ* attribute), 114
relation_embeddings (*dicее.models.DeCaL* attribute), 125
relation_embeddings (*dicее.models.DualE* attribute), 137
relation_embeddings (*dicее.models.dualE.DualE* attribute), 70

- `relation_embeddings` (*dicee.models.FMult* attribute), 134
- `relation_embeddings` (*dicee.models.FMult2* attribute), 135
- `relation_embeddings` (*dicee.models.function_space.FMult* attribute), 72
- `relation_embeddings` (*dicee.models.function_space.FMult2* attribute), 73
- `relation_embeddings` (*dicee.models.function_space.GFMult* attribute), 72
- `relation_embeddings` (*dicee.models.function_space.LFMult* attribute), 74
- `relation_embeddings` (*dicee.models.function_space.LFMult1* attribute), 73
- `relation_embeddings` (*dicee.models.GFMult* attribute), 134
- `relation_embeddings` (*dicee.models.LFMult* attribute), 136
- `relation_embeddings` (*dicee.models.LFMult1* attribute), 135
- `relation_embeddings` (*dicee.models.pykeen_models.PykeenKGE* attribute), 78
- `relation_embeddings` (*dicee.models.PykeenKGE* attribute), 130
- `relation_embeddings` (*dicee.models.quaternion.AConvQ* attribute), 82
- `relation_embeddings` (*dicee.models.quaternion.ConvQ* attribute), 81
- `relation_embeddings` (*dicee.PykeenKGE* attribute), 181
- `relation_to_idx` (*dicee.knowledge_graph.KG* attribute), 45
- `relations_str` (*dicee.knowledge_graph.KG* property), 46
- `reload_dataset()` (in module *dicee*), 195
- `reload_dataset()` (in module *dicee.dataset_classes*), 29
- `report` (*dicee.DICE_Trainer* attribute), 188
- `report` (*dicee.evaluator.Evaluator* attribute), 42
- `report` (*dicee.Execute* attribute), 194
- `report` (*dicee.executer.Execute* attribute), 43
- `report` (*dicee.trainer.DICE_Trainer* attribute), 159
- `report` (*dicee.trainer.dice_trainer.DICE_Trainer* attribute), 154
- `reports` (*dicee.callbacks.Eval* attribute), 23
- `requires_grad_for_interactions` (*dicee.Keci* attribute), 164
- `requires_grad_for_interactions` (*dicee.KeciBase* attribute), 164
- `requires_grad_for_interactions` (*dicee.models.clifford.Keci* attribute), 61
- `requires_grad_for_interactions` (*dicee.models.clifford.KeciBase* attribute), 64
- `requires_grad_for_interactions` (*dicee.models.Keci* attribute), 122
- `requires_grad_for_interactions` (*dicee.models.KeciBase* attribute), 124
- `resid_dropout` (*dicee.models.transformers.CausalSelfAttention* attribute), 87
- `residual_convolution()` (*dicee.AConEx* method), 173
- `residual_convolution()` (*dicee.AConvO* method), 173
- `residual_convolution()` (*dicee.AConvQ* method), 174
- `residual_convolution()` (*dicee.ConEx* method), 176
- `residual_convolution()` (*dicee.ConvO* method), 176
- `residual_convolution()` (*dicee.ConvQ* method), 175
- `residual_convolution()` (*dicee.models.AConEx* method), 108
- `residual_convolution()` (*dicee.models.AConvO* method), 121
- `residual_convolution()` (*dicee.models.AConvQ* method), 115
- `residual_convolution()` (*dicee.models.complex.AConEx* method), 68
- `residual_convolution()` (*dicee.models.complex.ConEx* method), 68
- `residual_convolution()` (*dicee.models.ConEx* method), 107
- `residual_convolution()` (*dicee.models.ConvO* method), 120
- `residual_convolution()` (*dicee.models.ConvQ* method), 114
- `residual_convolution()` (*dicee.models.octonion.AConvO* method), 78
- `residual_convolution()` (*dicee.models.octonion.ConvO* method), 77
- `residual_convolution()` (*dicee.models.quaternion.AConvQ* method), 82
- `residual_convolution()` (*dicee.models.quaternion.ConvQ* method), 81
- `retrieve_embeddings()` (in module *dicee.scripts.serve*), 148
- `return_multi_hop_query_results()` (*dicee.KGE* method), 192
- `return_multi_hop_query_results()` (*dicee.knowledge_graph_embeddings.KGE* method), 49
- `root()` (in module *dicee.scripts.serve*), 148
- `roots` (*dicee.models.FMult* attribute), 134
- `roots` (*dicee.models.function_space.FMult* attribute), 72
- `roots` (*dicee.models.function_space.GFMult* attribute), 72
- `roots` (*dicee.models.GFMult* attribute), 134
- `runtime` (*dicee.analyse_experiments.Experiment* attribute), 19

S

- `sample_counter` (*dicee.abstracts.AbstractPPECallback* attribute), 17
- `sample_entity()` (*dicee.abstracts.BaseInteractiveKGE* method), 14
- `sample_relation()` (*dicee.abstracts.BaseInteractiveKGE* method), 14
- `sample_triples_ratio` (*dicee.config.Namespace* attribute), 27
- `sample_triples_ratio` (*dicee.knowledge_graph.KG* attribute), 45

sanity_checking_with_arguments() (in module *dicee.sanity_checkers*), 147
save() (*dicee.abstracts.BaseInteractiveKGE* method), 14
save() (*dicee.read_preprocess_save_load_kg.LoadSaveToDisk* method), 146
save() (*dicee.read_preprocess_save_load_kg.save_load_disk.LoadSaveToDisk* method), 141
save_checkpoint() (*dicee.abstracts.AbstractTrainer* static method), 13
save_checkpoint_model() (in module *dicee*), 187
save_checkpoint_model() (in module *dicee.static_funcs*), 150
save_embeddings() (in module *dicee*), 187
save_embeddings() (in module *dicee.static_funcs*), 151
save_embeddings_as_csv() (*dicee.config.Namespace* attribute), 26
save_experiment() (*dicee.analyse_experiments.Experiment* method), 19
save_model_at_every_epoch() (*dicee.config.Namespace* attribute), 27
save_numpy_ndarray() (in module *dicee*), 187
save_numpy_ndarray() (in module *dicee.read_preprocess_save_load_kg.util*), 144
save_numpy_ndarray() (in module *dicee.static_funcs*), 150
save_pickle() (in module *dicee*), 187
save_pickle() (in module *dicee.read_preprocess_save_load_kg.util*), 145
save_pickle() (in module *dicee.static_funcs*), 150
save_queries() (*dicee.query_generator.QueryGenerator* method), 139
save_queries() (*dicee.QueryGenerator* method), 207
save_queries_and_answers() (*dicee.query_generator.QueryGenerator* static method), 139
save_queries_and_answers() (*dicee.QueryGenerator* static method), 207
save_trained_model() (*dicee.Execute* method), 194
save_trained_model() (*dicee.executer.Execute* method), 43
scalar_batch_NN() (*dicee.LFMMult* method), 180
scalar_batch_NN() (*dicee.models.function_space.LFMMult* method), 74
scalar_batch_NN() (*dicee.models.LFMMult* method), 136
scaler (*dicee.callbacks.Perturb* attribute), 25
scaler (*dicee.trainer.torch_trainer_ddp.NodeTrainer* attribute), 158
score() (*dicee.ComplEx* static method), 172
score() (*dicee.DistMult* method), 164
score() (*dicee.Keci* method), 167
score() (*dicee.models.clifford.Keci* method), 63
score() (*dicee.models.ComplEx* static method), 109
score() (*dicee.models.complex.ComplEx* static method), 69
score() (*dicee.models.DistMult* method), 104
score() (*dicee.models.Keci* method), 124
score() (*dicee.models.octonion.OMult* method), 76
score() (*dicee.models.OMult* method), 119
score() (*dicee.models.QMult* method), 113
score() (*dicee.models.quaternion.QMult* method), 81
score() (*dicee.models.real.DistMult* method), 83
score() (*dicee.models.real.TransE* method), 83
score() (*dicee.models.TransE* method), 104
score() (*dicee.OMult* method), 179
score() (*dicee.QMult* method), 178
score() (*dicee.TransE* method), 167
score_func (*dicee.models.FMMult2* attribute), 135
score_func (*dicee.models.function_space.FMMult2* attribute), 73
scoring_technique (*dicee.analyse_experiments.Experiment* attribute), 19
scoring_technique (*dicee.config.Namespace* attribute), 27
search() (*dicee.scripts.serve.NeuralSearcher* method), 148
search_embeddings() (in module *dicee.scripts.serve*), 148
seed (*dicee.query_generator.QueryGenerator* attribute), 138
seed (*dicee.QueryGenerator* attribute), 206
select_model() (in module *dicee*), 187
select_model() (in module *dicee.static_funcs*), 150
selected_optimizer (*dicee.BaseKGE* attribute), 184
selected_optimizer (*dicee.models.base_model.BaseKGE* attribute), 58
selected_optimizer (*dicee.models.BaseKGE* attribute), 99, 102, 106, 110, 116, 129, 132
separator (*dicee.config.Namespace* attribute), 27
separator (*dicee.knowledge_graph.KG* attribute), 46
sequential_vocabulary_construction() (*dicee.read_preprocess_save_load_kg.PreprocessKG* method), 146
sequential_vocabulary_construction() (*dicee.read_preprocess_save_load_kg.preprocess.PreprocessKG* method), 140
set_global_seed() (*dicee.query_generator.QueryGenerator* method), 138
set_global_seed() (*dicee.QueryGenerator* method), 206
set_model_eval_mode() (*dicee.abstracts.BaseInteractiveKGE* method), 14
set_model_train_mode() (*dicee.abstracts.BaseInteractiveKGE* method), 14

- setup() (*dicее.CVDataModule* method), 203
- setup() (*dicее.dataset_classes.CVDataModule* method), 38
- setup_executor() (*dicее.Execute* method), 194
- setup_executor() (*dicее.executer.Execute* method), 43
- Shallom (*class in dicее*), 179
- Shallom (*class in dicее.models*), 104
- Shallom (*class in dicее.models.real*), 83
- shallom (*dicее.models.real.Shallom* attribute), 83
- shallom (*dicее.models.Shallom* attribute), 104
- shallom (*dicее.Shallom* attribute), 179
- single_hop_query_answering() (*dicее.KGE* method), 192
- single_hop_query_answering() (*dicее.knowledge_graph_embeddings.KGE* method), 49
- sparql_endpoint (*dicее.config.Namespace* attribute), 26
- sparql_endpoint (*dicее.knowledge_graph.KG* attribute), 45
- start() (*dicее.DICE_Trainer* method), 189
- start() (*dicее.Execute* method), 194
- start() (*dicее.executer.Execute* method), 44
- start() (*dicее.read_preprocess_save_load_kg.PreprocessKG* method), 145
- start() (*dicее.read_preprocess_save_load_kg.preprocess.PreprocessKG* method), 139
- start() (*dicее.read_preprocess_save_load_kg.read_from_disk.ReadFromDisk* method), 140
- start() (*dicее.read_preprocess_save_load_kg.ReadFromDisk* method), 146
- start() (*dicее.trainer.DICE_Trainer* method), 160
- start() (*dicее.trainer.dice_trainer.DICE_Trainer* method), 155
- start_time (*dicее.callbacks.PrintCallback* attribute), 20
- start_time (*dicее.Execute* attribute), 194
- start_time (*dicее.executer.Execute* attribute), 43
- step() (*dicее.EnsembleKGE* method), 186
- step() (*dicее.models.ADOPT* method), 92
- step() (*dicее.models.adopt.ADOPT* method), 51
- step() (*dicее.models.ensemble.EnsembleKGE* method), 71
- storage_path (*dicее.config.Namespace* attribute), 26
- storage_path (*dicее.DICE_Trainer* attribute), 188
- storage_path (*dicее.trainer.DICE_Trainer* attribute), 159
- storage_path (*dicее.trainer.dice_trainer.DICE_Trainer* attribute), 154
- store() (*in module dicее*), 187
- store() (*in module dicее.static_funcs*), 151
- store_ensemble() (*dicее.abstracts.AbstractPPECallback* method), 17
- strategy (*dicее.abstracts.AbstractTrainer* attribute), 12
- swa (*dicее.config.Namespace* attribute), 28

T

- T() (*dicее.DualE* method), 171
- T() (*dicее.models.DualE* method), 137
- T() (*dicее.models.dualE.DualE* method), 71
- t_conorm() (*dicее.KGE* method), 192
- t_conorm() (*dicее.knowledge_graph_embeddings.KGE* method), 49
- t_norm() (*dicее.KGE* method), 192
- t_norm() (*dicее.knowledge_graph_embeddings.KGE* method), 49
- target_dim (*dicее.AllvsAll* attribute), 198
- target_dim (*dicее.dataset_classes.AllvsAll* attribute), 33
- target_dim (*dicее.dataset_classes.MultiLabelDataset* attribute), 30
- target_dim (*dicее.dataset_classes.OnevsAllDataset* attribute), 31
- target_dim (*dicее.knowledge_graph.KG* attribute), 46
- target_dim (*dicее.MultiLabelDataset* attribute), 196
- target_dim (*dicее.OnevsAllDataset* attribute), 197
- temperature (*dicее.BytE* attribute), 182
- temperature (*dicее.models.transformers.BytE* attribute), 85
- tensor_t_norm() (*dicее.KGE* method), 192
- tensor_t_norm() (*dicее.knowledge_graph_embeddings.KGE* method), 49
- TensorParallel (*class in dicее.trainer.model_parallelism*), 156
- test_data_loader() (*dicее.models.base_model.BaseKGELightning* method), 54
- test_data_loader() (*dicее.models.BaseKGELightning* method), 94
- test_epoch_end() (*dicее.models.base_model.BaseKGELightning* method), 54
- test_epoch_end() (*dicее.models.BaseKGELightning* method), 94
- test_h1 (*dicее.analyse_experiments.Experiment* attribute), 19
- test_h3 (*dicее.analyse_experiments.Experiment* attribute), 19
- test_h10 (*dicее.analyse_experiments.Experiment* attribute), 19

test_mrr (*dicee.analyse_experiments.Experiment* attribute), 19
 test_path (*dicee.query_generator.QueryGenerator* attribute), 138
 test_path (*dicee.QueryGenerator* attribute), 206
 timeit () (*in module dicee*), 187, 195
 timeit () (*in module dicee.read_preprocess_save_load_kg.util*), 144
 timeit () (*in module dicee.static_funcs*), 150
 timeit () (*in module dicee.static_preprocess_funcs*), 153
 to () (*dicee.EnsembleKGE* method), 186
 to () (*dicee.KGE* method), 190
 to () (*dicee.knowledge_graph_embeddings.KGE* method), 46
 to () (*dicee.models.ensemble.EnsembleKGE* method), 71
 to_df () (*dicee.analyse_experiments.Experiment* method), 19
 topk (*dicee.BytE* attribute), 182
 topk (*dicee.models.transformers.BytE* attribute), 85
 torch_ordered_shaped_bpe_entities (*dicee.dataset_classes.MultiLabelDataset* attribute), 30
 torch_ordered_shaped_bpe_entities (*dicee.MultiLabelDataset* attribute), 196
 TorchDDPTrainer (*class in dicee.trainer.torch_trainer_ddp*), 158
 TorchTrainer (*class in dicee.trainer.torch_trainer*), 156
 train () (*dicee.KGE* method), 193
 train () (*dicee.knowledge_graph_embeddings.KGE* method), 50
 train () (*dicee.trainer.torch_trainer_ddp.NodeTrainer* method), 159
 train_data (*dicee.AllvsAll* attribute), 198
 train_data (*dicee.dataset_classes.AllvsAll* attribute), 33
 train_data (*dicee.dataset_classes.KvsAll* attribute), 32
 train_data (*dicee.dataset_classes.KvsSampleDataset* attribute), 35
 train_data (*dicee.dataset_classes.MultiClassClassificationDataset* attribute), 31
 train_data (*dicee.dataset_classes.OnevsAllDataset* attribute), 31
 train_data (*dicee.dataset_classes.OnevsSample* attribute), 33, 34
 train_data (*dicee.KvsAll* attribute), 197
 train_data (*dicee.KvsSampleDataset* attribute), 201
 train_data (*dicee.MultiClassClassificationDataset* attribute), 196
 train_data (*dicee.OnevsAllDataset* attribute), 197
 train_data (*dicee.OnevsSample* attribute), 199
 train_data_loader () (*dicee.CVDataModule* method), 203
 train_data_loader () (*dicee.dataset_classes.CVDataModule* method), 37
 train_data_loader () (*dicee.models.base_model.BaseKGELightning* method), 55
 train_data_loader () (*dicee.models.BaseKGELightning* method), 96
 train_data_loaders (*dicee.trainer.torch_trainer.TorchTrainer* attribute), 157
 train_dataset_loader (*dicee.trainer.torch_trainer_ddp.NodeTrainer* attribute), 158
 train_h1 (*dicee.analyse_experiments.Experiment* attribute), 18
 train_h3 (*dicee.analyse_experiments.Experiment* attribute), 18
 train_h10 (*dicee.analyse_experiments.Experiment* attribute), 18
 train_indices_target (*dicee.dataset_classes.MultiLabelDataset* attribute), 30
 train_indices_target (*dicee.MultiLabelDataset* attribute), 196
 train_k_vs_all () (*dicee.KGE* method), 193
 train_k_vs_all () (*dicee.knowledge_graph_embeddings.KGE* method), 50
 train_mode (*dicee.EnsembleKGE* attribute), 186
 train_mode (*dicee.models.ensemble.EnsembleKGE* attribute), 71
 train_mrr (*dicee.analyse_experiments.Experiment* attribute), 18
 train_path (*dicee.query_generator.QueryGenerator* attribute), 138
 train_path (*dicee.QueryGenerator* attribute), 206
 train_set (*dicee.BPE_NegativeSamplingDataset* attribute), 195
 train_set (*dicee.dataset_classes.BPE_NegativeSamplingDataset* attribute), 29
 train_set (*dicee.dataset_classes.MultiLabelDataset* attribute), 30
 train_set (*dicee.dataset_classes.NegSampleDataset* attribute), 36
 train_set (*dicee.dataset_classes.TriplePredictionDataset* attribute), 36
 train_set (*dicee.MultiLabelDataset* attribute), 196
 train_set (*dicee.NegSampleDataset* attribute), 201
 train_set (*dicee.TriplePredictionDataset* attribute), 202
 train_set_idx (*dicee.CVDataModule* attribute), 203
 train_set_idx (*dicee.dataset_classes.CVDataModule* attribute), 37
 train_set_target (*dicee.knowledge_graph.KG* attribute), 46
 train_target (*dicee.AllvsAll* attribute), 198
 train_target (*dicee.dataset_classes.AllvsAll* attribute), 33
 train_target (*dicee.dataset_classes.KvsAll* attribute), 32
 train_target (*dicee.dataset_classes.KvsSampleDataset* attribute), 35
 train_target (*dicee.KvsAll* attribute), 198
 train_target (*dicee.KvsSampleDataset* attribute), 201

train_target_indices (*dicee.knowledge_graph.KG attribute*), 46
 train_triples() (*dicee.KGE method*), 193
 train_triples() (*dicee.knowledge_graph_embeddings.KGE method*), 50
 trained_model (*dicee.Execute attribute*), 193
 trained_model (*dicee.executer.Execute attribute*), 43
 trainer (*dicee.config.Namespace attribute*), 27
 trainer (*dicee.DICE_Trainer attribute*), 188
 trainer (*dicee.Execute attribute*), 193
 trainer (*dicee.executer.Execute attribute*), 43
 trainer (*dicee.trainer.DICE_Trainer attribute*), 159
 trainer (*dicee.trainer.dice_trainer.DICE_Trainer attribute*), 154
 trainer (*dicee.trainer.torch_trainer_ddp.NodeTrainer attribute*), 158
 training_step (*dicee.trainer.torch_trainer.TorchTrainer attribute*), 157
 training_step() (*dicee.BytE method*), 182
 training_step() (*dicee.models.base_model.BaseKGELightning method*), 52
 training_step() (*dicee.models.BaseKGELightning method*), 93
 training_step() (*dicee.models.transformers.BytE method*), 85
 training_step_outputs (*dicee.models.base_model.BaseKGELightning attribute*), 52
 training_step_outputs (*dicee.models.BaseKGELightning attribute*), 93
 training_technique (*dicee.knowledge_graph.KG attribute*), 45
 TransE (*class in dicee*), 167
 TransE (*class in dicee.models*), 104
 TransE (*class in dicee.models.real*), 83
 transfer_batch_to_device() (*dicee.CVDDataModule method*), 204
 transfer_batch_to_device() (*dicee.dataset_classes.CVDDataModule method*), 38
 transformer (*dicee.BytE attribute*), 182
 transformer (*dicee.models.transformers.BytE attribute*), 85
 transformer (*dicee.models.transformers.GPT attribute*), 90
 trapezoid() (*dicee.models.FMult2 method*), 135
 trapezoid() (*dicee.models.function_space.FMult2 method*), 73
 tri_score() (*dicee.LFMult method*), 180
 tri_score() (*dicee.models.function_space.LFMult method*), 74
 tri_score() (*dicee.models.function_space.LFMult1 method*), 74
 tri_score() (*dicee.models.LFMult method*), 136
 tri_score() (*dicee.models.LFMult1 method*), 135
 triple_score() (*dicee.KGE method*), 192
 triple_score() (*dicee.knowledge_graph_embeddings.KGE method*), 48
 TriplePredictionDataset (*class in dicee*), 201
 TriplePredictionDataset (*class in dicee.dataset_classes*), 36
 tuple2list() (*dicee.query_generator.QueryGenerator method*), 138
 tuple2list() (*dicee.QueryGenerator method*), 206

U

unlabelled_size (*dicee.callbacks.PseudoLabellingCallback attribute*), 22
 unmap() (*dicee.query_generator.QueryGenerator method*), 139
 unmap() (*dicee.QueryGenerator method*), 207
 unmap_query() (*dicee.query_generator.QueryGenerator method*), 139
 unmap_query() (*dicee.QueryGenerator method*), 207

V

val_aswa (*dicee.callbacks.ASWA attribute*), 23
 val_dataloader() (*dicee.models.base_model.BaseKGELightning method*), 54
 val_dataloader() (*dicee.models.BaseKGELightning method*), 95
 val_h1 (*dicee.analyse_experiments.Experiment attribute*), 18
 val_h3 (*dicee.analyse_experiments.Experiment attribute*), 18
 val_h10 (*dicee.analyse_experiments.Experiment attribute*), 18
 val_mrr (*dicee.analyse_experiments.Experiment attribute*), 18
 val_path (*dicee.query_generator.QueryGenerator attribute*), 138
 val_path (*dicee.QueryGenerator attribute*), 206
 validate_knowledge_graph() (*in module dicee.sanity_checkers*), 146
 vocab_preparation() (*dicee.evaluator.Evaluator method*), 42
 vocab_size (*dicee.models.transformers.GPTConfig attribute*), 89
 vocab_to_parquet() (*in module dicee*), 188
 vocab_to_parquet() (*in module dicee.static_funcs*), 151
 vtp_score() (*dicee.LFMult method*), 180
 vtp_score() (*dicee.models.function_space.LFMult method*), 74
 vtp_score() (*dicee.models.function_space.LFMult1 method*), 74

`vtp_score()` (*dicee.models.LFMult* method), 136
`vtp_score()` (*dicee.models.LFMultI* method), 135

W

`weight` (*dicee.models.transformers.LayerNorm* attribute), 86
`weight_decay` (*dicee.BaseKGE* attribute), 184
`weight_decay` (*dicee.config.Namespace* attribute), 27
`weight_decay` (*dicee.models.base_model.BaseKGE* attribute), 58
`weight_decay` (*dicee.models.BaseKGE* attribute), 99, 102, 106, 110, 116, 129, 132
`weights` (*dicee.models.FMult* attribute), 134
`weights` (*dicee.models.function_space.FMult* attribute), 72
`weights` (*dicee.models.function_space.GFMult* attribute), 73
`weights` (*dicee.models.GFMult* attribute), 134
`write_csv_from_model_parallel()` (in module *dicee*), 188
`write_csv_from_model_parallel()` (in module *dicee.static_funcs*), 152
`write_links()` (*dicee.query_generator.QueryGenerator* method), 139
`write_links()` (*dicee.QueryGenerator* method), 207
`write_report()` (*dicee.Execute* method), 194
`write_report()` (*dicee.executer.Execute* method), 44

X

`x_values` (*dicee.LFMult* attribute), 179
`x_values` (*dicee.models.function_space.LFMult* attribute), 74
`x_values` (*dicee.models.LFMult* attribute), 136