
DICE Embeddings

Release 0.1.3.2

Caglar Demir

Jan 14, 2026

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	215
14.3 Classes	215
14.4 Package Contents	215
Python Module Index	227

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

1 Dicee Manual

Version: dicee 0.2.0

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

Publisher and maintainer: Caglar Demir²

Contact: caglar.demir@upb.de

License: OSI Approved :: MIT License

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. **Pandas³ & Co.** to use parallelism at preprocessing a large knowledge graph,
2. **PyTorch⁴ & Co.** to learn knowledge graph embeddings via multi-CPUs, GPUs, TPUs or computing cluster, and
3. **Huggingface⁵** 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 PyTorch⁸ & PytorchLightning⁹. 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 Huggingface¹⁰? Seamlessly deploy and share pre-trained embedding models through the Huggingface ecosystem.

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/>

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 parallel 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
```

(continues on next page)

(continued from previous page)

```
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
<hr/>				
dicee/__init__.py	7	0	100%	
dicee/abstracts.py	338	115	66%	112-113, ..

(continues on next page)

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

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

(continued from previous page)

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

(continues on next page)

(continued from previous page)

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

13 How to cite

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

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

(continues on next page)

(continued from previous page)

```
author={Demir, Caglar and Ngonga Ngomo, Axel-Cyrille},
booktitle={Joint European Conference on Machine Learning and Knowledge Discovery in
→Databases},
pages={567--582},
year={2023},
organization={Springer}
}
# LitCQD
@inproceedings{demir2023litcqd,
    title={LitCQD: Multi-Hop Reasoning in Incomplete Knowledge Graphs with Numeric
→Literals},
    author={Demir, Caglar and Wiebesiek, Michel and Lu, Renzhong and Ngonga Ngomo, Axel-
→Cyrille and Heindorf, Stefan},
    booktitle={Joint European Conference on Machine Learning and Knowledge Discovery in
→Databases},
    pages={617--633},
    year={2023},
    organization={Springer}
}
# DICE Embedding Framework
@article{demir2022hardware,
    title={Hardware-agnostic computation for large-scale knowledge graph embeddings},
    author={Demir, Caglar and Ngomo, Axel-Cyrille Ngonga},
    journal={Software Impacts},
    year={2022},
    publisher={Elsevier}
}
# KronE
@inproceedings{demir2022kronecker,
    title={Kronecker decomposition for knowledge graph embeddings},
    author={Demir, Caglar and Lienen, Julian and Ngonga Ngomo, Axel-Cyrille},
    booktitle={Proceedings of the 33rd ACM Conference on Hypertext and Social Media},
    pages={1--10},
    year={2022}
}
# QMult, OMult, ConvQ, ConvO
@InProceedings{pmlr-v157-demir21a,
    title = {Convolutional Hypercomplex Embeddings for Link Prediction},
    author = {Demir, Caglar and Moussallem, Diego and Heindorf, Stefan and Ngonga
→Ngomo, Axel-Cyrille},
    booktitle = {Proceedings of The 13th Asian Conference on Machine Learning},
    pages = {656--671},
    year = {2021},
    editor = {Balasubramanian, Vineeth N. and Tsang, Ivor},
    volume = {157},
    series = {Proceedings of Machine Learning Research},
    month = {17--19 Nov},
    publisher = {PMLR},
    pdf = {https://proceedings.mlr.press/v157/demir21a/demir21a.pdf},
    url = {https://proceedings.mlr.press/v157/demir21a.html},
}
# ConEx
```

(continues on next page)

(continued from previous page)

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

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

14 dicee

DICE Embeddings - Knowledge Graph Embedding Library.

A library for training and using knowledge graph embedding models with support for various scoring techniques and training strategies.

Submodules:

`evaluation`: Model evaluation functions and Evaluator class
`models`: KGE model implementations
`trainer`: Training orchestration scripts
`utils`: Utility scripts

14.1 Submodules

`dicee.__main__`

`dicee.abstracts`

`Classes`

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

Module Contents

```
class dicee.abstracts.AbstractTrainer(args, callbacks)
Abstract class for Trainer class for knowledge graph embedding models
```

Parameter

```
args
    [str] ?

callbacks: list
    ?

attributes

callbacks

is_global_zero = True

global_rank = 0

local_rank = 0

strategy = None

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

A function to call callbacks before the training starts.

Parameter

```
args

kwargs

rtype
    None

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

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

Parameter

```
args

kwargs

rtype
    None

on_train_epoch_start(*args, **kwargs)
```

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

Parameter

args

kwargs

rtype

None

on_train_epoch_end(*args, **kwargs)

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

Parameter

args

kwargs

rtype

None

on_train_batch_end(*args, **kwargs)

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

Parameter

args

kwargs

rtype

None

static save_checkpoint(full_path: str, model) → None

A static function to save a model into disk

Parameter

full_path : str

model:

rtype

None

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

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

Parameter

path_of_pretrained_model_dir

[str] ?

construct_ensemble: boolean

?

model_name: str apply_semantic_constraint : boolean

```

construct_ensemble = False
apply_semantic_constraint = False
configs
get_eval_report () → dict
get_bpe_token_representation (str_entity_or_relation: List[str] | str) → List[List[int]] | List[int]

```

Parameters

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

Return type

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

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

Parameters

triples

```
set_model_train_mode () → None
```

Setting the model into training mode

Parameter

```
set_model_eval_mode () → None
```

Setting the model into eval mode

Parameter

```
property name
```

```
sample_entity (n: int) → List[str]
```

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

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

```
save () → None
```

```
get_entity_index (x: str)
```

```
get_relation_index (x: str)
```

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

Index Triple

Parameter

head_entity: List[str]

String representation of selected entities.

relation: List[str]

String representation of selected relations.

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

Returns: Tuple

pytorch tensor of triple score

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

`get_entity_embeddings (items: List[str])`

Return embedding of an entity given its string representation

Parameter

`items:`
entities

`get_relation_embeddings (items: List[str])`

Return embedding of a relation given its string representation

Parameter

`items:`
relations

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

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

`parameters ()`

`class dicee.abstracts.InteractiveQueryDecomposition`

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

`tensor_t_norm (subquery_scores: torch.FloatTensor, tnorm: str = 'min') → torch.FloatTensor`

Compute T-norm over $[0,1]^{\{n \text{ times } d\}}$ where n denotes the number of hops and d denotes number of entities

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

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

`class dicee.abstracts.AbstractCallback`

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

Abstract class for Callback class for knowledge graph embedding models

Parameter

`on_init_start (*args, **kwargs)`

Parameter

trainer:

model:

rtype

None

on_init_end(*args, **kwargs)

Call at the beginning of the training.

Parameter

trainer:

model:

rtype

None

on_fit_start(trainer, model)

Call at the beginning of the training.

Parameter

trainer:

model:

rtype

None

on_train_epoch_end(trainer, model)

Call at the end of each epoch during training.

Parameter

trainer:

model:

rtype

None

on_train_batch_end(*args, **kwargs)

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

Parameter

trainer:

model:

rtype

None

on_fit_end(*args, **kwargs)

Call at the end of the training.

Parameter

trainer:

model:

rtype

None

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

Bases: *AbstractCallback*

Abstract class for Callback class for knowledge graph embedding models

Parameter

num_epochs

path

sample_counter = 0

epoch_count = 0

alphas = None

on_fit_start (trainer, model)

Call at the beginning of the training.

Parameter

trainer:

model:

rtype

None

on_fit_end (trainer, model)

Call at the end of the training.

Parameter

trainer:

model:

rtype

None

store_ensemble (param_ensemble) → None

```
class dicee.abstracts.BaseInteractiveTrainKGE
```

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

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

```

train_k_vs_all(h, r, iteration=1, lr=0.001)
    Train k vs all :param head_entity: :param relation: :param iteration: :param lr: :return:
train(kg, lr=0.1, epoch=10, batch_size=32, neg_sample_ratio=10, num_workers=1) → None
    Retrained a pretrain model on an input KG via negative sampling.

train_literals(train_file_path: str = None, num_epochs: int = 100, lit_lr: float = 0.001,
    lit_normalization_type: str = 'z-norm', batch_size: int = 1024, sampling_ratio: float = None,
    random_seed=1, loader_backend: str = 'pandas', freeze_entity_embeddings: bool = True,
    gate_residual: bool = True, device: str = None, shuffle_data: bool = True)
    Trains the Literal Embeddings model using literal data.

```

Parameters

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

dicee.analyse_experiments

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

Classes

Experiment

Functions

get_default_arguments()

analyse(args)

Module Contents

```
dicee.analyse_experiments.get_default_arguments()

class dicee.analyse_experiments.Experiment

    model_name = []
    callbacks = []
    embedding_dim = []
    num_params = []
    num_epochs = []
    batch_size = []
    lr = []
    byte_pair_encoding = []
    aswa = []
    path_dataset_folder = []
    full_storage_path = []
    pq = []
    train_mrr = []
    train_h1 = []
    train_h3 = []
    train_h10 = []
    val_mrr = []
    val_h1 = []
    val_h3 = []
    val_h10 = []
    test_mrr = []
    test_h1 = []
    test_h3 = []
    test_h10 = []
    runtime = []
    normalization = []
    scoring_technique = []
    save_experiment(x)
```

```
to_df()

dicee.analyse_experiments.analyse(args)
```

dicee.callbacks

Callbacks for training lifecycle events.

Provides callback classes for various training events including epoch end, model saving, weight averaging, and evaluation.

Classes

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

Functions

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

Module Contents

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

Bases: `dicee.abstracts.AbstractCallback`

Callback to store epoch losses to a CSV file.

Parameters

`path` – Directory path where the loss file will be saved.

`path`

`on_fit_end(trainer, model) → None`

Store epoch loss history to CSV file.

Parameters

- `trainer` – The trainer instance.

- **model** – The model being trained.

```
class dicee.callbacks.PrintCallback
Bases: dicee.abstracts.AbstractCallback
Abstract class for Callback class for knowledge graph embedding models
```

Parameter

start_time

on_fit_start (*trainer, pl_module*)

Call at the beginning of the training.

Parameter

trainer:

model:

rtype

None

on_fit_end (*trainer, pl_module*)

Call at the end of the training.

Parameter

trainer:

model:

rtype

None

on_train_batch_end (**args, **kwargs*)

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

Parameter

trainer:

model:

rtype

None

on_train_epoch_end (**args, **kwargs*)

Call at the end of each epoch during training.

Parameter

trainer:

model:

rtype

None

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

Bases: [dicee.abstracts.AbstractCallback](#)

Abstract class for Callback class for knowledge graph embedding models

Parameter

every_x_epoch

max_epochs

epoch_counter = 0

path

on_train_batch_end(*args, **kwargs)

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

Parameter

trainer:

model:

rtype

None

on_fit_start(trainer, pl_module)

Call at the beginning of the training.

Parameter

trainer:

model:

rtype

None

on_train_epoch_end(*args, **kwargs)

Call at the end of each epoch during training.

Parameter

trainer:

model:

rtype

None

on_fit_end(*args, **kwargs)

Call at the end of the training.

Parameter

trainer:

model:

rtype

None

on_epoch_end(model, trainer, **kwargs)

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

Bases: dicee.abstracts.AbstractCallback

Abstract class for Callback class for knowledge graph embedding models

Parameter

data_module

kg

num_of_epochs = 0

unlabelled_size

batch_size

create_random_data()

on_epoch_end(trainer, model)

dicee.callbacks.estimate_q(eps)

estimate rate of convergence q from sequence esp

dicee.callbacks.compute_convergence(seq, i)

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

Bases: dicee.abstracts.AbstractCallback

Abstract class for Callback class for knowledge graph embedding models

Parameter

path

reports = []

epoch_ratio = None

epoch_counter = 0

on_fit_start(trainer, model)

Call at the beginning of the training.

Parameter

trainer:

model:

rtype

None

on_fit_end(*trainer, model*)

Call at the end of the training.

Parameter

trainer:

model:

rtype

None

on_train_epoch_end(*trainer, model*)

Call at the end of each epoch during training.

Parameter

trainer:

model:

rtype

None

on_train_batch_end(*args, **kwargs)

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

Parameter

trainer:

model:

rtype

None

class dicee.callbacks.Krone

Bases: *dicee.abstracts.AbstractCallback*

Abstract class for Callback class for knowledge graph embedding models

Parameter

f = None

static batch_kronecker_product(*a, b*)

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

```
get_kronecker_triple_representation(indexed_triple: torch.LongTensor)
```

Get kronecker embeddings

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

Call at the beginning of the training.

Parameter

trainer:

model:

rtype

None

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

Bases: *dicee.abstracts.AbstractCallback*

A callback for a three-Level Perturbation

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

Parameter Perturbation:

Output Perturbation:

```
level = 'input'  
ratio = 0.0  
method = None  
scaler = None  
frequency = None
```

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

Called when the train batch begins.

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

Bases: *dicee.abstracts.AbstractCallback*

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

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

```
experiment_dir
```

```
max_epochs
```

```
epoch_counter = 0
```

```
save_model_every_n_epoch = True
```

```
reports
```

```

n_epochs_eval_model = 'val_test'

default_eval_model = None

eval_epochs

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

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

class dicee.callbacks.LRScheduler(adaptive_lr_config: dict, total_epochs: int, experiment_dir: str,
    eta_max: float = 0.1, snapshot_dir: str = 'snapshots')
Bases: dicee.abstracts.AbstractCallback

Callback for managing learning rate scheduling and model snapshots.

Supports cosine annealing ("cca"), MMCCLR ("mmcclr"), and their deferred (warmup) variants: - "deferred_cca"
- "deferred_mmcclr"

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

total_epochs

experiment_dir

snapshot_dir

batches_per_epoch = None

total_steps = None

cycle_length = None

warmup_steps = None

lr_lambda = None

scheduler = None

step_count = 0

snapshot_loss

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

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

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

```

Parameter

trainer:

model:

rtype

None

dicee.config

Configuration module for DICE embeddings.

Provides the Namespace class with default configuration values for training knowledge graph embedding models.

Classes

<i>Namespace</i>	Extended Namespace with default KGE training configuration.
------------------	---

Module Contents

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

Bases: argparse.Namespace

Extended Namespace with default KGE training configuration.

Provides sensible defaults for all training parameters while allowing easy customization through command-line arguments or direct assignment.

```
dataset_dir: str = None
```

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

```
save_embeddings_as_csv: bool = False
```

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

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

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

```
path_to_store_single_run: str = None
```

A single directory created that contains related data about embeddings.

```
path_single_kg = None
```

Path of a file corresponding to the input knowledge graph

```
sparql_endpoint = None
```

An endpoint of a triple store.

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

KGE model

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

Optimizer

```
embedding_dim: int = 64
```

Size of continuous vector representation of an entity/relation

```
num_epochs: int = 150
```

Number of pass over the training data

```
batch_size: int = 1024
```

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

```
lr: float = 0.1
```

Learning rate

```

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

gpus = None
    Number GPUs to be used during training

callbacks
    10} }

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

Type
    { "last_percent_to_consider"

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

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

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

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

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

weight_decay: float = 0.0
    Weight decay for all trainable params

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

init_param: str = None
    xavier_normal or None

gradient_accumulation_steps: int = 0
    Not tested e

num_folds_for_cv: int = 0
    Number of folds for CV

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

Type
    Evaluate trained model choices

save_model_at_every_epoch: int = None
    Not tested

label_smoothing_rate: float = 0.0

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

```

```

random_seed: int = 0
    Random Seed

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

read_only_few: int = None
    Read only first few triples

pykeen_model_kwargs
    Additional keyword arguments for pykeen models

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

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

p: int = 0
    P parameter of Clifford Embeddings

q: int = 1
    Q parameter of Clifford Embeddings

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

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

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

byte_pair_encoding: bool = False
    Byte pair encoding

    Type
        WIP

adaptive_swa: bool = False
    Adaptive stochastic weight averaging

swa: bool = False
    Stochastic weight averaging

swag: bool = False
    Stochastic weight averaging - Gaussian

ema: bool = False
    Exponential Moving Average

twa: bool = False
    Trainable weight averaging

block_size: int = None
    block size of LLM

continual_learning = None
    Path of a pretrained model size of LLM

```

```

auto_batch_finding = False
A flag for using auto batch finding

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

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

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

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

adaptive_lr
    "cca"}}

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

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

swa_c_epochs: int = 1
Number of epochs to average over for SWA, SWAG, EMA, TWA.

__iter__()

```

dicee.dataset_classes

Classes

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

Functions

<i>reload_dataset</i> (path, form_of_labelling, ...)	Reload the files from disk to construct the Pytorch dataset continues on next page
--	---

Table 8 – continued from previous page

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

Module Contents

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

Reload the files from disk to construct the Pytorch dataset

`dicee.dataset_classes.construct_dataset`(* (Keyword-only parameters separator (PEP 3102)), *train_set: numpy.ndarray | list, valid_set=None, test_set=None, ordered_bpe_entities=None, train_target_indices=None, target_dim: int = None, entity_to_idx: dict, relation_to_idx: dict, form_of_labelling: str, scoring_technique: str, neg_ratio: int, label_smoothing_rate: float, byte_pair_encoding=None, block_size: int = None*) → torch.utils.data.Dataset

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

Bases: torch.utils.data.Dataset

An abstract class representing a Dataset.

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

 **Note**

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

`train_set`

`ordered_bpe_entities`

`num_bpe_entities`

`neg_ratio`

`num_datapoints`

`__len__()`

`__getitem__(idx)`

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

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

Bases: torch.utils.data.Dataset

An abstract class representing a Dataset.

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

Note

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

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

class dicee.dataset_classes.MultiClassClassificationDataset(
    subword_units: numpy.ndarray, block_size: int = 8)
Bases: torch.utils.data.Dataset
Dataset for the 1vsALL training strategy
```

Parameters

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

Return type

`torch.utils.data.Dataset`

```
train_data
block_size = 8
num_of_data_points
collate_fn = None
__len__()
__getitem__(idx)
```

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

Bases: torch.utils.data.Dataset

Dataset for the 1vsALL training strategy

Parameters

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

Return type

torch.utils.data.Dataset

```
train_data
```

```
target_dim
```

```
collate_fn = None
```

```
__len__()
```

```
__getitem__(idx)
```

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

Bases: torch.utils.data.Dataset

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

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

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

Note

TODO

train_set_idx

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

entity_idxs

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

relation_idxs

[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_idxs, relation_idxs,
label_smoothing_rate=0.0)
Bases: torch.utils.data.Dataset

```

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

Let D denote a dataset for AllvsAll training and be defined as $D := \{(x,y)_i\}_{i=1}^N$, 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 $[0,1]^{|\mathcal{E}|}$ is a binary label.

overall $y_{-i} = 1$ s.t. $(h, r) \in E_i$ in KG

i Note

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

train_set_idx
[`numpy.ndarray`] n by 3 array representing n triples
entity_idxs
[`dictionary`] string representation of an entity to its integer id
relation_idxs
[`dictionary`] string representation of a relation to its integer id

self : `torch.utils.data.Dataset`

```

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

```

```

train_data = None
train_target = None
label_smoothing_rate
collate_fn = None
target_dim
__len__()
__getitem__(idx)

```

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

Bases: torch.utils.data.Dataset

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

Parameters

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

train_data

The input data converted into a PyTorch tensor.

Type

torch.Tensor

num_entities

Number of entities in the dataset.

Type

int

num_relations

Number of relations in the dataset.

Type

int

neg_sample_ratio

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

Type

int

label_smoothing_rate

The smoothing factor applied to the labels.

Type

torch.Tensor

collate_fn

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

Type

function, optional

train_data

num_entities

```

num_relations
neg_sample_ratio = None
label_smoothing_rate
collate_fn = None
__len__()  

    Returns the number of samples in the dataset.
__getitem__(idx)  

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

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

Returns
A tuple consisting of:  


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

```

Return type

tuple

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

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

Bases: torch.utils.data.Dataset

KvsSample a Dataset:

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

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

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

train_set_idx

Indexed triples for the training.

entity_idxs

mapping.

relation_idxs

mapping.

form

?

store

?

label_smoothing_rate

?

```

torch.utils.data.Dataset

train_data = None
train_target = None
neg_ratio = None
num_entities
label_smoothing_rate
collate_fn = None
max_num_of_classes

__len__()
__getitem__(idx)

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

```

Bases: torch.utils.data.Dataset

An abstract class representing a Dataset.

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

Note

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

```

neg_sample_ratio
train_triples
length
num_entities
num_relations
labels
train_set = []
__len__()
__getitem__(idx)

```

```

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

Triple Dataset

D:= {(x)_i}_i ^N, where
. x:(h,r, t) in KG is a unique h in E and a relation r in R and . 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_idxs
mapping.

relation_idxs
mapping.

form
?

store
?

label_smoothing_rate

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

label_smoothing_rate

neg_sample_ratio

train_set

length

num_entities

num_relations

__len__()

__getitem__(idx)

collate_fn(batch: List[torch.Tensor])


```

```

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

```

Create a Dataset for cross validation

Parameters

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

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

Return type

?

```
train_set_idx
num_entities
num_relations
neg_sample_ratio
batch_size
num_workers
train_dataloader() → torch.utils.data.DataLoader
```

An iterable or collection of iterables specifying training samples.

For more information about multiple dataloaders, see this section.

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

For data processing use the following pattern:

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

However, the above are only necessary for distributed processing.

⚠ Warning

do not assign state in `prepare_data`

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

ℹ Note

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

`setup(*args, **kwargs)`

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

Parameters

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

Example:

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

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

        # don't do this
        self.something = else

    def setup(self, stage):
        data = load_data(...)
        self.ll = 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):

```

(continues on next page)

(continued from previous page)

```
super().__init__()
self.prepare_data_per_node = True

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

This is called before requesting the dataloaders:

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

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

Bases: torch.utils.data.Dataset

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

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

train_file_path

Path to the training data file.

Type

str

normalization

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

Type

str

normalization_params

Parameters used for normalization.

Type

dict

sampling_ratio

Fraction of the training set to use for ablations.

Type

float

entity_to_idx

Mapping of entities to their indices.

Type

dict

```

num_entities
    Total number of entities.

    Type
        int

data_property_to_idx
    Mapping of data properties to their indices.

    Type
        dict

num_data_properties
    Total number of data properties.

    Type
        int

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

    Type
        str

train_file_path

loader_backend = 'pandas'

normalization_type = 'z-norm'

normalization_params

sampling_ratio = None

entity_to_idx = None

num_entities

__getitem__ (index)

__len__ ()

static load_and_validate_literal_data (file_path: str = None, loader_backend: str = 'pandas') → pandas.DataFrame
    Loads and validates the literal data file. :param file_path: Path to the literal data file. :type file_path: str

    Returns
        DataFrame containing the loaded and validated data.

    Return type
        pd.DataFrame

static denormalize (preds_norm, attributes, normalization_params) → numpy.ndarray
    Denormalizes the predictions based on the normalization type.

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

    Returns
        Denormalized predictions.

```

Return type
np.ndarray

dicee.eval_static_funcs

Static evaluation functions for KGE models.

This module provides backward compatibility by re-exporting from the new dicee.evaluation module.

Deprecated since version Use: dicee.evaluation submodules instead. This module will be removed in a future version.

Functions

<code>evaluate_link_prediction_performance(→ Dict[str, float])</code>	Evaluate link prediction performance with head and tail prediction.
<code>evaluate_link_prediction_performance_with_reciprocals(→ Dict[str, float])</code>	Evaluate link prediction with reciprocal relations.
<code>evaluate_link_prediction_performance_with_bpe(→ Dict[str, float])</code>	Evaluate link prediction with BPE encoding (head and tail).
<code>evaluate_link_prediction_performance_with_reciprocal_bpe(→ Dict[str, float])</code>	Evaluate link prediction with BPE encoding and reciprocals.
<code>evaluate_lp_bpe_k_vs_all(→ Dict[str, float])</code>	Evaluate BPE link prediction with KvsAll scoring.
<code>evaluate_literal_prediction(→ Op[Dict[pandas.DataFrame], pandas.DataFrame])</code>	Evaluate trained literal prediction model on a test file.
<code>evaluate_ensemble_link_prediction_performance(→ Dict[str, float])</code>	Evaluate link prediction performance of an ensemble of KGE models.

Module Contents

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

Evaluate link prediction performance with head and tail prediction.

Performs filtered evaluation where known correct answers are filtered out before computing ranks.

Parameters

- `model` – KGE model wrapper with entity/relation mappings.
- `triples` – Test triples as list of (head, relation, tail) strings.
- `er_vocab` – Mapping (entity, relation) -> list of valid tail entities.
- `re_vocab` – Mapping (relation, entity) -> list of valid head entities.

Returns

Dictionary with H@1, H@3, H@10, and MRR metrics.

`dicee.eval_static_funcs.evaluate_link_prediction_performance_with_reciprocals(model, triples, er_vocab: Dict[Tuple, List]) → Dict[str, float]`

Evaluate link prediction with reciprocal relations.

Optimized for models trained with reciprocal triples where only tail prediction is needed.

Parameters

- `model` – KGE model wrapper.
- `triples` – Test triples as list of (head, relation, tail) strings.

- **er_vocab** – Mapping (entity, relation) -> list of valid tail entities.

Returns

Dictionary with H@1, H@3, H@10, and MRR metrics.

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

Evaluate link prediction with BPE encoding (head and tail).

Parameters

- **model** – KGE model wrapper with BPE support.
- **within_entities** – List of entities to evaluate within.
- **triples** – Test triples as list of (head, relation, tail) tuples.
- **er_vocab** – Mapping (entity, relation) -> list of valid tail entities.
- **re_vocab** – Mapping (relation, entity) -> list of valid head entities.

Returns

Dictionary with H@1, H@3, H@10, and MRR metrics.

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

Evaluate link prediction with BPE encoding and reciprocals.

Parameters

- **model** – KGE model wrapper with BPE support.
- **within_entities** – List of entities to evaluate within.
- **triples** – Test triples as list of [head, relation, tail] strings.
- **er_vocab** – Mapping (entity, relation) -> list of valid tail entities.

Returns

Dictionary with H@1, H@3, H@10, and MRR metrics.

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

Evaluate BPE link prediction with KvsAll scoring.

Parameters

- **model** – The KGE model wrapper.
- **triples** – List of string triples.
- **er_vocab** – Entity-relation vocabulary for filtering.
- **batch_size** – Batch size for processing.
- **func_triple_to_bpe_representation** – Function to convert triples to BPE.
- **str_to_bpe_entity_to_idx** – Mapping from string entities to BPE indices.

Returns

Dictionary with H@1, H@3, H@10, and MRR metrics.

Raises

ValueError – If batch_size is not provided.

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

Evaluate trained literal prediction model on a test file.

Evaluates the literal prediction capabilities of a KGE model by computing MAE and RMSE metrics for each attribute.

Parameters

- **kge_model** – Trained KGE model with literal prediction capability.
- **eval_file_path** – Path to the evaluation file containing test literals.
- **store_lit_preds** – If True, stores predictions to CSV file.
- **eval_literals** – If True, evaluates and prints error metrics.
- **loader_backend** – Backend for loading dataset ('pandas' or 'rdflib').
- **return_attr_error_metrics** – If True, returns the metrics DataFrame.

Returns

DataFrame with per-attribute MAE and RMSE if return_attr_error_metrics is True, otherwise None.

Raises

- **RuntimeError** – If the KGE model doesn't have a trained literal model.
- **AssertionError** – If model is invalid or test set has no valid data.

Example

```
>>> from dicee import KGE  
>>> from dicee.evaluation import evaluate_literal_prediction  
>>> model = KGE(path="pretrained_model")  
>>> metrics = evaluate_literal_prediction(  
...     model,  
...     eval_file_path="test_literals.csv",  
...     return_attr_error_metrics=True  
... )  
>>> print(metrics)
```

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

Evaluate link prediction performance of an ensemble of KGE models.

Combines predictions from multiple models using weighted or simple averaging, with optional score normalization.

Parameters

- **models** – List of KGE models (e.g., snapshots from training).
- **triples** – Test triples as numpy array or list, shape (N, 3), with integer indices (head, relation, tail).
- **er_vocab** – Mapping (head_idx, rel_idx) -> list of tail indices for filtered evaluation.

- **weights** – Weights for model averaging. Required if weighted_averaging is True. Must sum to 1 for proper averaging.
- **batch_size** – Batch size for processing triples.
- **weighted_averaging** – If True, use weighted averaging of predictions. If False, use simple mean.
- **normalize_scores** – If True, normalize scores to [0, 1] range per sample before averaging.

Returns

Dictionary with H@1, H@3, H@10, and MRR metrics.

Raises

AssertionError – If weighted_averaging is True but weights are not provided or have wrong length.

Example

```
>>> from dicee.evaluation import evaluate_ensemble_link_prediction_performance
>>> models = [model1, model2, model3]
>>> weights = [0.5, 0.3, 0.2]
>>> results = evaluate_ensemble_link_prediction_performance(
...     models, test_triples, er_vocab,
...     weights=weights, weighted_averaging=True
... )
>>> print(f"MRR: {results['MRR']:.4f}")
```

dicee.evaluation

Evaluation module for knowledge graph embedding models.

This module provides comprehensive evaluation capabilities for KGE models, including link prediction, literal prediction, and ensemble evaluation.

Modules:

link_prediction: Functions for evaluating link prediction performance
literal_prediction: Functions for evaluating literal/attribute prediction
ensemble: Functions for ensemble model evaluation
evaluator: Main Evaluator class for integrated evaluation
utils: Shared utility functions for evaluation

Example

```
>>> from dicee.evaluation import Evaluator
>>> from dicee.evaluation.link_prediction import evaluate_link_prediction_performance
>>> from dicee.evaluation.ensemble import evaluate_ensemble_link_prediction_
    ↵performance
```

Submodules

dicee.evaluation.ensemble

Ensemble evaluation functions.

This module provides functions for evaluating ensemble models, including weighted averaging and score normalization.

Functions

```
evaluate_ensemble_link_prediction_performance
```

Evaluate link prediction performance of an ensemble of KGE models.

Module Contents

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

Evaluate link prediction performance of an ensemble of KGE models.

Combines predictions from multiple models using weighted or simple averaging, with optional score normalization.

Parameters

- **models** – List of KGE models (e.g., snapshots from training).
- **triples** – Test triples as numpy array or list, shape (N, 3), with integer indices (head, relation, tail).
- **er_vocab** – Mapping (head_idx, rel_idx) -> list of tail indices for filtered evaluation.
- **weights** – Weights for model averaging. Required if weighted_averaging is True. Must sum to 1 for proper averaging.
- **batch_size** – Batch size for processing triples.
- **weighted_averaging** – If True, use weighted averaging of predictions. If False, use simple mean.
- **normalize_scores** – If True, normalize scores to [0, 1] range per sample before averaging.

Returns

Dictionary with H@1, H@3, H@10, and MRR metrics.

Raises

AssertionError – If weighted_averaging is True but weights are not provided or have wrong length.

Example

```
>>> from dicee.evaluation import evaluate_ensemble_link_prediction_performance
>>> models = [model1, model2, model3]
>>> weights = [0.5, 0.3, 0.2]
>>> results = evaluate_ensemble_link_prediction_performance(
...     models, test_triples, er_vocab,
...     weights=weights, weighted_averaging=True
... )
>>> print(f"MRR: {results['MRR']:.4f}")
```

dicee.evaluation.evaluator

Main Evaluator class for KGE model evaluation.

This module provides the Evaluator class which orchestrates evaluation of knowledge graph embedding models across different datasets and scoring techniques.

Attributes

```
VALID_SCORING_TECHNIQUES
```

Classes

```
Evaluator
```

Evaluator class for KGE models in various downstream tasks.

Module Contents

```
dicee.evaluation.evaluator.VALID_SCORING_TECHNIQUES
```

```
class dicee.evaluation.evaluator.Evaluator(args, is_continual_training: bool = False)
```

Evaluator class for KGE models in various downstream tasks.

Orchestrates link prediction evaluation with different scoring techniques including standard evaluation and byte-pair encoding based evaluation.

```
er_vocab
```

Entity-relation to tail vocabulary for filtered ranking.

```
re_vocab
```

Relation-entity (tail) to head vocabulary.

```
ee_vocab
```

Entity-entity to relation vocabulary.

```
num_entities
```

Total number of entities in the knowledge graph.

```
num_relations
```

Total number of relations in the knowledge graph.

```
args
```

Configuration arguments.

```
report
```

Dictionary storing evaluation results.

```
during_training
```

Whether evaluation is happening during training.

Example

```
>>> from dicee.evaluation import Evaluator
>>> evaluator = Evaluator(args)
>>> results = evaluator.eval(dataset, model, 'EntityPrediction')
>>> print(f"Test MRR: {results['Test']['MRR']:.4f}")
```

```
re_vocab: Dict | None = None
```

```

er_vocab: Dict | None = None
ee_vocab: Dict | None = None
func_triple_to_bpe_representation = None
is_continual_training = False
num_entities: int | None = None
num_relations: int | None = None
domain_constraints_per_rel = None
range_constraints_per_rel = None
args
report: Dict
during_training = False
vocab_preparation(dataset) → None

```

Prepare vocabularies from the dataset for evaluation.

Resolves any future objects and saves vocabularies to disk.

Parameters

dataset – Knowledge graph dataset with vocabulary attributes.

eval (dataset, trained_model, form_of_labelling: str, during_training: bool = False) → Dict | None

Evaluate the trained model on the dataset.

Parameters

- **dataset** – Knowledge graph dataset (KG instance).
- **trained_model** – The trained KGE model.
- **form_of_labelling** – Type of labelling ('EntityPrediction' or 'RelationPrediction').
- **during_training** – Whether evaluation is during training.

Returns

Dictionary of evaluation metrics, or None if evaluation is skipped.

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

Evaluate with negative sampling scoring.

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

Evaluate with BPE-encoded entities and negative sampling.

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

Evaluate BytE model with generation.

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

Evaluate with BPE and KvsAll scoring.

```
eval_with_vs_all(*, train_set, valid_set=None, test_set=None, trained_model, form_of_labelling)
    → None
```

Evaluate with KvsAll or 1vsAll scoring.

```
evaluate_lp_k_vs_all(model, triple_idx, info: str | None = None,
    form_of_labelling: str | None = None) → Dict[str, float]
```

Filtered link prediction evaluation with KvsAll scoring.

Parameters

- **model** – The trained model to evaluate.
- **triple_idx** – Integer-indexed test triples.
- **info** – Description to print.
- **form_of_labelling** – ‘EntityPrediction’ or ‘RelationPrediction’.

Returns

Dictionary with H@1, H@3, H@10, and MRR metrics.

```
evaluate_lp_with_byte(model, triples: List[List[str]], info: str | None = None) → Dict[str, float]
```

Evaluate BytE model with text generation.

Parameters

- **model** – BytE model.
- **triples** – String triples.
- **info** – Description to print.

Returns

Dictionary with placeholder metrics (-1 values).

```
evaluate_lp_bpe_k_vs_all(model, triples: List[List[str]], info: str | None = None,
    form_of_labelling: str | None = None) → Dict[str, float]
```

Evaluate BPE model with KvsAll scoring.

Parameters

- **model** – BPE-enabled model.
- **triples** – String triples.
- **info** – Description to print.
- **form_of_labelling** – Type of labelling.

Returns

Dictionary with H@1, H@3, H@10, and MRR metrics.

```
evaluate_lp(model, triple_idx, info: str) → Dict[str, float]
```

Evaluate link prediction with negative sampling.

Parameters

- **model** – The model to evaluate.
- **triple_idx** – Integer-indexed triples.
- **info** – Description to print.

Returns

Dictionary with H@1, H@3, H@10, and MRR metrics.

dummy_eval (*trained_model*, *form_of_labelling*: str) → None

Run evaluation from saved data (for continual training).

Parameters

- **trained_model** – The trained model.
- **form_of_labelling** – Type of labelling.

eval_with_data (*dataset*, *trained_model*, *triple_idx*: numpy.ndarray, *form_of_labelling*: str)
→ Dict[str, float]

Evaluate a trained model on a given dataset.

Parameters

- **dataset** – Knowledge graph dataset.
- **trained_model** – The trained model.
- **triple_idx** – Integer-indexed triples to evaluate.
- **form_of_labelling** – Type of labelling.

Returns

Dictionary with evaluation metrics.

Raises

ValueError – If scoring technique is invalid.

dicee.evaluation.link_prediction

Link prediction evaluation functions.

This module provides various functions for evaluating link prediction performance of knowledge graph embedding models.

Functions

<code>evaluate_link_prediction_performance</code> (→ Dict[str, float])	Evaluate link prediction performance with head and tail prediction.
<code>evaluate_link_prediction_performance_with_</code>	Evaluate link prediction with reciprocal relations.
<code>evaluate_link_prediction_performance_with_j</code>	Evaluate link prediction with BPE encoding and reciprocals.
<code>evaluate_link_prediction_performance_with_ij</code>	Evaluate link prediction with BPE encoding (head and tail).
<code>evaluate_lp</code> (→ Dict[str, float])	Evaluate link prediction with batched processing.
<code>evaluate_bpe_lp</code> (→ Dict[str, float])	Evaluate link prediction with BPE-encoded entities.
<code>evaluate_lp_bpe_k_vs_all</code> (→ Dict[str, float])	Evaluate BPE link prediction with KvsAll scoring.

Module Contents

`dicee.evaluation.link_prediction.evaluate_link_prediction_performance` (*model*, *triples*, *er_vocab*: Dict[Tuple, List], *re_vocab*: Dict[Tuple, List]) → Dict[str, float]

Evaluate link prediction performance with head and tail prediction.

Performs filtered evaluation where known correct answers are filtered out before computing ranks.

Parameters

- **model** – KGE model wrapper with entity/relation mappings.

- **triples** – Test triples as list of (head, relation, tail) strings.
- **er_vocab** – Mapping (entity, relation) -> list of valid tail entities.
- **re_vocab** – Mapping (relation, entity) -> list of valid head entities.

Returns

Dictionary with H@1, H@3, H@10, and MRR metrics.

```
dicee.evaluation.link_prediction.  
    evaluate_link_prediction_performance_with_reciprocals(model, triples,  
    er_vocab: Dict[Tuple, List]) → Dict[str, float]
```

Evaluate link prediction with reciprocal relations.

Optimized for models trained with reciprocal triples where only tail prediction is needed.

Parameters

- **model** – KGE model wrapper.
- **triples** – Test triples as list of (head, relation, tail) strings.
- **er_vocab** – Mapping (entity, relation) -> list of valid tail entities.

Returns

Dictionary with H@1, H@3, H@10, and MRR metrics.

```
dicee.evaluation.link_prediction.  
    evaluate_link_prediction_performance_with_bpe_reciprocals(model,  
    within_entities: List[str], triples: List[List[str]], er_vocab: Dict[Tuple, List]) → Dict[str, float]
```

Evaluate link prediction with BPE encoding and reciprocals.

Parameters

- **model** – KGE model wrapper with BPE support.
- **within_entities** – List of entities to evaluate within.
- **triples** – Test triples as list of [head, relation, tail] strings.
- **er_vocab** – Mapping (entity, relation) -> list of valid tail entities.

Returns

Dictionary with H@1, H@3, H@10, and MRR metrics.

```
dicee.evaluation.link_prediction.evaluate_link_prediction_performance_with_bpe(  
    model, within_entities: List[str], triples: List[Tuple[str]], er_vocab: Dict[Tuple, List],  
    re_vocab: Dict[Tuple, List]) → Dict[str, float]
```

Evaluate link prediction with BPE encoding (head and tail).

Parameters

- **model** – KGE model wrapper with BPE support.
- **within_entities** – List of entities to evaluate within.
- **triples** – Test triples as list of (head, relation, tail) tuples.
- **er_vocab** – Mapping (entity, relation) -> list of valid tail entities.
- **re_vocab** – Mapping (relation, entity) -> list of valid head entities.

Returns

Dictionary with H@1, H@3, H@10, and MRR metrics.

```
dicee.evaluation.link_prediction.evaluate_lp(model, triple_idx, num_entities: int,  
er_vocab: Dict[Tuple, List], re_vocab: Dict[Tuple, List], info: str = 'Eval Starts',  
batch_size: int = 128, chunk_size: int = 1000) → Dict[str, float]
```

Evaluate link prediction with batched processing.

Memory-efficient evaluation using chunked entity scoring.

Parameters

- **model** – The KGE model to evaluate.
- **triple_idx** – Integer-indexed triples as numpy array.
- **num_entities** – Total number of entities.
- **er_vocab** – Mapping (head_idx, rel_idx) -> list of tail indices.
- **re_vocab** – Mapping (rel_idx, tail_idx) -> list of head indices.
- **info** – Description to print.
- **batch_size** – Batch size for triple processing.
- **chunk_size** – Chunk size for entity scoring.

Returns

Dictionary with H@1, H@3, H@10, and MRR metrics.

```
dicee.evaluation.link_prediction.evaluate_bpe_lp(model, triple_idx: List[Tuple],  
all_bpe_shaped_entities, er_vocab: Dict[Tuple, List], re_vocab: Dict[Tuple, List],  
info: str = 'Eval Starts') → Dict[str, float]
```

Evaluate link prediction with BPE-encoded entities.

Parameters

- **model** – The KGE model to evaluate.
- **triple_idx** – List of BPE-encoded triple tuples.
- **all_bpe_shaped_entities** – All entities with BPE representations.
- **er_vocab** – Mapping for tail filtering.
- **re_vocab** – Mapping for head filtering.
- **info** – Description to print.

Returns

Dictionary with H@1, H@3, H@10, and MRR metrics.

```
dicee.evaluation.link_prediction.evaluate_lp_bpe_k_vs_all(model, triples: List[List[str]],  
er_vocab: Dict | None = None, batch_size: int | None = None,  
func_triple_to_bpe_representation: Callable | None = None,  
str_to_bpe_entity_to_idx: Dict | None = None) → Dict[str, float]
```

Evaluate BPE link prediction with KvsAll scoring.

Parameters

- **model** – The KGE model wrapper.
- **triples** – List of string triples.
- **er_vocab** – Entity-relation vocabulary for filtering.
- **batch_size** – Batch size for processing.
- **func_triple_to_bpe_representation** – Function to convert triples to BPE.

- `str_to_bpe_entity_to_idx` – Mapping from string entities to BPE indices.

Returns

Dictionary with H@1, H@3, H@10, and MRR metrics.

Raises

`ValueError` – If batch_size is not provided.

dicee.evaluation.literal_prediction

Literal prediction evaluation functions.

This module provides functions for evaluating literal/attribute prediction performance of knowledge graph embedding models.

Functions

<code>evaluate_literal_prediction</code> (→ tional[pandas.DataFrame])	Op-	Evaluate trained literal prediction model on a test file.
--	-----	---

Module Contents

```
dicee.evaluation.literal_prediction.evaluate_literal_prediction(kge_model,  
eval_file_path: str = None, store_lit_preds: bool = True, eval_literals: bool = True,  
loader_backend: str = 'pandas', return_attr_error_metrics: bool = False)  
→ pandas.DataFrame | None
```

Evaluate trained literal prediction model on a test file.

Evaluates the literal prediction capabilities of a KGE model by computing MAE and RMSE metrics for each attribute.

Parameters

- `kge_model` – Trained KGE model with literal prediction capability.
- `eval_file_path` – Path to the evaluation file containing test literals.
- `store_lit_preds` – If True, stores predictions to CSV file.
- `eval_literals` – If True, evaluates and prints error metrics.
- `loader_backend` – Backend for loading dataset ('pandas' or 'rdflib').
- `return_attr_error_metrics` – If True, returns the metrics DataFrame.

Returns

DataFrame with per-attribute MAE and RMSE if return_attr_error_metrics is True, otherwise None.

Raises

- `RuntimeError` – If the KGE model doesn't have a trained literal model.
- `AssertionError` – If model is invalid or test set has no valid data.

Example

```
>>> from dicee import KGE
>>> from dicee.evaluation import evaluate_literal_prediction
>>> model = KGE(path="pretrained_model")
>>> metrics = evaluate_literal_prediction(
...     model,
...     eval_file_path="test_literals.csv",
...     return_attr_error_metrics=True
... )
>>> print(metrics)
```

dicee.evaluation.utils

Utility functions for evaluation module.

This module contains shared helper functions used across different evaluation components.

Attributes

`DEFAULT_HITS_RANGE`

`ALL_HITS_RANGE`

Functions

<code>make_iterable_verbose</code> (→ Iterable)	Wrap an iterable with tqdm progress bar if verbose is True.
<code>compute_metrics_from_ranks</code> (→ Dict[str, float])	Compute standard link prediction metrics from ranks.
<code>compute_metrics_from_ranks_simple</code> (→ Dict[str, float])	Compute link prediction metrics without scaling factor.
<code>update_hits</code> (→ None)	Update hits dictionary based on rank.
<code>create_hits_dict</code> (→ Dict[int, List[float]])	Create an initialized hits dictionary.
<code>efficient_zero_grad</code> (→ None)	Efficiently zero gradients using parameter.grad = None.

Module Contents

`dicee.evaluation.utils.DEFAULT_HITS_RANGE: List[int] = [1, 3, 10]`

`dicee.evaluation.utils.ALL_HITS_RANGE: List[int]`

`dicee.evaluation.utils.make_iterable_verbose`(*iterable_object: Iterable, verbose: bool, desc: str = 'Default', position: int | None = None, leave: bool = True*) → Iterable

Wrap an iterable with tqdm progress bar if verbose is True.

Parameters

- **iterable_object** – The iterable to potentially wrap.
- **verbose** – Whether to show progress bar.
- **desc** – Description for the progress bar.

- **position** – Position of the progress bar.
- **leave** – Whether to leave the progress bar after completion.

Returns

The original iterable or a tqdm-wrapped version.

```
dicee.evaluation.utils.compute_metrics_from_ranks(ranks: List[int], num_triples: int,
    hits_dict: Dict[int, List[float]], scale_factor: int = 1) → Dict[str, float]
```

Compute standard link prediction metrics from ranks.

Parameters

- **ranks** – List of ranks for each prediction.
- **num_triples** – Total number of triples evaluated.
- **hits_dict** – Dictionary mapping hit levels to lists of hits.
- **scale_factor** – Factor to scale the denominator (e.g., 2 for head+tail).

Returns

Dictionary containing H@1, H@3, H@10, and MRR metrics.

```
dicee.evaluation.utils.compute_metrics_from_ranks_simple(ranks: List[int], num_triples: int,
    hits_dict: Dict[int, List[float]]) → Dict[str, float]
```

Compute link prediction metrics without scaling factor.

Parameters

- **ranks** – List of ranks for each prediction.
- **num_triples** – Total number of triples evaluated.
- **hits_dict** – Dictionary mapping hit levels to lists of hits.

Returns

Dictionary containing H@1, H@3, H@10, and MRR metrics.

```
dicee.evaluation.utils.update_hits(hits: Dict[int, List[float]], rank: int,
    hits_range: List[int] | None = None) → None
```

Update hits dictionary based on rank.

Parameters

- **hits** – Dictionary to update in-place.
- **rank** – The rank to check against hit levels.
- **hits_range** – List of hit levels to check (default: ALL_HITS_RANGE).

```
dicee.evaluation.utils.create_hits_dict(hits_range: List[int] | None = None)
    → Dict[int, List[float]]
```

Create an initialized hits dictionary.

Parameters

hits_range – List of hit levels to initialize (default: ALL_HITS_RANGE).

Returns

Dictionary with empty lists for each hit level.

```
dicee.evaluation.utils.efficient_zero_grad(model) → None
```

Efficiently zero gradients using parameter.grad = None.

This is more efficient than optimizer.zero_grad() as it avoids memory operations.

See: https://pytorch.org/tutorials/recipes/recipes/tuning_guide.html

Parameters

`model` – PyTorch model to zero gradients for.

Attributes

`DEFAULT_HITS_RANGE`

`ALL_HITS_RANGE`

Classes

`Evaluator`

Evaluator class for KGE models in various downstream tasks.

Functions

<code>evaluate_link_prediction_performance(→ Dict[str, float])</code>	Evaluate link prediction performance with head and tail prediction.
<code>evaluate_link_prediction_performance_with_</code>	Evaluate link prediction with reciprocal relations.
<code>evaluate_link_prediction_performance_with_j</code>	Evaluate link prediction with BPE encoding (head and tail).
<code>evaluate_link_prediction_performance_with_ij</code>	Evaluate link prediction with BPE encoding and reciprocals.
<code>evaluate_lp(→ Dict[str, float])</code>	Evaluate link prediction with batched processing.
<code>evaluate_lp_bpe_k_vs_all(→ Dict[str, float])</code>	Evaluate BPE link prediction with KvsAll scoring.
<code>evaluate_bpe_lp(→ Dict[str, float])</code>	Evaluate link prediction with BPE-encoded entities.
<code>evaluate_literal_prediction(→ Op-tional[pandas.DataFrame])</code>	Evaluate trained literal prediction model on a test file.
<code>evaluate_ensemble_link_prediction_performanc</code>	Evaluate link prediction performance of an ensemble of KGE models.
<code>compute_metrics_from_ranks(→ Dict[str, float])</code>	Compute standard link prediction metrics from ranks.
<code>compute_metrics_from_ranks_simple(→ Dict[str, float])</code>	Compute link prediction metrics without scaling factor.
<code>make_iterable_verbose(→ Iterable)</code>	Wrap an iterable with tqdm progress bar if verbose is True.
<code>update_hits(→ None)</code>	Update hits dictionary based on rank.
<code>create_hits_dict(→ Dict[int, List[float]])</code>	Create an initialized hits dictionary.

Package Contents

`class dicee.evaluation.Evaluator(args, is_continual_training: bool = False)`

Evaluator class for KGE models in various downstream tasks.

Orchestrates link prediction evaluation with different scoring techniques including standard evaluation and byte-pair encoding based evaluation.

er_vocab
Entity-relation to tail vocabulary for filtered ranking.

re_vocab
Relation-entity (tail) to head vocabulary.

ee_vocab
Entity-entity to relation vocabulary.

num_entities
Total number of entities in the knowledge graph.

num_relations
Total number of relations in the knowledge graph.

args
Configuration arguments.

report
Dictionary storing evaluation results.

during_training
Whether evaluation is happening during training.

Example

```
>>> from dicee.evaluation import Evaluator
>>> evaluator = Evaluator(args)
>>> results = evaluator.eval(dataset, model, 'EntityPrediction')
>>> print(f"Test MRR: {results['Test']['MRR']:.4f}")
```

```
re_vocab: Dict | None = None
er_vocab: Dict | None = None
ee_vocab: Dict | None = None
func_triple_to_bpe_representation = None
is_continual_training = False
num_entities: int | None = None
num_relations: int | None = None
domain_constraints_per_rel = None
range_constraints_per_rel = None
args
report: Dict
during_training = False
```

vocab_preparation(*dataset*) → None

Prepare vocabularies from the dataset for evaluation.

Resolves any future objects and saves vocabularies to disk.

Parameters

• **dataset** – Knowledge graph dataset with vocabulary attributes.

eval(*dataset, trained_model, form_of_labelling: str, during_training: bool = False*) → Dict | None

Evaluate the trained model on the dataset.

Parameters

- **dataset** – Knowledge graph dataset (KG instance).
- **trained_model** – The trained KGE model.
- **form_of_labelling** – Type of labelling ('EntityPrediction' or 'RelationPrediction').
- **during_training** – Whether evaluation is during training.

Returns

Dictionary of evaluation metrics, or None if evaluation is skipped.

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

Evaluate with negative sampling scoring.

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

Evaluate with BPE-encoded entities and negative sampling.

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

Evaluate ByTE model with generation.

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

Evaluate with BPE and KvsAll scoring.

eval_with_vs_all(**, train_set, valid_set=None, test_set=None, trained_model, form_of_labelling*)
→ None

Evaluate with KvsAll or 1vsAll scoring.

evaluate_lp_k_vs_all(*model, triple_idx, info: str | None = None,
form_of_labelling: str | None = None*) → Dict[str, float]

Filtered link prediction evaluation with KvsAll scoring.

Parameters

- **model** – The trained model to evaluate.
- **triple_idx** – Integer-indexed test triples.
- **info** – Description to print.
- **form_of_labelling** – 'EntityPrediction' or 'RelationPrediction'.

Returns

Dictionary with H@1, H@3, H@10, and MRR metrics.

evaluate_lp_with_byte (*model*, *triples*: *List[List[str]]*, *info*: *str* | *None* = *None*) → *Dict[str, float]*

Evaluate BytE model with text generation.

Parameters

- **model** – BytE model.
- **triples** – String triples.
- **info** – Description to print.

Returns

Dictionary with placeholder metrics (-1 values).

evaluate_lp_bpe_k_vs_all (*model*, *triples*: *List[List[str]]*, *info*: *str* | *None* = *None*, *form_of_labelling*: *str* | *None* = *None*) → *Dict[str, float]*

Evaluate BPE model with KvsAll scoring.

Parameters

- **model** – BPE-enabled model.
- **triples** – String triples.
- **info** – Description to print.
- **form_of_labelling** – Type of labelling.

Returns

Dictionary with H@1, H@3, **H@10**, and MRR metrics.

evaluate_lp (*model*, *triple_idx*, *info*: *str*) → *Dict[str, float]*

Evaluate link prediction with negative sampling.

Parameters

- **model** – The model to evaluate.
- **triple_idx** – Integer-indexed triples.
- **info** – Description to print.

Returns

Dictionary with H@1, H@3, **H@10**, and MRR metrics.

dummy_eval (*trained_model*, *form_of_labelling*: *str*) → *None*

Run evaluation from saved data (for continual training).

Parameters

- **trained_model** – The trained model.
- **form_of_labelling** – Type of labelling.

eval_with_data (*dataset*, *trained_model*, *triple_idx*: *numpy.ndarray*, *form_of_labelling*: *str*)
→ *Dict[str, float]*

Evaluate a trained model on a given dataset.

Parameters

- **dataset** – Knowledge graph dataset.
- **trained_model** – The trained model.
- **triple_idx** – Integer-indexed triples to evaluate.
- **form_of_labelling** – Type of labelling.

Returns

Dictionary with evaluation metrics.

Raises

ValueError – If scoring technique is invalid.

```
dicee.evaluation.evaluate_link_prediction_performance(model, triples,  
er_vocab: Dict[Tuple, List], re_vocab: Dict[Tuple, List]) → Dict[str, float]
```

Evaluate link prediction performance with head and tail prediction.

Performs filtered evaluation where known correct answers are filtered out before computing ranks.

Parameters

- **model** – KGE model wrapper with entity/relation mappings.
- **triples** – Test triples as list of (head, relation, tail) strings.
- **er_vocab** – Mapping (entity, relation) -> list of valid tail entities.
- **re_vocab** – Mapping (relation, entity) -> list of valid head entities.

Returns

Dictionary with H@1, H@3, H@10, and MRR metrics.

```
dicee.evaluation.evaluate_link_prediction_performance_with_reciprocals(model, triples,  
er_vocab: Dict[Tuple, List]) → Dict[str, float]
```

Evaluate link prediction with reciprocal relations.

Optimized for models trained with reciprocal triples where only tail prediction is needed.

Parameters

- **model** – KGE model wrapper.
- **triples** – Test triples as list of (head, relation, tail) strings.
- **er_vocab** – Mapping (entity, relation) -> list of valid tail entities.

Returns

Dictionary with H@1, H@3, H@10, and MRR metrics.

```
dicee.evaluation.evaluate_link_prediction_performance_with_bpe(model,  
within_entities: List[str], triples: List[Tuple[str]], er_vocab: Dict[Tuple, List],  
re_vocab: Dict[Tuple, List]) → Dict[str, float]
```

Evaluate link prediction with BPE encoding (head and tail).

Parameters

- **model** – KGE model wrapper with BPE support.
- **within_entities** – List of entities to evaluate within.
- **triples** – Test triples as list of (head, relation, tail) tuples.
- **er_vocab** – Mapping (entity, relation) -> list of valid tail entities.
- **re_vocab** – Mapping (relation, entity) -> list of valid head entities.

Returns

Dictionary with H@1, H@3, H@10, and MRR metrics.

```
dicee.evaluation.evaluate_link_prediction_performance_with_bpe_reciprocals(model,  
within_entities: List[str], triples: List[List[str]], er_vocab: Dict[Tuple, List]) → Dict[str, float]
```

Evaluate link prediction with BPE encoding and reciprocals.

Parameters

- **model** – KGE model wrapper with BPE support.
- **within_entities** – List of entities to evaluate within.
- **triples** – Test triples as list of [head, relation, tail] strings.
- **er_vocab** – Mapping (entity, relation) -> list of valid tail entities.

Returns

Dictionary with H@1, H@3, H@10, and MRR metrics.

```
dicee.evaluation.evaluate_lp(model, triple_idx, num_entities: int, er_vocab: Dict[Tuple, List],  
    re_vocab: Dict[Tuple, List], info: str = 'Eval Starts', batch_size: int = 128, chunk_size: int = 1000)  
    → Dict[str, float]
```

Evaluate link prediction with batched processing.

Memory-efficient evaluation using chunked entity scoring.

Parameters

- **model** – The KGE model to evaluate.
- **triple_idx** – Integer-indexed triples as numpy array.
- **num_entities** – Total number of entities.
- **er_vocab** – Mapping (head_idx, rel_idx) -> list of tail indices.
- **re_vocab** – Mapping (rel_idx, tail_idx) -> list of head indices.
- **info** – Description to print.
- **batch_size** – Batch size for triple processing.
- **chunk_size** – Chunk size for entity scoring.

Returns

Dictionary with H@1, H@3, H@10, and MRR metrics.

```
dicee.evaluation.evaluate_lp_bpe_k_vs_all(model, triples: List[List[str]],  
    er_vocab: Dict[None, None] = None, batch_size: int | None = None,  
    func_triple_to_bpe_representation: Callable[None, None] = None,  
    str_to_bpe_entity_to_idx: Dict[None, None] = None) → Dict[str, float]
```

Evaluate BPE link prediction with KvsAll scoring.

Parameters

- **model** – The KGE model wrapper.
- **triples** – List of string triples.
- **er_vocab** – Entity-relation vocabulary for filtering.
- **batch_size** – Batch size for processing.
- **func_triple_to_bpe_representation** – Function to convert triples to BPE.
- **str_to_bpe_entity_to_idx** – Mapping from string entities to BPE indices.

Returns

Dictionary with H@1, H@3, H@10, and MRR metrics.

Raises

ValueError – If batch_size is not provided.

```
dicee.evaluation.evaluate_bpe_lp(model, triple_idx: List[Tuple], all_bpe_shaped_entities,  
er_vocab: Dict[Tuple, List], re_vocab: Dict[Tuple, List], info: str = 'Eval Starts') → Dict[str, float]  
Evaluate link prediction with BPE-encoded entities.
```

Parameters

- **model** – The KGE model to evaluate.
- **triple_idx** – List of BPE-encoded triple tuples.
- **all_bpe_shaped_entities** – All entities with BPE representations.
- **er_vocab** – Mapping for tail filtering.
- **re_vocab** – Mapping for head filtering.
- **info** – Description to print.

Returns

Dictionary with H@1, H@3, H@10, and MRR metrics.

```
dicee.evaluation.evaluate_literal_prediction(kge_model, eval_file_path: str = None,  
store_lit_preds: bool = True, eval_literals: bool = True, loader_backend: str = 'pandas',  
return_attr_error_metrics: bool = False) → pandas.DataFrame | None
```

Evaluate trained literal prediction model on a test file.

Evaluates the literal prediction capabilities of a KGE model by computing MAE and RMSE metrics for each attribute.

Parameters

- **kge_model** – Trained KGE model with literal prediction capability.
- **eval_file_path** – Path to the evaluation file containing test literals.
- **store_lit_preds** – If True, stores predictions to CSV file.
- **eval_literals** – If True, evaluates and prints error metrics.
- **loader_backend** – Backend for loading dataset ('pandas' or 'rdflib').
- **return_attr_error_metrics** – If True, returns the metrics DataFrame.

Returns

DataFrame with per-attribute MAE and RMSE if return_attr_error_metrics is True, otherwise None.

Raises

- **RuntimeError** – If the KGE model doesn't have a trained literal model.
- **AssertionError** – If model is invalid or test set has no valid data.

Example

```
>>> from dicee import KGE  
>>> from dicee.evaluation import evaluate_literal_prediction  
>>> model = KGE(path="pretrained_model")  
>>> metrics = evaluate_literal_prediction(  
...     model,  
...     eval_file_path="test_literals.csv",  
...     return_attr_error_metrics=True  
... )  
>>> print(metrics)
```

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

Evaluate link prediction performance of an ensemble of KGE models.

Combines predictions from multiple models using weighted or simple averaging, with optional score normalization.

Parameters

- **models** – List of KGE models (e.g., snapshots from training).
- **triples** – Test triples as numpy array or list, shape (N, 3), with integer indices (head, relation, tail).
- **er_vocab** – Mapping (head_idx, rel_idx) -> list of tail indices for filtered evaluation.
- **weights** – Weights for model averaging. Required if weighted_averaging is True. Must sum to 1 for proper averaging.
- **batch_size** – Batch size for processing triples.
- **weighted_averaging** – If True, use weighted averaging of predictions. If False, use simple mean.
- **normalize_scores** – If True, normalize scores to [0, 1] range per sample before averaging.

Returns

Dictionary with H@1, H@3, H@10, and MRR metrics.

Raises

AssertionError – If weighted_averaging is True but weights are not provided or have wrong length.

Example

```
>>> from dicee.evaluation import evaluate_ensemble_link_prediction_performance  
>>> models = [model1, model2, model3]  
>>> weights = [0.5, 0.3, 0.2]  
>>> results = evaluate_ensemble_link_prediction_performance(  
...     models, test_triples, er_vocab,  
...     weights=weights, weighted_averaging=True  
... )  
>>> print(f'MRR: {results["MRR"]:.4f}')
```

```
dicee.evaluation.compute_metrics_from_ranks(ranks: List[int], num_triples: int,  
hits_dict: Dict[int, List[float]], scale_factor: int = 1) → Dict[str, float]
```

Compute standard link prediction metrics from ranks.

Parameters

- **ranks** – List of ranks for each prediction.
- **num_triples** – Total number of triples evaluated.
- **hits_dict** – Dictionary mapping hit levels to lists of hits.
- **scale_factor** – Factor to scale the denominator (e.g., 2 for head+tail).

Returns

Dictionary containing H@1, H@3, H@10, and MRR metrics.

```
dicee.evaluation.compute_metrics_from_ranks_simple(ranks: List[int], num_triples: int,  
hits_dict: Dict[int, List[float]]) → Dict[str, float]
```

Compute link prediction metrics without scaling factor.

Parameters

- **ranks** – List of ranks for each prediction.
- **num_triples** – Total number of triples evaluated.
- **hits_dict** – Dictionary mapping hit levels to lists of hits.

Returns

Dictionary containing H@1, H@3, H@10, and MRR metrics.

```
dicee.evaluation.make_iterable_verbose(iterable_object: Iterable, verbose: bool, desc: str = 'Default',  
position: int | None = None, leave: bool = True) → Iterable
```

Wrap an iterable with tqdm progress bar if verbose is True.

Parameters

- **iterable_object** – The iterable to potentially wrap.
- **verbose** – Whether to show progress bar.
- **desc** – Description for the progress bar.
- **position** – Position of the progress bar.
- **leave** – Whether to leave the progress bar after completion.

Returns

The original iterable or a tqdm-wrapped version.

```
dicee.evaluation.update_hits(hits: Dict[int, List[float]], rank: int, hits_range: List[int] | None = None)  
→ None
```

Update hits dictionary based on rank.

Parameters

- **hits** – Dictionary to update in-place.
- **rank** – The rank to check against hit levels.
- **hits_range** – List of hit levels to check (default: ALL_HITS_RANGE).

```
dicee.evaluation.create_hits_dict(hits_range: List[int] | None = None) → Dict[int, List[float]]
```

Create an initialized hits dictionary.

Parameters

hits_range – List of hit levels to initialize (default: ALL_HITS_RANGE).

Returns

Dictionary with empty lists for each hit level.

```
dicee.evaluation.DEFAULT_HITS_RANGE: List[int] = [1, 3, 10]
```

```
dicee.evaluation.ALL_HITS_RANGE: List[int]
```

dicee.evaluator

Evaluator module for knowledge graph embedding models.

This module provides backward compatibility by re-exporting from the new dicee.evaluation module.

Deprecated since version Use: `dicee.evaluation.Evaluator` instead. This module will be removed in a future version.

Classes

<code>Evaluator</code>	Evaluator class for KGE models in various downstream tasks.
------------------------	---

Module Contents

`class dicee.evaluator.Evaluator(args, is_continual_training: bool = False)`

Evaluator class for KGE models in various downstream tasks.

Orchestrates link prediction evaluation with different scoring techniques including standard evaluation and byte-pair encoding based evaluation.

`er_vocab`

Entity-relation to tail vocabulary for filtered ranking.

`re_vocab`

Relation-entity (tail) to head vocabulary.

`ee_vocab`

Entity-entity to relation vocabulary.

`num_entities`

Total number of entities in the knowledge graph.

`num_relations`

Total number of relations in the knowledge graph.

`args`

Configuration arguments.

`report`

Dictionary storing evaluation results.

`during_training`

Whether evaluation is happening during training.

Example

```
>>> from dicee.evaluation import Evaluator
>>> evaluator = Evaluator(args)
>>> results = evaluator.eval(dataset, model, 'EntityPrediction')
>>> print(f"Test MRR: {results['Test']['MRR']:.4f}")
```

`re_vocab: Dict | None = None`

`er_vocab: Dict | None = None`

`ee_vocab: Dict | None = None`

`func_triple_to_bpe_representation = None`

```

is_continual_training = False

num_entities: int | None = None

num_relations: int | None = None

domain_constraints_per_rel = None

range_constraints_per_rel = None

args

report: Dict

during_training = False

vocab_preparation(dataset) → None
    Prepare vocabularies from the dataset for evaluation.

    Resolves any future objects and saves vocabularies to disk.

Parameters
    dataset – Knowledge graph dataset with vocabulary attributes.

eval(dataset, trained_model, form_of_labelling: str, during_training: bool = False) → Dict | None
    Evaluate the trained model on the dataset.

Parameters
    • dataset – Knowledge graph dataset (KG instance).
    • trained_model – The trained KGE model.
    • form_of_labelling – Type of labelling ('EntityPrediction' or 'RelationPrediction').
    • during_training – Whether evaluation is during training.

Returns
    Dictionary of evaluation metrics, or None if evaluation is skipped.

eval_rank_of_head_and_tail_entity(*train_set, valid_set=None, test_set=None, trained_model)
    → None
    Evaluate with negative sampling scoring.

eval_rank_of_head_and_tail_byte_pair_encoded_entity(*train_set=None, valid_set=None,
    test_set=None, ordered_bpe_entities, trained_model) → None
    Evaluate with BPE-encoded entities and negative sampling.

eval_with_byte(*raw_train_set, raw_valid_set=None, raw_test_set=None, trained_model,
    form_of_labelling) → None
    Evaluate ByTE model with generation.

eval_with_bpe_vs_all(*raw_train_set, raw_valid_set=None, raw_test_set=None, trained_model,
    form_of_labelling) → None
    Evaluate with BPE and KvsAll scoring.

eval_with_vs_all(*train_set, valid_set=None, test_set=None, trained_model, form_of_labelling)
    → None
    Evaluate with KvsAll or 1vsAll scoring.

```

```
evaluate_lp_k_vs_all (model, triple_idx, info: str | None = None,  
form_of_labelling: str | None = None) → Dict[str, float]
```

Filtered link prediction evaluation with KvsAll scoring.

Parameters

- **model** – The trained model to evaluate.
- **triple_idx** – Integer-indexed test triples.
- **info** – Description to print.
- **form_of_labelling** – ‘EntityPrediction’ or ‘RelationPrediction’.

Returns

Dictionary with H@1, H@3, H@10, and MRR metrics.

```
evaluate_lp_with_byte (model, triples: List[List[str]], info: str | None = None) → Dict[str, float]
```

Evaluate BytE model with text generation.

Parameters

- **model** – BytE model.
- **triples** – String triples.
- **info** – Description to print.

Returns

Dictionary with placeholder metrics (-1 values).

```
evaluate_lp_bpe_k_vs_all (model, triples: List[List[str]], info: str | None = None,  
form_of_labelling: str | None = None) → Dict[str, float]
```

Evaluate BPE model with KvsAll scoring.

Parameters

- **model** – BPE-enabled model.
- **triples** – String triples.
- **info** – Description to print.
- **form_of_labelling** – Type of labelling.

Returns

Dictionary with H@1, H@3, H@10, and MRR metrics.

```
evaluate_lp (model, triple_idx, info: str) → Dict[str, float]
```

Evaluate link prediction with negative sampling.

Parameters

- **model** – The model to evaluate.
- **triple_idx** – Integer-indexed triples.
- **info** – Description to print.

Returns

Dictionary with H@1, H@3, H@10, and MRR metrics.

```
dummy_eval (trained_model, form_of_labelling: str) → None
```

Run evaluation from saved data (for continual training).

Parameters

- **trained_model** – The trained model.

- **form_of_labelling** – Type of labelling.

eval_with_data (*dataset, trained_model, triple_idx: numpy.ndarray, form_of_labelling: str*)
 → Dict[str, float]

Evaluate a trained model on a given dataset.

Parameters

- **dataset** – Knowledge graph dataset.
- **trained_model** – The trained model.
- **triple_idx** – Integer-indexed triples to evaluate.
- **form_of_labelling** – Type of labelling.

Returns

Dictionary with evaluation metrics.

Raises

ValueError – If scoring technique is invalid.

dicee.executer

Executor module for training, retraining and evaluating KGE models.

This module provides the Execute and ContinuousExecute classes for managing the full lifecycle of knowledge graph embedding model training.

Classes

<i>Execute</i>	Executor class for training, retraining and evaluating KGE models.
<i>ContinuousExecute</i>	A subclass of Execute Class for retraining

Module Contents

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

Executor class for training, retraining and evaluating KGE models.

Handles the complete workflow: 1. Loading & Preprocessing & Serializing input data 2. Training & Validation & Testing 3. Storing all necessary information

args

Processed input arguments.

distributed

Whether distributed training is enabled.

rank

Process rank in distributed training.

world_size

Total number of processes.

local_rank

Local GPU rank.

```

trainer
    Training handler instance.

trained_model
    The trained model after training completes.

knowledge_graph
    The loaded knowledge graph.

report
    Dictionary storing training metrics and results.

evaluator
    Model evaluation handler.

distributed

args

is_continual_training = False

trainer: dicee.trainer.DICE_Trainer | None = None

trained_model = None

knowledge_graph: dicee.knowledge_graph.KG | None = None

report: Dict

evaluator: dicee.evaluator.Evaluator | None = None

start_time: float | None = None

is_rank_zero() → bool

cleanup()

setup_executor() → None
    Set up storage directories for the experiment.

    Creates or reuses experiment directories based on configuration. Saves the configuration to a JSON file.

create_and_store_kg() → None
    Create knowledge graph and store as memory-mapped file.

    Only executed on rank 0 in distributed training. Skips if memmap already exists.

load_from_memmap() → None
    Load knowledge graph from memory-mapped file.

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

Knowledge Graph module for data loading and preprocessing.

Provides the KG class for handling knowledge graph data including loading, preprocessing, and indexing operations.

Classes

`KG`

Knowledge Graph container and processor.

Module Contents

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

Knowledge Graph container and processor.

Handles loading, preprocessing, and indexing of knowledge graph data from various sources including files, SPARQL endpoints, and serialized formats.

dataset_dir

Path to directory containing train/valid/test files.

num_entities

Total number of unique entities.

num_relations

Total number of unique relations.

train_set

Indexed training triples as numpy array.

valid_set

Indexed validation triples (optional).

test_set

Indexed test triples (optional).

entity_to_idx

Mapping from entity strings to indices.

relation_to_idx

Mapping from relation strings to indices.

dataset_dir = None

```
sparql_endpoint = None
path_single_kg = None
byte_pair_encoding = False
ordered_shaped_bpe_tokens = None
add_noise_rate = None
num_entities: int | None = None
num_relations: int | None = None
path_for_deserialization = None
add_reciprocal = None
eval_model = None
read_only_few = None
sample_triples_ratio = None
path_for_serialization = None
entity_to_idx = None
relation_to_idx = None
backend = 'pandas'
training_technique = None
separator = None
raw_train_set = None
raw_valid_set = None
raw_test_set = None
train_set = None
valid_set = None
test_set = None
idx_entity_to_bpe_shaped: Dict
enc
num_tokens
num_bpe_entities: int | None = None
padding = False
dummy_id
max_length_subword_tokens: int | None = None
```

```

train_set_target = None
target_dim: int | None = None
train_target_indices = None
ordered_bpe_entities = None
description_of_input = None
describe() → None
    Generate a description string of the dataset statistics.

property entities_str: List[str]
    Get list of all entity strings.

property relations_str: List[str]
    Get list of all relation strings.

exists(h: str, r: str, t: str) → bool
    Check if a triple exists in the training set.

```

Parameters

- **h** – Head entity string.
- **r** – Relation string.
- **t** – Tail entity string.

Returns

True if the triple exists, False otherwise.

```

__iter__() → Iterator[Tuple[str, str, str]]
    Iterate over training triples as string tuples.

__len__() → int
    Return number of triples in the raw training set.

func_triple_to_bpe_representation(triple: List[str])

```

dicee.knowledge_graph_embeddings

Classes

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

Module Contents

```

class dicee.knowledge_graph_embeddings.KGE(path=None, url=None, construct_ensemble=False,
                                              model_name=None)
Bases:                                         dicee.abstracts.BaseInteractiveKGE,           dicee.abstracts.
                                                InteractiveQueryDecomposition, dicee.abstracts.BaseInteractiveTrainKGE
Knowledge Graph Embedding Class for interactive usage of pre-trained models

__str__()

```

```

to (device: str) → None

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

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

generate (h='', r='')

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

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

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

    argmax_{e in E} f(e,r,t), where r in R, t in E.

```

Parameter

relation: Union[List[str], str]
 String representation of selected relations.

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

k: int
 Highest ranked k entities.

Returns: Tuple

Highest K scores and entities

```

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

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

    argmax_{r in R} f(h,r,t), where h, t in E.

```

Parameter

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

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

k: int
 Highest ranked k entities.

Returns: Tuple

Highest K scores and entities

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

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

argmax_{e in E} f(h,r,e), where h in E and r in R.

Parameter

head_entity: List[str]

String representation of selected entities.

tail_entity: List[str]

String representation of selected entities.

Returns: Tuple

scores

```
predict(*: h: List[str] | str = None, r: List[str] | str = None, t: List[str] | str = None, within=None,  
    logits=True) → torch.FloatTensor
```

Parameters

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

```
predict_topk(*: h: str | List[str] = None, r: str | List[str] = None, t: str | List[str] = None, topk: int = 10,  
    within: List[str] = None, batch_size: int = 1024)
```

Predict missing item in a given triple.

Returns

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

```
triple_score(h: List[str] | str = None, r: List[str] | str = None, t: List[str] | str = None, logits=False)  
    → torch.FloatTensor
```

Predict triple score

Parameter

head_entity: List[str]

String representation of selected entities.

relation: List[str]

String representation of selected relations.

tail_entity: List[str]

String representation of selected entities.

logits: bool

If logits is True, unnormalized score returned

Returns: Tuple

pytorch tensor of triple score

```
return_multi_hop_query_results (aggregated_query_for_all_entities, k: int, only_scores)
```

```
single_hop_query_answering (query: tuple, only_scores: bool = True, k: int = None)
```

```
answer_multi_hop_query (query_type: str = None, query: Tuple[str | Tuple[str, str], Ellipsis] = None,
queries: List[Tuple[str | Tuple[str, str], Ellipsis]] = None, tnorm: str = 'prod',
neg_norm: str = 'standard', lambda_: float = 0.0, k: int = 10, only_scores=False)
→ List[Tuple[str, torch.Tensor]]
```

@TODO: Refactoring is needed # @TODO: Score computation for each query type should be done in a static function

Find an answer set for EPFO queries including negation and disjunction

Parameter

query_type: str The type of the query, e.g., “2p”.

query: Union[str, Tuple[str, Tuple[str, 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 descending 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

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

otin G

predict_literals (*entity: List[str] | str = None, attribute: List[str] | str = None, denormalize_preds: bool = True*) → numpy.ndarray

Predicts literal values for given entities and attributes.

Parameters

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

Returns

Predictions for the given entities and attributes.

Return type

numpy ndarray

dicee.models

Submodules

dicee.models.adopt

ADOPT Optimizer Implementation.

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

ADOPT Overview:

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

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

Algorithm Comparison:

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

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

Classes:

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

Functions:

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

Performance:

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

Example:

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

References:

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

Notes:

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

Classes

`ADOPT`

ADOPT Optimizer.

Functions

`adopt`(`params`, `grads`, `exp_avgs`, `exp_avg_sqs`, `Functional API that performs ADOPT algorithm computation.`
`state_steps`)

Module Contents

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

Bases: `torch.optim.optimizer.Optimizer`

ADOPT Optimizer.

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

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

Mathematical formulation:

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

where:

- θ_t : parameter at step t
- g_t : gradient at step t
- m_t : first moment estimate (momentum)
- v_t : second moment estimate (variance)
- α : learning rate
- β_1, β_2 : exponential decay rates
- `clip()`: optional gradient clipping function

Reference:

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

Parameters

- **params** (`ParamsT`) – Iterable of parameters to optimize or dicts defining parameter groups.
- **lr** (`float` or `Tensor`, `optional`) – Learning rate. Can be a float or 1-element Tensor. Default: 1e-3
- **betas** (`Tuple[float, float]`, `optional`) – Coefficients (β_1, β_2) for computing running averages of gradient and its square. β_1 controls momentum, β_2 controls variance. Default: (0.9, 0.9999)
- **eps** (`float`, `optional`) – Term added to denominator to improve numerical stability. Default: 1e-6
- **clip_lambda** (`Callable[[int], float]`, `optional`) – Function that takes the step number and returns the gradient clipping threshold. Common choices: - lambda step: $\text{step}^{**0.25}$ (default, gradually increases clipping threshold) - lambda step: 1.0 (constant clipping) - None (no clipping) Default: lambda step: $\text{step}^{**0.25}$
- **weight_decay** (`float`, `optional`) – Weight decay coefficient (L2 penalty). Default: 0.0

- **decouple** (*bool, optional*) – If True, uses decoupled weight decay (AdamW-style), applying weight decay directly to parameters. If False, adds weight decay to gradients (L2 regularization). Default: False
- **foreach** (*bool, optional*) – If True, uses the faster foreach implementation for multi-tensor operations. Default: None (auto-select)
- **maximize** (*bool, optional*) – If True, maximizes parameters instead of minimizing. Useful for reinforcement learning. Default: False
- **capturable** (*bool, optional*) – If True, the optimizer is safe to capture in a CUDA graph. Requires learning rate as Tensor. Default: False
- **differentiable** (*bool, optional*) – If True, the optimization step can be differentiated. Useful for meta-learning. Default: False
- **fused** (*bool, optional*) – If True, uses fused kernel implementation (currently not supported). Default: None

Raises

- **ValueError** – If learning rate, epsilon, betas, or weight_decay are invalid.
- **RuntimeError** – If fused is enabled (not currently supported).
- **RuntimeError** – If lr is a Tensor with foreach=True and capturable=False.

Example

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

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

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

Note

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

clip_lambda

__setstate__(state)

Restore optimizer state from a checkpoint.

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

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

Parameters

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

Note

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

step (*closure=None*)

Perform a single optimization step.

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

1. Optionally evaluates a closure to recompute the loss (useful for algorithms like LBFGS or when loss needs multiple evaluations)
2. For each parameter group: - Collects parameters with gradients and their associated state - Extracts hyperparameters (betas, learning rate, etc.) - Calls the functional `adopt()` API to perform the actual update
3. Returns the loss value if a closure was provided

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

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

Parameters

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

Returns

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

Return type

`Optional[Tensor]`

Example

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

```

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

```

Note

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

```

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

```

Functional API that performs ADOPT algorithm computation.

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

1. **Single-tensor mode** (default): Updates parameters one at a time - Compatible with `torch.jit.script` - More flexible but slower - Used when `foreach=False` or automatically for small models
2. **Multi-tensor (foreach) mode**: Batches operations across tensors - 2-3x faster on GPU through vectorization - Groups tensors by device/dtype automatically - Used when `foreach=True`
3. **Fused mode**: Uses specialized fused kernels (not yet implemented) - Would provide maximum performance - Currently raises `RuntimeError` if enabled

Algorithm overview (ADOPT):

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

Mathematical formulation:

```

# Normalize gradient by its historical variance normed_g_t = g_t / sqrt(v_t + ε)
# Optional gradient clipping for stability normed_g_t = clip(normed_g_t, threshold(t))
# Momentum on normalized gradients (key difference from Adam) m_t = β₁ * m_{t-1} + (1 - β₁) * normed_g_t
# Parameter update θ_t = θ_{t-1} - α * m_t
# Update variance estimate v_t = β₂ * v_{t-1} + (1 - β₂) * g_t²

```

where:

- θ : parameters

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

Automatic mode selection:

When foreach and fused are both None (default), the function automatically selects the best implementation based on:

- Parameter types and devices
- Whether differentiable mode is enabled
- Capturable mode requirements

```

param params
    Parameters to optimize.

type params
    List[Tensor]

param grads
    Gradients for each parameter.

type grads
    List[Tensor]

param exp_avgs
    First moment estimates (momentum).

type exp_avgs
    List[Tensor]

param exp_avg_sqs
    Second moment estimates (variance).

type exp_avg_sqs
    List[Tensor]

param state_steps
    Step counters (must be singleton tensors).

type state_steps
    List[Tensor]

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

type foreach
    Optional[bool]

param capturable
    If True, ensure CUDA graph capture safety.

type capturable
    bool

param differentiable
    If True, allow gradients through optimization step.

```

```

type differentiable
    bool

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

type fused
    Optional[bool]

param grad_scale
    Gradient scaler for AMP training.

type grad_scale
    Optional[Tensor]

param found_inf
    Flag for inf/nan detection in AMP.

type found_inf
    Optional[Tensor]

param has_complex
    Whether any parameters are complex-valued.

type has_complex
    bool

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

type beta1
    float

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

type beta2
    float

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

type lr
    Union[float, Tensor]

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

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

param weight_decay
    Weight decay coefficient (L2 penalty).

type weight_decay
    float

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

type decouple
    bool

```

param eps
Small constant for numerical stability in normalization.

type eps
float

param maximize
If True, maximize objective instead of minimize.

type maximize
bool

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

raises RuntimeError
If state_steps contains non-tensor elements.

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

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

Example

```
>>> # Typically called by ADOPT optimizer, not directly
>>> adopt(
...     params=[p1, p2],
...     grads=[g1, g2],
...     exp_avgs=[m1, m2],
...     exp_avg_sqs=[v1, v2],
...     state_steps=[step1, step2],
...     beta1=0.9,
...     beta2=0.9999,
...     lr=0.001,
...     clip_lambda=lambda s: s**0.25,
...     weight_decay=0.01,
...     decouple=True,
...     eps=1e-6,
...     maximize=False,
... )
```

Note

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

See also

- ADOPT class: High-level optimizer interface
- `_single_tensor_adopt`: Single-tensor implementation details
- `_multi_tensor_adopt`: Multi-tensor implementation details

dicee.models.base_model

Classes

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

Module Contents

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

Bases: `lightning.LightningModule`

Base class for all neural network modules.

Your models should also subclass this class.

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

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

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

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

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

Note

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

Variables

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

```
training_step_outputs = []
```

```
mem_of_model() → Dict
```

Size of model in MB and number of params

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

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

Parameters

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

Returns

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

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

Example:

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

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

```
def __init__(self):  
    super().__init__()  
    self.automatic_optimization = False  
  
    # Multiple optimizers (e.g.: GANs)  
def training_step(self, batch, batch_idx):  
    opt1, opt2 = self.optimizers()  
  
    # do training_step with encoder  
    ...  
    opt1.step()  
    # do training_step with decoder  
    ...  
    opt2.step()
```

Note

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

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

Parameters

- `yhat_batch`
- `y_batch`

`on_train_epoch_end(*args, **kwargs)`

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

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

```
class MyLightningModule(L.LightningModule):  
    def __init__(self):  
        super().__init__()  
        self.training_step_outputs = []  
  
    def training_step(self):  
        loss = ...  
        self.training_step_outputs.append(loss)  
        return loss  
  
    def on_train_epoch_end(self):  
        # 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.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.reload_dataloaders_every_n_epochs`` to a positive integer.

For data processing use the following pattern:

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

However, the above are only necessary for distributed processing.

Warning

do not assign state in `prepare_data`

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

Note

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

`configure_optimizers(parameters=None)`

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

Returns

Any of these 6 options.

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

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

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

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

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

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

Note

Some things to know:

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

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

Bases: *BaseKGELightning*

Base class for all neural network modules.

Your models should also subclass this class.

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

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

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

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

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

Note

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

Variables

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

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

```

kernel_size = None
num_of_output_channels = None
weight_decay = None
loss
selected_optimizer = None
normalizer_class = None
normalize_head_entity_embeddings
normalize_relation_embeddings
normalize_tail_entity_embeddings
hidden_normalizer
param_init
input_dp_ent_real
input_dp_rel_real
hidden_dropout
loss_history = []
byte_pair_encoding
max_length_subword_tokens
block_size
forward_byte_pair_encoded_k_vs_all(x: torch.LongTensor)

Parameters
  x (B x 2 x T)

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

Parameters
-----
init_params_with_sanity_checking()

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

Parameters
  • x
  • y_idx
  • ordered_bpe_entities

```

```

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

Parameters
    x

forward_k_vs_all (*args, **kwargs)

forward_k_vs_sample (*args, **kwargs)

get_triple_representation (idx_hrt)

get_head_relation_representation (indexed_triple)

get_sentence_representation (x: torch.LongTensor)

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

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

Parameters
    x (B x 2 x T)

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

```

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

Bases: torch.nn.Module

Base class for all neural network modules.

Your models should also subclass this class.

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

```

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

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

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

```

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

Note

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

Variables

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

```
args = None
__call__(x)
static forward(x)
```

dicee.models.clifford

Classes

`Keci`

Base class for all neural network modules.

`CKeci`

Without learning dimension scaling

`DeCaL`

Base class for all neural network modules.

Module Contents

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

Bases: `dicee.models.base_model.BaseKGE`

Base class for all neural network modules.

Your models should also subclass this class.

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

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

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

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

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

Note

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

Variables

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

```
name = 'Keci'

p
q
r

requires_grad_for_interactions = True

compute_sigma_pp(hp, rp)
    Compute sigma_{pp} = sum_{i=1}^{p-1} sum_{k=i+1}^p (h_i r_k - h_k r_i) e_i e_k
    sigma_{pp} captures the interactions between along p bases For instance, let p e_1, e_2, e_3, we compute
    interactions between e_1 e_2, e_1 e_3 , and e_2 e_3 This can be implemented with a nested two for loops
    results = [] for i in range(p - 1):
        for k in range(i + 1, p):
            results.append(hp[:, :, i] * rp[:, :, k] - hp[:, :, k] * rp[:, :, i])
    sigma_pp = torch.stack(results, dim=2) assert sigma_pp.shape == (b, r, int((p * (p - 1)) / 2))
```

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

e2e1, e2e2, e2e3, e3e1, e3e2, e3e3

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

```
compute_sigma_qq(hq, rq)
    Compute sigma_{qq} = sum_{j=1}^{p+q-1} sum_{k=j+1}^{p+q} (h_j r_k - h_k r_j) e_j e_k sigma_{q}
    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
    r = r_0 + sum_{i=1}^p r_i e_i +
    sum_{j=p+1}^{p+q} r_j e_j
    ei ^2 = +1 for i <= p ej ^2 = -1 for p < j <= p+q ei ej = -eje1 for i
    eq j
    h r = sigma_0 + sigma_p + sigma_q + sigma_{pp} + sigma_{q} + sigma_{pq} where
    (1) sigma_0 = h_0 r_0 + sum_{i=1}^p (h_0 r_i) e_i - sum_{j=p+1}^{p+q} (h_j r_j) e_j
    (2) sigma_p = sum_{i=1}^p (h_0 r_i + h_i r_0) e_i
    (3) sigma_q = sum_{j=p+1}^{p+q} (h_0 r_j + h_j r_0) e_j
    (4) sigma_{pp} = sum_{i=1}^{p-1} sum_{k=i+1}^p (h_i r_k - h_k r_i) e_i e_k
    (5) sigma_{qq} = sum_{j=1}^{p+q-1} sum_{k=j+1}^{p+q} (h_j r_k - h_k r_j) e_j e_k
    (6) sigma_{pq} = sum_{i=1}^p sum_{j=p+1}^{p+q} (h_i r_j - h_j r_i) e_i e_j

construct_cl_multivector (x: torch.FloatTensor, r: int, p: int, q: int)
    → tuple[torch.FloatTensor, torch.FloatTensor, torch.FloatTensor]
Construct a batch of multivectors Cl_{p,q}(mathbb{R})^d

```

Parameter

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

returns

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

forward_k_vs_with_explicit (x: torch.Tensor)

k_vs_all_score (bpe_head_ent_emb, bpe_rel_ent_emb, E)

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

Kvsall training

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

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

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

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

Parameter

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

returns

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

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

Parameter

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

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

rtype

torch.FloatTensor with (n, k) shape

```
score(h, r, t)
```

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

Parameter

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

rtype

torch.FloatTensor with (n) shape

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

Bases: *Keci*

Without learning dimension scaling

```
name = 'CKeci'
```

```
requires_grad_for_interactions = False
```

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

Bases: *dicee.models.base_model.BaseKGE*

Base class for all neural network modules.

Your models should also subclass this class.

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

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

(continues on next page)

```

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

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

```

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

Note

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

Variables

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

```

name = 'DeCaL'

entity_embeddings

relation_embeddings

p

q

r

re

forward_triples(x: torch.Tensor) -> torch.FloatTensor

```

Parameter

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

rtype

`torch.FloatTensor with (n) shape`

`cl_pqr(a: torch.tensor) -> torch.tensor`

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

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

compute_sigmas_single (*list_h_emb*, *list_r_emb*, *list_t_emb*)

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

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

and return:

$$\text{sigma}_0 t = \sigma_0 \cdot t_0 = s0 + s1 - s2s3, s4 \text{ and } s5$$

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

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

For different base vector interactions, we have

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

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 $\text{Cl}_{\{p,q,r\}}(\mathbb{R}^d)$.
- (3) Perform Cl multiplication
- (4) Inner product of (3) and all entity embeddings

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

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

Multiplying a base vector with its scalar coefficient

construct_cl_multivector (*x*: *torch.FloatTensor*, *re*: int, *p*: int, *q*: int, *r*: int)

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

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

Parameter

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

returns

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

```
compute_sigma_pp(hp, rp)
```

Compute .. math:

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

σ_{pp} captures the interactions between along p bases For instance, let $p = 1, 2, 3$, we compute interactions between $e_1 e_2, e_1 e_3, e_2 e_3$. 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

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

σ_{qq} captures the interactions between along q bases For instance, let $q = 1, 2, 3$, we compute interactions between $e_1 e_2, e_1 e_3, e_2 e_3$. 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., $e_1 e_1, e_1 e_2, e_1 e_3, e_2 e_1, e_2 e_2, e_2 e_3, e_3 e_1, e_3 e_2, e_3 e_3$

e2e1, e2e2, e2e3, e3e1, e3e2, e3e3

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

```
compute_sigma_rr(hk, rk)
```

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

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

Compute

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

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

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

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

```

print(sigma_pq.shape)

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


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


results = [] sigma_pq = torch.zeros(b, r, p, q) for i in range(p):
    for j in range(q):
        sigma_pq[:, :, i, j] = hp[:, :, i] * rq[:, :, j] - hq[:, :, j] * rp[:, :, i]
    print(sigma_pq.shape)

compute_sigma_qr(*hq, hk, rq, rk)


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


results = [] sigma_pq = torch.zeros(b, r, p, q) for i in range(p):
    for j in range(q):
        sigma_pq[:, :, i, j] = hp[:, :, i] * rq[:, :, j] - hq[:, :, j] * rp[:, :, i]
    print(sigma_pq.shape)

```

dicee.models.complex

Classes

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

Module Contents

```

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

name = 'ConEx'

conv2d

fc_num_input

fc1

norm_fc1

bn_conv2d

feature_map_dropout

```

```

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

Parameters
    x

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

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

    conv2d
    fc_num_input
    fc1
    norm_fc1
    bn_conv2d
    feature_map_dropout

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

Parameters
    x

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

class dicee.models.complex.ComplEx(args)
    Bases: dicee.models.base_model.BaseKGE
    Base class for all neural network modules.
    Your models should also subclass this class.
    Modules can also contain other Modules, allowing them to be nested in a tree structure. You can assign the sub-modules as regular attributes:

```

```

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

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

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

```

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

Note

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

Variables

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

```

name = 'ComplEx'

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

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

```

Parameters

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

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

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

dicee.models.dualE

Classes

DualE

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

Module Contents

```
class dicee.models.dualE(args)
Bases: dicee.models.base_model.BaseKGE
Dual Quaternion Knowledge Graph Embeddings (https://ojs.aaai.org/index.php/AAAI/article/download/16850/16657)
name = 'DualE'

entity_embeddings
relation_embeddings
num_ent = None

kvsall_score(e_1_h, e_2_h, e_3_h, e_4_h, e_5_h, e_6_h, e_7_h, e_8_h, e_1_t, e_2_t, e_3_t, e_4_t,
              e_5_t, e_6_t, e_7_t, e_8_t, r_1, r_2, r_3, r_4, r_5, r_6, r_7, r_8) → torch.tensor
    KvsAll scoring function
```

Input

x: torch.LongTensor with (n,) shape

Output

torch.FloatTensor with (n) shape

```
forward_triples(idx_triple: torch.tensor) → torch.tensor
```

Negative Sampling forward pass:

Input

x: torch.LongTensor with (n,) shape

Output

torch.FloatTensor with (n) shape

```
forward_k_vs_all(x)
```

KvsAll forward pass

Input

x: torch.LongTensor with (n,) shape

Output

torch.FloatTensor with (n) shape

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

Transpose function

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

dicee.models.ensemble

Classes

`EnsembleKGE`

Module Contents

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

`name`

`train_mode = True`

`args`

`named_children()`

`property example_input_array`

`parameters()`

`modules()`

`__iter__()`

`__len__()`

`eval()`

`to(device)`

`state_dict()`

Return the state dict of the ensemble.

`load_state_dict(state_dict, strict=True)`

Load the state dict into the ensemble.

`mem_of_model()`

`__call__(x_batch)`

`step()`

`get_embeddings()`

`__str__()`

dicee.models.function_space

Classes

`FMult`

Learning Knowledge Neural Graphs

continues on next page

Table 31 – continued from previous page

<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:  $f(x) = \sum_{k=0}^n \{k=d-1\} w_k e^{ikx}$ . and use the three different scoring function as in the paper to evaluate the score

    name = 'LFMult1'

    entity_embeddings

    relation_embeddings

    forward_triples (idx_triple)

Parameters
    x

```

```

tri_score(h, r, t)

vtp_score(h, r, t)

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

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

name = 'LFMult'

entity_embeddings
relation_embeddings
degree
m
x_values
forward_triples(idx_triple)

Parameters
x
construct_multi_coeff(x)

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

linear(x, w, b)

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

tri_score(coeff_h, coeff_r, coeff_t)
this part implements the trilinear scoring techniques:
score(h,r,t) =  $\int_0^1 h(x)r(x)t(x) dx = \sum_{i,j,k=0}^{d-1} \frac{a_i b_j c_k}{(1+i+j+k)^d}$ 
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 implements the vector triple product scoring techniques:
score(h,r,t) =  $\int_0^1 h(x)r(x)t(x) dx = \sum_{i,j,k=0}^{d-1} \frac{a_i c_j b_k - b_i c_j a_k}{((1+i+j+k)(1+k))^{d-1}}$ 
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 the denominator and take the sum

```

4. take the sum over each batch

comp_func (*h, r, t*)

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

polynomial (*coeff, x, degree*)

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

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

pop (*coeff, x, degree*)

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

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

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

dicee.models.literal

Classes

LiteralEmbeddings

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

Module Contents

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

Bases: `torch.nn.Module`

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

num_of_data_properties

Number of data properties (attributes).

Type

int

embedding_dims

Dimension of the embeddings.

Type

int

entity_embeddings

Pre-trained entity embeddings.

Type

`torch.tensor`

dropout

Dropout rate for regularization.

Type

float

```

gate_residual
    Whether to use gated residual connections.

    Type
        bool

freeze_entity_embeddings
    Whether to freeze the entity embeddings during training.

    Type
        bool

embedding_dim

num_of_data_properties

hidden_dim

gate_residual = True

freeze_entity_embeddings = True

entity_embeddings

data_property_embeddings

fc

fc_out

dropout

gated_residual_proj

layer_norm

forward(entity_idx, attr_idx)

```

Parameters

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

Returns

scalar predictions.

Return type

Tensor

property device

dicee.models.octonion

Classes

OMult

Base class for all neural network modules.

ConvO

Base class for all neural network modules.

continues on next page

Table 33 – continued from previous page

<i>AConvO</i>	Additive Convolutional Octonion Knowledge Graph Embeddings
---------------	--

Functions

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

Module Contents

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

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

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

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

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

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

Note

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

Variables

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

```

name = 'OMult'

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

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

k_vs_all_score(bpe_head_ent_emb, bpe_rel_ent_emb, E)

forward_k_vs_all(x)

```

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

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

Bases: *dicee.models.base_model.BaseKGE*

Base class for all neural network modules.

Your models should also subclass this class.

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

```

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

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

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

```

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

Note

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

Variables

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

```

name = 'ConvO'

conv2d

fc_num_input

```

```

fc1
bn_conv2d
norm_fc1
feature_map_dropout

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

residual_convolution(O_1, O_2)

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

    Parameters
        x

forward_k_vs_all(x: torch.Tensor)

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

class dicee.models.octonion.AConvO(args: dict)
Bases: dicee.models.base\_model.BaseKGE

Additive Convolutional Octonion Knowledge Graph Embeddings

name = 'AConvO'

conv2d
fc_num_input
fc1
bn_conv2d
norm_fc1
feature_map_dropout

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

residual_convolution(O_1, O_2)

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

    Parameters
        x

forward_k_vs_all(x: torch.Tensor)

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

```

dicee.models.pykeen_models

Classes

`PykeenKGE`

A class for using knowledge graph embedding models implemented in Pykeen

Module Contents

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

Bases: `dicee.models.base_model.BaseKGE`

A class for using knowledge graph embedding models implemented in Pykeen

Notes: Pykeen_DistMult: C Pykeen_ComplEx: Pykeen_QuatE: Pykeen_MuRE: Pykeen_CP: Pykeen_Hole: Pykeen_HolE: Pykeen_HolE: Pykeen_TransD: Pykeen_TransE: Pykeen_TransF: Pykeen_TransH: Pykeen_TransR:

`model_kwargs`

`name`

`model`

`loss_history = []`

`args`

`entity_embeddings = None`

`relation_embeddings = None`

`forward_k_vs_all (x: torch.LongTensor)`

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

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

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

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

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

`else:`

t = self.entity_embeddings.weight

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

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

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

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

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

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

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

dicee.models.quaternion

Classes

<i>QM</i> ult	Base class for all neural network modules.
<i>ConvQ</i>	Convolutional Quaternion Knowledge Graph Embeddings
<i>AConvQ</i>	Additive Convolutional Quaternion Knowledge Graph Embeddings

Functions

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

Module Contents

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

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

Bases: `dicee.models.base_model.BaseKGE`

Base class for all neural network modules.

Your models should also subclass this class.

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

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

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

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

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

Note

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

Variables

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

```
name = 'QMult'  
  
explicit = True  
  
quaternion_multiplication_followed_by_inner_product (h, r, t)
```

Parameters

- `h` – shape: (`*batch_dims, dim`) The head representations.
- `r` – shape: (`*batch_dims, dim`) The head representations.
- `t` – shape: (`*batch_dims, dim`) The tail representations.

Returns

Triple scores.

`static quaternion_normalizer (x: torch.FloatTensor) → torch.FloatTensor`

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

Absolute value of a quaternion

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

L2 norm of quaternion vector:

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

Parameters

`x` – The vector.

Returns

The normalized vector.

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

`k_vs_all_score (bpe_head_ent_emb, bpe_rel_ent_emb, E)`

Parameters

- `bpe_head_ent_emb`
- `bpe_rel_ent_emb`
- `E`

`forward_k_vs_all (x)`

Parameters

`x`

```

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

class dicee.models.quaternion.ConvQ(args)
Bases: dicee.models.base_model.BaseKGE

Convolutional Quaternion Knowledge Graph Embeddings

name = 'ConvQ'

entity_embeddings

relation_embeddings

conv2d

fc_num_input

fc1

bn_conv1

bn_conv2

feature_map_dropout

residual_convolution(Q_1, Q_2)

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

Parameters
x

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

class dicee.models.quaternion.AConvQ(args)
Bases: dicee.models.base_model.BaseKGE

Additive Convolutional Quaternion Knowledge Graph Embeddings

name = 'AConvQ'

entity_embeddings

relation_embeddings

conv2d

fc_num_input

fc1

bn_conv1

bn_conv2

```

```

feature_map_dropout
residual_convolution(Q_1, Q_2)
forward_triples(indexed_triple: torch.Tensor) → torch.Tensor

```

Parameters

x

forward_k_vs_all(*x*: torch.Tensor)

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

dicee.models.real

Classes

<i>DistMult</i>	Embedding Entities and Relations for Learning and Inference in Knowledge Bases
<i>TransE</i>	Translating Embeddings for Modeling
<i>Shallow</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>CoKEConfig</i>	Configuration for the CoKE (Contextualized Knowledge Graph Embedding) model.
<i>CoKE</i>	Contextualized Knowledge Graph Embedding (CoKE) model.

Module Contents

```

class dicee.models.real.DistMult(args)
Bases: dicee.models.base_model.BaseKGE
Embedding Entities and Relations for Learning and Inference in Knowledge Bases https://arxiv.org/abs/1412.6575

name = 'DistMult'

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

Parameters

- emb_h
- emb_r
- emb_E

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

```

```

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

    name = 'TransE'

    margin = 4

    score(head_ent_emb, rel_ent_emb, tail_ent_emb)

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

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

    shallom

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

    forward_k_vs_all(x) → torch.FloatTensor

    forward_triples(x) → torch.FloatTensor

Parameters
    x

Returns

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

    dist_func

    margin = 1.0

    forward_triples(x: torch.LongTensor)

Parameters
    x

class dicee.models.real.CoKEConfig
Configuration for the CoKE (Contextualized Knowledge Graph Embedding) model.

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

vocab_size
    Total vocabulary size (num_entities + num_relations)

n_layer
    Number of transformer layers

```

```

n_head
    Number of attention heads per layer

n_embd
    Embedding dimension (set to match model embedding_dim)

dropout
    Dropout rate applied throughout the model

bias
    Whether to use bias in linear layers

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

block_size: int = 3

vocab_size: int = None

n_layer: int = 6

n_head: int = 8

n_embd: int = None

dropout: float = 0.3

bias: bool = True

causal: bool = False

class dicee.models.real.CoKE(args, config: CoKEConfig = CoKEConfig())
Bases: dicee.models.base_model.BaseKGE

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

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

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

name = 'CoKE'

config

pos_emb

mask_emb

blocks

ln_f

coke_dropout

forward_k_vs_all(x: torch.Tensor)

score(emb_h, emb_r, emb_t)

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

```

dicee.models.static_funcs

Functions

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

Module Contents

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

dicee.models.transformers

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

Classes

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

Module Contents

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

Bases: *dicee.models.base_model.BaseKGE*

Base class for all neural network modules.

Your models should also subclass this class.

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

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

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

(continues on next page)

(continued from previous page)

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

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

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

Note

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

Variables

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

```
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.SelfAttention(config)
```

Bases: torch.nn.Module

Base class for all neural network modules.

Your models should also subclass this class.

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

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

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

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

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

Note

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

Variables

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

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

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

Bases: `torch.nn.Module`

Base class for all neural network modules.

Your models should also subclass this class.

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

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

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

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

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

Note

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

Variables

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

`c_fc`

`gelu`

`c_proj`

`dropout`

`forward(x)`

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

Bases: `torch.nn.Module`

Base class for all neural network modules.

Your models should also subclass this class.

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

```

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

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

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

```

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

Note

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

Variables

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

```

ln_1

attn

ln_2

mlp

forward(x)

class dicee.models.transformers.GPTConfig

block_size: int = 1024
vocab_size: int = 50304
n_layer: int = 12
n_head: int = 12
n_embd: int = 768
dropout: float = 0.0
bias: bool = False
causal: bool = True

```

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

Bases: `torch.nn.Module`

Base class for all neural network modules.

Your models should also subclass this class.

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

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

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

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

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

Note

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

Variables

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

`config`

`transformer`

`lm_head`

`get_num_params` (`non_embedding=True`)

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

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

`crop_block_size` (`block_size`)

`classmethod from_pretrained` (`model_type, override_args=None`)

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

`estimate_mfu` (`fwdbwd_per_iter, dt`)

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

Classes

<i>ADOPT</i>	ADOPT Optimizer.
<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>Block</i>	Base class for all neural network modules.
<i>DistMult</i>	Embedding Entities and Relations for Learning and Inference in Knowledge Bases
<i>TransE</i>	Translating Embeddings for Modeling
<i>Shallow</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>CoKEConfig</i>	Configuration for the CoKE (Contextualized Knowledge Graph Embedding) model.
<i>CoKE</i>	Contextualized Knowledge Graph Embedding (CoKE) model.
<i>BaseKGE</i>	Base class for all neural network modules.
<i>ConEx</i>	Convolutional ComplEx Knowledge Graph Embeddings
<i>AConEx</i>	Additive Convolutional ComplEx Knowledge Graph Embeddings
<i>ComplEx</i>	Base class for all neural network modules.
<i>BaseKGE</i>	Base class for all neural network modules.
<i>IdentityClass</i>	Base class for all neural network modules.
<i>QMult</i>	Base class for all neural network modules.
<i>ConvQ</i>	Convolutional Quaternion Knowledge Graph Embeddings
<i>AConvQ</i>	Additive Convolutional Quaternion Knowledge Graph Embeddings
<i>BaseKGE</i>	Base class for all neural network modules.
<i>IdentityClass</i>	Base class for all neural network modules.
<i>OMult</i>	Base class for all neural network modules.
<i>ConvO</i>	Base class for all neural network modules.
<i>AConvO</i>	Additive Convolutional Octonion Knowledge Graph Embeddings
<i>Keci</i>	Base class for all neural network modules.
<i>CKeci</i>	Without learning dimension scaling
<i>DeCaL</i>	Base class for all neural network modules.
<i>BaseKGE</i>	Base class for all neural network modules.
<i>PykeenKGE</i>	A class for using knowledge graph embedding models implemented in Pykeen
<i>BaseKGE</i>	Base class for all neural network modules.
<i>FMult</i>	Learning Knowledge Neural Graphs
<i>GFMult</i>	Learning Knowledge Neural Graphs
<i>FMult2</i>	Learning Knowledge Neural Graphs
<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:

continues on next page

Table 41 – continued from previous page

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

Functions

<i>quaternion_mul</i> (→ Tuple[torch.Tensor, torch.Tensor, ...]) <i>quaternion_mul_with_unit_norm</i> (*, Q_1, Q_2)	Perform quaternion multiplication
<i>octonion_mul</i> (*, O_1, O_2)	
<i>octonion_mul_norm</i> (*, O_1, O_2)	

Package Contents

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

Bases: `torch.optim.optimizer.Optimizer`

ADOPT Optimizer.

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

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

Mathematical formulation:

$$m_t = \beta_1 * m_{t-1} + (1 - \beta_1) * \text{clip}(g_t / \sqrt{v_t})$$

where:

- θ_t : parameter at step t
- g_t : gradient at step t
- m_t : first moment estimate (momentum)
- v_t : second moment estimate (variance)
- α : learning rate
- β_1, β_2 : exponential decay rates
- `clip()`: optional gradient clipping function

Reference:

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

Parameters

- **params** (*ParamsT*) – Iterable of parameters to optimize or dicts defining parameter groups.
- **lr** (*float or Tensor, optional*) – Learning rate. Can be a float or 1-element Tensor. Default: 1e-3
- **betas** (*Tuple[float, float], optional*) – Coefficients (β_1, β_2) for computing running averages of gradient and its square. β_1 controls momentum, β_2 controls variance. Default: (0.9, 0.9999)
- **eps** (*float, optional*) – Term added to denominator to improve numerical stability. Default: 1e-6
- **clip_lambda** (*Callable[[int], float], optional*) – Function that takes the step number and returns the gradient clipping threshold. Common choices: - lambda step: $\text{step}^{**0.25}$ (default, gradually increases clipping threshold) - lambda step: 1.0 (constant clipping) - None (no clipping) Default: lambda step: $\text{step}^{**0.25}$
- **weight_decay** (*float, optional*) – Weight decay coefficient (L2 penalty). Default: 0.0
- **decouple** (*bool, optional*) – If True, uses decoupled weight decay (AdamW-style), applying weight decay directly to parameters. If False, adds weight decay to gradients (L2 regularization). Default: False
- **foreach** (*bool, optional*) – If True, uses the faster foreach implementation for multi-tensor operations. Default: None (auto-select)
- **maximize** (*bool, optional*) – If True, maximizes parameters instead of minimizing. Useful for reinforcement learning. Default: False
- **capturable** (*bool, optional*) – If True, the optimizer is safe to capture in a CUDA graph. Requires learning rate as Tensor. Default: False
- **differentiable** (*bool, optional*) – If True, the optimization step can be differentiated. Useful for meta-learning. Default: False
- **fused** (*bool, optional*) – If True, uses fused kernel implementation (currently not supported). Default: None

Raises

- **ValueError** – If learning rate, epsilon, betas, or weight_decay are invalid.
- **RuntimeError** – If fused is enabled (not currently supported).
- **RuntimeError** – If lr is a Tensor with foreach=True and capturable=False.

Example

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

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

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

Note

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

`clip_lambda`

`__setstate__(state)`

Restore optimizer state from a checkpoint.

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

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

Parameters

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

Note

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

`step(closure=None)`

Perform a single optimization step.

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

1. Optionally evaluates a closure to recompute the loss (useful for algorithms like LBFGS or when loss needs multiple evaluations)
2. For each parameter group: - Collects parameters with gradients and their associated state - Extracts hyperparameters (betas, learning rate, etc.) - Calls the functional `adopt()` API to perform the actual update
3. Returns the loss value if a closure was provided

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

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

Parameters

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

- Enable gradients (torch.enable_grad())
- Compute forward pass
- Compute loss
- Compute backward pass
- Return the loss value Example: lambda: (loss := model(x), loss.backward(), loss)[-1]

Default: None

Returns

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

Return type

Optional[Tensor]

Example

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

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

Note

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

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

Bases: lightning.LightningModule

Base class for all neural network modules.

Your models should also subclass this class.

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

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

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

(continues on next page)

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

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

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

Note

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

Variables

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

`training_step_outputs` = []

`mem_of_model()` → Dict

Size of model in MB and number of params

`training_step` (batch, batch_idx=None)

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

Parameters

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

Returns

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

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

Example:

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

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

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

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

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

Note

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

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

Parameters

- `yhat_batch`
- `y_batch`

`on_train_epoch_end(*args, **kwargs)`

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

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

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

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

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

`test_epoch_end(outputs: List[Any])`

`test_dataloader() → None`

An iterable or collection of iterables specifying test samples.

For more information about multiple dataloaders, see this section.

For data processing use the following pattern:

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

However, the above are only necessary for distributed processing.

⚠ Warning

do not assign state in `prepare_data`

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

ℹ Note

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

ℹ Note

If you don't need a 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.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.reload_dataloaders_every_n_epochs`` to a positive integer.

For data processing use the following pattern:

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

However, the above are only necessary for distributed processing.

Warning

do not assign state in `prepare_data`

- `fit()`

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

Note

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

`configure_optimizers(parameters=None)`

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

Returns

Any of these 6 options.

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

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

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

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

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

Note

Some things to know:

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

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

Bases: `BaseKG``Lightning`

Base class for all neural network modules.

Your models should also subclass this class.

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

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

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

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

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

Note

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

Variables

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

`args`

`embedding_dim = None`

`num_entities = None`

`num_relations = None`

`num_tokens = None`

`learning_rate = None`

`apply_unit_norm = None`

`input_dropout_rate = None`

`hidden_dropout_rate = None`

`optimizer_name = None`

`feature_map_dropout_rate = None`

`kernel_size = None`

`num_of_output_channels = None`

`weight_decay = None`

`loss`

`selected_optimizer = None`

`normalizer_class = None`

`normalize_head_entity_embeddings`

`normalize_relation_embeddings`

`normalize_tail_entity_embeddings`

`hidden_normalizer`

`param_init`

`input_dp_ent_real`

`input_dp_rel_real`

`hidden_dropout`

`loss_history = []`

`byte_pair_encoding`

```

max_length_subword_tokens
block_size

forward_byte_pair_encoded_k_vs_all(x: torch.LongTensor)
```

Parameters

- **x** (*B* × 2 × *T*)

```

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

Parameters

```

init_params_with_sanity_checking()
```

```

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

Parameters

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

```

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

Parameters

- **x**

```

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

```

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

```

get_triple_representation(idx_hrt)
```

```

get_head_relation_representation(indexed_triple)
```

```

get_sentence_representation(x: torch.LongTensor)
```

Parameters

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

```

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

Parameters

- **x** (*B* × 2 × *T*)

```

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

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

Bases: torch.nn.Module

Base class for all neural network modules.

Your models should also subclass this class.

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

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

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

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

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

Note

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

Variables

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

```
args = None

__call__(x)

static forward(x)

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

Bases: `BaseKGELightning`

Base class for all neural network modules.

Your models should also subclass this class.

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

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

class Model(nn.Module):
```

(continues on next page)

```

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

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

```

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

Note

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

Variables

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

```

args

embedding_dim = None

num_entities = None

num_relations = None

num_tokens = None

learning_rate = None

apply_unit_norm = None

input_dropout_rate = None

hidden_dropout_rate = None

optimizer_name = None

feature_map_dropout_rate = None

kernel_size = None

num_of_output_channels = None

weight_decay = None

loss

selected_optimizer = None

normalizer_class = None

normalize_head_entity_embeddings

```

```

normalize_relation_embeddings
normalize_tail_entity_embeddings
hidden_normalizer
param_init
input_dp_ent_real
input_dp_rel_real
hidden_dropout
loss_history = []
byte_pair_encoding
max_length_subword_tokens
block_size
forward_byte_pair_encoded_k_vs_all(x: torch.LongTensor)

Parameters
    x (B x 2 x T)

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

Parameters
-----
init_params_with_sanity_checking()

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

Parameters
    • x
    • y_idx
    • ordered_bpe_entities

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

Parameters
    x

forward_k_vs_all(*args, **kwargs)

forward_k_vs_sample(*args, **kwargs)

get_triple_representation(idx_hrt)

get_head_relation_representation(indexed_triple)

```

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

Parameters

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

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

→ Tuple[torch.FloatTensor, torch.FloatTensor]

Parameters

x (B x 2 x T)

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

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

Bases: torch.nn.Module

Base class for all neural network modules.

Your models should also subclass this class.

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

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

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

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

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

Note

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

Variables

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

`ln_1`

`attn`

```

ln_2

mlp

forward(x)

class dicee.models.DistMult(args)
Bases: dicee.models.base_model.BaseKGE
Embedding Entities and Relations for Learning and Inference in Knowledge Bases https://arxiv.org/abs/1412.6575

name = 'DistMult'

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

Parameters

- emb_h
- emb_r
- emb_E

forward_k_vs_all(x: torch.LongTensor)

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

score(h, r, t)

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

name = 'TransE'

margin = 4

score(head_ent_emb, rel_ent_emb, tail_ent_emb)

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

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

shallow

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

forward_k_vs_all(x) → torch.FloatTensor

forward_triples(x) → torch.FloatTensor

Parameters
x

Returns

```

```

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

    A Physical Embedding Model for Knowledge Graphs

    name = 'Pyke'

    dist_func

    margin = 1.0

    forward_triples(x: torch.LongTensor)
```

Parameters

x

```

class dicee.models.CoKEConfig
    Configuration for the CoKE (Contextualized Knowledge Graph Embedding) model.

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

    vocab_size
        Total vocabulary size (num_entities + num_relations)

    n_layer
        Number of transformer layers

    n_head
        Number of attention heads per layer

    n_embd
        Embedding dimension (set to match model embedding_dim)

    dropout
        Dropout rate applied throughout the model

    bias
        Whether to use bias in linear layers

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

    block_size: int = 3

    vocab_size: int = None

    n_layer: int = 6

    n_head: int = 8

    n_embd: int = None

    dropout: float = 0.3

    bias: bool = True

    causal: bool = False
```

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

Bases: *dicee.models.base_model.BaseKGE*

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

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

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

```
name = 'CoKE'
```

```
config
```

```
pos_emb
```

```
mask_emb
```

```
blocks
```

```
ln_f
```

```
coke_dropout
```

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

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

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

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

Bases: *BaseKGLightning*

Base class for all neural network modules.

Your models should also subclass this class.

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

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

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

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

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

Note

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

Variables

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

```
args

embedding_dim = None

num_entities = None

num_relations = None

num_tokens = None

learning_rate = None

apply_unit_norm = None

input_dropout_rate = None

hidden_dropout_rate = None

optimizer_name = None

feature_map_dropout_rate = None

kernel_size = None

num_of_output_channels = None

weight_decay = None

loss

selected_optimizer = None

normalizer_class = None

normalize_head_entity_embeddings

normalize_relation_embeddings

normalize_tail_entity_embeddings

hidden_normalizer

param_init

input_dp_ent_real

input_dp_rel_real

hidden_dropout

loss_history = []
```

```

byte_pair_encoding
max_length_subword_tokens
block_size

forward_byte_pair_encoded_k_vs_all(x: torch.LongTensor) → torch.FloatTensor

    Parameters
        x (B × 2 × T)
    forward_byte_pair_encoded_triple(x: Tuple[torch.LongTensor, torch.LongTensor]) → torch.FloatTensor

        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) → torch.FloatTensor

    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) → torch.FloatTensor

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

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

    Parameters
        x (B × 2 × T)
    get_embeddings() → Tuple[numpy.ndarray, numpy.ndarray]

```

```

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

    Convolutional ComplEx Knowledge Graph Embeddings

    name = 'ConEx'

    conv2d

    fc_num_input

    fc1

    norm_fc1

    bn_conv2d

    feature_map_dropout

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

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

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

    Parameters
    x

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

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

    Additive Convolutional ComplEx Knowledge Graph Embeddings

    name = 'AConEx'

    conv2d

    fc_num_input

    fc1

    norm_fc1

    bn_conv2d

    feature_map_dropout

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

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

```

```

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

Parameters
    x

```

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

```

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

```

Base class for all neural network modules.

Your models should also subclass this class.

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

```

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

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

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

```

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

Note

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

Variables

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

```

name = 'ComplEx'

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

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

```

Parameters

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

```

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

dicee.models.quaternion_mul(*Q_1, Q_2)
    → Tuple[torch.Tensor, torch.Tensor, torch.Tensor, torch.Tensor]
Perform quaternion multiplication :param Q_1: :param Q_2: :return:

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

Base class for all neural network modules.

Your models should also subclass this class.

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

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

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

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

```

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

Note

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

Variables

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

```

args

embedding_dim = None

num_entities = None

num_relations = None

num_tokens = None

learning_rate = None

apply_unit_norm = None

```

```

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

```

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

Parameters

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

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

Parameters

x

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

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

```
get_triple_representation(idx_hrt)
```

```
get_head_relation_representation(indexed_triple)
```

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

Parameters

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

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

Parameters

x (B x 2 x T)

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

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

Bases: torch.nn.Module

Base class for all neural network modules.

Your models should also subclass this class.

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

```
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)

(continued from previous page)

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

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

Note

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

Variables

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

```
args = None

__call__(x)

static forward(x)

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

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

Base class for all neural network modules.

Your models should also subclass this class.

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

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

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

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

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

Note

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

Variables

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

```
name = 'QMult'

explicit = True

quaternion_multiplication_followed_by_inner_product(h, r, t)
```

Parameters

- `h` – shape: (`*batch_dims, dim`) The head representations.
- `r` – shape: (`*batch_dims, dim`) The head representations.
- `t` – shape: (`*batch_dims, dim`) The tail representations.

Returns

Triple scores.

`static quaternion_normalizer(x: torch.FloatTensor) → torch.FloatTensor`

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

Absolute value of a quaternion

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

L2 norm of quaternion vector:

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

Parameters

`x` – The vector.

Returns

The normalized vector.

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

`k_vs_all_score(bpe_head_ent_emb, bpe_rel_ent_emb, E)`

Parameters

- `bpe_head_ent_emb`
- `bpe_rel_ent_emb`
- `E`

`forward_k_vs_all(x)`

Parameters

`x`

`forward_k_vs_sample(x, target_entity_idx)`

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

```

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

entity_embeddings
relation_embeddings
conv2d
fc_num_input
fc1
bn_conv1
bn_conv2
feature_map_dropout
residual_convolution(Q_1, Q_2)

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

Parameters
x

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

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

entity_embeddings
relation_embeddings
conv2d
fc_num_input
fc1
bn_conv1
bn_conv2
feature_map_dropout
residual_convolution(Q_1, Q_2)

```

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

Parameters

x

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

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

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

Bases: *BaseKGLightning*

Base class for all neural network modules.

Your models should also subclass this class.

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

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

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

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

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

Note

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

Variables

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

`args`

```
embedding_dim = None
```

```
num_entities = None
```

```
num_relations = None
```

```
num_tokens = None
```

```
learning_rate = None
```

```

apply_unit_norm = None
input_dropout_rate = None
hidden_dropout_rate = None
optimizer_name = None
feature_map_dropout_rate = None
kernel_size = None
num_of_output_channels = None
weight_decay = None
loss
selected_optimizer = None
normalizer_class = None
normalize_head_entity_embeddings
normalize_relation_embeddings
normalize_tail_entity_embeddings
hidden_normalizer
param_init
input_dp_ent_real
input_dp_rel_real
hidden_dropout
loss_history = []
byte_pair_encoding
max_length_subword_tokens
block_size
forward_byte_pair_encoded_k_vs_all(x: torch.LongTensor)

Parameters
  x (B x 2 x T)

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

Parameters
-----
init_params_with_sanity_checking()

```

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

Parameters

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

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

Parameters

x

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

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

```
get_triple_representation(idx_hrt)
```

```
get_head_relation_representation(indexed_triple)
```

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

Parameters

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

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

Parameters

x (B x 2 x T)

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

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

Bases: torch.nn.Module

Base class for all neural network modules.

Your models should also subclass this class.

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

```
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)

(continued from previous page)

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

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

Note

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

Variables

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

```
args = None

__call__(x)

static forward(x)

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

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

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

Bases: `dicee.models.base_model.BaseKGE`

Base class for all neural network modules.

Your models should also subclass this class.

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

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

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

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

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

Note

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

Variables

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

`name = 'OMult'`

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

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

`k_vs_all_score(bpe_head_ent_emb, bpe_rel_ent_emb, E)`

`forward_k_vs_all(x)`

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

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

Bases: `dicee.models.base_model.BaseKGE`

Base class for all neural network modules.

Your models should also subclass this class.

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

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

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

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

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

Note

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

Variables

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

```
name = 'ConvO'

conv2d

fc_num_input

fc1

bn_conv2d

norm_fc1

feature_map_dropout

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

residual_convolution(O_1, O_2)

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

Parameters

`x`

`forward_k_vs_all(x: torch.Tensor)`

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

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

Bases: `dicee.models.base_model.BaseKGE`

Additive Convolutional Octonion Knowledge Graph Embeddings

`name = 'AConvO'`

`conv2d`

`fc_num_input`

`fc1`

`bn_conv2d`

`norm_fc1`

`feature_map_dropout`

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

`residual_convolution(O_1, O_2)`

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

Parameters

`x`

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

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

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

Base class for all neural network modules.

Your models should also subclass this class.

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

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

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

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

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

i Note

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

Variables

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

```
name = 'Keci'

p
q
r

requires_grad_for_interactions = True

compute_sigma_pp(hp, rp)
Compute sigma_{pp} = sum_{i=1}^{p-1} sum_{k=i+1}^p (h_i r_k - h_k r_i) e_i e_k

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

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

```

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

```

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

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

`e2e1, e2e2, e2e3, e3e1, e3e2, e3e3`

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

compute_sigma_qq(hq, rq)

Compute `sigma_qq = sum_{j=1}^{p+q-1} sum_{k=j+1}^{p+q} (h_j r_k - h_k r_j) e_j e_k` sigma_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 r = r_0 + sum_{i=1}^p r_i e_i + sum_{j=p+1}^{p+q} r_j e_j`

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

`eq j`

`h r = sigma_0 + sigma_p + sigma_q + sigma_pp + sigma_qq + sigma_pq` where

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

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

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

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

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

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

construct_cl_multivector (*x*: *torch.FloatTensor*, *r*: *int*, *p*: *int*, *q*: *int*)
 \rightarrow tuple[*torch.FloatTensor*, *torch.FloatTensor*, *torch.FloatTensor*]
Construct a batch of multivectors $Cl_{\{p,q\}}(\mathbb{R}^d)$

Parameter

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

returns

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

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

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

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

Kvsall training

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

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

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

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

Parameter

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

returns

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

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

Parameter

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

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

rtype

torch.FloatTensor with (n, k) shape

```

score(h, r, t)
forward_triples(x: torch.Tensor) → torch.FloatTensor

```

Parameter

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

rtype

torch.FloatTensor with (n) shape

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

Bases: *Keci*

Without learning dimension scaling

```
name = 'CKeci'
```

```
requires_grad_for_interactions = False
```

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

Bases: *dicee.models.base_model.BaseKGE*

Base class for all neural network modules.

Your models should also subclass this class.

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

```

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

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

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

```

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

Note

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

Variables

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

```
name = 'DeCaL'
```

```

entity_embeddings
relation_embeddings

p



q



r



re



forward_triples (x: torch.Tensor) → torch.FloatTensor


```

Parameter

x: *torch.LongTensor* with (n,) shape

rtype

torch.FloatTensor with (n) shape

c1_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:

$$\sigma_0 t = \sigma_0 \cdot t_0 = s0 + s1 - s2s3, s4ands5$$

compute_sigmas_multivect (*list_h_emb*, *list_r_emb*)

Here we compute and return all the sums with vectors interaction for the same and different bases.

For same bases vectors interaction we have

$$\sigma_{pp} = \sum_{i=1}^{p-1} \sum_{i'=i+1}^p (h_i r_{i'} - h_{i'} r_i) (modelsthe interactions between e_i and e'_{i'} for 1 \leq i, i' \leq p) \sigma_{qq} = \sum_{j=p+1}^{p+q-1} \sum_{j'=j+1}^{p+q} (h_j r_{j'} - h_{j'} r_j)$$

For different base vector interactions, we have

$$\sigma_{pq} = \sum_{i=1}^p \sum_{j=p+1}^{p+q} (h_i r_j - h_j r_i) (interactions n between e_i and e_j for 1 \leq i \leq p and p+1 \leq j \leq p+q) \sigma_{pr} = \sum_{i=1}^p \sum_{j=p+1}^{p+q} (h_i r_j - h_j r_i) (interactions n between e_i and e_j for 1 \leq i \leq p and p+1 \leq j \leq p+q)$$

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 funcitons are identical Parameter ——— *x*: *torch.LongTensor* with (n,) shape :*dtype*: *torch.FloatTensor* with (n, |E|) shape

apply_coefficients (*h0, hp, hq, hk, r0, rp, rq, rk*)

Multiplying a base vector with its scalar coefficient

construct_cl_multivector (*x*: *torch.FloatTensor*, *re*: int, *p*: int, *q*: int, *r*: int)
 → tuple[*torch.FloatTensor*, *torch.FloatTensor*, *torch.FloatTensor*]

Construct a batch of multivectors $\text{Cl}_{\{p,q,r\}}(\mathbb{R}^d)$

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 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

$$\sigma_{q,q}^* = \sum_{j=p+1}^{p+q-1} \sum_{j'=j+1}^{p+q} (x_j y_{j'} - x_{j'} y_j) \quad \text{Eq.16}$$

`sigma_{q}` captures the interactions between along q bases For instance, let q e_1, e_2, e_3, we compute interactions between e_1 e_2, e_1 e_3 , and e_2 e_3 This can be implemented with a nested two for loops

results = [] for j in range(q - 1):

for k in range(j + 1, q):

results.append(hq[:, :, j] * rq[:, :, k] - hq[:, :, k] * rq[:, :, j])

sigma_qq = torch.stack(results, dim=2) assert sigma_qq.shape == (b, r, int((q * (q - 1)) / 2))

Yet, this computation would be quite inefficient. Instead, we compute interactions along all p, e.g., e1e1, e1e2, e1e3,

e2e1, e2e2, e2e3, e3e1, e3e2, e3e3

Then select the triangular matrix without diagonals: e1e2, e1e3, e2e3.

compute_sigma_rr(hk, rk)

$$\sigma_{r,r}^* = \sum_{k=p+q+1}^{p+q+r-1} \sum_{k'=k+1}^p (x_k y_{k'} - x_{k'} y_k)$$

compute_sigma_pq(* hp, hq, rp, rq)

Compute

$$\sum_{i=1}^p \sum_{j=p+1}^{p+q} (h_i r_j - h_j r_i) e_i e_j$$

results = [] sigma_pq = torch.zeros(b, r, p, q) for i in range(p):

for j in range(q):

sigma_pq[:, :, i, j] = hp[:, :, i] * rq[:, :, j] - hq[:, :, j] * rp[:, :, i]

print(sigma_pq.shape)

compute_sigma_pr(* hp, hk, rp, rk)

Compute

$$\sum_{i=1}^p \sum_{j=p+1}^{p+q} (h_i r_j - h_j r_i) e_i e_j$$

results = [] sigma_pq = torch.zeros(b, r, p, q) for i in range(p):

for j in range(q):

sigma_pq[:, :, i, j] = hp[:, :, i] * rq[:, :, j] - hq[:, :, j] * rp[:, :, i]

print(sigma_pq.shape)

compute_sigma_qr(* hq, hk, rq, rk)

$$\sum_{i=1}^p \sum_{j=p+1}^{p+q} (h_i r_j - h_j r_i) e_i e_j$$

results = [] sigma_pq = torch.zeros(b, r, p, q) for i in range(p):

for j in range(q):

sigma_pq[:, :, i, j] = hp[:, :, i] * rq[:, :, j] - hq[:, :, j] * rp[:, :, i]

print(sigma_pq.shape)

```
class dicee.models.BaseKGE(args: dict)
```

Bases: `BaseKGELightning`

Base class for all neural network modules.

Your models should also subclass this class.

Modules can also contain other Modules, allowing them to be nested in a tree structure. You can assign the sub-modules as regular attributes:

```
import torch.nn as nn
import torch.nn.functional as F

class Model(nn.Module):
    def __init__(self) -> None:
        super().__init__()
        self.conv1 = nn.Conv2d(1, 20, 5)
        self.conv2 = nn.Conv2d(20, 20, 5)

    def forward(self, x):
        x = F.relu(self.conv1(x))
        return F.relu(self.conv2(x))
```

Submodules assigned in this way will be registered, and will also have their parameters converted when you call `to()`, etc.

Note

As per the example above, an `__init__()` call to the parent class must be made before assignment on the child.

Variables

`training (bool)` – Boolean represents whether this module is in training or evaluation mode.

```
args
embedding_dim = None
num_entities = None
num_relations = None
num_tokens = None
learning_rate = None
apply_unit_norm = None
input_dropout_rate = None
hidden_dropout_rate = None
optimizer_name = None
feature_map_dropout_rate = None
```

```

kernel_size = None
num_of_output_channels = None
weight_decay = None
loss
selected_optimizer = None
normalizer_class = None
normalize_head_entity_embeddings
normalize_relation_embeddings
normalize_tail_entity_embeddings
hidden_normalizer
param_init
input_dp_ent_real
input_dp_rel_real
hidden_dropout
loss_history = []
byte_pair_encoding
max_length_subword_tokens
block_size
forward_byte_pair_encoded_k_vs_all(x: torch.LongTensor)

Parameters
  x (B x 2 x T)

forward_byte_pair_encoded_triple(x: Tuple[torch.LongTensor, torch.LongTensor])
  byte pair encoded neural link predictors

Parameters
-----
init_params_with_sanity_checking()

forward(x: torch.LongTensor | Tuple[torch.LongTensor, torch.LongTensor],
      y_idx: torch.LongTensor = None)

Parameters
  • x
  • y_idx
  • ordered_bpe_entities

```

```
forward_triples (x: torch.LongTensor) → torch.Tensor
```

Parameters

x

```
forward_k_vs_all (*args, **kwargs)
```

```
forward_k_vs_sample (*args, **kwargs)
```

```
get_triple_representation (idx_hrt)
```

```
get_head_relation_representation (indexed_triple)
```

```
get_sentence_representation (x: torch.LongTensor)
```

Parameters

- (b (x shape)

- 3

- t)

```
get_bpe_head_and_relation_representation (x: torch.LongTensor)
```

→ Tuple[torch.FloatTensor, torch.FloatTensor]

Parameters

x (B x 2 x T)

```
get_embeddings () → Tuple[numpy.ndarray, numpy.ndarray]
```

```
class dicee.models.PykeenKGE (args: dict)
```

Bases: dicee.models.base_model.BaseKGE

A class for using knowledge graph embedding models implemented in Pykeen

Notes: Pykeen_DistMult: C Pykeen_ComplEx: Pykeen_QuatE: Pykeen_MuRE: Pykeen_CP: Pykeen_HolE: Pykeen_HolE: Pykeen_HolE: Pykeen_TransD: Pykeen_TransE: Pykeen_TransF: Pykeen_TransH: Pykeen_TransR:

```
model_kwargs
```

```
name
```

```
model
```

```
loss_history = []
```

```
args
```

```
entity_embeddings = None
```

```
relation_embeddings = None
```

```
forward_k_vs_all (x: torch.LongTensor)
```

=> Explicit version by this we can apply bn and dropout

(1) Retrieve embeddings of heads and relations + apply Dropout & Normalization if given. h, r = self.get_head_relation_representation(x) # (2) Reshape (1). if self.last_dim > 0:

```
h = h.reshape(len(x), self.embedding_dim, self.last_dim) r = r.reshape(len(x), self.embedding_dim, self.last_dim)
```

(3) Reshape all entities. if self.last_dim > 0:

```

t = self.entity_embeddings.weight.reshape(self.num_entities, self.embedding_dim, self.last_dim)

else:
    t = self.entity_embeddings.weight

# (4) Call the score_t from interactions to generate triple scores. return self.interaction.score_t(h=h, r=r,
all_entities=t, slice_size=1)

forward_triples (x: torch.LongTensor) → torch.FloatTensor
# => Explicit version by this we can apply bn and dropout
# (1) Retrieve embeddings of heads, relations and tails and apply Dropout & Normalization if given. h, r, t =
self.get_triple_representation(x) # (2) Reshape (1). if self.last_dim > 0:
    h = h.reshape(len(x), self.embedding_dim, self.last_dim) r = r.reshape(len(x), self.embedding_dim,
    self.last_dim) t = t.reshape(len(x), self.embedding_dim, self.last_dim)
# (3) Compute the triple score return self.interaction.score(h=h, r=r, t=t, slice_size=None, slice_dim=0)

abstractmethod forward_k_vs_sample (x: torch.LongTensor, target_entity_idx)

class dicee.models.BaseKGE (args: dict)
Bases: BaseKGELightning

Base class for all neural network modules.

Your models should also subclass this class.

Modules can also contain other Modules, allowing them to be nested in a tree structure. You can assign the sub-
modules as regular attributes:

```

```

import torch.nn as nn
import torch.nn.functional as F

class Model(nn.Module):
    def __init__(self) -> None:
        super().__init__()
        self.conv1 = nn.Conv2d(1, 20, 5)
        self.conv2 = nn.Conv2d(20, 20, 5)

    def forward(self, x):
        x = F.relu(self.conv1(x))
        return F.relu(self.conv2(x))

```

Submodules assigned in this way will be registered, and will also have their parameters converted when you call `to()`, etc.

Note

As per the example above, an `__init__()` call to the parent class must be made before assignment on the child.

Variables

`training (bool)` – Boolean represents whether this module is in training or evaluation mode.

```

args
embedding_dim = None
num_entities = None
num_relations = None
num_tokens = None
learning_rate = None
apply_unit_norm = None
input_dropout_rate = None
hidden_dropout_rate = None
optimizer_name = None
feature_map_dropout_rate = None
kernel_size = None
num_of_output_channels = None
weight_decay = None
loss
selected_optimizer = None
normalizer_class = None
normalize_head_entity_embeddings
normalize_relation_embeddings
normalize_tail_entity_embeddings
hidden_normalizer
param_init
input_dp_ent_real
input_dp_rel_real
hidden_dropout
loss_history = []
byte_pair_encoding
max_length_subword_tokens
block_size
forward_byte_pair_encoded_k_vs_all(x: torch.LongTensor)

```

Parameters

x ($B \times 2 \times T$)

```

forward_byte_pair_encoded_triple(x: Tuple[torch.LongTensor, torch.LongTensor])
    byte pair encoded neural link predictors

    Parameters
    -----
    init_params_with_sanity_checking()

forward(x: torch.LongTensor | Tuple[torch.LongTensor, torch.LongTensor],
        y_idx: torch.LongTensor = None)

    Parameters
    *
    * x
    * y_idx
    * ordered_bpe_entities

forward_triples(x: torch.LongTensor) → torch.Tensor

    Parameters
    x

forward_k_vs_all(*args, **kwargs)

forward_k_vs_sample(*args, **kwargs)

get_triple_representation(idx_hrt)
get_head_relation_representation(indexed_triple)
get_sentence_representation(x: torch.LongTensor)

    Parameters
    *
    * (b (x shape)
    * 3
    * t)

get_bpe_head_and_relation_representation(x: torch.LongTensor)
    → Tuple[torch.FloatTensor, torch.FloatTensor]

    Parameters
    x (B x 2 x T)
get_embeddings() → Tuple[numpy.ndarray, numpy.ndarray]

class dicee.models.FMult(args)
Bases: dicee.models.base_model.BaseKGE

Learning Knowledge Neural Graphs

name = 'FMult'

entity_embeddings

relation_embeddings

k

```

```

num_sample = 50
gamma
roots
weights

compute_func (weights: torch.FloatTensor, x) → torch.FloatTensor
chain_func (weights, x: torch.FloatTensor)
forward_triples (idx_triple: torch.Tensor) → torch.Tensor

Parameters
x

class dicee.models.GFMult (args)
Bases: dicee.models.base_model.BaseKGE
Learning Knowledge Neural Graphs
name = 'GFMult'
entity_embeddings
relation_embeddings
k
num_sample = 250
roots
weights

compute_func (weights: torch.FloatTensor, x) → torch.FloatTensor
chain_func (weights, x: torch.FloatTensor)
forward_triples (idx_triple: torch.Tensor) → torch.Tensor

Parameters
x

class dicee.models.FMult2 (args)
Bases: dicee.models.base_model.BaseKGE
Learning Knowledge Neural Graphs
name = 'FMult2'
n_layers = 3
k
n = 50
score_func = 'compositional'
discrete_points

```

```

entity_embeddings
relation_embeddings
build_func(Vec)
build_chain_funcs(list_Vec)
compute_func(W, b, x) → torch.FloatTensor
function(list_W, list_b)
trapezoid(list_W, list_b)
forward_triples(idx_triple: torch.Tensor) → torch.Tensor

```

Parameters

x

```
class dicee.models.LFMult1(args)
```

Bases: *dicee.models.base_model.BaseKGE*

Embedding with trigonometric functions. We represent all entities and relations in the complex number space as: $f(x) = \sum_{k=0}^d \{k=0\}^k w_k e^{ikx}$. and use the three different 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: $f(x) = \sum_{i=0}^d a_i x^i$ and use the three different scoring function as in the paper to evaluate the score. We also consider combining with Neural Networks.

```

name = 'LFMult'
entity_embeddings
relation_embeddings
degree
m
x_values

```

```

forward_triples (idx_triple)

Parameters
    x

construct_multi_coeff (x)

poly_NN (x, coefh, coefr, coeft)
    Constructing a 2 layers NN to represent the embeddings. h = sigma( $wh^T x + bh$ ), r = sigma( $wr^T x + br$ ), t = sigma( $wt^T x + bt$ )

linear (x, w, b)

scalar_batch_NN (a, b, c)
    element wise multiplication between a,b and c: Inputs : a, b, c =====> torch.tensor of size batch_size x m x d Output : a tensor of size batch_size x d

tri_score (coeff_h, coeff_r, coeff_t)
    this part implement the trilinear scoring techniques:
    score( $h, r, t$ ) =  $\int_{\{0\}} \{1\} h(x)r(x)t(x) dx = \sum_{\{i,j,k=0\}}^{d-1} \frac{a_i * b_j * c_k}{(1+(i+j+k)\%d)}$ 
    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:
    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 polynomials without for loops :) it takes a matrix tensor of coefficients (coeff), a matrix tensor of points x and range of integer [0,1,...d]
    and return a tensor ( $coeff[0][0] + coeff[0][1]x + ... + coeff[0][d]x^d$ )

coeff[1][0] + coeff[1][1]x +...+ coeff[1][d]x^d

class dicee.models.Duale (args)
Bases: dicee.models.base_model.BaseKGE

Dual Quaternion Knowledge Graph Embeddings (https://ojs.aaai.org/index.php/AAAI/article/download/16850/16657)

```

```
name = 'DualE'

entity_embeddings
relation_embeddings

num_ent = None

kvsall_score (e_1_h, e_2_h, e_3_h, e_4_h, e_5_h, e_6_h, e_7_h, e_8_h, e_1_t, e_2_t, e_3_t, e_4_t,
              e_5_t, e_6_t, e_7_t, e_8_t, r_1, r_2, r_3, r_4, r_5, r_6, r_7, r_8) → torch.tensor
    KvsAll scoring function
```

Input

x: torch.LongTensor with (n,) shape

Output

torch.FloatTensor with (n) shape

```
forward_triples (idx_triple: torch.tensor) → torch.tensor
```

Negative Sampling forward pass:

Input

x: torch.LongTensor with (n,) shape

Output

torch.FloatTensor with (n) shape

```
forward_k_vs_all (x)
```

KvsAll forward pass

Input

x: torch.LongTensor with (n,) shape

Output

torch.FloatTensor with (n) shape

```
T (x: torch.tensor) → torch.tensor
```

Transpose function

Input: Tensor with shape (nxm) Output: Tensor with shape (mxn)

dicee.query_generator

Classes

```
QueryGenerator
```

Module Contents

```
class dicee.query_generator.QueryGenerator (train_path: str, val_path: str, test_path: str,
    ent2id: Dict = None, rel2id: Dict = None, seed: int = 1, gen_valid: bool = False,
    gen_test: bool = True)

    train_path
    val_path
    test_path
    gen_valid = False
    gen_test = True
    seed = 1
    max_ans_num = 1000000.0
    mode
    ent2id = None
    rel2id: Dict = None
    ent_in: Dict
    ent_out: Dict
    query_name_to_struct
    list2tuple (list_data)
    tuple2list (x: List | Tuple) → List | Tuple
        Convert a nested tuple to a nested list.
    set_global_seed (seed: int)
        Set seed
    construct_graph (paths: List[str]) → Tuple[Dict, Dict]
        Construct graph from triples Returns dicts with incoming and outgoing edges
    fill_query (query_structure: List[str | List], ent_in: Dict, ent_out: Dict, answer: int) → bool
        Private method for fill_query logic.
    achieve_answer (query: List[str | List], ent_in: Dict, ent_out: Dict) → set
        Private method for achieve_answer logic. @TODO: Document the code
    write_links (ent_out, small_ent_out)
    ground_queries (query_structure: List[str | List], ent_in: Dict, ent_out: Dict, small_ent_in: Dict,
        small_ent_out: Dict, gen_num: int, query_name: str)
        Generating queries and achieving answers
    unmap (query_type, queries, tp_answers, fp_answers, fn_answers)
    unmap_query (query_structure, query, id2ent, id2rel)
```

```

generate_queries (query_struct: List, gen_num: int, query_type: str)
    Passing incoming and outgoing edges to ground queries depending on mode [train valid or text] and getting
    queries and answers in return @ TODO: create a class for each single query struct

save_queries (query_type: str, gen_num: int, save_path: str)

abstractmethod 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 byte pair encoding and add padding	
preprocess_with_pandas()	→ None
Preprocess with pandas: add reciprocal triples, construct vocabulary, and index datasets	
preprocess_with_polars()	→ None
Preprocess with polars: add reciprocal triples and create indexed datasets	

```
sequential_vocabulary_construction() → None  
    (1) Read input data into memory  
    (2) Remove triples with a condition  
    (3) Serialize vocabularies in a pandas dataframe where  
        => the index is integer and => a single column is string (e.g. URI)
```

dicee.read_preprocess_save_load_kg.read_from_disk

Classes

<i>ReadFromDisk</i>	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

<i>LoadSaveToDisk</i>

Module Contents

```
class dicee.read_preprocess_save_load_kg.save_load_disk.LoadSaveToDisk(kg)
```

kg

save()

load()

dicee.read_preprocess_save_load_kg.util

Functions

<code>polars_dataframe_indexer</code> (→ polars.DataFrame)	Replaces 'subject', 'relation', and 'object' columns in the input Polars DataFrame with their corresponding index values
<code>pandas_dataframe_indexer</code> (→ pandas.DataFrame)	Replaces 'subject', 'relation', and 'object' columns in the input Pandas DataFrame with their corresponding index values
<code>apply_reciprocal_or_noise</code> (add_reciprocal, eval_model) <code>timeit</code> (func)	Add reciprocal triples if conditions are met
<code>read_with_polars</code> (→ polars.DataFrame)	Load and Preprocess via Polars
<code>read_with_pandas</code> (data_path[, read_only_few, ...])	Load and Preprocess via Pandas
<code>read_from_disk</code> (→ Tuple[polars.DataFrame, pandas.DataFrame])	
<code>count_triples</code> (→ int)	Returns the total number of triples in the triple store.
<code>fetch_worker</code> (endpoint, offsets, chunk_size, ...)	Worker process: fetch assigned chunks and save to disk with per-worker tqdm.
<code>read_from_triple_store_with_polars</code> (endpoint[, ...])	Main function to read all triples in parallel, save as Parquet, and load into Polars dataframe.
<code>read_from_triple_store_with_pandas</code> ([endpoint])	Read triples from triple store into pandas dataframe
<code>get_er_vocab</code> (data[, file_path])	
<code>get_re_vocab</code> (data[, file_path])	
<code>get_ee_vocab</code> (data[, file_path])	
<code>create_constraints</code> (triples[, file_path])	
<code>load_with_pandas</code> (→ None)	Deserialize data
<code>save_numpy_ndarray</code> (* , data, file_path)	
<code>load_numpy_ndarray</code> (* , file_path)	
<code>save_pickle</code> (* , data[, file_path])	
<code>load_pickle</code> (*[, file_path])	
<code>create_reciprocal_triples</code> (x)	Add inverse triples into dask dataframe
<code>dataset_sanity_checking</code> (→ None)	

Module Contents

```
dicee.read_preprocess_save_load_kg.util.polars_dataframe_indexer(  
    df_polars: polars.DataFrame, idx_entity: polars.DataFrame, idx_relation: polars.DataFrame)  
    → polars.DataFrame  
Replaces 'subject', 'relation', and 'object' columns in the input Polars DataFrame with their corresponding index values from the entity and relation index DataFrames.
```

This function processes the DataFrame in three main steps: 1. Replace the ‘relation’ values with the corresponding index from *idx_relation*. 2. Replace the ‘subject’ values with the corresponding index from *idx_entity*. 3. Replace the ‘object’ values with the corresponding index from *idx_entity*.

Parameters:

df_polars

[polars.DataFrame] The input Polars DataFrame containing columns: ‘subject’, ‘relation’, and ‘object’.

idx_entity

[polars.DataFrame] A Polars DataFrame that contains the mapping between entity names and their corresponding indices. Must have columns: ‘entity’ and ‘index’.

idx_relation

[polars.DataFrame] A Polars DataFrame that contains the mapping between relation names and their corresponding indices. Must have columns: ‘relation’ and ‘index’.

Returns:

polars.DataFrame

A DataFrame with the ‘subject’, ‘relation’, and ‘object’ columns replaced by their corresponding indices.

Example Usage:

```
>>> df_polars = pl.DataFrame({
    "subject": ["Alice", "Bob", "Charlie"],
    "relation": ["knows", "works_with", "lives_in"],
    "object": ["Dave", "Eve", "Frank"]
})
>>> idx_entity = pl.DataFrame({
    "entity": ["Alice", "Bob", "Charlie", "Dave", "Eve", "Frank"],
    "index": [0, 1, 2, 3, 4, 5]
})
>>> idx_relation = pl.DataFrame({
    "relation": ["knows", "works_with", "lives_in"],
    "index": [0, 1, 2]
})
>>> polars_dataframe_indexer(df_polars, idx_entity, idx_relation)
```

Steps:

1. Join the input DataFrame *df_polars* on the ‘relation’ column with *idx_relation* to replace the relations with their indices.
2. Join on ‘subject’ to replace it with the corresponding entity index using a left join on *idx_entity*.
3. Join on ‘object’ to replace it with the corresponding entity index using a left join on *idx_entity*.
4. Select only the ‘subject’, ‘relation’, and ‘object’ columns to return the final result.

```
dicee.read_preprocess_save_load_kg.util.pandas_dataframe_indexer(
    df_pandas: pandas.DataFrame, idx_entity: pandas.DataFrame, idx_relation: pandas.DataFrame)
    → pandas.DataFrame
```

Replaces ‘subject’, ‘relation’, and ‘object’ columns in the input Pandas DataFrame with their corresponding index values from the entity and relation index DataFrames.

Parameters:

df_pandas

[pd.DataFrame] The input Pandas DataFrame containing columns: ‘subject’, ‘relation’, and ‘object’.

idx_entity

[pd.DataFrame] A Pandas DataFrame that contains the mapping between entity names and their corresponding indices. Must have columns: ‘entity’ and ‘index’.

idx_relation

[pd.DataFrame] A Pandas DataFrame that contains the mapping between relation names and their corresponding indices. Must have columns: ‘relation’ and ‘index’.

Returns:

pd.DataFrame

A DataFrame with the ‘subject’, ‘relation’, and ‘object’ columns replaced by their corresponding indices.

```
dicee.read_preprocess_save_load_kg.util.apply_reciprocal_or_noise(add_reciprocal: bool,  
eval_model: str, df: object = None, info: str = None)
```

Add reciprocal triples if conditions are met

```
dicee.read_preprocess_save_load_kg.util.timeit(func)
```

```
dicee.read_preprocess_save_load_kg.util.read_with_polars(data_path,  
read_only_few: int = None, sample_triples_ratio: float = None, separator: str = None)  
→ polars.DataFrame
```

Load and Preprocess via Polars

```
dicee.read_preprocess_save_load_kg.util.read_with_pandas(data_path,  
read_only_few: int = None, sample_triples_ratio: float = None, separator: str = None)
```

Load and Preprocess via Pandas

```
dicee.read_preprocess_save_load_kg.util.read_from_disk(data_path: str,  
read_only_few: int = None, sample_triples_ratio: float = None, backend: str = None,  
separator: str = None) → Tuple[polars.DataFrame, pandas.DataFrame]
```

```
dicee.read_preprocess_save_load_kg.util.count_triples(endpoint: str) → int
```

Returns the total number of triples in the triple store.

```
dicee.read_preprocess_save_load_kg.util.fetch_worker(endpoint: str, offsets: list[int],  
chunk_size: int, output_dir: str, worker_id: int)
```

Worker process: fetch assigned chunks and save to disk with per-worker tqdm.

```
dicee.read_preprocess_save_load_kg.util.read_from_triple_store_with_polars(  
endpoint: str, chunk_size: int = 500000, output_dir: str = 'triples_parquet')
```

Main function to read all triples in parallel, save as Parquet, and load into Polars dataframe.

```
dicee.read_preprocess_save_load_kg.util.read_from_triple_store_with_pandas(  
endpoint: str = None)
```

Read triples from triple store into pandas dataframe

```
dicee.read_preprocess_save_load_kg.util.get_er_vocab(data, file_path: str = None)
```

```
dicee.read_preprocess_save_load_kg.util.get_re_vocab(data, file_path: str = None)
```

```
dicee.read_preprocess_save_load_kg.util.get_ee_vocab(data, file_path: str = None)
```

```
dicee.read_preprocess_save_load_kg.util.create_constraints(triples, file_path: str = None)
```

(1) Extract domains and ranges of relations

(2) Store a mapping from relations to entities that are outside of the domain and range. 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

<code>PreprocessKG</code>	Preprocess the data in memory
<code>LoadSaveToDisk</code>	
<code>ReadFromDisk</code>	Read the data from disk into memory

Package Contents

```
class dicee.read_preprocess_save_load_kg.PreprocessKG(kg)
```

Preprocess the data in memory

`kg`

`start()` → None

Preprocess train, valid and test datasets stored in knowledge graph instance

Parameter

`rtype`

None

```

preprocess_with_byte_pair_encoding()
preprocess_with_byte_pair_encoding_with_padding() → None
    Preprocess with byte pair encoding and add padding

preprocess_with_pandas() → None
    Preprocess with pandas: add reciprocal triples, construct vocabulary, and index datasets

preprocess_with_polars() → None
    Preprocess with polars: add reciprocal triples and create indexed datasets

sequential_vocabulary_construction() → None
    (1) Read input data into memory
    (2) Remove triples with a condition
    (3) Serialize vocabularies in a pandas dataframe where
        => the index is integer and => a single column is string (e.g. URI)

class dicee.read_preprocess_save_load_kg.LoadSaveToDisk(kg)

    kg
    save()
    load()

class dicee.read_preprocess_save_load_kg.ReadFromDisk(kg)
    Read the data from disk into memory
    kg
    start() → None
        Read a knowledge graph from disk into memory
        Data will be available at the train_set, test_set, valid_set attributes.

```

Parameter

None

rtype

None

add_noisy_triples_into_training()

dicee.sanity_checkers

Functions

is_sparql_endpoint_alive([sparql_endpoint])

validate_knowledge_graph(args)
sanity_checking_with_arguments(args)

Validating the source of knowledge graph

sanity_check_callback_args(args) Perform sanity checks on callback-related arguments.

Module Contents

`dicee.sanity_checkers.is_sparql_endpoint_alive(sparql_endpoint: str = None)`

`dicee.sanity_checkers.validate_knowledge_graph(args)`

Validating the source of knowledge graph

`dicee.sanity_checkers.sanity_checking_with_arguments(args)`

`dicee.sanity_checkers.sanity_check_callback_args(args)`

Perform sanity checks on callback-related arguments.

`dicee.scripts`

Submodules

`dicee.scripts.index_serve`

```
$ docker pull qdrant/qdrant && docker run -p 6333:6333 -p 6334:6334 -v $(pwd)/qdrant_storage:/qdrant/storage:z  
qdrant/qdrant $ dicee_vector_db --index --serve --path CountryEmbeddings --collection "countries_vdb"
```

Attributes

`app`

`neural_searcher`

Classes

`NeuralSearcher`

`StringListRequest`

Functions

`get_default_arguments()`

`index(args)`

`root()`

`search_embeddings(q)`

`retrieve_embeddings(q)`

`search_embeddings_batch(request)`

continues on next page

Table 52 – continued from previous page

<code>serve(args)</code>
<code>main()</code>

Module Contents

```

dicee.scripts.index_serve.get_default_arguments()

dicee.scripts.index_serve.index(args)

dicee.scripts.index_serve.app

dicee.scripts.index_serve.neural_searcher = None

class dicee.scripts.index_serve.NeuralSearcher(args)

    collection_name

    entity_to_idx = None

    qdrant_client

    topk = 5

    retrieve_embedding(entity: str = None, entities: List[str] = None) → List

    search(entity: str)

async dicee.scripts.index_serve.root()

async dicee.scripts.index_serve.search_embeddings(q: str)

async dicee.scripts.index_serve.retrieve_embeddings(q: str)

class dicee.scripts.index_serve.StringListRequest
    Bases: pydantic.BaseModel

    queries: List[str]

    reducer: str | None = None

async dicee.scripts.index_serve.search_embeddings_batch(request: StringListRequest)

dicee.scripts.index_serve.serve(args)

dicee.scripts.index_serve.main()

```

dicee.scripts.run

Functions

<code>get_default_arguments([description])</code>	Extends pytorch_lightning Trainer's arguments with ours continues on next page
---	---

Table 53 – continued from previous page

`main()`

Module Contents

`dicee.scripts.run.get_default_arguments` (*description=None*)

Extends pytorch_lightning Trainer's arguments with ours

`dicee.scripts.run.main()`

`dicee.static_funcs`

Static utility functions for DICE embeddings.

This module provides utility functions for model initialization, data loading, serialization, and various helper operations.

Attributes

`MODEL_REGISTRY`

Functions

<code>create_reciprocal_triples</code> (→ das.DataFrame)	pan-	Add inverse triples to a DataFrame.
<code>get_er_vocab</code> (→ Dict[Tuple[int, int], List[int]])		Build entity-relation to tail vocabulary.
<code>get_re_vocab</code> (→ Dict[Tuple[int, int], List[int]])		Build relation-entity (tail) to head vocabulary.
<code>get_ee_vocab</code> (→ Dict[Tuple[int, int], List[int]])		Build entity-entity to relation vocabulary.
<code>timeit</code> (→ Callable)		Decorator to measure and print execution time and memory usage.
<code>save_pickle</code> (→ None)		Save data to a pickle file.
<code>load_pickle</code> (→ object)		Load data from a pickle file.
<code>load_term_mapping</code> (→ Union[dict, lars.DataFrame])	po-	Load term-to-index mapping from pickle or CSV file.
<code>select_model</code> (args[, is_continual_training, age_path])	stor-	
<code>load_model</code> (→ Tuple[object, Tuple[dict, dict]])		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</code> (* data, file_path)		
<code>numpy_data_type_changer</code> (→ numpy.ndarray)		Detect most efficient data type for a given triples
<code>save_checkpoint_model</code> (→ None)		Store Pytorch model into disk
<code>store</code> (→ None)		
<code>add_noisy_triples</code> (→ pandas.DataFrame)		Add randomly constructed triples
<code>read_or_load_kg</code> (args, cls)		

continues on next page

Table 55 – continued from previous page

<code>initialize_model(...)</code>	Initialize a knowledge graph embedding model.
<code>load_json(→ Dict)</code>	Load JSON file into a dictionary.
<code>save_embeddings(→ None)</code>	Save embeddings to a CSV file.
<code>vocab_to_parquet(vocab_to_idx, name, ...)</code>	
<code>create_experiment_folder(→ str)</code>	Create a timestamped experiment folder.
<code>continual_training_setup_executor(→ None)</code>	
<code>exponential_function(→ torch.FloatTensor)</code>	
<code>load_numpy(→ numpy.ndarray)</code>	
<code>evaluate(entity_to_idx, scores, easy_answers, # @TODO: CD: Renamed this function hard_answers)</code>	
<code>download_file(url[, destination_folder])</code>	
<code>download_files_from_url(→ None)</code>	
<code>download_pretrained_model(→ str)</code>	
<code>write_csv_from_model_parallel(path)</code>	Create
<code>from_pretrained_model_write_embeddings_int(None)</code>	

Module Contents

`dicee.static_funcs.MODEL_REGISTRY: Dict[str, Tuple[Type, str]]`
`dicee.static_funcs.create_reciprocal_triples(df: pandas.DataFrame) → pandas.DataFrame`
 Add inverse triples to a DataFrame.
 For each triple (s, p, o), creates an inverse triple (o, p_inverse, s).

Parameters

`df` – DataFrame with ‘subject’, ‘relation’, and ‘object’ columns.

Returns

DataFrame with original and inverse triples concatenated.

`dicee.static_funcs.get_er_vocab(data: numpy.ndarray, file_path: str | None = None)`
 → Dict[Tuple[int, int], List[int]]

Build entity-relation to tail vocabulary.

Parameters

- `data` – Array of triples with shape (n, 3) where columns are (head, relation, tail).
- `file_path` – Optional path to save the vocabulary as pickle.

Returns

Dictionary mapping (head, relation) pairs to list of tail entities.

`dicee.static_funcs.get_re_vocab(data: numpy.ndarray, file_path: str | None = None)`
 → Dict[Tuple[int, int], List[int]]

Build relation-entity (tail) to head vocabulary.

Parameters

- **data** – Array of triples with shape (n, 3) where columns are (head, relation, tail).
- **file_path** – Optional path to save the vocabulary as pickle.

Returns

Dictionary mapping (relation, tail) pairs to list of head entities.

```
dicee.static_funcs.get_ee_vocab(data: numpy.ndarray, file_path: str | None = None)
    → Dict[Tuple[int, int], List[int]]
```

Build entity-entity to relation vocabulary.

Parameters

- **data** – Array of triples with shape (n, 3) where columns are (head, relation, tail).
- **file_path** – Optional path to save the vocabulary as pickle.

Returns

Dictionary mapping (head, tail) pairs to list of relations.

```
dicee.static_funcs.timeit(func: Callable) → Callable
```

Decorator to measure and print execution time and memory usage.

Parameters

func – Function to be timed.

Returns

Wrapped function that prints timing information.

```
dicee.static_funcs.save_pickle(*, data: object | None = None, file_path: str) → None
```

Save data to a pickle file.

Note: Consider using more portable formats (JSON, Parquet) for new code.

Parameters

- **data** – Object to serialize. If None, nothing is saved.
- **file_path** – Path where the pickle file will be saved.

```
dicee.static_funcs.load_pickle(file_path: str) → object
```

Load data from a pickle file.

Note: Consider using more portable formats (JSON, Parquet) for new code.

Parameters

file_path – Path to the pickle file.

Returns

Deserialized object from the pickle file.

```
dicee.static_funcs.load_term_mapping(file_path: str) → dict | polars.DataFrame
```

Load term-to-index mapping from pickle or CSV file.

Attempts to load from pickle first, falls back to CSV if not found.

Parameters

file_path – Base path without extension.

Returns

Dictionary or Polars DataFrame containing the mapping.

```
dicee.static_funcs.select_model(args: dict, is_continual_training: bool = None,
    storage_path: str = None)
```

```

dicee.static_funcs.load_model(path_of_experiment_folder: str, model_name='model.pt', verbose=0)
    → Tuple[object, Tuple[dict, dict]]
Load weights and initialize pytorch module from namespace arguments

dicee.static_funcs.load_model_ensemble(path_of_experiment_folder: str)
    → Tuple[dicee.models.base_model.BaseKGE, Tuple[pandas.DataFrame, pandas.DataFrame]]
Construct Ensemble Of weights and initialize pytorch module from namespace arguments

(1) Detect models under given path
(2) Accumulate parameters of detected models
(3) Normalize parameters
(4) Insert (3) into model.

dicee.static_funcs.save_numpy_ndarray(*, data: numpy.ndarray, file_path: str)

dicee.static_funcs.numpy_data_type_changer(train_set: numpy.ndarray, num: int)
    → numpy.ndarray
Detect most efficient data type for a given triples :param train_set: :param num: :return:

dicee.static_funcs.save_checkpoint_model(model, path: str) → None
Store Pytorch model into disk

dicee.static_funcs.store(trained_model, model_name: str = 'model', full_storage_path: str = None,
    save_embeddings_as_csv=False) → None

dicee.static_funcs.add_noisy_triples(train_set: pandas.DataFrame, add_noise_rate: float)
    → pandas.DataFrame
Add randomly constructed triples :param train_set: :param add_noise_rate: :return:

dicee.static_funcs.read_or_load_kg(args, cls)

dicee.static_funcs.intialize_model(args: Dict, verbose: int = 0)
    → Tuple[dicee.models.base_model.BaseKGE, str]
Initialize a knowledge graph embedding model.

```

Parameters

- **args** – Dictionary containing model configuration including ‘model’ key.
- **verbose** – Verbosity level. If > 0, prints initialization message.

Returns

Tuple of (initialized model, form of labelling string).

Raises

ValueError – If the model name is not recognized.

```
dicee.static_funcs.load_json(path: str) → Dict
```

Load JSON file into a dictionary.

Parameters

path – Path to the JSON file.

Returns

Dictionary containing the JSON data.

Raises

- **FileNotFoundException** – If the file does not exist.

- `json.JSONDecodeError` – If the file contains invalid JSON.

`dicee.static_funcs.save_embeddings(embeddings: numpy.ndarray, indexes: List, path: str) → None`
Save embeddings to a CSV file.

Parameters

- `embeddings` – NumPy array of embeddings with shape (n_items, embedding_dim).
- `indexes` – List of index labels (entity/relation names).
- `path` – Output file path.

`dicee.static_funcs.vocab_to_parquet(vocab_to_idx, name, path_for_serialization, print_into)`

`dicee.static_funcs.create_experiment_folder(folder_name: str = 'Experiments') → str`
Create a timestamped experiment folder.

Parameters

`folder_name` – Base directory name for experiments.

Returns

Full path to the created experiment folder.

`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`

Training-related static functions.

This module provides backward compatibility by re-exporting evaluation functions from the new `dicee.evaluation` module, along with training utilities.

Deprecated since version Evaluation: functions have moved to `dicee.evaluation`. Use that module for new code. This module will continue to export training utilities.

Functions

<code>evaluate_lp</code> (→ Dict[str, float])	Evaluate link prediction with batched processing.
<code>evaluate_bpe_lp</code> (→ Dict[str, float])	Evaluate link prediction with BPE-encoded entities.
<code>make_iterable_verbose</code> (→ Iterable)	Wrap an iterable with tqdm progress bar if verbose is True.
<code>efficient_zero_grad</code> (→ None)	Efficiently zero gradients using parameter.grad = None.

Module Contents

```
dicee.static_funcs_training.evaluate_lp(model, triple_idx, num_entities: int,  
er_vocab: Dict[Tuple, List], re_vocab: Dict[Tuple, List], info: str = 'Eval Starts',  
batch_size: int = 128, chunk_size: int = 1000) → Dict[str, float]
```

Evaluate link prediction with batched processing.

Memory-efficient evaluation using chunked entity scoring.

Parameters

- **model** – The KGE model to evaluate.
- **triple_idx** – Integer-indexed triples as numpy array.
- **num_entities** – Total number of entities.
- **er_vocab** – Mapping (head_idx, rel_idx) -> list of tail indices.
- **re_vocab** – Mapping (rel_idx, tail_idx) -> list of head indices.
- **info** – Description to print.
- **batch_size** – Batch size for triple processing.
- **chunk_size** – Chunk size for entity scoring.

Returns

Dictionary with H@1, H@3, H@10, and MRR metrics.

```
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: str = 'Eval Starts') → Dict[str, float]
```

Evaluate link prediction with BPE-encoded entities.

Parameters

- **model** – The KGE model to evaluate.
- **triple_idx** – List of BPE-encoded triple tuples.
- **all_bpe_shaped_entities** – All entities with BPE representations.
- **er_vocab** – Mapping for tail filtering.
- **re_vocab** – Mapping for head filtering.
- **info** – Description to print.

Returns

Dictionary with H@1, H@3, H@10, and MRR metrics.

```
dicee.static_funcs_training.make_iterable_verbose(iterable_object: Iterable, verbose: bool,  
desc: str = 'Default', position: int | None = None, leave: bool = True) → Iterable
```

Wrap an iterable with tqdm progress bar if verbose is True.

Parameters

- **iterable_object** – The iterable to potentially wrap.
- **verbose** – Whether to show progress bar.
- **desc** – Description for the progress bar.
- **position** – Position of the progress bar.
- **leave** – Whether to leave the progress bar after completion.

Returns

The original iterable or a tqdm-wrapped version.

```
dicee.static_funcs_training.efficient_zero_grad(model) → None
```

Efficiently zero gradients using parameter.grad = None.

This is more efficient than optimizer.zero_grad() as it avoids memory operations.

See: https://pytorch.org/tutorials/recipes/recipes/tuning_guide.html

Parameters

model – PyTorch model to zero gradients for.

dicee.static_preprocess_funcs

Attributes

```
enable_log
```

Functions

```
timeit(func)
```

```
preprocesses_input_args(args)
```

Sanity Checking in input arguments

```
create_constraints(→ Tuple[dict, dict, dict, dict])
```

```
get_er_vocab(data)
```

```
get_re_vocab(data)
```

```
get_ee_vocab(data)
```

```
mapping_from_first_two_cols_to_third(train_se
```

Module Contents

```
dicee.static_preprocess_funcs.enable_log = False  
dicee.static_preprocess_funcs.timeit(func)  
dicee.static_preprocess_funcs.preprocesses_input_args(args)  
    Sanity Checking in input arguments  
dicee.static_preprocess_funcs.create_constraints(triples: numpy.ndarray)  
    → Tuple[dict, dict, dict, dict]  
  
(1) Extract domains and ranges of relations  
(2) Store a mapping from relations to entities that are outside of the domain and range. Create constraints entities based on the range of relations :param triples: :return:  
dicee.static_preprocess_funcs.get_er_vocab(data)  
dicee.static_preprocess_funcs.get_re_vocab(data)  
dicee.static_preprocess_funcs.get_ee_vocab(data)  
dicee.static_preprocess_funcs.mapping_from_first_two_cols_to_third(train_set_idx)
```

dicee.trainer

Submodules

dicee.trainer.dice_trainer

DICE Trainer module for knowledge graph embedding training.

Provides the DICE_Trainer class which supports multiple training backends including PyTorch Lightning, DDP, and custom CPU/GPU trainers.

Classes

<i>DICE_Trainer</i>	DICE_Trainer implement
---------------------	------------------------

Functions

<i>load_term_mapping</i> (→ polars.DataFrame)	Load term-to-index mapping from CSV file.
<i>initialize_trainer</i> (...)	Initialize the appropriate trainer based on configuration.
<i>get_callbacks</i> (→ List)	Create list of callbacks based on configuration.

Module Contents

```
dicee.trainer.dice_trainer.load_term_mapping(file_path: str) → polars.DataFrame  
    Load term-to-index mapping from CSV file.
```

Parameters

file_path – Base path without extension.

Returns

Polars DataFrame containing the mapping.

```
dicee.trainer.dice_trainer.initialize_trainer(args, callbacks: List)
```

```
    → dicee.trainer.torch_trainer.TorchTrainer | dicee.trainer.model_parallelism.TensorParallel | dicee.trainer.torch_trainer_ddp
```

Initialize the appropriate trainer based on configuration.

Parameters

- **args** – Configuration arguments containing trainer type.
- **callbacks** – List of training callbacks.

Returns

Initialized trainer instance.

Raises

AssertionError – If trainer is None after initialization.

```
dicee.trainer.dice_trainer.get_callbacks(args) → List
```

Create list of callbacks based on configuration.

Parameters

args – Configuration arguments.

Returns

List of callback instances.

```
class dicee.trainer.dice_trainer.DICE_Trainer(args, is_continual_training: bool, storage_path,  
evaluator=None)
```

DICE_Trainer implement

- 1- Pytorch Lightning trainer (<https://pytorch-lightning.readthedocs.io/en/stable/common/trainer.html>)
- 2- Multi-GPU Trainer(<https://pytorch.org/docs/stable/generated/torch.nn.parallel.DistributedDataParallel.html>)
- 3- CPU Trainer

args

is_continual_training:bool

storage_path:str

evaluator:

report:dict

report**args**

trainer = None

is_continual_training

storage_path

evaluator = None

form_of_labelling = None

continual_start (*knowledge_graph*)

- (1) Initialize training.
- (2) Load model
- (3) Load trainer (3) Fit model

Parameter

returns

- *model*
- **form_of_labelling** (*str*)

initialize_trainer (*callbacks: List*)

→ lightning.Trainer | dicee.trainer.model_parallelism.TensorParallel | dicee.trainer.torch_trainer.TorchTrainer | dicee.

Initialize Trainer from input arguments

initialize_or_load_model ()

init_dataloader (*dataset: torch.utils.data.Dataset*) → torch.utils.data.DataLoader

init_dataset () → torch.utils.data.Dataset

start (*knowledge_graph: dicee.knowledge_graph.KG* | *numpy.memmap*)

→ Tuple[dicee.models.base_model.BaseKGE, str]

Start the training

- (1) Initialize Trainer

- (2) Initialize or load a pretrained KGE model

in DDP setup, we need to load the memory map of already read/index KG.

k_fold_cross_validation (*dataset*) → Tuple[dicee.models.base_model.BaseKGE, str]

Perform K-fold Cross-Validation

1. Obtain K train and test splits.

2. **For each split,**

2.1 initialize trainer and model 2.2. Train model with configuration provided in args. 2.3. Compute the mean reciprocal rank (MRR) score of the model on the test respective split.

3. Report the mean and average MRR .

Parameters

- **self**
- **dataset**

Returns

model

dicee.trainer.model_parallelism

Classes

`TensorParallel`

Abstract class for Trainer class for knowledge graph embedding models

Functions

```
extract_input_outputs(z[, device])  
  
find_good_batch_size(train_loader,  
tp_ensemble_model)  
forward_backward_update_loss(→ float)
```

Module Contents

```
dicee.trainer.model_parallelism.extract_input_outputs (z: list, device=None)  
  
dicee.trainer.model_parallelism.find_good_batch_size (train_loader, tp_ensemble_model)  
  
dicee.trainer.model_parallelism.forward_backward_update_loss (z: Tuple, ensemble_model)  
    → float  
  
class dicee.trainer.model_parallelism.TensorParallel (args, callbacks)  
    Bases: dicee.abtracts.AbstractTrainer  
    Abstract class for Trainer class for knowledge graph embedding models
```

Parameter

args
[str] ?

callbacks: list
?

fit (*args, **kwargs)
Train model

dicee.trainer.torch_trainer

Classes

`TorchTrainer`

TorchTrainer for using single GPU or multi CPUs on a single node

Module Contents

```
class dicee.trainer.torch_trainer.TorchTrainer (args, callbacks)  
    Bases: dicee.abtracts.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
NodeTrainer

A Trainer based on torch.nn.parallel.DistributedDataParallel

Functions

```
make_iterable_verbose(→ Iterable)
```

Module Contents

```
dicee.trainer.torch_trainer_ddp.make_iterable_verbose(iterable_object, verbose,
desc='Default', position=None, leave=True) → Iterable
```

```
class dicee.trainer.torch_trainer_ddp.TorchDDPTrainer(args, callbacks)
```

Bases: `dicee.abstracts.AbstractTrainer`

A Trainer based on `torch.nn.parallel.DistributedDataParallel`

Arguments

entity_idxs

mapping.

relation_idxs

mapping.

form

?

store

?

label_smoothing_rate

Using hard targets (0,1) drives weights to infinity. An outlier produces enormous gradients.

Return type

`torch.utils.data.Dataset`

fit(*args, **kwargs)

Train model

```
class dicee.trainer.torch_trainer_ddp.NodeTrainer(trainer, model: torch.nn.Module,
train_dataset_loader: torch.utils.data.DataLoader, callbacks, num_epochs: int)
```

trainer

local_rank

global_rank

optimizer

train_dataset_loader

loss_func

callbacks

model

num_epochs

loss_history = []

```

ctx
scaler
extract_input_outputs(z: list)
train()
    Training loop for DDP

```

Classes

<i>DICE_Trainer</i>	DICE_Trainer implement
---------------------	------------------------

Package Contents

```

class dicee.trainer.DICE_Trainer(args, is_continual_training: bool, storage_path, evaluator=None)

DICE_Trainer implement
    1- Pytorch Lightning trainer (https://pytorch-lightning.readthedocs.io/en/stable/common/trainer.html)
    2- Multi-GPU Trainer(https://pytorch.org/docs/stable/generated/torch.nn.parallel.DistributedDataParallel.html)
    3- CPU Trainer

    args
    is_continual_training:bool
    storage_path:str
    evaluator:
    report:dict

report

args

trainer = None

is_continual_training

storage_path

evaluator = None

form_of_labelling = None

continual_start(knowledge_graph)
    (1) Initialize training.
    (2) Load model
    (3) Load trainer (3) Fit model

```

Parameter

returns

- *model*
- **form_of_labelling** (*str*)

initialize_trainer (*callbacks: List*)

→ lightning.Trainer | 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

dicee.weight_averaging

Classes

<i>ASWA</i>	Adaptive stochastic weight averaging
<i>SWA</i>	Stochastic Weight Averaging callback.
<i>SWAG</i>	Stochastic Weight Averaging - Gaussian (SWAG).
<i>EMA</i>	Exponential Moving Average (EMA) callback.
<i>TWA</i>	Train with Weight Averaging (TWA) using subspace projection + averaging.

Module Contents

```
class dicee.weight_averaging.ASWA(num_epochs, path)
```

Bases: `dicee.abstracts.AbstractCallback`

Adaptive stochastic weight averaging ASWE keeps track of the validation performance and update s the ensemble model accordingly.

path

num_epochs

initial_eval_setting = None

epoch_count = 0

alphas = []

val_aswa = -1

on_fit_end(*trainer, model*)

Call at the end of the training.

Parameter

trainer:

model:

rtype

None

```
static compute_mrr(trainer, model) → float
```

```
get_aswa_state_dict(model)
```

```
decide(running_model_state_dict, ensemble_state_dict, val_running_model,
       mrr_updated_ensemble_model)
```

Perform Hard Update, software or rejection

Parameters

- `running_model_state_dict`
- `ensemble_state_dict`
- `val_running_model`
- `mrr_updated_ensemble_model`

```
on_train_epoch_end(trainer, model)
```

Call at the end of each epoch during training.

Parameter

trainer:

model:

rtype

None

```

class dicee.weight_averaging.SWA (swa_start_epoch, swa_c_epochs: int = 1, lr_init: float = 0.1,
    swa_lr: float = 0.05, max_epochs: int = None)
Bases: dicee.abstracts.AbstractCallback

Stochastic Weight Averaging callback.

Initialize SWA callback.

    swa_start_epoch: int
        The epoch at which to start SWA.

    swa_c_epochs: int
        The number of epochs to use for SWA.

    lr_init: float
        The initial learning rate.

    swa_lr: float
        The learning rate to use during SWA.

    max_epochs: int
        The maximum number of epochs. args.num_epochs

    swa_start_epoch
    swa_c_epochs = 1
    swa_lr = 0.05
    lr_init = 0.1
    max_epochs = None
    swa_model = None
    swa_n = 0
    current_epoch = -1

    static moving_average (swa_model, running_model, alpha)
        Update SWA model with moving average of current model. Math: # SWA update: #  $\theta_{\text{swa}} \leftarrow (1 - \alpha) * \theta_{\text{swa}} + \alpha * \theta$  #  $\alpha = 1 / (n + 1)$ , where  $n$  = number of models already averaged #  $\alpha$  is tracked via self.swa_n in code

    on_train_epoch_start (trainer, model)
        Update learning rate according to SWA schedule.

    on_train_epoch_end (trainer, model)
        Apply SWA averaging if conditions are met.

    on_fit_end (trainer, model)
        Replace main model with SWA model at the end of training.

class dicee.weight_averaging.SWAG (swa_start_epoch, swa_c_epochs: int = 1, lr_init: float = 0.1,
    swa_lr: float = 0.05, max_epochs: int = None, max_num_models: int = 20,
    var_clamp: float = 1e-30)
Bases: dicee.abstracts.AbstractCallback

Stochastic Weight Averaging - Gaussian (SWAG). Parameters

    swa_start_epoch
        [int] Epoch at which to start collecting weights.

```

```

swa_c_epochs
    [int] Interval of epochs between updates.

lr_init
    [float] Initial LR.

swa_lr
    [float] LR in SWA / GSWA phase.

max_epochs
    [int] Total number of epochs.

max_num_models
    [int] Number of models to keep for low-rank covariance approx.

var_clamp
    [float] Clamp low variance for stability.

swa_start_epoch

swa_c_epochs = 1

swa_lr = 0.05

lr_init = 0.1

max_epochs = None

max_num_models = 20

var_clamp = 1e-30

mean = None

sq_mean = None

deviations = []

gswa_n = 0

current_epoch = -1

get_mean_and_var()
    Return mean + variance (diagonal part).

sample (base_model, scale=0.5)
    Sample new model from SWAG posterior distribution.

    Math: # From SWAG, posterior is approximated as: #  $\theta \sim N(\text{mean}, \Sigma)$  # where  $\Sigma \approx \text{diag}(\text{var}) + (1/(K-1)) * D D^T$  # - mean = running average of weights # - var = elementwise variance ( $\text{sq\_mean} - \text{mean}^2$ ) # - D = [dev_1, dev_2, ..., dev_K], deviations from mean (low-rank approx) # - K = number of collected models

    # Sampling step: # 1.  $\theta_{\text{diag}} = \text{mean} + \text{scale} * \text{std} \odot \varepsilon$ , where  $\varepsilon \sim N(0, I)$  # 2.  $\theta_{\text{lowrank}} = \theta_{\text{diag}} + (D z) / \sqrt{K-1}$ , where  $z \sim N(0, I_K)$  # Final sample =  $\theta_{\text{lowrank}}$ 

on_train_epoch_start (trainer, model)
    Update LR schedule (same as SWA).

on_train_epoch_end (trainer, model)
    Collect Gaussian stats at the end of epochs after swa_start.

```

`on_fit_end`(*trainer, model*)

Set model weights to the collected SWAG mean at the end of training.

```
class dicee.weight_averaging.EMA(ema_start_epoch: int, decay: float = 0.999,
                                 max_epochs: int = None, ema_c_epochs: int = 1)
```

Bases: `dicee.abstracts.AbstractCallback`

Exponential Moving Average (EMA) callback.

Parameters

- `ema_start_epoch` (`int`) – Epoch to start EMA.
- `decay` (`float`) – EMA decay rate (typical: 0.99 - 0.9999) Math: $\theta_{\text{ema}} \leftarrow \text{decay} * \theta_{\text{ema}} + (1 - \text{decay}) * \theta$
- `max_epochs` (`int`) – Maximum number of epochs.

`ema_start_epoch`

`decay = 0.999`

`max_epochs = None`

`ema_c_epochs = 1`

`ema_model = None`

`current_epoch = -1`

```
static ema_update(ema_model, running_model, decay: float)
```

Update EMA model with exponential moving average of current model. Math: # EMA update: # $\theta_{\text{ema}} \leftarrow (1 - \alpha) * \theta_{\text{ema}} + \alpha * \theta$ # alpha = 1 - decay, where decay is the EMA smoothing factor (typical 0.99 - 0.999) # alpha controls how much of the current model θ contributes to the EMA # decay is fixed in code -> can be extended to scheduled

`on_train_epoch_start`(*trainer, model*)

Track current epoch.

`on_train_epoch_end`(*trainer, model*)

Update EMA if past start epoch.

`on_fit_end`(*trainer, model*)

Replace main model with EMA model at the end of training.

```
class dicee.weight_averaging.TWA(twa_start_epoch: int, lr_init: float, num_samples: int = 5,
                                   reg_lambda: float = 0.0, max_epochs: int = None, twa_c_epochs: int = 1)
```

Bases: `dicee.abstracts.AbstractCallback`

Train with Weight Averaging (TWA) using subspace projection + averaging.

Parameters

`twa_start_epoch`

[int] Epoch to start TWA.

`lr_init`

[float] Learning rate used for β updates.

`num_samples`

[int] Number of sampled weight snapshots to build projection subspace.

```

reg_lambda
    [float] Regularization coefficient for  $\beta$  updates.

max_epochs
    [int] Total number of training epochs.

twa_c_epochs
    [int] Interval of epochs between TWA updates.

twa_start_epoch

num_samples = 5

reg_lambda = 0.0

max_epochs = None

lr_init

twa_c_epochs = 1

current_epoch = -1

weight_samples = []

twa_model = None

base_weights = None

P = None

beta = None

sample_weights (model)
    Collect sampled weights from the current model and maintain rolling buffer.

build_projection (weight_samples, k=None)
    Build projection subspace from collected weight samples. :param weight_samples: list of flat weight tensors [(D,), ...] :param k: number of basis vectors to keep. Defaults to min(N, D).

Returns
    (D,) base weight vector (average) P: (D, k) projection matrix with top-k basis directions

Return type
    mean_w

on_train_epoch_start (trainer, model)
    Track epoch.

on_train_epoch_end (trainer, model)
    Main TWA logic: build subspace and update in  $\beta$  space.

    # Math: # TWA weight update: # w_twa = mean_w + P * beta # mean_w = (1/n) * sum_i w_i (SWA baseline)
    # beta <- (1 - eta * lambda) * beta - eta * P^T * g # g = gradient of training loss w.r.t. full model weights
    # eta = learning rate, lambda = ridge regularization # P = orthonormal basis spanning sampled checkpoints
    {w_i}

on_fit_end (trainer, model)
    Replace with TWA model at the end.

```

14.2 Attributes

—version—

14.3 Classes

<i>Execute</i>	Executor class for training, retraining and evaluating KGE models.
<i>KGE</i>	Knowledge Graph Embedding Class for interactive usage of pre-trained models
<i>QueryGenerator</i>	
<i>DICE_Trainer</i>	DICE_Trainer implement
<i>Evaluator</i>	Evaluator class for KGE models in various downstream tasks.

14.4 Package Contents

class dicee.**Execute**(args, continuous_training: bool = False)

Executor class for training, retraining and evaluating KGE models.

Handles the complete workflow: 1. Loading & Preprocessing & Serializing input data 2. Training & Validation & Testing 3. Storing all necessary information

args

Processed input arguments.

distributed

Whether distributed training is enabled.

rank

Process rank in distributed training.

world_size

Total number of processes.

local_rank

Local GPU rank.

trainer

Training handler instance.

trained_model

The trained model after training completes.

knowledge_graph

The loaded knowledge graph.

report

Dictionary storing training metrics and results.

evaluator

Model evaluation handler.

```

distributed
args
is_continual_training = False
trainer: dicee.trainer.DICE_Trainer | None = None
trained_model = None
knowledge_graph: dicee.knowledge_graph.KG | None = None
report: Dict
evaluator: dicee.evaluator.Evaluator | None = None
start_time: float | None = None
is_rank_zero() → bool
cleanup()

setup_executor() → None
    Set up storage directories for the experiment.

    Creates or reuses experiment directories based on configuration. Saves the configuration to a JSON file.

create_and_store_kg() → None
    Create knowledge graph and store as memory-mapped file.

    Only executed on rank 0 in distributed training. Skips if memmap already exists.

load_from_memmap() → None
    Load knowledge graph from memory-mapped file.

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.KGE(path=None, url=None, construct_ensemble=False, model_name=None)

Bases: *dicee.abstracts.BaseInteractiveKGE*, *dicee.abstracts.InteractiveQueryDecomposition*, *dicee.abstracts.BaseInteractiveTrainKGE*

Knowledge Graph Embedding Class for interactive usage of pre-trained models

__str__()

to(device: str) → None

get_transductive_entity_embeddings(indices: torch.LongTensor | List[str], as_pytorch=False, as_numpy=False, as_list=True) → torch.FloatTensor | numpy.ndarray | List[float]

create_vector_database(collection_name: str, distance: str, location: str = 'localhost', port: int = 6333)

generate(h='', r='')

eval_lp_performance(dataset=List[Tuple[str, str, str]], filtered=True)

predict_missing_head_entity(relation: List[str] | str, tail_entity: List[str] | str, within=None, batch_size=2, topk=1, return_indices=False) → Tuple

Given a relation and a tail entity, return top k ranked head entity.

argmax_{e in E} f(e,r,t), where r in R, t in E.

Parameter

relation: Union[List[str], str]

String representation of selected relations.

tail_entity: Union[List[str], str]

String representation of selected entities.

k: int

Highest ranked k entities.

Returns: Tuple

Highest K scores and entities

```
predict_missing_relations(head_entity: List[str] | str, tail_entity: List[str] | str, within=None,  
batch_size=2, topk=1, return_indices=False) → Tuple
```

Given a head entity and a tail entity, return top k ranked relations.

argmax_{r in R} f(h,r,t), where h, t in E.

Parameter

head_entity: List[str]

String representation of selected entities.

tail_entity: List[str]

String representation of selected entities.

k: int

Highest ranked k entities.

Returns: Tuple

Highest K scores and entities

```
predict_missing_tail_entity(head_entity: List[str] | str, relation: List[str] | str,  
within: List[str] = None, batch_size=2, topk=1, return_indices=False) → torch.FloatTensor
```

Given a head entity and a relation, return top k ranked entities

argmax_{e in E} f(h,r,e), where h in E and r in R.

Parameter

head_entity: List[str]

String representation of selected entities.

tail_entity: List[str]

String representation of selected entities.

Returns: Tuple

scores

```
predict(*: h: List[str] | str = None, r: List[str] | str = None, t: List[str] | str = None, within=None,  
logits=True) → torch.FloatTensor
```

Parameters

- **logits**
- **h**
- **r**
- **t**
- **within**

```
predict_topk (*, h: str | List[str] = None, r: str | List[str] = None, t: str | List[str] = None, topk: int = 10,  
    within: List[str] = None, batch_size: int = 1024)
```

Predict missing item in a given triple.

Returns

- If you query a single (h, r, ?) or (? , r, t) or (h, ?, t), returns List[(item, score)]
- If you query a batch of B, returns List of B such lists.

```
triple_score (h: List[str] | str = None, r: List[str] | str = None, t: List[str] | str = None, logits=False)  
    → torch.FloatTensor
```

Predict triple score

Parameter

head_entity: List[str]

String representation of selected entities.

relation: List[str]

String representation of selected relations.

tail_entity: List[str]

String representation of selected entities.

logits: bool

If logits is True, unnormalized score returned

Returns: Tuple

pytorch tensor of triple score

```
return_multi_hop_query_results (aggregated_query_for_all_entities, k: int, only_scores)
```

```
single_hop_query_answering (query: tuple, only_scores: bool = True, k: int = None)
```

```
answer_multi_hop_query (query_type: str = None, query: Tuple[str | Tuple[str, str], Ellipsis] = None,  
    queries: List[Tuple[str | Tuple[str, str], Ellipsis]] = None, tnorm: str = 'prod',  
    neg_norm: str = 'standard', lambda_: float = 0.0, k: int = 10, only_scores=False)  
    → List[Tuple[str, torch.Tensor]]
```

@TODO: Refactoring is needed # @TODO: Score computation for each query type should be done in a static function

Find an answer set for EPFO queries including negation and disjunction

Parameter

query_type: str The type of the query, e.g., “2p”.

query: Union[str, Tuple[str, Tuple[str, 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 descending 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

predict_literals (*entity: List[str] | str = None, attribute: List[str] | str = None, denormalize_preds: bool = True*) → numpy.ndarray

Predicts literal values for given entities and attributes.

Parameters

- **entity** (*Union[List[str], str]*) – Entity or list of entities to predict literals for.
- **attribute** (*Union[List[str], str]*) – Attribute or list of attributes to predict literals for.
- **denormalize_preds** (*bool*) – If True, denormalizes the predictions.

Returns

Predictions for the given entities and attributes.

Return type

numpy ndarray

class dicee.QueryGenerator (*train_path, val_path: str, test_path: str, ent2id: Dict = None, rel2id: Dict = None, seed: int = 1, gen_valid: bool = False, gen_test: bool = True*)

train_path

val_path

test_path

gen_valid = False

gen_test = True

```

seed = 1

max_ans_num = 1000000.0

mode

ent2id = None

rel2id: Dict = None

ent_in: Dict

ent_out: Dict

query_name_to_struct

list2tuple(list_data)

tuple2list(x: List | Tuple) → List | Tuple
    Convert a nested tuple to a nested list.

set_global_seed(seed: int)
    Set seed

construct_graph(paths: List[str]) → Tuple[Dict, Dict]
    Construct graph from triples Returns dicts with incoming and outgoing edges

fill_query(query_structure: List[str | List], ent_in: Dict, ent_out: Dict, answer: int) → bool
    Private method for fill_query logic.

achieve_answer(query: List[str | List], ent_in: Dict, ent_out: Dict) → set
    Private method for achieve_answer logic. @TODO: Document the code

write_links(ent_out, small_ent_out)

ground_queries(query_structure: List[str | List], ent_in: Dict, ent_out: Dict, small_ent_in: Dict,
    small_ent_out: Dict, gen_num: int, query_name: str)
    Generating queries and achieving answers

unmap(query_type, queries, tp_answers, fp_answers, fn_answers)

unmap_query(query_structure, query, id2ent, id2rel)

generate_queries(query_struct: List, gen_num: int, query_type: str)
    Passing incoming and outgoing edges to ground queries depending on mode [train valid or text] and getting
    queries and answers in return @ TODO: create a class for each single query struct

save_queries(query_type: str, gen_num: int, save_path: str)

abstractmethod 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

```

```
class dicee.DICE_Trainer(args, is_continual_training: bool, storage_path, evaluator=None)
```

DICE_Trainer implement

- 1- Pytorch Lightning trainer (<https://pytorch-lightning.readthedocs.io/en/stable/common/trainer.html>)
- 2- Multi-GPU Trainer(<https://pytorch.org/docs/stable/generated/torch.nn.parallel.DistributedDataParallel.html>)
- 3- CPU Trainer

```
args
```

```
is_continual_training:bool
```

```
storage_path:str
```

```
evaluator:
```

```
report:dict
```

report

args

```
trainer = None
```

```
is_continual_training
```

```
storage_path
```

```
evaluator = None
```

```
form_of_labelling = None
```

```
continual_start(knowledge_graph)
```

- (1) Initialize training.
- (2) Load model
- (3) Load trainer (3) Fit model

Parameter

returns

- *model*
- **form_of_labelling** (*str*)

```
initialize_trainer(callbacks: List)
```

```
→ lightning.Trainer | dicee.trainer.model_parallelism.TensorParallel | dicee.trainer.torch_trainer.TorchTrainer | dicee.
```

Initialize Trainer from input arguments

```
initialize_or_load_model()
```

```
init_dataloader(dataset: torch.utils.data.Dataset) → torch.utils.data.DataLoader
```

```
init_dataset() → torch.utils.data.Dataset
```

```
start(knowledge_graph: dicee.knowledge_graph.KG | numpy.memmap)
```

```
→ Tuple[dicee.models.base_model.BaseKGE, str]
```

Start the training

- (1) Initialize Trainer

(2) Initialize or load a pretrained KGE model

in DDP setup, we need to load the memory map of already read/index KG.

k_fold_cross_validation (*dataset*) → Tuple[*dicee.models.base_model.BaseKGE*, str]

Perform K-fold Cross-Validation

1. Obtain K train and test splits.

2. **For each split,**

2.1 initialize trainer and model 2.2. Train model with configuration provided in args. 2.3. Compute the mean reciprocal rank (MRR) score of the model on the test respective split.

3. Report the mean and average MRR .

Parameters

- **self**
- **dataset**

Returns

model

class dicee.Evaluator (*args*, *is_continual_training*: bool = False)

Evaluator class for KGE models in various downstream tasks.

Orchestrates link prediction evaluation with different scoring techniques including standard evaluation and byte-pair encoding based evaluation.

er_vocab

Entity-relation to tail vocabulary for filtered ranking.

re_vocab

Relation-entity (tail) to head vocabulary.

ee_vocab

Entity-entity to relation vocabulary.

num_entities

Total number of entities in the knowledge graph.

num_relations

Total number of relations in the knowledge graph.

args

Configuration arguments.

report

Dictionary storing evaluation results.

during_training

Whether evaluation is happening during training.

Example

```
>>> from dicee.evaluation import Evaluator
>>> evaluator = Evaluator(args)
>>> results = evaluator.eval(dataset, model, 'EntityPrediction')
>>> print(f"Test MRR: {results['Test']['MRR']:.4f}")
```

```

re_vocab: Dict | None = None
er_vocab: Dict | None = None
ee_vocab: Dict | None = None
func_triple_to_bpe_representation = None
is_continual_training = False
num_entities: int | None = None
num_relations: int | None = None
domain_constraints_per_rel = None
range_constraints_per_rel = None
args
report: Dict
during_training = False

```

vocab_preparation(*dataset*) → None

Prepare vocabularies from the dataset for evaluation.

Resolves any future objects and saves vocabularies to disk.

Parameters

dataset – Knowledge graph dataset with vocabulary attributes.

eval(*dataset, trained_model, form_of_labelling: str, during_training: bool = False*) → Dict | None

Evaluate the trained model on the dataset.

Parameters

- **dataset** – Knowledge graph dataset (KG instance).
- **trained_model** – The trained KGE model.
- **form_of_labelling** – Type of labelling ('EntityPrediction' or 'RelationPrediction').
- **during_training** – Whether evaluation is during training.

Returns

Dictionary of evaluation metrics, or None if evaluation is skipped.

eval_rank_of_head_and_tail_entity(**, train_set, valid_set=None, test_set=None, trained_model*)
→ None

Evaluate with negative sampling scoring.

eval_rank_of_head_and_tail_byte_pair_encoded_entity(**, train_set=None, valid_set=None, test_set=None, ordered_bpe_entities, trained_model*) → None

Evaluate with BPE-encoded entities and negative sampling.

eval_with_byte(**, raw_train_set, raw_valid_set=None, raw_test_set=None, trained_model, form_of_labelling*) → None

Evaluate ByteE model with generation.

```
eval_with_bpe_vs_all(*, raw_train_set, raw_valid_set=None, raw_test_set=None, trained_model,  
form_of_labelling) → None
```

Evaluate with BPE and KvsAll scoring.

```
eval_with_vs_all(*, train_set, valid_set=None, test_set=None, trained_model, form_of_labelling)  
→ None
```

Evaluate with KvsAll or 1vsAll scoring.

```
evaluate_lp_k_vs_all(model, triple_idx, info: str | None = None,  
form_of_labelling: str | None = None) → Dict[str, float]
```

Filtered link prediction evaluation with KvsAll scoring.

Parameters

- **model** – The trained model to evaluate.
- **triple_idx** – Integer-indexed test triples.
- **info** – Description to print.
- **form_of_labelling** – ‘EntityPrediction’ or ‘RelationPrediction’.

Returns

Dictionary with H@1, H@3, **H@10**, and MRR metrics.

```
evaluate_lp_with_byte(model, triples: List[List[str]], info: str | None = None) → Dict[str, float]
```

Evaluate BytE model with text generation.

Parameters

- **model** – BytE model.
- **triples** – String triples.
- **info** – Description to print.

Returns

Dictionary with placeholder metrics (-1 values).

```
evaluate_lp_bpe_k_vs_all(model, triples: List[List[str]], info: str | None = None,  
form_of_labelling: str | None = None) → Dict[str, float]
```

Evaluate BPE model with KvsAll scoring.

Parameters

- **model** – BPE-enabled model.
- **triples** – String triples.
- **info** – Description to print.
- **form_of_labelling** – Type of labelling.

Returns

Dictionary with H@1, H@3, **H@10**, and MRR metrics.

```
evaluate_lp(model, triple_idx, info: str) → Dict[str, float]
```

Evaluate link prediction with negative sampling.

Parameters

- **model** – The model to evaluate.
- **triple_idx** – Integer-indexed triples.
- **info** – Description to print.

Returns

Dictionary with H@1, H@3, H@10, and MRR metrics.

dummy_eval (*trained_model*, *form_of_labelling*: str) → None

Run evaluation from saved data (for continual training).

Parameters

- **trained_model** – The trained model.
- **form_of_labelling** – Type of labelling.

eval_with_data (*dataset*, *trained_model*, *triple_idx*: numpy.ndarray, *form_of_labelling*: str)

→ Dict[str, float]

Evaluate a trained model on a given dataset.

Parameters

- **dataset** – Knowledge graph dataset.
- **trained_model** – The trained model.
- **triple_idx** – Integer-indexed triples to evaluate.
- **form_of_labelling** – Type of labelling.

Returns

Dictionary with evaluation metrics.

Raises

ValueError – If scoring technique is invalid.

dicee.__version__ = '0.2.1'

Python Module Index

d

 dicee, 12
 dicee.__main__, 12
 dicee.abstracts, 12
 dicee.analyse_experiments, 19
 dicee.callbacks, 21
 dicee.config, 28
 dicee.dataset_classes, 31
 dicee.eval_static_funcs, 45
 dicee.evaluation, 48
 dicee.evaluation.ensemble, 48
 dicee.evaluation.evaluator, 49
 dicee.evaluation.link_prediction, 53
 dicee.evaluation.literal_prediction, 56
 dicee.evaluation.utils, 57
 dicee.evaluator, 67
 dicee.executer, 71
 dicee.knowledge_graph, 74
 dicee.knowledge_graph_embeddings, 76
 dicee.models, 80
 dicee.models.adopt, 80
 dicee.models.base_model, 89
 dicee.models.clifford, 98
 dicee.models.complex, 105
 dicee.models.dualE, 107
 dicee.models.ensemble, 109
 dicee.models.function_space, 109
 dicee.models.literal, 113
 dicee.models.octonion, 114
 dicee.models.pykeen_models, 118
 dicee.models.quaternion, 119
 dicee.models.real, 122
 dicee.models.static_funcs, 125
 dicee.models.transformers, 125
 dicee.query_generator, 184
 dicee.read_preprocess_save_load_kg, 186
 dicee.read_preprocess_save_load_kg.preprocess,
 186
 dicee.read_preprocess_save_load_kg.read_from_disk,
 187
 dicee.read_preprocess_save_load_kg.save_load_disk,
 187
 dicee.read_preprocess_save_load_kg.util,
 188
 dicee.sanity_checkers, 192
 dicee.scripts, 193
 dicee.scripts.index_serve, 193
 dicee.scripts.run, 194
 dicee.static_funcs, 195
 dicee.static_funcs_training, 199
 dicee.static_preprocess_funcs, 201
 dicee.trainer, 202
 dicee.trainer.dice_trainer, 202
 dicee.trainer.model_parallelism, 204
 dicee.trainer.torch_trainer, 205
 dicee.trainer.torch_trainer_ddp, 206
 dicee.weight_averaging, 209

Index

Non-alphabetical

`__call__()` (*dicee.models.base_model.IdentityClass method*), 98
`__call__()` (*dicee.models.ensemble.EnsembleKGE method*), 109
`__call__()` (*dicee.models.IdentityClass method*), 145, 159, 165
`__getitem__()` (*dicee.dataset_classes.AllvsAll method*), 35
`__getitem__()` (*dicee.dataset_classes.BPE_NegativeSamplingDataset method*), 32
`__getitem__()` (*dicee.dataset_classes.KvsAll method*), 35
`__getitem__()` (*dicee.dataset_classes.KvsSampleDataset method*), 38
`__getitem__()` (*dicee.dataset_classes.LiteralDataset method*), 44
`__getitem__()` (*dicee.dataset_classes.MultiClassClassificationDataset method*), 33
`__getitem__()` (*dicee.dataset_classes.MultiLabelDataset method*), 33
`__getitem__()` (*dicee.dataset_classes.NegSampleDataset method*), 38
`__getitem__()` (*dicee.dataset_classes.OnevsAllDataset method*), 34
`__getitem__()` (*dicee.dataset_classes.OnevsSample method*), 37
`__getitem__()` (*dicee.dataset_classes.TriplePredictionDataset method*), 39
`__iter__()` (*dicee.config.Namespace method*), 31
`__iter__()` (*dicee.knowledge_graph.KG method*), 76
`__iter__()` (*dicee.models.ensemble.EnsembleKGE method*), 109
`__len__()` (*dicee.dataset_classes.AllvsAll method*), 35
`__len__()` (*dicee.dataset_classes.BPE_NegativeSamplingDataset method*), 32
`__len__()` (*dicee.dataset_classes.KvsAll method*), 35
`__len__()` (*dicee.dataset_classes.KvsSampleDataset method*), 38
`__len__()` (*dicee.dataset_classes.LiteralDataset method*), 44
`__len__()` (*dicee.dataset_classes.MultiClassClassificationDataset method*), 33
`__len__()` (*dicee.dataset_classes.MultiLabelDataset method*), 33
`__len__()` (*dicee.dataset_classes.NegSampleDataset method*), 38
`__len__()` (*dicee.dataset_classes.OnevsAllDataset method*), 34
`__len__()` (*dicee.dataset_classes.OnevsSample method*), 37
`__len__()` (*dicee.dataset_classes.TriplePredictionDataset method*), 39
`__len__()` (*dicee.knowledge_graph.KG method*), 76
`__len__()` (*dicee.models.ensemble.EnsembleKGE method*), 109
`__setstate__()` (*dicee.models.ADOPT method*), 135
`__setstate__()` (*dicee.models.adopt.ADOPT method*), 83
`__str__()` (*dicee.KGE method*), 217
`__str__()` (*dicee.knowledge_graph_embeddings.KGE method*), 76
`__str__()` (*dicee.models.ensemble.EnsembleKGE method*), 109
`__version__` (*in module dicee*), 226

A

`AbstractCallback` (*class in dicee.abstracts*), 16
`AbstractPPECallback` (*class in dicee.abstracts*), 18
`AbstractTrainer` (*class in dicee.abstracts*), 13
`AccumulateEpochLossCallback` (*class in dicee.callbacks*), 21
`achieve_answer()` (*dicee.query_generator.QueryGenerator method*), 185
`achieve_answer()` (*dicee.QueryGenerator method*), 221
`AConEx` (*class in dicee.models*), 154
`AConEx` (*class in dicee.models.complex*), 106
`AConvO` (*class in dicee.models*), 167
`AConvO` (*class in dicee.models.octonion*), 117
`AConvQ` (*class in dicee.models*), 161
`AConvQ` (*class in dicee.models.quaternion*), 121
`adaptive_lr` (*dicee.config.Namespace attribute*), 31
`adaptive_swa` (*dicee.config.Namespace attribute*), 30
`add_new_entity_embeddings()` (*dicee.abstracts.BaseInteractiveKGE method*), 16
`add_noise_rate` (*dicee.config.Namespace attribute*), 28
`add_noise_rate` (*dicee.knowledge_graph.KG attribute*), 75
`add_noisy_triples()` (*in module dicee.static_funcs*), 198
`add_noisy_triples_into_training()` (*dicee.read_preprocess_save_load_kg.read_from_disk.ReadFromDisk method*), 187
`add_noisy_triples_into_training()` (*dicee.read_preprocess_save_load_kg.ReadFromDisk method*), 192
`add_reciprocal` (*dicee.knowledge_graph.KG attribute*), 75
`ADOPT` (*class in dicee.models*), 133
`ADOPT` (*class in dicee.models.adopt*), 82
`adopt()` (*in module dicee.models.adopt*), 85
`ALL_HITS_RANGE` (*in module dicee.evaluation*), 67
`ALL_HITS_RANGE` (*in module dicee.evaluation.utils*), 57

AllvsAll (*class in dicee.dataset_classes*), 35
 alphas (*dicee.abstracts.AbstractPPECallback attribute*), 18
 alphas (*dicee.weight_averaging.ASWA attribute*), 210
 analyse () (*in module dicee.analyse_experiments*), 21
 answer_multi_hop_query () (*dicee.KGE method*), 219
 answer_multi_hop_query () (*dicee.knowledge_graph_embeddings.KGE method*), 79
 app (*in module dicee.scripts.index_serve*), 194
 apply_coefficients () (*dicee.models.clifford.DeCaL method*), 103
 apply_coefficients () (*dicee.models.clifford.Keci method*), 100
 apply_coefficients () (*dicee.models.DeCaL method*), 173
 apply_coefficients () (*dicee.models.Keci method*), 169
 apply_reciprocal_or_noise () (*in module dicee.read_preprocess_save_load_kg.util*), 190
 apply_semantic_constraint (*dicee.abstracts.BaseInteractiveKGE attribute*), 15
 apply_unit_norm (*dicee.models.base_model.BaseKGE attribute*), 95
 apply_unit_norm (*dicee.models.BaseKGE attribute*), 143, 146, 152, 156, 162, 175, 179
 args (*dicee.DICE_Trainer attribute*), 222
 args (*dicee.evaluation.Evaluator attribute*), 60
 args (*dicee.evaluation.evaluator.Evaluator attribute*), 50, 51
 args (*dicee.Evaluator attribute*), 223, 224
 args (*dicee.evaluator.Evaluator attribute*), 68, 69
 args (*dicee.Execute attribute*), 215, 216
 args (*dicee.executor.Execute attribute*), 71, 72
 args (*dicee.models.base_model.BaseKGE attribute*), 95
 args (*dicee.models.base_model.IdentityClass attribute*), 98
 args (*dicee.models.BaseKGE attribute*), 143, 146, 152, 156, 162, 175, 178
 args (*dicee.models.ensemble.EnsembleKGE attribute*), 109
 args (*dicee.models.IdentityClass attribute*), 145, 159, 165
 args (*dicee.models.pykeen_models.PykeenKGE attribute*), 118
 args (*dicee.models.PykeenKGE attribute*), 177
 args (*dicee.trainer.DICE_Trainer attribute*), 208
 args (*dicee.trainer.dice_trainer.DICE_Trainer attribute*), 203
 ASWA (*class in dicee.weight_averaging*), 210
 awsa (*dicee.analyse_experiments.Experiment attribute*), 20
 attn (*dicee.models.Block attribute*), 148
 attn (*dicee.models.transformers.Block attribute*), 130
 attn_dropout (*dicee.models.transformers.SelfAttention attribute*), 128
 attributes (*dicee.abstracts.AbstractTrainer attribute*), 13
 auto_batch_finding (*dicee.config.Namespace attribute*), 30

B

backend (*dicee.config.Namespace attribute*), 29
 backend (*dicee.knowledge_graph.KG attribute*), 75
 base_weights (*dicee.weight_averaging.TWA attribute*), 214
 BaseInteractiveKGE (*class in dicee.abstracts*), 14
 BaseInteractiveTrainKGE (*class in dicee.abstracts*), 18
 BaseKGE (*class in dicee.models*), 142, 145, 151, 156, 162, 174, 178
 BaseKGE (*class in dicee.models.base_model*), 94
 BaseKGELightning (*class in dicee.models*), 136
 BaseKGELightning (*class in dicee.models.base_model*), 89
 batch_kronecker_product () (*dicee.callbacks.KronE static method*), 25
 batch_size (*dicee.analyse_experiments.Experiment attribute*), 20
 batch_size (*dicee.callbacks.PseudoLabellingCallback attribute*), 24
 batch_size (*dicee.config.Namespace attribute*), 28
 batch_size (*dicee.dataset_classes.CVDataModule attribute*), 40
 batches_per_epoch (*dicee.callbacks.LRScheduler attribute*), 27
 beta (*dicee.weight_averaging.TWA attribute*), 214
 bias (*dicee.models.CoKEConfig attribute*), 150
 bias (*dicee.models.real.CoKEConfig attribute*), 124
 bias (*dicee.models.transformers.GPTConfig attribute*), 130
 bias (*dicee.models.transformers.LayerNorm attribute*), 127
 Block (*class in dicee.models*), 148
 Block (*class in dicee.models.transformers*), 129
 block_size (*dicee.config.Namespace attribute*), 30
 block_size (*dicee.dataset_classes.MultiClassClassificationDataset attribute*), 33
 block_size (*dicee.models.base_model.BaseKGE attribute*), 96
 block_size (*dicee.models.BaseKGE attribute*), 144, 147, 153, 157, 163, 176, 179
 block_size (*dicee.models.CoKEConfig attribute*), 150

block_size (*dicee.models.real.CoKEConfig attribute*), 123, 124
 block_size (*dicee.models.transformers.GPTConfig attribute*), 130
 blocks (*dicee.models.CoKE attribute*), 151
 blocks (*dicee.models.real.CoKE attribute*), 124
 bn_conv1 (*dicee.models.AConvQ attribute*), 161
 bn_conv1 (*dicee.models.ConvQ attribute*), 161
 bn_conv1 (*dicee.models.quaternion.AConvQ attribute*), 121
 bn_conv1 (*dicee.models.quaternion.ConvQ attribute*), 121
 bn_conv2 (*dicee.models.AConvQ attribute*), 161
 bn_conv2 (*dicee.models.ConvQ attribute*), 161
 bn_conv2 (*dicee.models.quaternion.AConvQ attribute*), 121
 bn_conv2 (*dicee.models.quaternion.ConvQ attribute*), 121
 bn_conv2d (*dicee.models.AConEx attribute*), 154
 bn_conv2d (*dicee.models.AConvO attribute*), 167
 bn_conv2d (*dicee.models.complex.AConEx attribute*), 106
 bn_conv2d (*dicee.models.complex.ConEx attribute*), 105
 bn_conv2d (*dicee.models.ConEx attribute*), 154
 bn_conv2d (*dicee.models.ConvO attribute*), 167
 bn_conv2d (*dicee.models.octonion.AConvO attribute*), 117
 bn_conv2d (*dicee.models.octonion.ConvO attribute*), 117
 BPE_NegativeSamplingDataset (*class in dicee.dataset_classes*), 32
 build_chain_funcs () (*dicee.models.FMult2 method*), 182
 build_chain_funcs () (*dicee.models.function_space.FMult2 method*), 111
 build_func () (*dicee.models.FMult2 method*), 182
 build_func () (*dicee.models.function_space.FMult2 method*), 111
 build_projection () (*dicee.weight_averaging.TWA method*), 214
 Byte (*class in dicee.models.transformers*), 125
 byte_pair_encoding (*dicee.analyse_experiments.Experiment attribute*), 20
 byte_pair_encoding (*dicee.config.Namespace attribute*), 30
 byte_pair_encoding (*dicee.knowledge_graph.KG attribute*), 75
 byte_pair_encoding (*dicee.models.base_model.BaseKGE attribute*), 96
 byte_pair_encoding (*dicee.models.BaseKGE attribute*), 143, 147, 152, 157, 163, 176, 179

C

c_attn (*dicee.models.transformers.SelfAttention attribute*), 128
 c_fc (*dicee.models.transformers.MLP attribute*), 129
 c_proj (*dicee.models.transformers.MLP attribute*), 129
 c_proj (*dicee.models.transformers.SelfAttention attribute*), 128
 callbacks (*dicee.abstracts.AbstractTrainer attribute*), 13
 callbacks (*dicee.analyse_experiments.Experiment attribute*), 20
 callbacks (*dicee.config.Namespace attribute*), 29
 callbacks (*dicee.trainer.torch_trainer_ddp.NodeTrainer attribute*), 207
 causal (*dicee.models.CoKEConfig attribute*), 150
 causal (*dicee.models.real.CoKEConfig attribute*), 124
 causal (*dicee.models.transformers.GPTConfig attribute*), 130
 causal (*dicee.models.transformers.SelfAttention attribute*), 128
 chain_func () (*dicee.models.FMult method*), 181
 chain_func () (*dicee.models.function_space.FMult method*), 110
 chain_func () (*dicee.models.function_space.GFMult method*), 111
 chain_func () (*dicee.models.GFMult method*), 181
 CKeci (*class in dicee.models*), 171
 CKeci (*class in dicee.models.clifford*), 101
 cl_pqr () (*dicee.models.clifford.DeCaL method*), 102
 cl_pqr () (*dicee.models.DeCaL method*), 172
 cleanup () (*dicee.Execute method*), 216
 cleanup () (*dicee.executer.Execute method*), 72
 clifford_multiplication () (*dicee.models.clifford.Keci method*), 100
 clifford_multiplication () (*dicee.models.Keci method*), 169
 clip_lambda (*dicee.models.ADOPT attribute*), 135
 clip_lambda (*dicee.models.adopt.ADOPT attribute*), 83
 CoKE (*class in dicee.models*), 150
 CoKE (*class in dicee.models.real*), 124
 coke_dropout (*dicee.models.CoKE attribute*), 151
 coke_dropout (*dicee.models.real.CoKE attribute*), 124
 CoKEConfig (*class in dicee.models*), 150
 CoKEConfig (*class in dicee.models.real*), 123
 collate_fn (*dicee.dataset_classes.AllvsAll attribute*), 35

```

collate_fn (dicee.dataset_classes.KvsAll attribute), 35
collate_fn (dicee.dataset_classes.KvsSampleDataset attribute), 38
collate_fn (dicee.dataset_classes.MultiClassClassificationDataset attribute), 33
collate_fn (dicee.dataset_classes.MultiLabelDataset attribute), 33
collate_fn (dicee.dataset_classes.OnevsAllDataset attribute), 34
collate_fn (dicee.dataset_classes.OnevsSample attribute), 36, 37
collate_fn () (dicee.dataset_classes.BPE_NegativeSamplingDataset method), 32
collate_fn () (dicee.dataset_classes.TriplePredictionDataset method), 39
collection_name (dicee.scripts.index_serve.NeuralSearcher attribute), 194
comp_func () (dicee.models.function_space.LFMult method), 113
comp_func () (dicee.models.LFMult method), 183
ComplEx (class in dicee.models), 155
ComplEx (class in dicee.models.complex), 106
compute_convergence () (in module dicee.callbacks), 24
compute_func () (dicee.models.FMult method), 181
compute_func () (dicee.models.FMult2 method), 182
compute_func () (dicee.models.function_space.FMult method), 110
compute_func () (dicee.models.function_space.FMult2 method), 111
compute_func () (dicee.models.function_space.GFMult method), 110
compute_func () (dicee.models.GFMult method), 181
compute_metrics_from_ranks () (in module dicee.evaluation), 66
compute_metrics_from_ranks () (in module dicee.evaluation.utils), 58
compute_metrics_from_ranks_simple () (in module dicee.evaluation), 66
compute_metrics_from_ranks_simple () (in module dicee.evaluation.utils), 58
compute_mrr () (dicee.weight_averaging.ASWA static method), 210
compute_sigma_pp () (dicee.models.clifford.DeCaL method), 103
compute_sigma_pp () (dicee.models.clifford.Keci method), 99
compute_sigma_pp () (dicee.models.DeCaL method), 173
compute_sigma_pp () (dicee.models.Keci method), 168
compute_sigma_pq () (dicee.models.clifford.DeCaL method), 104
compute_sigma_pq () (dicee.models.clifford.Keci method), 99
compute_sigma_pq () (dicee.models.DeCaL method), 174
compute_sigma_pq () (dicee.models.Keci method), 169
compute_sigma_pr () (dicee.models.clifford.DeCaL method), 105
compute_sigma_pr () (dicee.models.DeCaL method), 174
compute_sigma_qq () (dicee.models.clifford.DeCaL method), 104
compute_sigma_qq () (dicee.models.clifford.Keci method), 99
compute_sigma_qq () (dicee.models.DeCaL method), 173
compute_sigma_qq () (dicee.models.Keci method), 169
compute_sigma_qr () (dicee.models.clifford.DeCaL method), 105
compute_sigma_qr () (dicee.models.DeCaL method), 174
compute_sigma_rr () (dicee.models.clifford.DeCaL method), 104
compute_sigma_rr () (dicee.models.DeCaL method), 174
compute_sigmas_multivect () (dicee.models.clifford.DeCaL method), 103
compute_sigmas_multivect () (dicee.models.DeCaL method), 172
compute_sigmas_single () (dicee.models.clifford.DeCaL method), 102
compute_sigmas_single () (dicee.models.DeCaL method), 172
ConEx (class in dicee.models), 153
ConEx (class in dicee.models.complex), 105
config (dicee.models.CoKE attribute), 151
config (dicee.models.real.CoKE attribute), 124
config (dicee.models.transformers.ByTE attribute), 126
config (dicee.models.transformers.GPT attribute), 131
configs (dicee.abstracts.BaseInteractiveKGE attribute), 15
configure_optimizers () (dicee.models.base_model.BaseKGELightning method), 93
configure_optimizers () (dicee.models.BaseKGELightning method), 141
configure_optimizers () (dicee.models.transformers.GPT method), 131
construct_batch_selected_cl_multivector () (dicee.models.clifford.Keci method), 100
construct_batch_selected_cl_multivector () (dicee.models.Keci method), 170
construct_cl_multivector () (dicee.models.clifford.DeCaL method), 103
construct_cl_multivector () (dicee.models.clifford.Keci method), 100
construct_cl_multivector () (dicee.models.DeCaL method), 173
construct_cl_multivector () (dicee.models.Keci method), 170
construct_dataset () (in module dicee.dataset_classes), 32
construct_ensemble (dicee.abstracts.BaseInteractiveKGE attribute), 14
construct_graph () (dicee.query_generator.QueryGenerator method), 185
construct_graph () (dicee.QueryGenerator method), 221
construct_input_and_output () (dicee.abstracts.BaseInteractiveKGE method), 16

```

```

construct_multi_coeff() (dicee.models.function_space.LFMult method), 112
construct_multi_coeff() (dicee.models.LFMult method), 183
continual_learning (dicee.config.Namespace attribute), 30
continual_start() (dicee.DICE_Trainer method), 222
continual_start() (dicee.executor.ContinuousExecute method), 73
continual_start() (dicee.trainer.DICE_Trainer method), 208
continual_start() (dicee.trainer.dice_trainer.DICE_Trainer method), 203
continual_training_setup_executor() (in module dicee.static_funcs), 199
ContinuousExecute (class in dicee.executor), 73
conv2d (dicee.models.AConEx attribute), 154
conv2d (dicee.models.AConvO attribute), 167
conv2d (dicee.models.AConvQ attribute), 161
conv2d (dicee.models.complex.AConEx attribute), 106
conv2d (dicee.models.complex.ConEx attribute), 105
conv2d (dicee.models.ConEx attribute), 154
conv2d (dicee.models.ConvO attribute), 167
conv2d (dicee.models.ConvQ attribute), 161
conv2d (dicee.models.octonion.AConvO attribute), 117
conv2d (dicee.models.octonion.ConvO attribute), 116
conv2d (dicee.models.quaternion.AConvQ attribute), 121
conv2d (dicee.models.quaternion.ConvQ attribute), 121
ConvO (class in dicee.models), 166
ConvO (class in dicee.models.octonion), 116
ConvQ (class in dicee.models), 160
ConvQ (class in dicee.models.quaternion), 121
count_triples() (in module dicee.read_preprocess_save_load_kg.util), 190
create_and_store_kg() (dicee.Execute method), 216
create_and_store_kg() (dicee.executor.Execute method), 72
create_constraints() (in module dicee.read_preprocess_save_load_kg.util), 190
create_constraints() (in module dicee.static_funcs), 202
create_experiment_folder() (in module dicee.static_funcs), 199
create_hits_dict() (in module dicee.evaluation), 67
create_hits_dict() (in module dicee.evaluation.utils), 58
create_random_data() (dicee.callbacks.PseudoLabellingCallback method), 24
create_reciprocal_triples() (in module dicee.read_preprocess_save_load_kg.util), 191
create_reciprocal_triples() (in module dicee.static_funcs), 196
create_vector_database() (dicee.KGE method), 217
create_vector_database() (dicee.knowledge_graph_embeddings.KGE method), 77
crop_block_size() (dicee.models.transformers.GPT method), 131
ctx (dicee.trainer.torch_trainer_ddp.NodeTrainer attribute), 207
current_epoch (dicee.weight_averaging.EMA attribute), 213
current_epoch (dicee.weight_averaging.SWA attribute), 211
current_epoch (dicee.weight_averaging.SWAG attribute), 212
current_epoch (dicee.weight_averaging.TWA attribute), 214
CVDataModule (class in dicee.dataset_classes), 39
cycle_length (dicee.callbacks.LRScheduler attribute), 27

```

D

```

data_module (dicee.callbacks.PseudoLabellingCallback attribute), 24
data_property_embeddings (dicee.models.literal.LiteralEmbeddings attribute), 114
data_property_to_idx (dicee.dataset_classes.LiteralDataset attribute), 44
dataset_dir (dicee.config.Namespace attribute), 28
dataset_dir (dicee.knowledge_graph.KG attribute), 74
dataset_sanity_checking() (in module dicee.read_preprocess_save_load_kg.util), 191
DeCaL (class in dicee.models), 171
DeCaL (class in dicee.models.clifford), 101
decay (dicee.weight_averaging.EMA attribute), 213
decide() (dicee.weight_averaging.ASWA method), 210
default_eval_model (dicee.callbacks.PeriodicEvalCallback attribute), 27
DEFAULT_HITS_RANGE (in module dicee.evaluation), 67
DEFAULT_HITS_RANGE (in module dicee.evaluation.utils), 57
degree (dicee.models.function_space.LFMult attribute), 112
degree (dicee.models.LFMult attribute), 182
denormalize() (dicee.dataset_classes.LiteralDataset static method), 44
describe() (dicee.knowledge_graph.KG method), 76
description_of_input (dicee.knowledge_graph.KG attribute), 76
deviations (dicee.weight_averaging.SWAG attribute), 212

```

```
device (dicee.models.literal.LiteralEmbeddings property), 114
DICE_Trainer (class in dicee), 221
DICE_Trainer (class in dicee.trainer), 208
DICE_Trainer (class in dicee.trainer.dice_trainer), 203
dicee
    module, 12
dicee.__main__
    module, 12
dicee.abstracts
    module, 12
dicee.analyse_experiments
    module, 19
dicee.callbacks
    module, 21
dicee.config
    module, 28
dicee.dataset_classes
    module, 31
dicee.eval_static_funcs
    module, 45
dicee.evaluation
    module, 48
dicee.evaluation.ensemble
    module, 48
dicee.evaluation.evaluator
    module, 49
dicee.evaluation.link_prediction
    module, 53
dicee.evaluation.literal_prediction
    module, 56
dicee.evaluation.utils
    module, 57
dicee.evaluator
    module, 67
dicee.executor
    module, 71
dicee.knowledge_graph
    module, 74
dicee.knowledge_graph_embeddings
    module, 76
dicee.models
    module, 80
dicee.models.adopt
    module, 80
dicee.models.base_model
    module, 89
dicee.models.clifford
    module, 98
dicee.models.complex
    module, 105
dicee.models.dualE
    module, 107
dicee.models.ensemble
    module, 109
dicee.models.function_space
    module, 109
dicee.models.literal
    module, 113
dicee.models.octonion
    module, 114
dicee.models.pykeen_models
    module, 118
dicee.models.quaternion
    module, 119
dicee.models.real
    module, 122
dicee.models.static_funcs
    module, 125
```

```

dicee.models.transformers
    module, 125
dicee.query_generator
    module, 184
dicee.read_preprocess_save_load_kg
    module, 186
dicee.read_preprocess_save_load_kg.preprocess
    module, 186
dicee.read_preprocess_save_load_kg.read_from_disk
    module, 187
dicee.read_preprocess_save_load_kg.save_load_disk
    module, 187
dicee.read_preprocess_save_load_kg.util
    module, 188
dicee.sanity_checkers
    module, 192
dicee.scripts
    module, 193
dicee.scripts.index_serve
    module, 193
dicee.scripts.run
    module, 194
dicee.static_funcs
    module, 195
dicee.static_funcs_training
    module, 199
dicee.static_preprocess_funcs
    module, 201
dicee.trainer
    module, 202
dicee.trainer.dice_trainer
    module, 202
dicee.trainer.model_parallelism
    module, 204
dicee.trainer.torch_trainer
    module, 205
dicee.trainer.torch_trainer_ddp
    module, 206
dicee.weight_averaging
    module, 209
discrete_points (dicee.models.FMult2 attribute), 181
discrete_points (dicee.models.function_space.FMult2 attribute), 111
dist_func (dicee.models.Pyke attribute), 150
dist_func (dicee.models.real.Pyke attribute), 123
DistMult (class in dicee.models), 149
DistMult (class in dicee.models.real), 122
distributed (dicee.Execute attribute), 215
distributed (dicee.executer.Execute attribute), 71, 72
domain_constraints_per_rel (dicee.evaluation.Evaluator attribute), 60
domain_constraints_per_rel (dicee.evaluation.evaluator.Evaluator attribute), 51
domain_constraints_per_rel (dicee.Evaluator attribute), 224
domain_constraints_per_rel (dicee.evaluator.Evaluator attribute), 69
download_file() (in module dicee.static_funcs), 199
download_files_from_url() (in module dicee.static_funcs), 199
download_pretrained_model() (in module dicee.static_funcs), 199
dropout (dicee.models.CoKEConfig attribute), 150
dropout (dicee.models.literal.LiteralEmbeddings attribute), 113, 114
dropout (dicee.models.real.CoKEConfig attribute), 124
dropout (dicee.models.transformers.GPTConfig attribute), 130
dropout (dicee.models.transformers.MLP attribute), 129
dropout (dicee.models.transformers.SelfAttention attribute), 128
DualE (class in dicee.models), 183
DualE (class in dicee.models.dualE), 108
dummy_eval() (dicee.evaluation.Evaluator method), 62
dummy_eval() (dicee.evaluation.evaluator.Evaluator method), 52
dummy_eval() (dicee.Evaluator method), 226
dummy_eval() (dicee.evaluator.Evaluator method), 70
dummy_id (dicee.knowledge_graph.KG attribute), 75

```

during_training (*dicee.evaluation.Evaluator attribute*), 60
 during_training (*dicee.evaluation.evaluator.Evaluator attribute*), 50, 51
 during_training (*dicee.Evaluator attribute*), 223, 224
 during_training (*dicee.evaluator.Evaluator attribute*), 68, 69

E

 ee_vocab (*dicee.evaluation.Evaluator attribute*), 60
 ee_vocab (*dicee.evaluation.evaluator.Evaluator attribute*), 50, 51
 ee_vocab (*dicee.Evaluator attribute*), 223, 224
 ee_vocab (*dicee.evaluator.Evaluator attribute*), 68
 efficient_zero_grad() (*in module dicee.evaluation.utils*), 58
 efficient_zero_grad() (*in module dicee.static_funcs_training*), 201
 EMA (*class in dicee.weight_averaging*), 213
 ema (*dicee.config.Namespace attribute*), 30
 ema_c_epochs (*dicee.weight_averaging.EMA attribute*), 213
 ema_model (*dicee.weight_averaging.EMA attribute*), 213
 ema_start_epoch (*dicee.weight_averaging.EMA attribute*), 213
 ema_update () (*dicee.weight_averaging.EMA static method*), 213
 embedding_dim (*dicee.analyse_experiments.Experiment attribute*), 20
 embedding_dim (*dicee.config.Namespace attribute*), 28
 embedding_dim (*dicee.models.base_model.BaseKGE attribute*), 95
 embedding_dim (*dicee.models.BaseKGE attribute*), 143, 146, 152, 156, 162, 175, 179
 embedding_dim (*dicee.models.literal.LiteralEmbeddings attribute*), 114
 embedding_dims (*dicee.models.literal.LiteralEmbeddings attribute*), 113
 enable_log (*in module dicee.static_preprocess_funcs*), 202
 enc (*dicee.knowledge_graph.KG attribute*), 75
 end () (*dicee.Execute method*), 216
 end () (*dicee.executer.Execute method*), 73
 EnsembleKGE (*class in dicee.models.ensemble*), 109
 ent2id (*dicee.query_generator.QueryGenerator attribute*), 185
 ent2id (*dicee.QueryGenerator attribute*), 221
 ent_in (*dicee.query_generator.QueryGenerator attribute*), 185
 ent_in (*dicee.QueryGenerator attribute*), 221
 ent_out (*dicee.query_generator.QueryGenerator attribute*), 185
 ent_out (*dicee.QueryGenerator attribute*), 221
 entities_str (*dicee.knowledge_graph.KG property*), 76
 entity_embeddings (*dicee.models.AConvQ attribute*), 161
 entity_embeddings (*dicee.models.clifford.DeCaL attribute*), 102
 entity_embeddings (*dicee.models.ConvQ attribute*), 161
 entity_embeddings (*dicee.models.DeCaL attribute*), 171
 entity_embeddings (*dicee.models.DualE attribute*), 184
 entity_embeddings (*dicee.models.dualE.DualE attribute*), 108
 entity_embeddings (*dicee.models.FMult attribute*), 180
 entity_embeddings (*dicee.models.FMult2 attribute*), 181
 entity_embeddings (*dicee.models.function_space.FMult attribute*), 110
 entity_embeddings (*dicee.models.function_space.FMult2 attribute*), 111
 entity_embeddings (*dicee.models.function_space.GFMult attribute*), 110
 entity_embeddings (*dicee.models.function_space.LFMult attribute*), 112
 entity_embeddings (*dicee.models.function_space.LFMult1 attribute*), 111
 entity_embeddings (*dicee.models.GFMult attribute*), 181
 entity_embeddings (*dicee.models.LFMult attribute*), 182
 entity_embeddings (*dicee.models.LFMult1 attribute*), 182
 entity_embeddings (*dicee.models.literal.LiteralEmbeddings attribute*), 113, 114
 entity_embeddings (*dicee.models.pykeen_models.PykeenKGE attribute*), 118
 entity_embeddings (*dicee.models.PykeenKGE attribute*), 177
 entity_embeddings (*dicee.models.quaternion.AConvQ attribute*), 121
 entity_embeddings (*dicee.models.quaternion.ConvQ attribute*), 121
 entity_to_idx (*dicee.dataset_classes.LiteralDataset attribute*), 43, 44
 entity_to_idx (*dicee.knowledge_graph.KG attribute*), 74, 75
 entity_to_idx (*dicee.scripts.index_serve.NeuralSearcher attribute*), 194
 epoch_count (*dicee.abstracts.AbstractPPECallback attribute*), 18
 epoch_count (*dicee.weight_averaging.ASWA attribute*), 210
 epoch_counter (*dicee.callbacks.Eval attribute*), 24
 epoch_counter (*dicee.callbacks.KGESaveCallback attribute*), 23
 epoch_counter (*dicee.callbacks.PeriodicEvalCallback attribute*), 26
 epoch_ratio (*dicee.callbacks.Eval attribute*), 24
 er_vocab (*dicee.evaluation.Evaluator attribute*), 59, 60

er_vocab (*dicee.evaluation.evaluator.Evaluator* attribute), 50
er_vocab (*dicee.Evaluator* attribute), 223, 224
er_vocab (*dicee.evaluator.Evaluator* attribute), 68
estimate_mfu () (*dicee.models.transformers.GPT* method), 131
estimate_q () (*in module dicee.callbacks*), 24
Eval (*class in dicee.callbacks*), 24
eval () (*dicee.evaluation.Evaluator* method), 61
eval () (*dicee.evaluation.evaluator.Evaluator* method), 51
eval () (*dicee.Evaluator* method), 224
eval () (*dicee.evaluator.Evaluator* method), 69
eval () (*dicee.models.ensemble.EnsembleKGE* method), 109
eval_at_epochs (*dicee.config.Namespace* attribute), 31
eval_epochs (*dicee.callbacks.PeriodicEvalCallback* attribute), 27
eval_every_n_epochs (*dicee.config.Namespace* attribute), 31
eval_lp_performance () (*dicee.KGE* method), 217
eval_lp_performance () (*dicee.knowledge_graph_embeddings.KGE* method), 77
eval_model (*dicee.config.Namespace* attribute), 29
eval_model (*dicee.knowledge_graph.KG* attribute), 75
eval_rank_of_head_and_tail_byte_pair_encoded_entity () (*dicee.evaluation.Evaluator* method), 61
eval_rank_of_head_and_tail_byte_pair_encoded_entity () (*dicee.evaluation.evaluator.Evaluator* method), 51
eval_rank_of_head_and_tail_byte_pair_encoded_entity () (*dicee.Evaluator* method), 224
eval_rank_of_head_and_tail_byte_pair_encoded_entity () (*dicee.evaluator.Evaluator* method), 69
eval_rank_of_head_and_tail_entity () (*dicee.evaluation.Evaluator* method), 61
eval_rank_of_head_and_tail_entity () (*dicee.evaluation.evaluator.Evaluator* method), 51
eval_rank_of_head_and_tail_entity () (*dicee.Evaluator* method), 224
eval_rank_of_head_and_tail_entity () (*dicee.evaluator.Evaluator* method), 69
eval_with_bpe_vs_all () (*dicee.evaluation.Evaluator* method), 61
eval_with_bpe_vs_all () (*dicee.evaluation.evaluator.Evaluator* method), 51
eval_with_bpe_vs_all () (*dicee.Evaluator* method), 224
eval_with_bpe_vs_all () (*dicee.evaluator.Evaluator* method), 69
eval_with_byte () (*dicee.evaluation.Evaluator* method), 61
eval_with_byte () (*dicee.evaluation.evaluator.Evaluator* method), 51
eval_with_byte () (*dicee.Evaluator* method), 224
eval_with_byte () (*dicee.evaluator.Evaluator* method), 69
eval_with_data () (*dicee.evaluation.Evaluator* method), 62
eval_with_data () (*dicee.evaluation.evaluator.Evaluator* method), 53
eval_with_data () (*dicee.Evaluator* method), 226
eval_with_data () (*dicee.evaluator.Evaluator* method), 71
eval_with_vs_all () (*dicee.evaluation.Evaluator* method), 61
eval_with_vs_all () (*dicee.evaluation.evaluator.Evaluator* method), 51
eval_with_vs_all () (*dicee.Evaluator* method), 225
eval_with_vs_all () (*dicee.evaluator.Evaluator* method), 69
evaluate () (*in module dicee.static_funcs*), 199
evaluate_bpe_lp () (*in module dicee.evaluation*), 64
evaluate_bpe_lp () (*in module dicee.evaluation.link_prediction*), 55
evaluate_bpe_lp () (*in module dicee.static_funcs_training*), 200
evaluate_ensemble_link_prediction_performance () (*in module dicee.eval_static_funcs*), 47
evaluate_ensemble_link_prediction_performance () (*in module dicee.evaluation*), 65
evaluate_ensemble_link_prediction_performance () (*in module dicee.evaluation.ensemble*), 49
evaluate_link_prediction_performance () (*in module dicee.eval_static_funcs*), 45
evaluate_link_prediction_performance () (*in module dicee.evaluation*), 63
evaluate_link_prediction_performance () (*in module dicee.evaluation.link_prediction*), 53
evaluate_link_prediction_performance_with_bpe () (*in module dicee.eval_static_funcs*), 46
evaluate_link_prediction_performance_with_bpe () (*in module dicee.evaluation*), 63
evaluate_link_prediction_performance_with_bpe () (*in module dicee.evaluation.link_prediction*), 54
evaluate_link_prediction_performance_with_reciprocals () (*in module dicee.eval_static_funcs*), 46
evaluate_link_prediction_performance_with_reciprocals () (*in module dicee.evaluation*), 63
evaluate_link_prediction_performance_with_reciprocals () (*in module dicee.evaluation.link_prediction*), 54
evaluate_link_prediction_performance_with_reciprocals () (*in module dicee.eval_static_funcs*), 45
evaluate_link_prediction_performance_with_reciprocals () (*in module dicee.evaluation*), 63
evaluate_link_prediction_performance_with_reciprocals () (*in module dicee.evaluation.link_prediction*), 54
evaluate_literal_prediction () (*in module dicee.eval_static_funcs*), 47
evaluate_literal_prediction () (*in module dicee.evaluation*), 65
evaluate_literal_prediction () (*in module dicee.evaluation.literal_prediction*), 56
evaluate_lp () (*dicee.evaluation.Evaluator* method), 62
evaluate_lp () (*dicee.evaluation.evaluator.Evaluator* method), 52
evaluate_lp () (*dicee.Evaluator* method), 225
evaluate_lp () (*dicee.evaluator.Evaluator* method), 70

```

evaluate_lp() (in module dicee.evaluation), 64
evaluate_lp() (in module dicee.evaluation.link_prediction), 54
evaluate_lp() (in module dicee.static_funcs_training), 200
evaluate_lp_bpe_k_vs_all() (dicee.evaluation.Evaluator method), 62
evaluate_lp_bpe_k_vs_all() (dicee.evaluation.evaluator.Evaluator method), 52
evaluate_lp_bpe_k_vs_all() (dicee.Evaluator method), 225
evaluate_lp_bpe_k_vs_all() (dicee.evaluator.Evaluator method), 70
evaluate_lp_bpe_k_vs_all() (in module dicee.eval_static_funcs), 46
evaluate_lp_bpe_k_vs_all() (in module dicee.evaluation), 64
evaluate_lp_bpe_k_vs_all() (in module dicee.evaluation.link_prediction), 55
evaluate_lp_k_vs_all() (dicee.evaluation.Evaluator method), 61
evaluate_lp_k_vs_all() (dicee.evaluation.evaluator.Evaluator method), 52
evaluate_lp_k_vs_all() (dicee.Evaluator method), 225
evaluate_lp_k_vs_all() (dicee.evaluator.Evaluator method), 69
evaluate_lp_with_byte() (dicee.evaluation.Evaluator method), 61
evaluate_lp_with_byte() (dicee.evaluation.evaluator.Evaluator method), 52
evaluate_lp_with_byte() (dicee.Evaluator method), 225
evaluate_lp_with_byte() (dicee.evaluator.Evaluator method), 70
Evaluator (class in dicee), 223
Evaluator (class in dicee.evaluation), 59
Evaluator (class in dicee.evaluation.evaluator), 50
Evaluator (class in dicee.evaluator), 68
evaluator (dicee.DICE_Trainer attribute), 222
evaluator (dicee.Execute attribute), 215, 216
evaluator (dicee.executer.Execute attribute), 72
evaluator (dicee.trainer.DICE_Trainer attribute), 208
evaluator (dicee.trainer.dice_trainer.DICE_Trainer attribute), 203
every_x_epoch (dicee.callbacks.KGESaveCallback attribute), 23
example_input_array (dicee.models.ensemble.EnsembleKGE property), 109
Execute (class in dicee), 215
Execute (class in dicee.executer), 71
exists() (dicee.knowledge_graph.KG method), 76
Experiment (class in dicee.analyse_experiments), 20
experiment_dir (dicee.callbacks.LRScheduler attribute), 27
experiment_dir (dicee.callbacks.PeriodicEvalCallback attribute), 26
explicit (dicee.models.QMult attribute), 160
explicit (dicee.models.quaternion.QMult attribute), 120
exponential_function() (in module dicee.static_funcs), 199
extract_input_outputs() (dicee.trainer.torch_trainer_ddp.NodeTrainer method), 208
extract_input_outputs() (in module dicee.trainer.model_parallelism), 205
extract_input_outputs_set_device() (dicee.trainer.torch_trainer.TorchTrainer method), 206

```

F

```

f (dicee.callbacks.KronE attribute), 25
fc (dicee.models.literal.LiteralEmbeddings attribute), 114
fc1 (dicee.models.AConEx attribute), 154
fc1 (dicee.models.AConvO attribute), 167
fc1 (dicee.models.AConvQ attribute), 161
fc1 (dicee.models.complex.AConEx attribute), 106
fc1 (dicee.models.complex.ConEx attribute), 105
fc1 (dicee.models.ConEx attribute), 154
fc1 (dicee.models.ConvO attribute), 167
fc1 (dicee.models.ConvQ attribute), 161
fc1 (dicee.models.octonion.AConvO attribute), 117
fc1 (dicee.models.octonion.ConvO attribute), 116
fc1 (dicee.models.quaternion.AConvQ attribute), 121
fc1 (dicee.models.quaternion.ConvQ attribute), 121
fc_num_input (dicee.models.AConEx attribute), 154
fc_num_input (dicee.models.AConvO attribute), 167
fc_num_input (dicee.models.AConvQ attribute), 161
fc_num_input (dicee.models.complex.AConEx attribute), 106
fc_num_input (dicee.models.complex.ConEx attribute), 105
fc_num_input (dicee.models.ConEx attribute), 154
fc_num_input (dicee.models.ConvO attribute), 167
fc_num_input (dicee.models.ConvQ attribute), 161
fc_num_input (dicee.models.octonion.AConvO attribute), 117
fc_num_input (dicee.models.octonion.ConvO attribute), 116

```

fc_num_input (*dicee.models.quaternion.AConvQ attribute*), 121
 fc_num_input (*dicee.models.quaternion.ConvQ attribute*), 121
 fc_out (*dicee.models.literal.LiteralEmbeddings attribute*), 114
 feature_map_dropout (*dicee.models.AConEx attribute*), 154
 feature_map_dropout (*dicee.models.AConvO attribute*), 167
 feature_map_dropout (*dicee.models.AConvQ attribute*), 161
 feature_map_dropout (*dicee.models.complex.AConEx attribute*), 106
 feature_map_dropout (*dicee.models.complex.ConEx attribute*), 105
 feature_map_dropout (*dicee.models.ConEx attribute*), 154
 feature_map_dropout (*dicee.models.ConvO attribute*), 167
 feature_map_dropout (*dicee.models.ConvQ attribute*), 161
 feature_map_dropout (*dicee.models.octonion.AConvO attribute*), 117
 feature_map_dropout (*dicee.models.octonion.ConvO attribute*), 117
 feature_map_dropout (*dicee.models.quaternion.AConvQ attribute*), 121
 feature_map_dropout (*dicee.models.quaternion.ConvQ attribute*), 121
 feature_map_dropout_rate (*dicee.config.Namespace attribute*), 30
 feature_map_dropout_rate (*dicee.models.base_model.BaseKGE attribute*), 95
 feature_map_dropout_rate (*dicee.models.BaseKGE attribute*), 143, 146, 152, 157, 163, 175, 179
 fetch_worker () (*in module dicee.read_preprocess_save_load_kg.util*), 190
 fill_query () (*dicee.query_generator.QueryGenerator method*), 185
 fill_query () (*dicee.QueryGenerator method*), 221
 find_good_batch_size () (*in module dicee.trainer.model_parallelism*), 205
 find_missing_triples () (*dicee.KGE method*), 220
 find_missing_triples () (*dicee.knowledge_graph_embeddings.KGE method*), 79
 fit () (*dicee.trainer.model_parallelism.TensorParallel method*), 205
 fit () (*dicee.trainer.torch_trainer_ddp.TorchDDPTrainer method*), 207
 fit () (*dicee.trainer.torch_trainer.TorchTrainer method*), 206
 flash (*dicee.models.transformers.SelfAttention attribute*), 128
 FMult (*class in dicee.models*), 180
 FMult (*class in dicee.models.function_space*), 110
 FMult2 (*class in dicee.models*), 181
 FMult2 (*class in dicee.models.function_space*), 111
 form_of_labelling (*dicee.DICE_Trainer attribute*), 222
 form_of_labelling (*dicee.trainer.DICE_Trainer attribute*), 208
 form_of_labelling (*dicee.trainer.dice_trainer.DICE_Trainer attribute*), 203
 forward () (*dicee.models.base_model.BaseKGE method*), 96
 forward () (*dicee.models.base_model.IdentityClass static method*), 98
 forward () (*dicee.models.BaseKGE method*), 144, 147, 153, 157, 163, 176, 180
 forward () (*dicee.models.Block method*), 149
 forward () (*dicee.models.IdentityClass static method*), 145, 159, 165
 forward () (*dicee.models.literal.LiteralEmbeddings method*), 114
 forward () (*dicee.models.transformers.Block method*), 130
 forward () (*dicee.models.transformers.BytE method*), 126
 forward () (*dicee.models.transformers.GPT method*), 131
 forward () (*dicee.models.transformers.LayerNorm method*), 127
 forward () (*dicee.models.transformers.MLP method*), 129
 forward () (*dicee.models.transformers.SelfAttention method*), 128
 forward_backward_update () (*dicee.trainer.torch_trainer.TorchTrainer method*), 206
 forward_backward_update_loss () (*in module dicee.trainer.model_parallelism*), 205
 forward_byte_pair_encoded_k_vs_all () (*dicee.models.base_model.BaseKGE method*), 96
 forward_byte_pair_encoded_k_vs_all () (*dicee.models.BaseKGE method*), 144, 147, 153, 157, 163, 176, 179
 forward_byte_pair_encoded_triple () (*dicee.models.base_model.BaseKGE method*), 96
 forward_byte_pair_encoded_triple () (*dicee.models.BaseKGE method*), 144, 147, 153, 157, 163, 176, 179
 forward_k_vs_all () (*dicee.models.AConEx method*), 154
 forward_k_vs_all () (*dicee.models.AConvO method*), 167
 forward_k_vs_all () (*dicee.models.AConvQ method*), 162
 forward_k_vs_all () (*dicee.models.base_model.BaseKGE method*), 97
 forward_k_vs_all () (*dicee.models.BaseKGE method*), 144, 147, 153, 158, 164, 177, 180
 forward_k_vs_all () (*dicee.models.clifford.DeCaL method*), 103
 forward_k_vs_all () (*dicee.models.clifford.Keci method*), 100
 forward_k_vs_all () (*dicee.models.CoKE method*), 151
 forward_k_vs_all () (*dicee.models.ComplEx method*), 155
 forward_k_vs_all () (*dicee.models.complex.AConEx method*), 106
 forward_k_vs_all () (*dicee.models.complex.ComplEx method*), 107
 forward_k_vs_all () (*dicee.models.complex.ConEx method*), 106
 forward_k_vs_all () (*dicee.models.ConEx method*), 154
 forward_k_vs_all () (*dicee.models.ConvO method*), 167
 forward_k_vs_all () (*dicee.models.ConvQ method*), 161

```

forward_k_vs_all() (dicee.models.DeCaL method), 172
forward_k_vs_all() (dicee.models.DistMult method), 149
forward_k_vs_all() (dicee.models.DualE method), 184
forward_k_vs_all() (dicee.models.dualE.DualE method), 108
forward_k_vs_all() (dicee.models.Keci method), 170
forward_k_vs_all() (dicee.models.octonion.AConvO method), 117
forward_k_vs_all() (dicee.models.octonion.ConvO method), 117
forward_k_vs_all() (dicee.models.octonion.QMult method), 116
forward_k_vs_all() (dicee.models.QMult method), 166
forward_k_vs_all() (dicee.models.pykeen_models.PykeenKGE method), 118
forward_k_vs_all() (dicee.models.PykeenKGE method), 177
forward_k_vs_all() (dicee.models.QMult method), 160
forward_k_vs_all() (dicee.models.quaternion.AConvQ method), 122
forward_k_vs_all() (dicee.models.quaternion.ConvQ method), 121
forward_k_vs_all() (dicee.models.quaternion.QMult method), 120
forward_k_vs_all() (dicee.models.real.CoKE method), 124
forward_k_vs_all() (dicee.models.real.DistMult method), 122
forward_k_vs_all() (dicee.models.real.Shallom method), 123
forward_k_vs_all() (dicee.models.real.TransE method), 123
forward_k_vs_all() (dicee.models.Shallom method), 149
forward_k_vs_all() (dicee.models.TransE method), 149
forward_k_vs_sample() (dicee.models.AConEx method), 155
forward_k_vs_sample() (dicee.models.base_model.BaseKGE method), 97
forward_k_vs_sample() (dicee.models.BaseKGE method), 144, 147, 153, 158, 164, 177, 180
forward_k_vs_sample() (dicee.models.clifford.Keci method), 101
forward_k_vs_sample() (dicee.models.CoKE method), 151
forward_k_vs_sample() (dicee.models.ComplEx method), 156
forward_k_vs_sample() (dicee.models.complex.AConEx method), 106
forward_k_vs_sample() (dicee.models.complex.ComplEx method), 107
forward_k_vs_sample() (dicee.models.complex.ConEx method), 106
forward_k_vs_sample() (dicee.models.ConEx method), 154
forward_k_vs_sample() (dicee.models.DistMult method), 149
forward_k_vs_sample() (dicee.models.Keci method), 170
forward_k_vs_sample() (dicee.models.pykeen_models.PykeenKGE method), 119
forward_k_vs_sample() (dicee.models.PykeenKGE method), 178
forward_k_vs_sample() (dicee.models.QMult method), 160
forward_k_vs_sample() (dicee.models.quaternion.QMult method), 120
forward_k_vs_sample() (dicee.models.real.CoKE method), 124
forward_k_vs_sample() (dicee.models.real.DistMult method), 122
forward_k_vs_with_explicit() (dicee.models.clifford.Keci method), 100
forward_k_vs_with_explicit() (dicee.models.Keci method), 170
forward_triples() (dicee.models.AConEx method), 154
forward_triples() (dicee.models.AConvO method), 167
forward_triples() (dicee.models.AConvQ method), 161
forward_triples() (dicee.models.base_model.BaseKGE method), 96
forward_triples() (dicee.models.BaseKGE method), 144, 147, 153, 158, 164, 176, 180
forward_triples() (dicee.models.clifford.DeCaL method), 102
forward_triples() (dicee.models.clifford.Keci method), 101
forward_triples() (dicee.models.complex.AConEx method), 106
forward_triples() (dicee.models.complex.ConEx method), 106
forward_triples() (dicee.models.ConEx method), 154
forward_triples() (dicee.models.ConvO method), 167
forward_triples() (dicee.models.ConvQ method), 161
forward_triples() (dicee.models.DeCaL method), 172
forward_triples() (dicee.models.DualE method), 184
forward_triples() (dicee.models.dualE.DualE method), 108
forward_triples() (dicee.models.FMult method), 181
forward_triples() (dicee.models.FMult2 method), 182
forward_triples() (dicee.models.function_space.FMult method), 110
forward_triples() (dicee.models.function_space.FMult2 method), 111
forward_triples() (dicee.models.function_space.GFMult method), 111
forward_triples() (dicee.models.function_space.LFMult method), 112
forward_triples() (dicee.models.function_space.LFMult1 method), 111
forward_triples() (dicee.models.GFMult method), 181
forward_triples() (dicee.models.Keci method), 171
forward_triples() (dicee.models.LFMult method), 182
forward_triples() (dicee.models.LFMult1 method), 182
forward_triples() (dicee.models.octonion.AConvO method), 117

```

```

forward_triples() (dicee.models.octonion.ConvO method), 117
forward_triples() (dicee.models.Pyke method), 150
forward_triples() (dicee.models.pykeen_models.PykeenKGE method), 118
forward_triples() (dicee.models.PykeenKGE method), 178
forward_triples() (dicee.models.quaternion.ACConvQ method), 122
forward_triples() (dicee.models.quaternion.ConvQ method), 121
forward_triples() (dicee.models.real.Pyke method), 123
forward_triples() (dicee.models.real.Shallom method), 123
forward_triples() (dicee.models.Shallom method), 149
freeze_entity_embeddings (dicee.models.literal.LiteralEmbeddings attribute), 114
frequency (dicee.callbacks.Perturb attribute), 26
from_pretrained() (dicee.models.transformers.GPT class method), 131
from_pretrained_model_write_embeddings_into_csv() (in module dicee.static_funcs), 199
full_storage_path (dicee.analyse_experiments.Experiment attribute), 20
func_triple_to_bpe_representation (dicee.evaluation.Evaluator attribute), 60
func_triple_to_bpe_representation (dicee.evaluation.evaluator.Evaluator attribute), 51
func_triple_to_bpe_representation (dicee.Evaluator attribute), 224
func_triple_to_bpe_representation (dicee.evaluator.Evaluator attribute), 68
func_triple_to_bpe_representation() (dicee.knowledge_graph.KG method), 76
function() (dicee.models.FMult2 method), 182
function() (dicee.models.function_space.FMult2 method), 111

```

G

```

gamma (dicee.models.FMult attribute), 181
gamma (dicee.models.function_space.FMult attribute), 110
gate_residual (dicee.models.literal.LiteralEmbeddings attribute), 113, 114
gated_residual_proj (dicee.models.literal.LiteralEmbeddings attribute), 114
gelu (dicee.models.transformers.MLP attribute), 129
gen_test (dicee.query_generator.QueryGenerator attribute), 185
gen_test (dicee.QueryGenerator attribute), 220
gen_valid (dicee.query_generator.QueryGenerator attribute), 185
gen_valid (dicee.QueryGenerator attribute), 220
generate() (dicee.KGE method), 217
generate() (dicee.knowledge_graph_embeddings.KGE method), 77
generate() (dicee.models.transformers.ByE method), 126
generate_queries() (dicee.query_generator.QueryGenerator method), 185
generate_queries() (dicee.QueryGenerator method), 221
get_aswa_state_dict() (dicee.weight_averaging.ASWA method), 210
get_bpe_head_and_relation_representation() (dicee.models.base_model.BaseKGE method), 97
get_bpe_head_and_relation_representation() (dicee.models.BaseKGE method), 144, 148, 153, 158, 164, 177, 180
get_bpe_token_representation() (dicee.abstracts.BaseInteractiveKGE method), 15
get_callbacks() (in module dicee.trainer.dice_trainer), 203
get_default_arguments() (in module dicee.analyse_experiments), 20
get_default_arguments() (in module dicee.scripts.index_serve), 194
get_default_arguments() (in module dicee.scripts.run), 195
get_ee_vocab() (in module dicee.read_preprocess_save_load_kg.util), 190
get_ee_vocab() (in module dicee.static_funcs), 197
get_ee_vocab() (in module dicee.static_preprocess_funcs), 202
get_embeddings() (dicee.models.base_model.BaseKGE method), 97
get_embeddings() (dicee.models.BaseKGE method), 144, 148, 153, 158, 164, 177, 180
get_embeddings() (dicee.models.ensemble.EnsembleKGE method), 109
get_embeddings() (dicee.models.real.Shallom method), 123
get_embeddings() (dicee.models.Shallom method), 149
get_entity_embeddings() (dicee.abstracts.BaseInteractiveKGE method), 16
get_entity_index() (dicee.abstracts.BaseInteractiveKGE method), 15
get_er_vocab() (in module dicee.read_preprocess_save_load_kg.util), 190
get_er_vocab() (in module dicee.static_funcs), 196
get_er_vocab() (in module dicee.static_preprocess_funcs), 202
get_eval_report() (dicee.abstracts.BaseInteractiveKGE method), 15
get_head_relation_representation() (dicee.models.base_model.BaseKGE method), 97
get_head_relation_representation() (dicee.models.BaseKGE method), 144, 147, 153, 158, 164, 177, 180
get_kronecker_triple_representation() (dicee.callbacks.KronE method), 25
get_mean_and_var() (dicee.weight_averaging.SWAG method), 212
get_num_params() (dicee.models.transformers.GPT method), 131
get_padded_bpe_triple_representation() (dicee.abstracts.BaseInteractiveKGE method), 15
get_queries() (dicee.query_generator.QueryGenerator method), 186
get_queries() (dicee.QueryGenerator method), 221

```

get_re_vocab() (in module dicee.read_preprocess_save_load_kg.util), 190
get_re_vocab() (in module dicee.static_funcs), 196
get_re_vocab() (in module dicee.static_preprocess_funcs), 202
get_relation_embeddings() (dicee.abstracts.BaseInteractiveKGE method), 16
get_relation_index() (dicee.abstracts.BaseInteractiveKGE method), 15
get_sentence_representation() (dicee.models.base_model.BaseKGE method), 97
get_sentence_representation() (dicee.models.BaseKGE method), 144, 147, 153, 158, 164, 177, 180
get_transductive_entity_embeddings() (dicee.KGE method), 217
get_transductive_entity_embeddings() (dicee.knowledge_graph_embeddings.KGE method), 77
get_triple_representation() (dicee.models.base_model.BaseKGE method), 97
get_triple_representation() (dicee.models.BaseKGE method), 144, 147, 153, 158, 164, 177, 180
GFMult (class in dicee.models), 181
GFMult (class in dicee.models.function_space), 110
global_rank (dicee.abstracts.AbstractTrainer attribute), 13
global_rank (dicee.trainer.torch_trainer_ddp.NodeTrainer attribute), 207
GPT (class in dicee.models.transformers), 130
GPTConfig (class in dicee.models.transformers), 130
gpus (dicee.config.Namespace attribute), 29
gradient_accumulation_steps (dicee.config.Namespace attribute), 29
ground_queries() (dicee.query_generator.QueryGenerator method), 185
ground_queries() (dicee.QueryGenerator method), 221
gswa_n (dicee.weight_averaging.SWAG attribute), 212

H

hidden_dim (dicee.models.literal.LiteralEmbeddings attribute), 114
hidden_dropout (dicee.models.base_model.BaseKGE attribute), 96
hidden_dropout (dicee.models.BaseKGE attribute), 143, 147, 152, 157, 163, 176, 179
hidden_dropout_rate (dicee.config.Namespace attribute), 30
hidden_dropout_rate (dicee.models.base_model.BaseKGE attribute), 95
hidden_dropout_rate (dicee.models.BaseKGE attribute), 143, 146, 152, 157, 163, 175, 179
hidden_normalizer (dicee.models.base_model.BaseKGE attribute), 96
hidden_normalizer (dicee.models.BaseKGE attribute), 143, 147, 152, 157, 163, 176, 179

I

IdentityClass (class in dicee.models), 144, 158, 164
IdentityClass (class in dicee.models.base_model), 97
idx_entity_to_bpe_shaped (dicee.knowledge_graph.KG attribute), 75
index() (in module dicee.scripts.index_serve), 194
index_triple() (dicee.abstracts.BaseInteractiveKGE method), 15
init_dataloader() (dicee.DICE_Trainer method), 222
init_dataloader() (dicee.trainer.DICE_Trainer method), 209
init_dataloader() (dicee.trainer.dice_trainer.DICE_Trainer method), 204
init_dataset() (dicee.DICE_Trainer method), 222
init_dataset() (dicee.trainer.DICE_Trainer method), 209
init_dataset() (dicee.trainer.dice_trainer.DICE_Trainer method), 204
init_param (dicee.config.Namespace attribute), 29
init_params_with_sanity_checking() (dicee.models.base_model.BaseKGE method), 96
init_params_with_sanity_checking() (dicee.models.BaseKGE method), 144, 147, 153, 157, 163, 176, 180
initial_eval_setting (dicee.weight_averaging.ASWA attribute), 210
initialize_or_load_model() (dicee.DICE_Trainer method), 222
initialize_or_load_model() (dicee.trainer.DICE_Trainer method), 209
initialize_or_load_model() (dicee.trainer.dice_trainer.DICE_Trainer method), 204
initialize_trainer() (dicee.DICE_Trainer method), 222
initialize_trainer() (dicee.trainer.DICE_Trainer method), 209
initialize_trainer() (dicee.trainer.dice_trainer.DICE_Trainer method), 204
initialize_trainer() (in module dicee.trainer.dice_trainer), 203
input_dp_ent_real (dicee.models.base_model.BaseKGE attribute), 96
input_dp_ent_real (dicee.models.BaseKGE attribute), 143, 147, 152, 157, 163, 176, 179
input_dp_rel_real (dicee.models.base_model.BaseKGE attribute), 96
input_dp_rel_real (dicee.models.BaseKGE attribute), 143, 147, 152, 157, 163, 176, 179
input_dropout_rate (dicee.config.Namespace attribute), 30
input_dropout_rate (dicee.models.base_model.BaseKGE attribute), 95
input_dropout_rate (dicee.models.BaseKGE attribute), 143, 146, 152, 156, 163, 175, 179
InteractiveQueryDecomposition (class in dicee.abstracts), 16
initialize_model() (in module dicee.static_funcs), 198
is_continual_training (dicee.DICE_Trainer attribute), 222
is_continual_training (dicee.evaluation.Evaluator attribute), 60

is_continual_training (*dicee.evaluation.evaluator.Evaluator* attribute), 51
is_continual_training (*dicee.Evaluator* attribute), 224
is_continual_training (*dicee.evaluator.Evaluator* attribute), 68
is_continual_training (*dicee.Execute* attribute), 216
is_continual_training (*dicee.executer.Execute* attribute), 72
is_continual_training (*dicee.trainer.DICE_Trainer* attribute), 208
is_continual_training (*dicee.trainer.dice_trainer.DICE_Trainer* attribute), 203
is_global_zero (*dicee.absts.AbstractTrainer* attribute), 13
is_rank_zero () (*dicee.Execute* method), 216
is_rank_zero () (*dicee.executer.Execute* method), 72
is_seen () (*dicee.absts.BaseInteractiveKGE* method), 15
is_sparql_endpoint_alive () (*in module dicee.sanity_checkers*), 193

K

k (*dicee.models.FMult* attribute), 180
k (*dicee.models.FMult2* attribute), 181
k (*dicee.models.function_space.FMult* attribute), 110
k (*dicee.models.function_space.FMult2* attribute), 111
k (*dicee.models.function_space.GFMult* attribute), 110
k (*dicee.models.GFMult* attribute), 181
k_fold_cross_validation () (*dicee.DICE_Trainer* method), 223
k_fold_cross_validation () (*dicee.trainer.DICE_Trainer* method), 209
k_fold_cross_validation () (*dicee.trainer.dice_trainer.DICE_Trainer* method), 204
k_vs_all_score () (*dicee.models.clifford.Keci* method), 100
k_vs_all_score () (*dicee.models.ComplEx* static method), 155
k_vs_all_score () (*dicee.models.complex.ComplEx* static method), 107
k_vs_all_score () (*dicee.models.DistMult* method), 149
k_vs_all_score () (*dicee.models.Keci* method), 170
k_vs_all_score () (*dicee.models.octonion.OMult* method), 116
k_vs_all_score () (*dicee.models.OMult* method), 166
k_vs_all_score () (*dicee.models.QMult* method), 160
k_vs_all_score () (*dicee.models.quaternion.QMult* method), 120
k_vs_all_score () (*dicee.models.real.DistMult* method), 122
Keci (*class in dicee.models*), 168
Keci (*class in dicee.models.clifford*), 98
kernel_size (*dicee.config.Namespace* attribute), 30
kernel_size (*dicee.models.base_model.BaseKGE* attribute), 95
kernel_size (*dicee.models.BaseKGE* attribute), 143, 146, 152, 157, 163, 175, 179
KG (*class in dicee.knowledge_graph*), 74
kg (*dicee.callbacks.PseudoLabellingCallback* attribute), 24
kg (*dicee.read_preprocess_save_load_kg.LoadSaveToDisk* attribute), 192
kg (*dicee.read_preprocess_save_load_kg.PreprocessKG* attribute), 191
kg (*dicee.read_preprocess_save_load_kg.preprocess.PreprocessKG* attribute), 186
kg (*dicee.read_preprocess_save_load_kg.read_from_disk.ReadFromDisk* attribute), 187
kg (*dicee.read_preprocess_save_load_kg.ReadFromDisk* attribute), 192
kg (*dicee.read_preprocess_save_load_kg.save_load_disk.LoadSaveToDisk* attribute), 187
KGE (*class in dicee*), 217
KGE (*class in dicee.knowledge_graph_embeddings*), 76
KGESaveCallback (*class in dicee.callbacks*), 22
knowledge_graph (*dicee.Execute* attribute), 215, 216
knowledge_graph (*dicee.executer.Execute* attribute), 72
KronE (*class in dicee.callbacks*), 25
KvsAll (*class in dicee.dataset_classes*), 34
kvsall_score () (*dicee.models.DualE* method), 184
kvsall_score () (*dicee.models.dualE.DualE* method), 108
KvsSampleDataset (*class in dicee.dataset_classes*), 37

L

label_smoothing_rate (*dicee.config.Namespace* attribute), 29
label_smoothing_rate (*dicee.dataset_classes.AllvsAll* attribute), 35
label_smoothing_rate (*dicee.dataset_classes.KvsAll* attribute), 35
label_smoothing_rate (*dicee.dataset_classes.KvsSampleDataset* attribute), 38
label_smoothing_rate (*dicee.dataset_classes.OnesvsSample* attribute), 36, 37
label_smoothing_rate (*dicee.dataset_classes.TriplePredictionDataset* attribute), 39
labels (*dicee.dataset_classes.NegSampleDataset* attribute), 38
layer_norm (*dicee.models.literal.LiteralEmbeddings* attribute), 114
LayerNorm (*class in dicee.models.transformers*), 127

learning_rate (*dicee.models.base_model.BaseKGE* attribute), 95
 learning_rate (*dicee.models.BaseKGE* attribute), 143, 146, 152, 156, 162, 175, 179
 length (*dicee.dataset_classes.NegSampleDataset* attribute), 38
 length (*dicee.dataset_classes.TriplePredictionDataset* attribute), 39
 level (*dicee.callbacks.Perturb* attribute), 26
 LFMult (class in *dicee.models*), 182
 LFMult (class in *dicee.models.function_space*), 112
 LFMult1 (class in *dicee.models*), 182
 LFMult1 (class in *dicee.models.function_space*), 111
 linear () (*dicee.models.function_space.LFMult* method), 112
 linear () (*dicee.models.LFMult* method), 183
 list2tuple () (*dicee.query_generator.QueryGenerator* method), 185
 list2tuple () (*dicee.QueryGenerator* method), 221
 LiteralDataset (class in *dicee.dataset_classes*), 43
 LiteralEmbeddings (class in *dicee.models.literal*), 113
 lm_head (*dicee.models.transformers.BytE* attribute), 126
 lm_head (*dicee.models.transformers.GPT* attribute), 131
 ln_1 (*dicee.models.Block* attribute), 148
 ln_1 (*dicee.models.transformers.Block* attribute), 130
 ln_2 (*dicee.models.Block* attribute), 148
 ln_2 (*dicee.models.transformers.Block* attribute), 130
 ln_f (*dicee.models.CoKE* attribute), 151
 ln_f (*dicee.models.real.CoKE* attribute), 124
 load () (*dicee.read_preprocess_save_load_kg.LoadSaveToDisk* method), 192
 load () (*dicee.read_preprocess_save_load_kg.save_load_disk.LoadSaveToDisk* method), 187
 load_and_validate_literal_data () (*dicee.dataset_classes.LiteralDataset* static method), 44
 load_from_memmap () (*dicee.Execute* method), 216
 load_from_memmap () (*dicee.executer.Execute* method), 72
 load_json () (in module *dicee.static_funcs*), 198
 load_model () (in module *dicee.static_funcs*), 197
 load_model_ensemble () (in module *dicee.static_funcs*), 198
 load_numpy () (in module *dicee.static_funcs*), 199
 load_numpy_ndarray () (in module *dicee.read_preprocess_save_load_kg.util*), 191
 load_pickle () (in module *dicee.read_preprocess_save_load_kg.util*), 191
 load_pickle () (in module *dicee.static_funcs*), 197
 load_queries () (*dicee.query_generator.QueryGenerator* method), 186
 load_queries () (*dicee.QueryGenerator* method), 221
 load_queries_and_answers () (*dicee.query_generator.QueryGenerator* static method), 186
 load_queries_and_answers () (*dicee.QueryGenerator* static method), 221
 load_state_dict () (*dicee.models.ensemble.EnsembleKGE* method), 109
 load_term_mapping () (in module *dicee.static_funcs*), 197
 load_term_mapping () (in module *dicee.trainer.dice_trainer*), 202
 load_with_pandas () (in module *dicee.read_preprocess_save_load_kg.util*), 191
 loader_backend (*dicee.dataset_classes.LiteralDataset* attribute), 44
 LoadSaveToDisk (class in *dicee.read_preprocess_save_load_kg*), 192
 LoadSaveToDisk (class in *dicee.read_preprocess_save_load_kg.save_load_disk*), 187
 local_rank (*dicee.abstracts.AbstractTrainer* attribute), 13
 local_rank (*dicee.Execute* attribute), 215
 local_rank (*dicee.executer.Execute* attribute), 71
 local_rank (*dicee.trainer.torch_trainer_ddp.NodeTrainer* attribute), 207
 loss (*dicee.models.base_model.BaseKGE* attribute), 96
 loss (*dicee.models.BaseKGE* attribute), 143, 146, 152, 157, 163, 176, 179
 loss_func (*dicee.trainer.torch_trainer_ddp.NodeTrainer* attribute), 207
 loss_function (*dicee.trainer.torch_trainer.TorchTrainer* attribute), 206
 loss_function () (*dicee.models.base_model.BaseKGELightning* method), 91
 loss_function () (*dicee.models.BaseKGELightning* method), 138
 loss_function () (*dicee.models.transformers.BytE* method), 126
 loss_history (*dicee.models.base_model.BaseKGE* attribute), 96
 loss_history (*dicee.models.BaseKGE* attribute), 143, 147, 152, 157, 163, 176, 179
 loss_history (*dicee.models.pykeen_models.PykeenKGE* attribute), 118
 loss_history (*dicee.models.PykeenKGE* attribute), 177
 loss_history (*dicee.trainer.torch_trainer_ddp.NodeTrainer* attribute), 207
 lr (*dicee.analyse_experiments.Experiment* attribute), 20
 lr (*dicee.config.Namespace* attribute), 28
 lr_init (*dicee.weight_averaging.SWA* attribute), 211
 lr_init (*dicee.weight_averaging.SWAG* attribute), 212
 lr_init (*dicee.weight_averaging.TWA* attribute), 214
 lr_lambda (*dicee.callbacks.LRScheduler* attribute), 27

LRScheduler (*class in dicee.callbacks*), 27

M

m (*dicee.models.function_space.LFMult attribute*), 112
m (*dicee.models.LFMult attribute*), 182
main () (*in module dicee.scripts.index_serve*), 194
main () (*in module dicee.scripts.run*), 195
make_iterable_verbose () (*in module dicee.evaluation*), 67
make_iterable_verbose () (*in module dicee.evaluation.utils*), 57
make_iterable_verbose () (*in module dicee.static_funcs_training*), 200
make_iterable_verbose () (*in module dicee.trainer.torch_trainer_ddp*), 207
mapping_from_first_two_cols_to_third () (*in module dicee.static_preprocess_funcs*), 202
margin (*dicee.models.Pyke attribute*), 150
margin (*dicee.models.real.Pyke attribute*), 123
margin (*dicee.models.real.TransE attribute*), 123
margin (*dicee.models.TransE attribute*), 149
mask_emb (*dicee.models.CoKE attribute*), 151
mask_emb (*dicee.models.real.CoKE attribute*), 124
max_ans_num (*dicee.query_generator.QueryGenerator attribute*), 185
max_ans_num (*dicee.QueryGenerator attribute*), 221
max_epochs (*dicee.callbacks.KGESaveCallback attribute*), 23
max_epochs (*dicee.callbacks.PeriodicEvalCallback attribute*), 26
max_epochs (*dicee.weight_averaging.EMA attribute*), 213
max_epochs (*dicee.weight_averaging.SWA attribute*), 211
max_epochs (*dicee.weight_averaging.SWAG attribute*), 212
max_epochs (*dicee.weight_averaging.TWA attribute*), 214
max_length_subword_tokens (*dicee.knowledge_graph.KG attribute*), 75
max_length_subword_tokens (*dicee.models.base_model.BaseKGE attribute*), 96
max_length_subword_tokens (*dicee.models.BaseKGE attribute*), 143, 147, 153, 157, 163, 176, 179
max_num_models (*dicee.weight_averaging.SWAG attribute*), 212
max_num_of_classes (*dicee.dataset_classes.KvsSampleDataset attribute*), 38
mean (*dicee.weight_averaging.SWAG attribute*), 212
mem_of_model () (*dicee.models.base_model.BaseKGELightning method*), 89
mem_of_model () (*dicee.models.BaseKGELightning method*), 137
mem_of_model () (*dicee.models.ensemble.EnsembleKGE method*), 109
method (*dicee.callbacks.Perturb attribute*), 26
MLP (*class in dicee.models.transformers*), 128
mlp (*dicee.models.Block attribute*), 149
mlp (*dicee.models.transformers.Block attribute*), 130
mode (*dicee.query_generator.QueryGenerator attribute*), 185
mode (*dicee.QueryGenerator attribute*), 221
model (*dicee.config.Namespace attribute*), 28
model (*dicee.models.pykeen_models.PykeenKGE attribute*), 118
model (*dicee.models.PykeenKGE attribute*), 177
model (*dicee.trainer.torch_trainer_ddp.NodeTrainer attribute*), 207
model (*dicee.trainer.torch_trainer.TorchTrainer attribute*), 206
model_kwarg (*dicee.models.pykeen_models.PykeenKGE attribute*), 118
model_kwarg (*dicee.models.PykeenKGE attribute*), 177
model_name (*dicee.analyse_experiments.Experiment attribute*), 20
MODEL_REGISTRY (*in module dicee.static_funcs*), 196
module
 dicee, 12
 dicee.__main__, 12
 dicee.abstracts, 12
 dicee.analyse_experiments, 19
 dicee.callbacks, 21
 dicee.config, 28
 dicee.dataset_classes, 31
 dicee.eval_static_funcs, 45
 dicee.evaluation, 48
 dicee.evaluation.ensemble, 48
 dicee.evaluation.evaluator, 49
 dicee.evaluation.link_prediction, 53
 dicee.evaluation.literal_prediction, 56
 dicee.evaluation.utils, 57
 dicee.evaluator, 67
 dicee.executer, 71

```

dicee.knowledge_graph, 74
dicee.knowledge_graph_embeddings, 76
dicee.models, 80
dicee.models.adopt, 80
dicee.models.base_model, 89
dicee.models.clifford, 98
dicee.models.complex, 105
dicee.models.dualE, 107
dicee.models.ensemble, 109
dicee.models.function_space, 109
dicee.models.literal, 113
dicee.models.octonion, 114
dicee.models.pykeen_models, 118
dicee.models.quaternion, 119
dicee.models.real, 122
dicee.models.static_funcs, 125
dicee.models.transformers, 125
dicee.query_generator, 184
dicee.read_preprocess_save_load_kg, 186
dicee.read_preprocess_save_load_kg.preprocess, 186
dicee.read_preprocess_save_load_kg.read_from_disk, 187
dicee.read_preprocess_save_load_kg.save_load_disk, 187
dicee.read_preprocess_save_load_kg.util, 188
dicee.sanity_checkers, 192
dicee.scripts, 193
dicee.scripts.index_serve, 193
dicee.scripts.run, 194
dicee.static_funcs, 195
dicee.static_funcs_training, 199
dicee.static_preprocess_funcs, 201
dicee.trainer, 202
dicee.trainer.dice_trainer, 202
dicee.trainer.model_parallelism, 204
dicee.trainer.torch_trainer, 205
dicee.trainer.torch_trainer_ddp, 206
dicee.weight_averaging, 209
modules() (dicee.models.ensemble.EnsembleKGE method), 109
moving_average() (dicee.weight_averaging.SWA static method), 211
MultiClassClassificationDataset (class in dicee.dataset_classes), 33
MultiLabelDataset (class in dicee.dataset_classes), 32

```

N

```

n (dicee.models.FMult2 attribute), 181
n (dicee.models.function_space.FMult2 attribute), 111
n_embd (dicee.models.CoKEConfig attribute), 150
n_embd (dicee.models.real.CoKEConfig attribute), 124
n_embd (dicee.models.transformers.GPTConfig attribute), 130
n_embd (dicee.models.transformers.SelfAttention attribute), 128
n_epochs_eval_model (dicee.callbacks.PeriodicEvalCallback attribute), 26
n_epochs_eval_model (dicee.config.Namespace attribute), 31
n_head (dicee.models.CoKEConfig attribute), 150
n_head (dicee.models.real.CoKEConfig attribute), 123, 124
n_head (dicee.models.transformers.GPTConfig attribute), 130
n_head (dicee.models.transformers.SelfAttention attribute), 128
n_layer (dicee.models.CoKEConfig attribute), 150
n_layer (dicee.models.real.CoKEConfig attribute), 123, 124
n_layer (dicee.models.transformers.GPTConfig attribute), 130
n_layers (dicee.models.FMult2 attribute), 181
n_layers (dicee.models.function_space.FMult2 attribute), 111
name (dicee.abstracts.BaseInteractiveKGE property), 15
name (dicee.models.AConEx attribute), 154
name (dicee.models.AConvO attribute), 167
name (dicee.models.AConvQ attribute), 161
name (dicee.models.CKeci attribute), 171
name (dicee.models.clifford.CKeci attribute), 101
name (dicee.models.clifford.DeCaL attribute), 102
name (dicee.models.clifford.Keci attribute), 99

```

name (*dicee.models.CoKE attribute*), 151
 name (*dicee.models.ComplEx attribute*), 155
 name (*dicee.models.complex.AConEx attribute*), 106
 name (*dicee.models.complex.ComplEx attribute*), 107
 name (*dicee.models.complex.ConEx attribute*), 105
 name (*dicee.models.ConEx attribute*), 154
 name (*dicee.models.ConvO attribute*), 167
 name (*dicee.models.ConvQ attribute*), 161
 name (*dicee.models.DeCaL attribute*), 171
 name (*dicee.models.DistMult attribute*), 149
 name (*dicee.models.DualE attribute*), 183
 name (*dicee.models.dualE.DualE attribute*), 108
 name (*dicee.models.ensemble.EnsembleKGE attribute*), 109
 name (*dicee.models.FMult attribute*), 180
 name (*dicee.models.FMult2 attribute*), 181
 name (*dicee.models.function_space.FMult attribute*), 110
 name (*dicee.models.function_space.FMult2 attribute*), 111
 name (*dicee.models.function_space.GFMult attribute*), 110
 name (*dicee.models.function_space.LFMult attribute*), 112
 name (*dicee.models.function_space.LFMult1 attribute*), 111
 name (*dicee.models.GFMult attribute*), 181
 name (*dicee.models.Keci attribute*), 168
 name (*dicee.models.LFMult attribute*), 182
 name (*dicee.models.LFMult1 attribute*), 182
 name (*dicee.models.octonion.ACConvO attribute*), 117
 name (*dicee.models.octonion.ConvO attribute*), 116
 name (*dicee.models.octonion.OMult attribute*), 115
 name (*dicee.models.OMult attribute*), 166
 name (*dicee.models.Pyke attribute*), 150
 name (*dicee.models.pykeen_models.PykeenKGE attribute*), 118
 name (*dicee.models.PykeenKGE attribute*), 177
 name (*dicee.models.QMult attribute*), 160
 name (*dicee.models.quaternion.ACConvQ attribute*), 121
 name (*dicee.models.quaternion.ConvQ attribute*), 121
 name (*dicee.models.quaternion.QMult attribute*), 120
 name (*dicee.models.real.CoKE attribute*), 124
 name (*dicee.models.real.DistMult attribute*), 122
 name (*dicee.models.real.Pyke attribute*), 123
 name (*dicee.models.real.Shallom attribute*), 123
 name (*dicee.models.real.TransE attribute*), 123
 name (*dicee.models.Shallom attribute*), 149
 name (*dicee.models.TransE attribute*), 149
 name (*dicee.models.transformers.BytE attribute*), 126
 named_children () (*dicee.models.ensemble.EnsembleKGE method*), 109
 Namespace (*class in dicee.config*), 28
 neg_ratio (*dicee.config.Namespace attribute*), 29
 neg_ratio (*dicee.dataset_classes.BPE_NegativeSamplingDataset attribute*), 32
 neg_ratio (*dicee.dataset_classes.KvsSampleDataset attribute*), 38
 neg_sample_ratio (*dicee.dataset_classes.CVDataModule attribute*), 40
 neg_sample_ratio (*dicee.dataset_classes.NegSampleDataset attribute*), 38
 neg_sample_ratio (*dicee.dataset_classes.OnevsSample attribute*), 36, 37
 neg_sample_ratio (*dicee.dataset_classes.TriplePredictionDataset attribute*), 39
 negnorm () (*dicee.abstracts.InteractiveQueryDecomposition method*), 16
 NegSampleDataset (*class in dicee.dataset_classes*), 38
 neural_searcher (*in module dicee.scripts.index_serve*), 194
 NeuralSearcher (*class in dicee.scripts.index_serve*), 194
 NodeTrainer (*class in dicee.trainer.torch_trainer_ddp*), 207
 norm_fc1 (*dicee.models.AConEx attribute*), 154
 norm_fc1 (*dicee.models.ACConvO attribute*), 167
 norm_fc1 (*dicee.models.complex.AConEx attribute*), 106
 norm_fc1 (*dicee.models.complex.ConEx attribute*), 105
 norm_fc1 (*dicee.models.ConEx attribute*), 154
 norm_fc1 (*dicee.models.ConvO attribute*), 167
 norm_fc1 (*dicee.models.octonion.ACConvO attribute*), 117
 norm_fc1 (*dicee.models.octonion.ConvO attribute*), 117
 normalization (*dicee.analyse_experiments.Experiment attribute*), 20
 normalization (*dicee.config.Namespace attribute*), 29
 normalization (*dicee.dataset_classes.LiteralDataset attribute*), 43

```

normalization_params (dicee.dataset_classes.LiteralDataset attribute), 43, 44
normalization_type (dicee.dataset_classes.LiteralDataset attribute), 44
normalize_head_entity_embeddings (dicee.models.base_model.BaseKGE attribute), 96
normalize_head_entity_embeddings (dicee.models.BaseKGE attribute), 143, 146, 152, 157, 163, 176, 179
normalize_relation_embeddings (dicee.models.base_model.BaseKGE attribute), 96
normalize_relation_embeddings (dicee.models.BaseKGE attribute), 143, 146, 152, 157, 163, 176, 179
normalize_tail_entity_embeddings (dicee.models.base_model.BaseKGE attribute), 96
normalize_tail_entity_embeddings (dicee.models.BaseKGE attribute), 143, 147, 152, 157, 163, 176, 179
normalizer_class (dicee.models.base_model.BaseKGE attribute), 96
normalizer_class (dicee.models.BaseKGE attribute), 143, 146, 152, 157, 163, 176, 179
num_bpe_entities (dicee.dataset_classes.BPE_NegativeSamplingDataset attribute), 32
num_bpe_entities (dicee.knowledge_graph.KG attribute), 75
num_core (dicee.config.Namespace attribute), 29
num_data_properties (dicee.dataset_classes.LiteralDataset attribute), 44
num_datapoints (dicee.dataset_classes.BPE_NegativeSamplingDataset attribute), 32
num_datapoints (dicee.dataset_classes.MultiLabelDataset attribute), 33
num_ent (dicee.models.DualE attribute), 184
num_ent (dicee.models.dualE.DualE attribute), 108
num_entities (dicee.dataset_classes.CVDataModule attribute), 40
num_entities (dicee.dataset_classes.KvsSampleDataset attribute), 38
num_entities (dicee.dataset_classes.LiteralDataset attribute), 43, 44
num_entities (dicee.dataset_classes.NegSampleDataset attribute), 38
num_entities (dicee.dataset_classes.OnevsSample attribute), 36
num_entities (dicee.dataset_classes.TriplePredictionDataset attribute), 39
num_entities (dicee.evaluation.Evaluator attribute), 60
num_entities (dicee.evaluation.evaluator.Evaluator attribute), 50, 51
num_entities (dicee.Evaluator attribute), 223, 224
num_entities (dicee.evaluator.Evaluator attribute), 68, 69
num_entities (dicee.knowledge_graph.KG attribute), 74, 75
num_entities (dicee.models.base_model.BaseKGE attribute), 95
num_entities (dicee.models.BaseKGE attribute), 143, 146, 152, 156, 162, 175, 179
num_epochs (dicee.abstracts.AbstractPPECallback attribute), 18
num_epochs (dicee.analyse_experiments.Experiment attribute), 20
num_epochs (dicee.config.Namespace attribute), 28
num_epochs (dicee.trainer.torch_trainer_ddp.NodeTrainer attribute), 207
num_epochs (dicee.weight_averaging.ASWA attribute), 210
num_folds_for_cv (dicee.config.Namespace attribute), 29
num_of_data_points (dicee.dataset_classes.MultiClassClassificationDataset attribute), 33
num_of_data_properties (dicee.models.literal.LiteralEmbeddings attribute), 113, 114
num_of_epochs (dicee.callbacks.PseudoLabellingCallback attribute), 24
num_of_output_channels (dicee.config.Namespace attribute), 30
num_of_output_channels (dicee.models.base_model.BaseKGE attribute), 96
num_of_output_channels (dicee.models.BaseKGE attribute), 143, 146, 152, 157, 163, 176, 179
num_params (dicee.analyse_experiments.Experiment attribute), 20
num_relations (dicee.dataset_classes.CVDataModule attribute), 40
num_relations (dicee.dataset_classes.NegSampleDataset attribute), 38
num_relations (dicee.dataset_classes.OnevsSample attribute), 36
num_relations (dicee.dataset_classes.TriplePredictionDataset attribute), 39
num_relations (dicee.evaluation.Evaluator attribute), 60
num_relations (dicee.evaluation.evaluator.Evaluator attribute), 50, 51
num_relations (dicee.Evaluator attribute), 223, 224
num_relations (dicee.evaluator.Evaluator attribute), 68, 69
num_relations (dicee.knowledge_graph.KG attribute), 74, 75
num_relations (dicee.models.base_model.BaseKGE attribute), 95
num_relations (dicee.models.BaseKGE attribute), 143, 146, 152, 156, 162, 175, 179
num_sample (dicee.models.FMult attribute), 180
num_sample (dicee.models.function_space.FMult attribute), 110
num_sample (dicee.models.function_space.GFMult attribute), 110
num_sample (dicee.models.GFMult attribute), 181
num_samples (dicee.weight_averaging.TWA attribute), 214
num_tokens (dicee.knowledge_graph.KG attribute), 75
num_tokens (dicee.models.base_model.BaseKGE attribute), 95
num_tokens (dicee.models.BaseKGE attribute), 143, 146, 152, 156, 162, 175, 179
num_workers (dicee.dataset_classes.CVDataModule attribute), 40
numpy_data_type_changer () (in module dicee.static_funcs), 198

```

O

octonion_mul () (in module dicee.models), 165
octonion_mul () (in module dicee.models.octonion), 115
octonion_mul_norm () (in module dicee.models), 165
octonion_mul_norm () (in module dicee.models.octonion), 115
octonion_normalizer () (dicee.models.AConvO static method), 167
octonion_normalizer () (dicee.models.ConvO static method), 167
octonion_normalizer () (dicee.models.octonion.AConvO static method), 117
octonion_normalizer () (dicee.models.octonion.ConvO static method), 117
octonion_normalizer () (dicee.models.octonion.OMult static method), 116
octonion_normalizer () (dicee.models.OMult static method), 166
OMult (class in dicee.models), 165
OMult (class in dicee.models.octonion), 115
on_epoch_end () (dicee.callbacks.KGESaveCallback method), 24
on_epoch_end () (dicee.callbacks.PseudoLabellingCallback method), 24
on_fit_end () (dicee.abstracts.AbstractCallback method), 17
on_fit_end () (dicee.abstracts.AbstractPPECallback method), 18
on_fit_end () (dicee.abstracts.AbstractTrainer method), 13
on_fit_end () (dicee.callbacks.AccumulateEpochLossCallback method), 21
on_fit_end () (dicee.callbacks.Eval method), 25
on_fit_end () (dicee.callbacks.KGESaveCallback method), 23
on_fit_end () (dicee.callbacks.LRScheduler method), 27
on_fit_end () (dicee.callbacks.PeriodicEvalCallback method), 27
on_fit_end () (dicee.callbacks.PrintCallback method), 22
on_fit_end () (dicee.weight_averaging.ASWA method), 210
on_fit_end () (dicee.weight_averaging.EMA method), 213
on_fit_end () (dicee.weight_averaging.SWA method), 211
on_fit_end () (dicee.weight_averaging.SWAG method), 212
on_fit_end () (dicee.weight_averaging.TWA method), 214
on_fit_start () (dicee.abstracts.AbstractCallback method), 17
on_fit_start () (dicee.abstracts.AbstractPPECallback method), 18
on_fit_start () (dicee.abstracts.AbstractTrainer method), 13
on_fit_start () (dicee.callbacks.Eval method), 24
on_fit_start () (dicee.callbacks.KGESaveCallback method), 23
on_fit_start () (dicee.callbacks.KronE method), 26
on_fit_start () (dicee.callbacks.PrintCallback method), 22
on_init_end () (dicee.abstracts.AbstractCallback method), 17
on_init_start () (dicee.abstracts.AbstractCallback method), 16
on_train_batch_end () (dicee.abstracts.AbstractCallback method), 17
on_train_batch_end () (dicee.abstracts.AbstractTrainer method), 14
on_train_batch_end () (dicee.callbacks.Eval method), 25
on_train_batch_end () (dicee.callbacks.KGESaveCallback method), 23
on_train_batch_end () (dicee.callbacks.LRScheduler method), 27
on_train_batch_end () (dicee.callbacks.PrintCallback method), 22
on_train_batch_start () (dicee.callbacks.Perturb method), 26
on_train_epoch_end () (dicee.abstracts.AbstractCallback method), 17
on_train_epoch_end () (dicee.abstracts.AbstractTrainer method), 14
on_train_epoch_end () (dicee.callbacks.Eval method), 25
on_train_epoch_end () (dicee.callbacks.KGESaveCallback method), 23
on_train_epoch_end () (dicee.callbacks.PeriodicEvalCallback method), 27
on_train_epoch_end () (dicee.callbacks.PrintCallback method), 22
on_train_epoch_end () (dicee.models.base_model.BaseKGELightning method), 91
on_train_epoch_end () (dicee.models.BaseKGELightning method), 138
on_train_epoch_end () (dicee.weight_averaging.ASWA method), 210
on_train_epoch_end () (dicee.weight_averaging.EMA method), 213
on_train_epoch_end () (dicee.weight_averaging.SWA method), 211
on_train_epoch_end () (dicee.weight_averaging.SWAG method), 212
on_train_epoch_end () (dicee.weight_averaging.TWA method), 214
on_train_epoch_start () (dicee.abstracts.AbstractTrainer method), 13
on_train_epoch_start () (dicee.weight_averaging.EMA method), 213
on_train_epoch_start () (dicee.weight_averaging.SWA method), 211
on_train_epoch_start () (dicee.weight_averaging.SWAG method), 212
on_train_epoch_start () (dicee.weight_averaging.TWA method), 214
on_train_start () (dicee.callbacks.LRScheduler method), 27
OnevsAllDataset (class in dicee.dataset_classes), 33
OnevsSample (class in dicee.dataset_classes), 35
optim (dicee.config.Namespace attribute), 28
optimizer (dicee.trainer.torch_trainer_ddp.NodeTrainer attribute), 207

```

optimizer (dicee.trainer.torch_trainer.TorchTrainer attribute), 206
optimizer_name (dicee.models.base_model.BaseKGE attribute), 95
optimizer_name (dicee.models.BaseKGE attribute), 143, 146, 152, 157, 163, 175, 179
ordered_bpe_entities (dicee.dataset_classes.BPE_NegativeSamplingDataset attribute), 32
ordered_bpe_entities (dicee.knowledge_graph.KG attribute), 76
ordered_shaped_bpe_tokens (dicee.knowledge_graph.KG attribute), 75

P

p (dicee.config.Namespace attribute), 30
p (dicee.models.clifford.DeCaL attribute), 102
p (dicee.models.clifford.Keci attribute), 99
p (dicee.models.DeCaL attribute), 172
p (dicee.models.Keci attribute), 168
p (dicee.weight_averaging.TWA attribute), 214
padding (dicee.knowledge_graph.KG attribute), 75
pandas_dataframe_indexer () (in module dicee.read_preprocess_save_load_kg.util), 189
param_init (dicee.models.base_model.BaseKGE attribute), 96
param_init (dicee.models.BaseKGE attribute), 143, 147, 152, 157, 163, 176, 179
parameters () (dicee.abstracts.BaseInteractiveKGE method), 16
parameters () (dicee.models.ensemble.EnsembleKGE method), 109
path (dicee.abstracts.AbstractPPECallback attribute), 18
path (dicee.callbacks.AccumulateEpochLossCallback attribute), 21
path (dicee.callbacks.Eval attribute), 24
path (dicee.callbacks.KGESaveCallback attribute), 23
path (dicee.weight_averaging.ASWA attribute), 210
path_dataset_folder (dicee.analyse_experiments.Experiment attribute), 20
path_for_deserialization (dicee.knowledge_graph.KG attribute), 75
path_for_serialization (dicee.knowledge_graph.KG attribute), 75
path_single_kg (dicee.config.Namespace attribute), 28
path_single_kg (dicee.knowledge_graph.KG attribute), 75
path_to_store_single_run (dicee.config.Namespace attribute), 28
PeriodicEvalCallback (class in dicee.callbacks), 26
Perturb (class in dicee.callbacks), 26
polars_dataframe_indexer () (in module dicee.read_preprocess_save_load_kg.util), 188
poly_NN () (dicee.models.function_space.LFMult method), 112
poly_NN () (dicee.models.LFMult method), 183
polynomial () (dicee.models.function_space.LFMult method), 113
polynomial () (dicee.models.LFMult method), 183
pop () (dicee.models.function_space.LFMult method), 113
pop () (dicee.models.LFMult method), 183
pos_emb (dicee.models.CoKE attribute), 151
pos_emb (dicee.models.real.CoKE attribute), 124
pq (dicee.analyse_experiments.Experiment attribute), 20
predict () (dicee.KGE method), 218
predict () (dicee.knowledge_graph_embeddings.KGE method), 78
predict_dataloader () (dicee.models.base_model.BaseKGELightning method), 92
predict_dataloader () (dicee.models.BaseKGELightning method), 140
predict_literals () (dicee.KGE method), 220
predict_literals () (dicee.knowledge_graph_embeddings.KGE method), 80
predict_missing_head_entity () (dicee.KGE method), 217
predict_missing_head_entity () (dicee.knowledge_graph_embeddings.KGE method), 77
predict_missing_relations () (dicee.KGE method), 218
predict_missing_relations () (dicee.knowledge_graph_embeddings.KGE method), 77
predict_missing_tail_entity () (dicee.KGE method), 218
predict_missing_tail_entity () (dicee.knowledge_graph_embeddings.KGE method), 77
predict_topk () (dicee.KGE method), 218
predict_topk () (dicee.knowledge_graph_embeddings.KGE method), 78
prepare_data () (dicee.dataset_classes.CVDataModule method), 42
preprocess_with_byte_pair_encoding () (dicee.read_preprocess_save_load_kg.PreprocessKG method), 191
preprocess_with_byte_pair_encoding () (dicee.read_preprocess_save_load_kg.preprocess.PreprocessKG method), 186
preprocess_with_byte_pair_encoding_with_padding () (dicee.read_preprocess_save_load_kg.PreprocessKG method), 192
preprocess_with_byte_pair_encoding_with_padding () (dicee.read_preprocess_save_load_kg.preprocess.PreprocessKG method), 186
preprocess_with_pandas () (dicee.read_preprocess_save_load_kg.PreprocessKG method), 192
preprocess_with_pandas () (dicee.read_preprocess_save_load_kg.preprocess.PreprocessKG method), 186
preprocess_with_polars () (dicee.read_preprocess_save_load_kg.PreprocessKG method), 192
preprocess_with_polars () (dicee.read_preprocess_save_load_kg.preprocess.PreprocessKG method), 186
preprocesses_input_args () (in module dicee.static_preprocess_funcs), 202

```

PreprocessKG (class in dicee.read_preprocess_save_load_kg), 191
PreprocessKG (class in dicee.read_preprocess_save_load_kg.preprocess), 186
PrintCallback (class in dicee.callbacks), 22
process (dicee.trainer.torch_trainer.TorchTrainer attribute), 206
PseudoLabellingCallback (class in dicee.callbacks), 24
Pyke (class in dicee.models), 149
Pyke (class in dicee.models.real), 123
pykeen_model_kwarg (dicee.config.Namespace attribute), 30
PykeenKGE (class in dicee.models), 177
PykeenKGE (class in dicee.models.pykeen_models), 118

Q

q (dicee.config.Namespace attribute), 30
q (dicee.models.clifford.DeCaL attribute), 102
q (dicee.models.clifford.Keci attribute), 99
q (dicee.models.DeCaL attribute), 172
q (dicee.models.Keci attribute), 168
qdant_client (dicee.scripts.index_serve.NeuralSearcher attribute), 194
QMult (class in dicee.models), 159
QMult (class in dicee.models.quaternion), 119
quaternion_mul () (in module dicee.models), 156
quaternion_mul () (in module dicee.models.static_funcs), 125
quaternion_mul_with_unit_norm () (in module dicee.models), 159
quaternion_mul_with_unit_norm () (in module dicee.models.quaternion), 119
quaternion_multiplication_followed_by_inner_product () (dicee.models.QMult method), 160
quaternion_multiplication_followed_by_inner_product () (dicee.models.quaternion.QMult method), 120
quaternion_normalizer () (dicee.models.QMult static method), 160
quaternion_normalizer () (dicee.models.quaternion.QMult static method), 120
queries (dicee.scripts.index_serve.StringListRequest attribute), 194
query_name_to_struct (dicee.query_generator.QueryGenerator attribute), 185
query_name_to_struct (dicee.QueryGenerator attribute), 221
QueryGenerator (class in dicee), 220
QueryGenerator (class in dicee.query_generator), 185

R

r (dicee.models.clifford.DeCaL attribute), 102
r (dicee.models.clifford.Keci attribute), 99
r (dicee.models.DeCaL attribute), 172
r (dicee.models.Keci attribute), 168
random_seed (dicee.config.Namespace attribute), 29
range_constraints_per_rel (dicee.evaluation.Evaluator attribute), 60
range_constraints_per_rel (dicee.evaluation.evaluator.Evaluator attribute), 51
range_constraints_per_rel (dicee.Evaluator attribute), 224
range_constraints_per_rel (dicee.evaluator.Evaluator attribute), 69
rank (dicee.Execute attribute), 215
rank (dicee.executer.Execute attribute), 71
ratio (dicee.callbacks.Perturb attribute), 26
raw_test_set (dicee.knowledge_graph.KG attribute), 75
raw_train_set (dicee.knowledge_graph.KG attribute), 75
raw_valid_set (dicee.knowledge_graph.KG attribute), 75
re (dicee.models.clifford.DeCaL attribute), 102
re (dicee.models.DeCaL attribute), 172
re_vocab (dicee.evaluation.Evaluator attribute), 60
re_vocab (dicee.evaluation.evaluator.Evaluator attribute), 50
re_vocab (dicee.Evaluator attribute), 223
re_vocab (dicee.evaluator.Evaluator attribute), 68
read_from_disk () (in module dicee.read_preprocess_save_load_kg.util), 190
read_from_triple_store_with_pandas () (in module dicee.read_preprocess_save_load_kg.util), 190
read_from_triple_store_with_polars () (in module dicee.read_preprocess_save_load_kg.util), 190
read_only_few (dicee.config.Namespace attribute), 30
read_only_few (dicee.knowledge_graph.KG attribute), 75
read_or_load_kg () (in module dicee.static_funcs), 198
read_with_pandas () (in module dicee.read_preprocess_save_load_kg.util), 190
read_with_polars () (in module dicee.read_preprocess_save_load_kg.util), 190
ReadFromDisk (class in dicee.read_preprocess_save_load_kg), 192
ReadFromDisk (class in dicee.read_preprocess_save_load_kg.read_from_disk), 187
reducer (dicee.scripts.index_serve.StringListRequest attribute), 194

reg_lambda (*dicee.weight_averaging.TWA attribute*), 214
 rel2id (*dicee.query_generator.QueryGenerator attribute*), 185
 rel2id (*dicee.QueryGenerator attribute*), 221
 relation_embeddings (*dicee.models.AConvQ attribute*), 161
 relation_embeddings (*dicee.models.clifford.DeCaL attribute*), 102
 relation_embeddings (*dicee.models.ConvQ attribute*), 161
 relation_embeddings (*dicee.models.DeCaL attribute*), 172
 relation_embeddings (*dicee.models.DualE attribute*), 184
 relation_embeddings (*dicee.models.dualE.DualE attribute*), 108
 relation_embeddings (*dicee.models.FMult attribute*), 180
 relation_embeddings (*dicee.models.FMult2 attribute*), 182
 relation_embeddings (*dicee.models.function_space.FMult attribute*), 110
 relation_embeddings (*dicee.models.function_space.FMult2 attribute*), 111
 relation_embeddings (*dicee.models.function_space.GFMult attribute*), 110
 relation_embeddings (*dicee.models.function_space.LFMult attribute*), 112
 relation_embeddings (*dicee.models.function_space.LFMultI attribute*), 111
 relation_embeddings (*dicee.models.GFMult attribute*), 181
 relation_embeddings (*dicee.models.LFMult attribute*), 182
 relation_embeddings (*dicee.models.LFMultI attribute*), 182
 relation_embeddings (*dicee.models.pykeen_models.PykeenKGE attribute*), 118
 relation_embeddings (*dicee.models.PykeenKGE attribute*), 177
 relation_embeddings (*dicee.models.quaternion.AConvQ attribute*), 121
 relation_embeddings (*dicee.models.quaternion.ConvQ attribute*), 121
 relation_to_idx (*dicee.knowledge_graph.KG attribute*), 74, 75
 relations_str (*dicee.knowledge_graph.KG property*), 76
 reload_dataset () (in module *dicee.dataset_classes*), 32
 report (*dicee.DICE_Trainer attribute*), 222
 report (*dicee.evaluation.Evaluator attribute*), 60
 report (*dicee.evaluation.evaluator.Evaluator attribute*), 50, 51
 report (*dicee.Evaluator attribute*), 223, 224
 report (*dicee.evaluator.Evaluator attribute*), 68, 69
 report (*dicee.Execute attribute*), 215, 216
 report (*dicee.executer.Execute attribute*), 72
 report (*dicee.trainer.DICE_Trainer attribute*), 208
 report (*dicee.trainer.dice_trainer.DICE_Trainer attribute*), 203
 reports (*dicee.callbacks.Eval attribute*), 24
 reports (*dicee.callbacks.PeriodicEvalCallback attribute*), 26
 requires_grad_for_interactions (*dicee.models.CKeci attribute*), 171
 requires_grad_for_interactions (*dicee.models.clifford.CKeci attribute*), 101
 requires_grad_for_interactions (*dicee.models.clifford.Keci attribute*), 99
 requires_grad_for_interactions (*dicee.models.Keci attribute*), 168
 resid_dropout (*dicee.models.transformers.SelfAttention attribute*), 128
 residual_convolution () (*dicee.models.AConEx method*), 154
 residual_convolution () (*dicee.models.AConvO method*), 167
 residual_convolution () (*dicee.models.AConvQ method*), 161
 residual_convolution () (*dicee.models.complex.AConEx method*), 106
 residual_convolution () (*dicee.models.complex.ConEx method*), 105
 residual_convolution () (*dicee.models.ConEx method*), 154
 residual_convolution () (*dicee.models.ConvO method*), 167
 residual_convolution () (*dicee.models.ConvQ method*), 161
 residual_convolution () (*dicee.models.octonion.AConvO method*), 117
 residual_convolution () (*dicee.models.octonion.ConvO method*), 117
 residual_convolution () (*dicee.models.quaternion.AConvQ method*), 122
 residual_convolution () (*dicee.models.quaternion.ConvQ method*), 121
 retrieve_embedding () (*dicee.scripts.index_serve.NeuralSearcher method*), 194
 retrieve_embeddings () (in module *dicee.scripts.index_serve*), 194
 return_multi_hop_query_results () (*dicee.KGE method*), 219
 return_multi_hop_query_results () (*dicee.knowledge_graph_embeddings.KGE method*), 79
 root () (in module *dicee.scripts.index_serve*), 194
 roots (*dicee.models.FMult attribute*), 181
 roots (*dicee.models.function_space.FMult attribute*), 110
 roots (*dicee.models.function_space.GFMult attribute*), 110
 roots (*dicee.models.GFMult attribute*), 181
 runtime (*dicee.analyse_experiments.Experiment attribute*), 20

S

sample () (*dicee.weight_averaging.SWAG method*), 212

sample_counter (*dicee.abstracts.AbstractPPECallback attribute*), 18
 sample_entity () (*dicee.abstracts.BaseInteractiveKGE method*), 15
 sample_relation () (*dicee.abstracts.BaseInteractiveKGE method*), 15
 sample_triples_ratio (*dicee.config.Namespace attribute*), 30
 sample_triples_ratio (*dicee.knowledge_graph.KG attribute*), 75
 sample_weights () (*dicee.weight_averaging.TWA method*), 214
 sampling_ratio (*dicee.dataset_classes.LiteralDataset attribute*), 43, 44
 sanity_check_callback_args () (*in module dicee.sanity_checkers*), 193
 sanity_checking_with_arguments () (*in module dicee.sanity_checkers*), 193
 save () (*dicee.abstracts.BaseInteractiveKGE method*), 15
 save () (*dicee.read_preprocess_save_load_kg.LoadSaveToDisk method*), 192
 save () (*dicee.read_preprocess_save_load_kg.save_load_disk.LoadSaveToDisk method*), 187
 save_checkpoint () (*dicee.abstracts.AbstractTrainer static method*), 14
 save_checkpoint_model () (*in module dicee.static_funcs*), 198
 save_embeddings () (*in module dicee.static_funcs*), 199
 save_embeddings_as_csv (*dicee.config.Namespace attribute*), 28
 save_every_n_epochs (*dicee.config.Namespace attribute*), 31
 save_experiment () (*dicee.analyse_experiments.Experiment method*), 20
 save_model_at_every_epoch (*dicee.config.Namespace attribute*), 29
 save_model_every_n_epoch (*dicee.callbacks.PeriodicEvalCallback attribute*), 26
 save_numpy_ndarray () (*in module dicee.read_preprocess_save_load_kg.util*), 191
 save_numpy_ndarray () (*in module dicee.static_funcs*), 198
 save_pickle () (*in module dicee.read_preprocess_save_load_kg.util*), 191
 save_pickle () (*in module dicee.static_funcs*), 197
 save_queries () (*dicee.query_generator.QueryGenerator method*), 186
 save_queries () (*dicee.QueryGenerator method*), 221
 save_queries_and_answers () (*dicee.query_generator.QueryGenerator static method*), 186
 save_queries_and_answers () (*dicee.QueryGenerator static method*), 221
 save_trained_model () (*dicee.Execute method*), 216
 save_trained_model () (*dicee.executer.Execute method*), 72
 scalar_batch_NN () (*dicee.models.function_space.LFMult method*), 112
 scalar_batch_NN () (*dicee.models.LFMult method*), 183
 scaler (*dicee.callbacks.Perturb attribute*), 26
 scaler (*dicee.trainer.torch_trainer_ddp.NodeTrainer attribute*), 208
 scheduler (*dicee.callbacks.LRScheduler attribute*), 27
 score () (*dicee.models.clifford.Keci method*), 101
 score () (*dicee.models.CoKE method*), 151
 score () (*dicee.models.ComplEx static method*), 155
 score () (*dicee.models.complex.ComplEx static method*), 107
 score () (*dicee.models.DistMult method*), 149
 score () (*dicee.models.Keci method*), 170
 score () (*dicee.models.octonion.OMult method*), 116
 score () (*dicee.models.OMult method*), 166
 score () (*dicee.models.QMult method*), 160
 score () (*dicee.models.quaternion.QMult method*), 120
 score () (*dicee.models.real.CoKE method*), 124
 score () (*dicee.models.real.DistMult method*), 122
 score () (*dicee.models.real.TransE method*), 123
 score () (*dicee.models.TransE method*), 149
 score_func (*dicee.models.FMult2 attribute*), 181
 score_func (*dicee.models.function_space.FMult2 attribute*), 111
 scoring_technique (*dicee.analyse_experiments.Experiment attribute*), 20
 scoring_technique (*dicee.config.Namespace attribute*), 29
 search () (*dicee.scripts.index_serve.NeuralSearcher method*), 194
 search_embeddings () (*in module dicee.scripts.index_serve*), 194
 search_embeddings_batch () (*in module dicee.scripts.index_serve*), 194
 seed (*dicee.query_generator.QueryGenerator attribute*), 185
 seed (*dicee.QueryGenerator attribute*), 220
 select_model () (*in module dicee.static_funcs*), 197
 selected_optimizer (*dicee.models.base_model.BaseKGE attribute*), 96
 selected_optimizer (*dicee.models.BaseKGE attribute*), 143, 146, 152, 157, 163, 176, 179
 SelfAttention (*class in dicee.models.transformers*), 127
 separator (*dicee.config.Namespace attribute*), 29
 separator (*dicee.knowledge_graph.KG attribute*), 75
 sequential_vocabulary_construction () (*dicee.read_preprocess_save_load_kg.PreprocessKG method*), 192
 sequential_vocabulary_construction () (*dicee.read_preprocess_save_load_kg.preprocess.PreprocessKG method*), 186
 serve () (*in module dicee.scripts.index_serve*), 194
 set_global_seed () (*dicee.query_generator.QueryGenerator method*), 185

```

set_global_seed() (dicee.QueryGenerator method), 221
set_model_eval_mode() (dicee.abstracts.BaseInteractiveKGE method), 15
set_model_train_mode() (dicee.abstracts.BaseInteractiveKGE method), 15
setup() (dicee.dataset_classes.CVDataModule method), 40
setup_executor() (dicee.Execute method), 216
setup_executor() (dicee.executer.Execute method), 72
Shallom (class in dicee.models), 149
Shallom (class in dicee.models.real), 123
shallom (dicee.models.real.Shallom attribute), 123
shallom (dicee.models.Shallom attribute), 149
single_hop_query_answering() (dicee.KGE method), 219
single_hop_query_answering() (dicee.knowledge_graph_embeddings.KGE method), 79
snapshot_dir (dicee.callbacks.LRScheduler attribute), 27
snapshot_loss (dicee.callbacks.LRScheduler attribute), 27
sparql_endpoint (dicee.config.Namespace attribute), 28
sparql_endpoint (dicee.knowledge_graph.KG attribute), 74
sq_mean (dicee.weight_averaging.SWAG attribute), 212
start() (dicee.DICE_Trainer method), 222
start() (dicee.Execute method), 217
start() (dicee.executer.Execute method), 73
start() (dicee.read_preprocess_save_load_kg.PreprocessKG method), 191
start() (dicee.read_preprocess_save_load_kg.preprocess.PreprocessKG method), 186
start() (dicee.read_preprocess_save_load_kg.read_from_disk.ReadFromDisk method), 187
start() (dicee.read_preprocess_save_load_kg.ReadFromDisk method), 192
start() (dicee.trainer.DICE_Trainer method), 209
start() (dicee.trainer.dice_trainer.DICE_Trainer method), 204
start_time (dicee.callbacks.PrintCallback attribute), 22
start_time (dicee.Execute attribute), 216
start_time (dicee.executer.Execute attribute), 72
state_dict() (dicee.models.ensemble.EnsembleKGE method), 109
step() (dicee.models.ADOPT method), 135
step() (dicee.models.adopt.ADOPT method), 84
step() (dicee.models.ensemble.EnsembleKGE method), 109
step_count (dicee.callbacks.LRScheduler attribute), 27
storage_path (dicee.config.Namespace attribute), 28
storage_path (dicee.DICE_Trainer attribute), 222
storage_path (dicee.trainer.DICE_Trainer attribute), 208
storage_path (dicee.trainer.dice_trainer.DICE_Trainer attribute), 203
store() (in module dicee.static_funcs), 198
store_ensemble() (dicee.abstracts.AbstractPPECallback method), 18
strategy (dicee.abstracts.AbstractTrainer attribute), 13
StringListRequest (class in dicee.scripts.index_serve), 194
SWA (class in dicee.weight_averaging), 210
swa (dicee.config.Namespace attribute), 30
swa_c_epochs (dicee.config.Namespace attribute), 31
swa_c_epochs (dicee.weight_averaging.SWA attribute), 211
swa_c_epochs (dicee.weight_averaging.SWAG attribute), 212
swa_lr (dicee.weight_averaging.SWA attribute), 211
swa_lr (dicee.weight_averaging.SWAG attribute), 212
swa_model (dicee.weight_averaging.SWA attribute), 211
swa_n (dicee.weight_averaging.SWA attribute), 211
swa_start_epoch (dicee.config.Namespace attribute), 31
swa_start_epoch (dicee.weight_averaging.SWA attribute), 211
swa_start_epoch (dicee.weight_averaging.SWAG attribute), 212
SWAG (class in dicee.weight_averaging), 211
swag (dicee.config.Namespace attribute), 30

```

T

```

T() (dicee.models.DualE method), 184
T() (dicee.models.dualE.DualE method), 108
t_conorm() (dicee.abstracts.InteractiveQueryDecomposition method), 16
t_norm() (dicee.abstracts.InteractiveQueryDecomposition method), 16
target_dim (dicee.dataset_classes.AllvsAll attribute), 35
target_dim (dicee.dataset_classes.MultiLabelDataset attribute), 33
target_dim (dicee.dataset_classes.OnevsAllDataset attribute), 34
target_dim (dicee.knowledge_graph.KG attribute), 76
temperature (dicee.models.transformers.BytE attribute), 126

```

tensor_t_norm() (*dicee.abstracts.InteractiveQueryDecomposition* method), 16
TensorParallel (*class in dicee.trainer.model_parallelism*), 205
test_dataloader() (*dicee.models.base_model.BaseKGELightning* method), 91
test_dataloader() (*dicee.models.BaseKGELightning* method), 139
test_epoch_end() (*dicee.models.base_model.BaseKGELightning* method), 91
test_epoch_end() (*dicee.models.BaseKGELightning* method), 138
test_h1 (*dicee.analyse_experiments.Experiment* attribute), 20
test_h3 (*dicee.analyse_experiments.Experiment* attribute), 20
test_h10 (*dicee.analyse_experiments.Experiment* attribute), 20
test_mrr (*dicee.analyse_experiments.Experiment* attribute), 20
test_path (*dicee.query_generator.QueryGenerator* attribute), 185
test_path (*dicee.QueryGenerator* attribute), 220
test_set (*dicee.knowledge_graph.KG* attribute), 74, 75
timeit() (*in module dicee.read_preprocess_save_load_kg.util*), 190
timeit() (*in module dicee.static_funcs*), 197
timeit() (*in module dicee.static_preprocess_funcs*), 202
to() (*dicee.KGE* method), 217
to() (*dicee.knowledge_graph_embeddings.KGE* method), 76
to() (*dicee.models.ensemble.EnsembleKGE* method), 109
to_df() (*dicee.analyse_experiments.Experiment* method), 20
topk (*dicee.models.transformers.BytE* attribute), 126
topk (*dicee.scripts.index_serve.NeuralSearcher* attribute), 194
torch_ordered_shaped_bpe_entities (*dicee.dataset_classes.MultiLabelDataset* attribute), 33
TorchDDPTrainer (*class in dicee.trainer.torch_trainer_ddp*), 207
TorchTrainer (*class in dicee.trainer.torch_trainer*), 205
total_epochs (*dicee.callbacks.LRScheduler* attribute), 27
total_steps (*dicee.callbacks.LRScheduler* attribute), 27
train() (*dicee.abstracts.BaseInteractiveTrainKGE* method), 19
train() (*dicee.trainer.torch_trainer_ddp.NodeTrainer* method), 208
train_data (*dicee.dataset_classes.AllvsAll* attribute), 35
train_data (*dicee.dataset_classes.KvsAll* attribute), 34
train_data (*dicee.dataset_classes.KvsSampleDataset* attribute), 38
train_data (*dicee.dataset_classes.MultiClassClassificationDataset* attribute), 33
train_data (*dicee.dataset_classes.OnevsAllDataset* attribute), 34
train_data (*dicee.dataset_classes.OnevsSample* attribute), 36
train_dataloader() (*dicee.dataset_classes.CVDataModule* method), 40
train_dataloader() (*dicee.models.base_model.BaseKGELightning* method), 93
train_dataloader() (*dicee.models.BaseKGELightning* method), 140
train_dataloaders (*dicee.trainer.torch_trainer.TorchTrainer* attribute), 206
train_dataset_loader (*dicee.trainer.torch_trainer_ddp.NodeTrainer* attribute), 207
train_file_path (*dicee.dataset_classes.LiteralDataset* attribute), 43, 44
train_h1 (*dicee.analyse_experiments.Experiment* attribute), 20
train_h3 (*dicee.analyse_experiments.Experiment* attribute), 20
train_h10 (*dicee.analyse_experiments.Experiment* attribute), 20
train_indices_target (*dicee.dataset_classes.MultiLabelDataset* attribute), 33
train_k_vs_all() (*dicee.abstracts.BaseInteractiveTrainKGE* method), 18
train_literals() (*dicee.abstracts.BaseInteractiveTrainKGE* method), 19
train_mode (*dicee.models.ensemble.EnsembleKGE* attribute), 109
train_mrr (*dicee.analyse_experiments.Experiment* attribute), 20
train_path (*dicee.query_generator.QueryGenerator* attribute), 185
train_path (*dicee.QueryGenerator* attribute), 220
train_set (*dicee.dataset_classes.BPE_NegativeSamplingDataset* attribute), 32
train_set (*dicee.dataset_classes.MultiLabelDataset* attribute), 33
train_set (*dicee.dataset_classes.NegSampleDataset* attribute), 38
train_set (*dicee.dataset_classes.TriplePredictionDataset* attribute), 39
train_set (*dicee.knowledge_graph.KG* attribute), 74, 75
train_set_idx (*dicee.dataset_classes.CVDataModule* attribute), 40
train_set_target (*dicee.knowledge_graph.KG* attribute), 75
train_target (*dicee.dataset_classes.AllvsAll* attribute), 35
train_target (*dicee.dataset_classes.KvsAll* attribute), 35
train_target (*dicee.dataset_classes.KvsSampleDataset* attribute), 38
train_target_indices (*dicee.knowledge_graph.KG* attribute), 76
train_triples (*dicee.dataset_classes.NegSampleDataset* attribute), 38
train_triples() (*dicee.abstracts.BaseInteractiveTrainKGE* method), 18
trained_model (*dicee.Execute* attribute), 215, 216
trained_model (*dicee.executer.Execute* attribute), 72
trainer (*dicee.config.Namespace* attribute), 29
trainer (*dicee.DICE_Trainer* attribute), 222

trainer (*dicee.Execute attribute*), 215, 216
trainer (*dicee.executer.Execute attribute*), 71, 72
trainer (*dicee.trainer.DICE_Trainer attribute*), 208
trainer (*dicee.trainer.dice_trainer.DICE_Trainer attribute*), 203
trainer (*dicee.trainer.torch_trainer_ddp.NodeTrainer attribute*), 207
training_step (*dicee.trainer.torch_trainer.TorchTrainer attribute*), 206
training_step () (*dicee.models.base_model.BaseKGELightning method*), 90
training_step () (*dicee.models.BaseKGELightning method*), 137
training_step () (*dicee.models.transformers.BytE method*), 126
training_step_outputs (*dicee.models.base_model.BaseKGELightning attribute*), 89
training_step_outputs (*dicee.models.BaseKGELightning attribute*), 137
training_technique (*dicee.knowledge_graph.KG attribute*), 75
TransE (*class in dicee.models*), 149
TransE (*class in dicee.models.real*), 122
transfer_batch_to_device () (*dicee.dataset_classes.CVDataModule method*), 41
transformer (*dicee.models.transformers.BytE attribute*), 126
transformer (*dicee.models.transformers.GPT attribute*), 131
trapezoid () (*dicee.models.FMult2 method*), 182
trapezoid () (*dicee.models.function_space.FMult2 method*), 111
tri_score () (*dicee.models.function_space.LFMult method*), 112
tri_score () (*dicee.models.function_space.LFMultI method*), 111
tri_score () (*dicee.models.LFMult method*), 183
tri_score () (*dicee.models.LFMultI method*), 182
triple_score () (*dicee.KGE method*), 219
triple_score () (*dicee.knowledge_graph_embeddings.KGE method*), 78
TriplePredictionDataset (*class in dicee.dataset_classes*), 38
tuple2list () (*dicee.query_generator.QueryGenerator method*), 185
tuple2list () (*dicee.QueryGenerator method*), 221
TWA (*class in dicee.weight_averaging*), 213
twa (*dicee.config.Namespace attribute*), 30
twa_c_epochs (*dicee.weight_averaging.TWA attribute*), 214
twa_model (*dicee.weight_averaging.TWA attribute*), 214
twa_start_epoch (*dicee.weight_averaging.TWA attribute*), 214

U

unlabelled_size (*dicee.callbacks.PseudoLabellingCallback attribute*), 24
unmap () (*dicee.query_generator.QueryGenerator method*), 185
unmap () (*dicee.QueryGenerator method*), 221
unmap_query () (*dicee.query_generator.QueryGenerator method*), 185
unmap_query () (*dicee.QueryGenerator method*), 221
update_hits () (*in module dicee.evaluation*), 67
update_hits () (*in module dicee.evaluation.utils*), 58

V

val_aswa (*dicee.weight_averaging.ASWA attribute*), 210
val_dataloader () (*dicee.models.base_model.BaseKGELightning method*), 92
val_dataloader () (*dicee.models.BaseKGELightning method*), 139
val_h1 (*dicee.analyse_experiments.Experiment attribute*), 20
val_h3 (*dicee.analyse_experiments.Experiment attribute*), 20
val_h10 (*dicee.analyse_experiments.Experiment attribute*), 20
val_mrr (*dicee.analyse_experiments.Experiment attribute*), 20
val_path (*dicee.query_generator.QueryGenerator attribute*), 185
val_path (*dicee.QueryGenerator attribute*), 220
VALID_SCORING_TECHNIQUES (*in module dicee.evaluation.evaluator*), 50
valid_set (*dicee.knowledge_graph.KG attribute*), 74, 75
validate_knowledge_graph () (*in module dicee.sanity_checkers*), 193
var_clamp (*dicee.weight_averaging.SWAG attribute*), 212
vocab_preparation () (*dicee.evaluation.Evaluator method*), 60
vocab_preparation () (*dicee.evaluation.evaluator.Evaluator method*), 51
vocab_preparation () (*dicee.Evaluator method*), 224
vocab_preparation () (*dicee.evaluator.Evaluator method*), 69
vocab_size (*dicee.models.CoKEConfig attribute*), 150
vocab_size (*dicee.models.real.CoKEConfig attribute*), 123, 124
vocab_size (*dicee.models.transformers.GPTConfig attribute*), 130
vocab_to_parquet () (*in module dicee.static_funcs*), 199
vtp_score () (*dicee.models.function_space.LFMult method*), 112
vtp_score () (*dicee.models.function_space.LFMultI method*), 112

`vtp_score()` (*dicee.models.LFMult method*), 183
`vtp_score()` (*dicee.models.LFMultI method*), 182

W

`warmup_steps` (*dicee.callbacks.LRScheduler attribute*), 27
`weight` (*dicee.models.transformers.LayerNorm attribute*), 127
`weight_decay` (*dicee.config.Namespace attribute*), 29
`weight_decay` (*dicee.models.base_model.BaseKGE attribute*), 96
`weight_decay` (*dicee.models.BaseKGE attribute*), 143, 146, 152, 157, 163, 176, 179
`weight_samples` (*dicee.weight_averaging.TWA attribute*), 214
`weights` (*dicee.models.FMult attribute*), 181
`weights` (*dicee.models.function_space.FMult attribute*), 110
`weights` (*dicee.models.function_space.GFMult attribute*), 110
`weights` (*dicee.models.GFMult attribute*), 181
`world_size` (*dicee.Execute attribute*), 215
`world_size` (*dicee.executer.Execute attribute*), 71
`write_csv_from_model_parallel()` (in module *dicee.static_funcs*), 199
`write_links()` (*dicee.query_generator.QueryGenerator method*), 185
`write_links()` (*dicee.QueryGenerator method*), 221
`write_report()` (*dicee.Execute method*), 217
`write_report()` (*dicee.executer.Execute method*), 73

X

`x_values` (*dicee.models.function_space.LFMult attribute*), 112
`x_values` (*dicee.models.LFMult attribute*), 182