

---

# DICE Embeddings

*Release 0.1.3.2*

**Caglar Demir**

**Dec 15, 2025**

## Contents:

<b>1 Dicee Manual</b>	<b>2</b>
<b>2 Installation</b>	<b>3</b>
2.1 Installation from Source . . . . .	3
<b>3 Download Knowledge Graphs</b>	<b>3</b>
<b>4 Knowledge Graph Embedding Models</b>	<b>3</b>
<b>5 How to Train</b>	<b>3</b>
<b>6 Creating an Embedding Vector Database</b>	<b>5</b>
6.1 Learning Embeddings . . . . .	5
6.2 Loading Embeddings into Qdrant Vector Database . . . . .	6
6.3 Launching Webservice . . . . .	6
<b>7 Answering Complex Queries</b>	<b>6</b>
<b>8 Predicting Missing Links</b>	<b>8</b>
<b>9 Downloading Pretrained Models</b>	<b>8</b>
<b>10 How to Deploy</b>	<b>8</b>
<b>11 Docker</b>	<b>8</b>
<b>12 Coverage Report</b>	<b>8</b>
<b>13 How to cite</b>	<b>10</b>
<b>14 dicee</b>	<b>12</b>
14.1 Submodules . . . . .	12
14.2 Attributes . . . . .	213
14.3 Classes . . . . .	213
14.4 Package Contents . . . . .	213
<b>Python Module Index</b>	<b>225</b>

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

## 1 Dicee Manual

**Version:** dicee 0.2.0

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

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

**Contact:** [caglar.demir@upb.de](mailto:caglar.demir@upb.de)

**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. **Pandas<sup>3</sup> & Co.** to use parallelism at preprocessing a large knowledge graph,
2. **PyTorch<sup>4</sup> & Co.** to learn knowledge graph embeddings via multi-CPUs, GPUs, TPUs or computing cluster, and
3. **Huggingface<sup>5</sup>** to ease the deployment of pre-trained models.

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

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

**Why Huggingface<sup>10</sup>?** Seamlessly deploy and share pre-trained embedding models through the Huggingface ecosystem.

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

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

<sup>3</sup> <https://pandas.pydata.org/>

<sup>4</sup> <https://pytorch.org/>

<sup>5</sup> <https://huggingface.co/>

<sup>6</sup> <https://pandas.pydata.org/>

<sup>7</sup> <https://pytorch.org/>

<sup>8</sup> <https://pytorch.org/>

<sup>9</sup> <https://www.pytorchlightning.ai/>

<sup>10</sup> <https://huggingface.co/>

## 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/](https://dice-research.org/projects/DiceEmbeddings/)<sup>11</sup>

## 10 How to Deploy

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

## 11 Docker

To build the Docker image:

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

To test the Docker image:

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

## 12 Coverage Report

The coverage report is generated using `coverage.py`<sup>12</sup>:

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

(continues on next page)

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

<sup>12</sup> <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](mailto: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:  
Utility scripts

### 14.1 Submodules

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

**dicee.abstracts**

**Classes**

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

## Module Contents

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

Abstract class for Trainer class for knowledge graph embedding models

### Parameter

```
args
```

[str] ?

```
callbacks: list
```

?

```
attributes
```

```
callbacks
```

```
is_global_zero = True
```

```
global_rank = 0
```

```
local_rank = 0
```

```
strategy = None
```

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

A function to call callbacks before the training starts.

### Parameter

```
args
```

```
kwargs
```

```
rtype
```

None

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

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

### Parameter

```
args
```

```
kwargs
```

```
rtype
```

None

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

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

### Parameter

```
args
```

```
kwargs
```

**rtype**  
None  
**on\_train\_epoch\_end**(\*args, \*\*kwargs)  
A function to call callbacks at the end of an epoch.

#### Parameter

args

kwargs

**rtype**  
None  
**on\_train\_batch\_end**(\*args, \*\*kwargs)  
A function to call callbacks at the end of each mini-batch during training.

#### Parameter

args

kwargs

**rtype**  
None  
**static save\_checkpoint**(full\_path: str, model) → None  
A static function to save a model into disk

#### Parameter

full\_path : str

model:

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

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

#### Parameter

**path\_of\_pretrained\_model\_dir**  
[str] ?

**construct\_ensemble: boolean**  
?

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

**construct\_ensemble = False**

**apply\_semantic\_constraint = False**

**configs**

**get\_eval\_report()** → dict

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

**Parameters**

**str\_entity\_or\_relation** (*corresponds to a str or a list of strings to be tokenized via BPE and shaped.*)

**Return type**

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

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

**Parameters**

**triples**

**set\_model\_train\_mode()** → None

Setting the model into training mode

**Parameter**

**set\_model\_eval\_mode()** → None

Setting the model into eval mode

**Parameter**

**property name**

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

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

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

**save()** → None

**get\_entity\_index(x: str)**

**get\_relation\_index(x: str)**

**index\_triple(head\_entity: List[str], relation: List[str], tail\_entity: List[str])**  
→ Tuple[torch.LongTensor, torch.LongTensor, torch.LongTensor]

Index Triple

**Parameter**

head\_entity: List[str]

String representation of selected entities.

relation: List[str]

String representation of selected relations.

tail\_entity: List[str]

String representation of selected entities.

### Returns: Tuple

pytorch tensor of triple score

**add\_new\_entity\_embeddings** (*entity\_name*: str = None, *embeddings*: torch.FloatTensor = None)

**get\_entity\_embeddings** (*items*: List[str])

Return embedding of an entity given its string representation

### Parameter

#### items:

entities

**get\_relation\_embeddings** (*items*: List[str])

Return embedding of a relation given its string representation

### Parameter

#### items:

relations

**construct\_input\_and\_output** (*head\_entity*: List[str], *relation*: List[str], *tail\_entity*: List[str], *labels*)

Construct a data point :param head\_entity: :param relation: :param tail\_entity: :param labels: :return:

**parameters** ()

**class** dicee.abstracts.**InteractiveQueryDecomposition**

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

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

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

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

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

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

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

Abstract class for Callback class for knowledge graph embedding models

### Parameter

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

### Parameter

trainer:

model:

**rtype**

None

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

Call at the beginning of the training.

### Parameter

trainer:

model:

**rtype**

None

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

Call at the beginning of the training.

### Parameter

trainer:

model:

**rtype**

None

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

Call at the end of each epoch during training.

### Parameter

trainer:

model:

**rtype**

None

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

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

### Parameter

trainer:

model:

**rtype**

None

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

Call at the end of the training.

### Parameter

trainer:

model:

**rtype**

None

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

Bases: [AbstractCallback](#)

Abstract class for Callback class for knowledge graph embedding models

### Parameter

**num\_epochs**

**path**

**sample\_counter** = 0

**epoch\_count** = 0

**alphas** = None

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

Call at the beginning of the training.

### Parameter

trainer:

model:

**rtype**

None

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

Call at the end of the training.

### Parameter

trainer:

model:

**rtype**

None

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

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

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

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

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

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

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

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

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

Trains the Literal Embeddings model using literal data.

#### Parameters

- **train\_file\_path** (*str*) – Path to the training data file.
- **num\_epochs** (*int*) – Number of training epochs.
- **lit\_lr** (*float*) – Learning rate for the literal model.
- **norm\_type** (*str*) – Normalization type to use ('z-norm', 'min-max', or None).
- **batch\_size** (*int*) – Batch size for training.
- **sampling\_ratio** (*float*) – Ratio of training triples to use.
- **loader\_backend** (*str*) – Backend for loading the dataset ('pandas' or 'rdflib').
- **freeze\_entity\_embeddings** (*bool*) – If True, freeze the entity embeddings during training.
- **gate\_residual** (*bool*) – If True, use gate residual connections in the model.
- **device** (*str*) – Device to use for training ('cuda' or 'cpu'). If None, will use available GPU or CPU.
- **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

<code>Namespace</code>	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

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

### Functions

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

## Module Contents

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

Reload the files from disk to construct the Pytorch dataset

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

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

Bases: torch.utils.data.Dataset

An abstract class representing a Dataset.

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

### Note

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

`train_set`

`ordered_bpe_entities`

`num_bpe_entities`

`neg_ratio`

`num_datapoints`

`__len__()`

`__getitem__(idx)`

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

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

Bases: torch.utils.data.Dataset

An abstract class representing a Dataset.

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

### Note

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

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

**class** dicee.dataset\_classes.**MultiClassClassificationDataset** (  
    *subword\_units: numpy.ndarray, block\_size: int = 8*)

Bases: `torch.utils.data.Dataset`

Dataset for the 1vsALL training strategy

#### Parameters

- **train\_set\_idx** – Indexed triples for the training.
- **entity\_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.

or all  $y_i = 1$  s.t.  $(h, r) \in E$

 **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  $[0,1]^{|\{E\}|}$  is a binary label.

or all  $y_{-i} = 1$  s.t.  $(h \ r \ E_{-i})$  in KG

### Note

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

**train\_set\_idx**  
[numpy.ndarray] n by 3 array representing n triples

**entity\_idxs**  
[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.

**orall y\_i =1 s.t. (h r E\_i) in KG**

**At each mini-batch construction, we subsample(y), hence n**  
 $|new\_y| << |E|$  new\_y contains all 1's if sum(y) < neg\_sample ratio new\_y contains

**train\_set\_idx**  
 Indexed triples for the training.

**entity\_idxs**  
 mapping.

**relation\_idxs**  
 mapping.

**form**  
 ?

**store**  
 ?

**label\_smoothing\_rate**  
 ?

torch.utils.data.Dataset

```
train_data = None
train_target = None
```

```

neg_ratio = None
num_entities
label_smoothing_rate
collate_fn = None
max_num_of_classes
__len__()
__getitem__(idx)

```

**class** dicee.dataset\_classes.NegSampleDataset (*train\_set: numpy.ndarray*, *num\_entities: int*,  
*num\_relations: int*, *neg\_sample\_ratio: int = 1*)

Bases: torch.utils.data.Dataset

An abstract class representing a Dataset.

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

### Note

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

```

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

```

**class** dicee.dataset\_classes.TriplePredictionDataset (*train\_set: numpy.ndarray*,  
*num\_entities: int*, *num\_relations: int*, *neg\_sample\_ratio: int = 1*, *label\_smoothing\_rate: float = 0.0*)

Bases: torch.utils.data.Dataset

Triple Dataset

**D:= {(x)\_i}\_i ^N, where**  
 . x:(h,r, t) in KG is a unique h in E and a relation r in R and . collect\_fn => Generates  
 negative triples

collect\_fn:

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

**train\_set\_idx**  
Indexed triples for the training.

**entity\_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.l1 = None

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

        # don't do this
        self.something = else

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

```

### `transfer_batch_to_device(*args, **kwargs)`

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

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

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

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

#### Note

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

#### Parameters

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

#### Returns

A reference to the data on the new device.

Example:

```

def transfer_batch_to_device(self, batch, device, dataloader_idx):
    if isinstance(batch, CustomBatch):
        # move all tensors in your custom data structure to the device
        batch.samples = batch.samples.to(device)
        batch.targets = batch.targets.to(device)
    elif dataloader_idx == 0:

```

(continues on next page)

(continued from previous page)

```
# skip device transfer for the first dataloader or anything you wish
# pass
else:
    batch = super().transfer_batch_to_device(batch, device, dataloader_
→idx)
return batch
```

### See also

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

## `prepare_data(*args, **kwargs)`

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

### ⚠ Warning

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

Example:

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

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

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

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

Example:

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

    # call on GLOBAL_RANK=0 (great for shared file systems)
```

(continues on next page)

(continued from previous page)

```
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&gt;tional[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, batch_size: int = None, func_triple_to_bpe_representation: Callable = None,  
    str_to_bpe_entity_to_idx: Dict = 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.

```
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, 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.

## Classes

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

## Module Contents

`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, form_of_labelling: str = 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*) → *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*, *form\_of\_labelling*: *str* = *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(→ 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 and reciprocals.
<code>evaluate_link_prediction_performance_with_i...</code>	Evaluate link prediction with BPE encoding (head and tail).
<code>evaluate_lp(→ Dict[str, float])</code>	Evaluate link prediction with batched processing.
<code>evaluate_bpe_lp(→ Dict[str, float])</code>	Evaluate link prediction with BPE-encoded entities.
<code>evaluate_lp_bpe_k_vs_all(→ Dict[str, float])</code>	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, batch_size: int = None, func_triple_to_bpe_representation: Callable = None,
    str_to_bpe_entity_to_idx: Dict = 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.

## 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(→ tional[pandas.DataFrame])</code>	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.

### 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>efficient_zero_grad</code> (→ None)	Efficiently zero gradients using parameter.grad = None.

### Module Contents

`dicee.evaluation.utils.make_iterable_verbose`(iterable\_object: Iterable, verbose: bool, desc: str = 'Default', position: int = 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
```

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: 1-10).

```
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](https://pytorch.org/tutorials/recipes/recipes/tuning_guide.html)

### Parameters

**model** – PyTorch model to zero gradients for.

## Classes

<code>Evaluator</code>	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_u</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>make_iterable_verbose(→ Iterable)</code>	Wrap an iterable with tqdm progress bar if verbose is True.

## 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, form_of_labelling: str = 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*) → *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*, *form\_of\_labelling*: *str* = *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,  
    batch_size: int = None, func_triple_to_bpe_representation: Callable = None,  
    str_to_bpe_entity_to_idx: Dict = 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.

```
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.make_iterable_verbose(iterable_object: Iterable, verbose: bool, desc: str = 'Default', position: int = 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.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, form_of_labelling: str = 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) → 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,
form_of_labelling: str = 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

<i>KG</i>	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

<code>KGE</code>	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  $f(e,r,x) > \text{confidence}$ .

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`,    `state_steps`)    Functional API that performs ADOPT algorithm computation.

---

## Module Contents

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

Bases: `torch.optim.optimizer.Optimizer`

ADOPT Optimizer.

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

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

### Mathematical formulation:

$$m_t = \beta_1 * m_{t-1} + (1 - \beta_1) * \text{clip}(g_t / \sqrt(v_t))$$

where:

- $\theta_t$ : parameter at step t
- $g_t$ : gradient at step t
- $m_t$ : first moment estimate (momentum)
- $v_t$ : second moment estimate (variance)
- $\alpha$ : learning rate
- $\beta_1, \beta_2$ : 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 ( $\beta_1, \beta_2$ ) for computing running averages of gradient and its square.  $\beta_1$  controls momentum,  $\beta_2$  controls variance. Default: (0.9, 0.9999)
- **eps** (*float, optional*) – Term added to denominator to improve numerical stability. Default: 1e-6
- **clip\_lambda** (*Callable[[int], float], optional*) – Function that takes the step number and returns the gradient clipping threshold. Common choices: - lambda step:  $step^{**0.25}$  (default, gradually increases clipping threshold) - lambda step: 1.0 (constant clipping) - None (no clipping) Default: lambda step:  $step^{**0.25}$
- **weight\_decay** (*float, optional*) – Weight decay coefficient (L2 penalty). Default: 0.0
- **decouple** (*bool, optional*) – If True, uses decoupled weight decay (AdamW-style), applying weight decay directly to parameters. If False, adds weight decay to gradients (L2 regularization). Default: False
- **foreach** (*bool, optional*) – If True, uses the faster foreach implementation for multi-tensor operations. Default: None (auto-select)
- **maximize** (*bool, optional*) – If True, maximizes parameters instead of minimizing. Useful for reinforcement learning. Default: False
- **capturable** (*bool, optional*) – If True, the optimizer is safe to capture in a CUDA graph. Requires learning rate as Tensor. Default: False
- **differentiable** (*bool, optional*) – If True, the optimization step can be differentiated. Useful for meta-learning. Default: False
- **fused** (*bool, optional*) – If True, uses fused kernel implementation (currently not supported). Default: None

#### Raises

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

#### Example

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

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

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

### Note

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

### `clip_lambda`

#### `__setstate__(state)`

Restore optimizer state from a checkpoint.

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

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

#### Parameters

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

### Note

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

### `step(closure=None)`

Perform a single optimization step.

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

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

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

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

## Parameters

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

- Enable gradients (torch.enable\_grad())
- Compute forward pass
- Compute loss
- Compute backward pass
- Return the loss value Example: lambda: (loss := model(x), loss.backward(), loss)[-1]

Default: None

## Returns

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

## Return type

Optional[Tensor]

## Example

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

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

### Note

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

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

Functional API that performs ADOPT algorithm computation.

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

1. **Single-tensor mode** (default): Updates parameters one at a time - Compatible with torch.jit.script - More flexible but slower - Used when foreach=False or automatically for small models
2. **Multi-tensor (foreach) mode**: Batches operations across tensors - 2-3x faster on GPU through vectorization - Groups tensors by device/dtype automatically - Used when foreach=True

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

### Algorithm overview (ADOPT):

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

#### Mathematical formulation:

```
# Normalize gradient by its historical variance normed_g_t = g_t / sqrt(v_t + 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
- β₁, β₂: exponential decay rates
- ε: numerical stability constant
- clip(): gradient clipping function based on step

### Automatic mode selection:

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

- Parameter types and devices
- Whether differentiable mode is enabled
- Learning rate type (float vs Tensor)
- Capturable mode requirements

```
param params
    Parameters to optimize.

type params
    List[Tensor]

param grads
    Gradients for each parameter.

type grads
    List[Tensor]

param exp_avgs
    First moment estimates (momentum).

type exp_avgs
    List[Tensor]

param exp_avg_sqs
    Second moment estimates (variance).
```

```

type exp_avg_sqs
    List[Tensor]

param state_steps
    Step counters (must be singleton tensors).

type state_steps
    List[Tensor]

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

type foreach
    Optional[bool]

param capturable
    If True, ensure CUDA graph capture safety.

type capturable
    bool

param differentiable
    If True, allow gradients through optimization step.

type differentiable
    bool

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

type fused
    Optional[bool]

param grad_scale
    Gradient scaler for AMP training.

type grad_scale
    Optional[Tensor]

param found_inf
    Flag for inf/nan detection in AMP.

type found_inf
    Optional[Tensor]

param has_complex
    Whether any parameters are complex-valued.

type has_complex
    bool

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

type beta1
    float

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

type beta2
    float

```

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

**type lr**  
Union[float, Tensor]

**param clip\_lambda**  
Function that maps step number to gradient clipping threshold. None disables clipping.

**type clip\_lambda**  
Optional[Callable[[int], float]]

**param weight\_decay**  
Weight decay coefficient (L2 penalty).

**type weight\_decay**  
float

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

**type decouple**  
bool

**param eps**  
Small constant for numerical stability in normalization.

**type eps**  
float

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

**type maximize**  
bool

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

**raises RuntimeError**  
If state\_steps contains non-tensor elements.

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

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

## Example

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

(continues on next page)

(continued from previous page)

```
...     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

`BaseKGELightning`

Base class for all neural network modules.

`BaseKGE`

Base class for all neural network modules.

`IdentityClass`

Base class for all neural network modules.

### Module Contents

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

Bases: `lightning.LightningModule`

Base class for all neural network modules.

Your models should also subclass this class.

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

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

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

(continues on next page)

```

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()`

### 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.base_model.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 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  $\sigma_{qq} = \sum_{j=1}^{p+q-1} \sum_{k=j+1}^{p+q} (h_j r_k - h_k r_j) e_j e_k$   $\sigma_{qq}$  captures the interactions between along q bases For instance, let  $q = 1, 2, 3$ , we compute interactions between  $e_1 e_2, e_1 e_3$ , 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  $p < j <= p+q$   $ei ej = -ejei$  for  $i = j$

eq j

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

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

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

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

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

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

(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  $\text{Cl}_{\{p,q\}}(\mathbb{R}^d)$ 
```

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

forward\_k\_vs\_with\_explicit and this funcitons are identical Parameter ——— x: torch.LongTensor with (n,2) shape :rtype: torch.FloatTensor with (n, |E|) shape

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

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

### 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

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

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

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

### Note

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

## Variables

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

```
name = 'DeCaL'
```

```
entity_embeddings
```

```
relation_embeddings
```

```


p



q



r



re



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


```

### Parameter

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

#### **rtype**

*torch.FloatTensor* with (n) shape

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

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

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

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

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

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

and return:

$$\sigma_0 t = \sigma_0 \cdot t_0 = s0 + s1 - s2s3, s4 and s5$$

**compute\_sigmas\_multivect** (*list\_h\_emb*, *list\_r\_emb*)

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

For same bases vectors interaction we have

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

For different base vector interactions, we have

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

**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 :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:

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

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

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

$\sigma_{qq}$  captures the interactions between along q bases For instance, let q e\_1, e\_2, e\_3, we compute interactions between e\_1 e\_2, e\_1 e\_3 , and e\_2 e\_3 This can be implemented with a nested two for loops

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

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

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

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

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

```
e2e1, e2e2, e2e3, e3e1, e3e2, e3e3
```

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

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

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

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

Compute

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

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

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

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

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

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

Compute

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

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

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

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

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

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

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

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

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

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

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

## dicee.models.complex

## Classes

<code>ConEx</code>	Convolutional ComplEx Knowledge Graph Embeddings
<code>AConEx</code>	Additive Convolutional ComplEx Knowledge Graph Embeddings
<code>ComplEx</code>	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.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

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

### Module Contents

```

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

Learning Knowledge Neural Graphs

name = 'FMult'

entity_embeddings

relation_embeddings

k

num_sample = 50

gamma

roots

weights

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

chain_func (weights, x: torch.FloatTensor)

```

```

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

    Parameters
        x

class dicee.models.function_space.GFMult (args)
    Bases: dicee.models.base_model.BaseKGE
    Learning Knowledge Neural Graphs
        name = 'GFMult'
        entity_embeddings
        relation_embeddings
        k
        num_sample = 250
        roots
        weights
        compute_func (weights: torch.FloatTensor, x) → torch.FloatTensor
        chain_func (weights, x: torch.FloatTensor)
        forward_triples (idx_triple: torch.Tensor) → torch.Tensor

    Parameters
        x

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

```

```

trapezoid(list_W, list_b)

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

    Parameters
        x

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

    Embedding with trigonometric functions. We represent all entities and relations in the complex number space as:  $f(x) = \sum_{k=0}^{\lfloor d/2 \rfloor} w_k e^{ikx}$ . 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:  $f(x) = \sum_{i=0}^{d-1} a_i x^{i \% d}$  and use the three different scoring function as in the paper to evaluate the score. We also consider combining with Neural Networks.

        name = 'LFMult'

        entity_embeddings

        relation_embeddings

        degree

        m

        x_values

        forward_triples(idx_triple)

    Parameters
        x

        construct_multi_coeff(x)

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

        linear(x, w, b)

```

**scalar\_batch\_NN**(*a, b, c*)  
 element wise multiplication between *a,b* and *c*: Inputs : *a, b, c* =====> torch.tensor of size batch\_size x m x d Output : a tensor of size batch\_size x d

**tri\_score**(*coeff\_h, coeff\_r, coeff\_t*)

this part implement the trilinear scoring techniques:

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

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

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

3. take the sum over each batch

**vtp\_score**(*h, r, t*)

this part implement the vector triple product scoring techniques:

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

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

2. Compute the first and second terms of the sum

3. Multiply with then denominator and take the sum

4. take the sum over each batch

**comp\_func**(*h, r, t*)

this part implement the function composition scoring techniques: i.e.  $\text{score} = \langle h, r, t \rangle$

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

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

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

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

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

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

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

## dicee.models.literal

### Classes

*LiteralEmbeddings*

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

### Module Contents

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

Bases: `torch.nn.Module`

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

**num\_of\_data\_properties**

Number of data properties (attributes).

**Type**

`int`

**embedding\_dims**

Dimension of the embeddings.

**Type**

`int`

**entity\_embeddings**

Pre-trained entity embeddings.

**Type**

`torch.tensor`

**dropout**

Dropout rate for regularization.

**Type**

`float`

**gate\_residual**

Whether to use gated residual connections.

**Type**

`bool`

**freeze\_entity\_embeddings**

Whether to freeze the entity embeddings during training.

**Type**

`bool`

**embedding\_dim**

**num\_of\_data\_properties**

**hidden\_dim**

**gate\_residual = True**

**freeze\_entity\_embeddings = True**

**entity\_embeddings**

**data\_property\_embeddings**

**fc**

**fc\_out**

**dropout**

```
gated_residual_proj  
layer_norm  
forward(entity_idx, attr_idx)
```

#### Parameters

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

#### Returns

scalar predictions.

#### Return type

*Tensor*

```
property device
```

## dicee.models.octonion

### Classes

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

### Functions

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

### Module Contents

```
dicee.models.octonion.octonion_mul(*, O_1, O_2)  
dicee.models.octonion.octonion_mul_norm(*, O_1, O_2)  
class dicee.models.octonion.OMult(args)  
Bases: dicee.models.base_model.BaseKGE  
Base class for all neural network modules.  
Your models should also subclass this class.  
Modules can also contain other Modules, allowing them to be nested in a tree structure. You can assign the sub-modules as regular attributes:
```

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

(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 = '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__()

```

(continues on next page)

(continued from previous 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.

```
name = 'ConvO'

conv2d

fc_num_input

fc1

bn_conv2d

norm_fc1

feature_map_dropout

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

residual_convolution(O_1, O_2)

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

### Parameters

`x`

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

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

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

Bases: `dicee.models.base_model.BaseKGE`

Additive Convolutional Octonion Knowledge Graph Embeddings

`name = 'AConvO'`

`conv2d`

```

fc_num_input
fc1
bn_conv2d
norm_fc1
feature_map_dropout
static octonion_normalizer(emb_rel_e0, emb_rel_e1, emb_rel_e2, emb_rel_e3, emb_rel_e4,
                           emb_rel_e5, emb_rel_e6, emb_rel_e7)
residual_convolution(O_1, O_2)
forward_triples(x: torch.Tensor) → torch.Tensor

Parameters
x

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


```

## dicee.models.pykeen\_models

### Classes

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

### Module Contents

```

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

model_kwargs
name
model
loss_history = []
args
entity_embeddings = None
relation_embeddings = None

```

```

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

    else:
        t = self.entity_embeddings.weight

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

forward_triples(x: torch.LongTensor) → torch.FloatTensor
    # => Explicit version by this we can apply bn and dropout
    # (1) Retrieve embeddings of heads, relations and tails and apply Dropout & Normalization if given. h, r, t =
    self.get_triple_representation(x) # (2) Reshape (1). if self.last_dim > 0:
        h = h.reshape(len(x), self.embedding_dim, self.last_dim) r = r.reshape(len(x), self.embedding_dim,
        self.last_dim) t = t.reshape(len(x), self.embedding_dim, self.last_dim)
    # (3) Compute the triple score return self.interaction.score(h=h, r=r, t=t, slice_size=None, slice_dim=0)

abstract forward_k_vs_sample(x: torch.LongTensor, target_entity_idx)

```

## dicee.models.quaternion

### Classes

<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

### Functions

---

<i>quaternion_mul_with_unit_norm</i> (*, 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 ( <a href="https://arxiv.org/abs/2101.09090">https://arxiv.org/abs/2101.09090</a> )
<i>Pyke</i>	A Physical Embedding Model for Knowledge Graphs
<i>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) → torch.Tensor

score(emb_h, emb_r, emb_t) → torch.Tensor

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

```

## dicee.models.static\_funcs

### Functions

<code><a href="#">quaternion_mul</a></code> (→ Tuple[ <i>torch.Tensor</i> , <i>torch.Tensor</i> , ...])	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](https://github.com/huggingface/transformers/blob/main/src/transformers/models/gpt2/modeling_gpt2.py)

### Classes

<code><a href="#">ByteE</a></code>	Base class for all neural network modules.
<code><a href="#">LayerNorm</a></code>	LayerNorm but with an optional bias. PyTorch doesn't support simply bias=False
<code><a href="#">SelfAttention</a></code>	Base class for all neural network modules.
<code><a href="#">MLP</a></code>	Base class for all neural network modules.
<code><a href="#">Block</a></code>	Base class for all neural network modules.
<code><a href="#">GPTConfig</a></code>	
<code><a href="#">GPT</a></code>	Base class for all neural network modules.

## Module Contents

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

Bases: `dicee.models.base_model.BaseKGE`

Base class for all neural network modules.

Your models should also subclass this class.

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

(continues on next page)

```
...  
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>Shallom</i>	A shallow neural model for relation prediction ( <a href="https://arxiv.org/abs/2101.09090">https://arxiv.org/abs/2101.09090</a> )
<i>Pyke</i>	A Physical Embedding Model for Knowledge Graphs
<i>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.

continues on next page

Table 1 – continued from previous page

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

## Functions

```

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

octonion_mul(*, O_1, O_2)

octonion_mul_norm(*, O_1, O_2)

```

## Package Contents

```

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

```

Bases: *torch.optim.optimizer.Optimizer*

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:

- $\theta_t$ : parameter at step t
- $g_t$ : gradient at step t
- $m_t$ : first moment estimate (momentum)
- $v_t$ : second moment estimate (variance)
- $\alpha$ : learning rate
- $\beta_1, \beta_2$ : 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 ( $\beta_1, \beta_2$ ) for computing running averages of gradient and its square.  $\beta_1$  controls momentum,  $\beta_2$  controls variance. Default: (0.9, 0.9999)
- `eps` (*float, optional*) – Term added to denominator to improve numerical stability. Default: 1e-6
- `clip_lambda` (*Callable[[int], float], optional*) – Function that takes the step number and returns the gradient clipping threshold. Common choices: - lambda step:  $step^{**0.25}$  (default, gradually increases clipping threshold) - lambda step: 1.0 (constant clipping) - None (no clipping) Default: lambda step:  $step^{**0.25}$
- `weight_decay` (*float, optional*) – Weight decay coefficient (L2 penalty). Default: 0.0
- `decouple` (*bool, optional*) – If True, uses decoupled weight decay (AdamW-style), applying weight decay directly to parameters. If False, adds weight decay to gradients (L2 regularization). Default: False
- `foreach` (*bool, optional*) – If True, uses the faster foreach implementation for multi-tensor operations. Default: None (auto-select)
- `maximize` (*bool, optional*) – If True, maximizes parameters instead of minimizing. Useful for reinforcement learning. Default: False
- `capturable` (*bool, optional*) – If True, the optimizer is safe to capture in a CUDA graph. Requires learning rate as Tensor. Default: False
- `differentiable` (*bool, optional*) – If True, the optimization step can be differentiated. Useful for meta-learning. Default: False
- `fused` (*bool, optional*) – If True, uses fused kernel implementation (currently not supported). Default: None

#### Raises

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

## Example

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

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

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

### **i** 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()`).

### **i** 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__()
        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 = ...
```

(continues on next page)

(continued from previous page)

```
    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()`

### ℹ Note

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

## `configure_optimizers(parameters=None)`

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

### Returns

Any of these 6 options.

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

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

```
lr_scheduler_config = {
    # REQUIRED: The scheduler instance
    "scheduler": lr_scheduler,
    # The unit of the scheduler's step size, could also be 'step'.
    # 'epoch' updates the scheduler on epoch end whereas 'step'
    # updates it after a optimizer update.
    "interval": "epoch",
    # How many epochs/steps should pass between calls to
    # `scheduler.step()`. 1 corresponds to updating the learning
    # rate after every epoch/step.
    "frequency": 1,
    # Metric to monitor for schedulers like `ReduceLROnPlateau`
    "monitor": "val_loss",
    # If set to `True`, will enforce that the value specified 'monitor'
```

(continues on next page)

(continued from previous page)

```
# 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)
```

(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
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 x 2 x T)

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

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

Bases: torch.nn.Module

Base class for all neural network modules.

Your models should also subclass this class.

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

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

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

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

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

#### Note

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

#### Variables

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

```
args = None

__call__(x)

static forward(x)

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

Bases: `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** ( $B \times 2 \times T$ )

```

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.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.**Shallom**(*args*)  
Bases: *dicee.models.base\_model.BaseKGE*  
A shallow neural model for relation prediction (<https://arxiv.org/abs/2101.09090>)

```

name = 'Shallom'
shallom
get_embeddings() → Tuple[numpy.ndarray, None]
forward_k_vs_all(x) → torch.FloatTensor
```

```

forward_triples (x) → torch.FloatTensor

Parameters
    x

Returns

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

dist_func

margin = 1.0

forward_triples (x: torch.LongTensor)

Parameters
    x

class dicee.models.CoKEConfig
Configuration for the CoKE (Contextualized Knowledge Graph Embedding) model.

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

vocab_size
    Total vocabulary size (num_entities + num_relations)

n_layer
    Number of transformer layers

n_head
    Number of attention heads per layer

n_embd
    Embedding dimension (set to match model embedding_dim)

dropout
    Dropout rate applied throughout the model

bias
    Whether to use bias in linear layers

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

block_size: int = 3

vocab_size: int = None

n_layer: int = 6

n_head: int = 8

n_embd: int = None

```

```

dropout: float = 0.3
bias: bool = True
causal: bool = False

class dicee.models.CoKE(args, config: CoKEConfig = CoKEConfig())
Bases: dicee.models.base_model.BaseKGE

```

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

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

The model creates a sequence [head\_emb, relation\_emb, mask\_emb], adds positional embeddings, and processes it through transformer layers to predict the tail entity.

```

name = 'CoKE'

config

pos_emb

mask_emb

blocks

ln_f

coke_dropout

forward_k_vs_all(x: torch.Tensor)
score(emb_h, emb_r, emb_t)

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

```

```

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

```

Base class for all neural network modules.

Your models should also subclass this class.

Modules can also contain other Modules, allowing them to be nested in a tree structure. You can assign the 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.ConEx(args)
    Bases: dicee.models.base_model.BaseKGE

    Convolutional ComplEx Knowledge Graph Embeddings

    name = 'ConEx'

    conv2d

    fc_num_input

    fc1

    norm_fc1

    bn_conv2d

    feature_map_dropout

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

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

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

    Parameters
        x

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

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

    Additive Convolutional ComplEx Knowledge Graph Embeddings

    name = 'AConEx'

    conv2d

    fc_num_input

    fc1

    norm_fc1

    bn_conv2d

    feature_map_dropout

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

```

```

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

Parameters
    x

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

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

```

Base class for all neural network modules.

Your models should also subclass this class.

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

```

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

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

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

```

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

### **Note**

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

### **Variables**

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

```

name = 'ComplEx'

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

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

```

### **Parameters**

- `emb_h`
- `emb_r`

- `emb_E`

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

`forward_k_vs_sample`(*x*: `torch.LongTensor`, *target\_entity\_idx*: `torch.LongTensor`)

`dicee.models.quaternion_mul`(\**Q\_1, Q\_2*)  
     → `Tuple[torch.Tensor, torch.Tensor, torch.Tensor, torch.Tensor]`

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

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

Bases: `BaseKGELightning`

Base class for all neural network modules.

Your models should also subclass this class.

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

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

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

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

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

### Note

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

### Variables

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

### args

```
embedding_dim = None
num_entities = None
num_relations = None
num_tokens = None
learning_rate = None
```

```

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

Parameters
  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:

$$\sigma_0 t = \sigma_0 \cdot t_0 = s0 + s1 - s2s3, s4 and s5$$

**compute\_sigmas\_multivect** (*list\_h\_emb*, *list\_r\_emb*)

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

For same bases vectors interaction we have

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

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:

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

$\sigma_{pp}$  captures the interactions between along p bases For instance, let p e\_1, e\_2, e\_3, we compute interactions between e\_1 e\_2, e\_1 e\_3 , and e\_2 e\_3 This can be implemented with a nested two for loops

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

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

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

e2e1, e2e2, e2e3, e3e1, e3e2, e3e3

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

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

Compute

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

`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)

abstract forward_k_vs_sample (x: torch.LongTensor, target_entity_idx)

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

Base class for all neural network modules.

Your models should also subclass this class.

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

```

```

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

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

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

```

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

### Note

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

### Variables

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

```

args
embedding_dim = None
num_entities = None
num_relations = None
num_tokens = None
learning_rate = None
apply_unit_norm = None
input_dropout_rate = None
hidden_dropout_rate = None
optimizer_name = None
feature_map_dropout_rate = None
kernel_size = None
num_of_output_channels = None
weight_decay = None
loss
selected_optimizer = None
normalizer_class = None
normalize_head_entity_embeddings
normalize_relation_embeddings
normalize_tail_entity_embeddings
hidden_normalizer
param_init
input_dp_ent_real
input_dp_rel_real
hidden_dropout
loss_history = []
byte_pair_encoding
max_length_subword_tokens
block_size
forward_byte_pair_encoded_k_vs_all(x: torch.LongTensor)

```

#### Parameters

**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)

abstract load_queries (path)

get_queries (query_type: str, gen_num: int)

static save_queries_and_answers (path: str, data: List[Tuple[str, Tuple[collections.defaultdict]]])
    → None
    Save Queries into Disk

static load_queries_and_answers (path: str) → List[Tuple[str, Tuple[collections.defaultdict]]]
    Load Queries from Disk to Memory

```

## dicee.read\_preprocess\_save\_load\_kg

### Submodules

## dicee.read\_preprocess\_save\_load\_kg.preprocess

### Classes

<i>PreprocessKG</i>	Preprocess the data in memory
---------------------	-------------------------------

### Module Contents

```

class dicee.read_preprocess_save_load_kg.preprocess.PreprocessKG (kg)
    Preprocess the data in memory

    kg

    start () → None
        Preprocess train, valid and test datasets stored in knowledge graph instance

```

### Parameter

<b>rtype</b>	
None	
<b>preprocess_with_byte_pair_encoding()</b>	
<b>preprocess_with_byte_pair_encoding_with_padding()</b>	→ None
Preprocess with byte pair encoding and add padding	
<b>preprocess_with_pandas()</b>	→ None
Preprocess with pandas: add reciprocal triples, construct vocabulary, and index datasets	
<b>preprocess_with_polars()</b>	→ 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)  
  
serve(args)  
  
main()
```

---

## Module Contents

```
dicee.scripts.index_serve.get_default_arguments()  
  
dicee.scripts.index_serve.index(args)  
  
dicee.scripts.index_serve.app  
  
dicee.scripts.index_serve.neural_searcher = None  
  
class dicee.scripts.index_serve.NeuralSearcher(args)  
  
    collection_name  
  
    entity_to_idx = None  
  
    qdrant_client  
  
    topk = 5  
  
    retrieve_embedding(entity: str = None, entities: List[str] = None) → List  
  
    search(entity: str)  
  
async dicee.scripts.index_serve.root()  
  
async dicee.scripts.index_serve.search_embeddings(q: str)  
  
async dicee.scripts.index_serve.retrieve_embeddings(q: str)  
  
class dicee.scripts.index_serve.StringListRequest  
    Bases: pydantic.BaseModel  
  
    queries: List[str]  
  
    reducer: str | None = None
```

```

async dicee.scripts.index_server.search_embeddings_batch(request: StringListRequest)
dicee.scripts.index_server.serve(args)
dicee.scripts.index_server.main()

```

## dicee.scripts.run

### Functions

<code>get_default_arguments([description])</code>	Extends pytorch_lightning Trainer's arguments with ours
<code>main()</code>	

## 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(→ das.DataFrame)</code>	pan-	Add inverse triples to a DataFrame.
<code>get_er_vocab(→ Dict[Tuple[int, int], List[int]])</code>		Build entity-relation to tail vocabulary.
<code>get_re_vocab(→ Dict[Tuple[int, int], List[int]])</code>		Build relation-entity (tail) to head vocabulary.
<code>get_ee_vocab(→ Dict[Tuple[int, int], List[int]])</code>		Build entity-entity to relation vocabulary.
<code>timeit(→ Callable)</code>		Decorator to measure and print execution time and memory usage.
<code>save_pickle(→ None)</code>		Save data to a pickle file.
<code>load_pickle(→ object)</code>		Load data from a pickle file.
<code>load_term_mapping(→ lars.DataFrame)</code>	po-	Load term-to-index mapping from pickle or CSV file.
<code>select_model(args[, is_continual_training, storage_path])</code>	stor-	
<code>load_model(→ Tuple[object, Tuple[dict, dict]])</code>	age	Load weights and initialize pytorch module from namespace arguments

continues on next page

Table 2 – continued from previous page

<code>load_model_ensemble(...)</code>	Construct Ensemble Of weights and initialize pytorch module from namespace arguments
<code>save_numpy_ndarray(*, data, file_path)</code>	
<code>numpy_data_type_changer(→ numpy.ndarray)</code>	Detect most efficient data type for a given triples
<code>save_checkpoint_model(→ None)</code>	Store Pytorch model into disk
<code>store(→ None)</code>	
<code>add_noisy_triples(→ pandas.DataFrame)</code>	Add randomly constructed triples
<code>read_or_load_kg(args, cls)</code>	
<code>intialize_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_recipriocal_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.initialize_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, 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](https://pytorch.org/tutorials/recipes/recipes/tuning_guide.html)

### Parameters

**model** – PyTorch model to zero gradients for.

## dicee.static\_preprocess\_funcs

### Attributes

---

<code>enable_log</code>
-------------------------

---

### Functions

---

<code>timeit(func)</code>
---------------------------

---

<code>preprocesses_input_args(args)</code>	Sanity Checking in input arguments
--	------------------------------------

---

<code>create_constraints(→ Tuple[dict, dict, dict, dict])</code>
--

---

<code>get_er_vocab(data)</code>
---------------------------------

---

<code>get_re_vocab(data)</code>
---------------------------------

---

<code>get_ee_vocab(data)</code>
---------------------------------

---

<code>mapping_from_first_two_cols_to_third(train_se</code>
--

---

## Module Contents

```
dicee.static_preprocess_funcs.enable_log = False  
dicee.static_preprocess_funcs.timeit(func)  
dicee.static_preprocess_funcs.preprocesses_input_args(args)  
    Sanity Checking in input arguments  
dicee.static_preprocess_funcs.create_constraints(triples: numpy.ndarray)  
    → Tuple[dict, dict, dict, dict]  
  
(1) Extract domains and ranges of relations  
(2) Store a mapping from relations to entities that are outside of the domain and range. Create constraints entities based on the range of relations :param triples: :return:  
dicee.static_preprocess_funcs.get_er_vocab(data)  
dicee.static_preprocess_funcs.get_re_vocab(data)  
dicee.static_preprocess_funcs.get_ee_vocab(data)  
dicee.static_preprocess_funcs.mapping_from_first_two_cols_to_third(train_set_idx)
```

## dicee.trainer

### Submodules

#### dicee.trainer.dice\_trainer

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.torch\_trainer.DiceeTorchTrainer*

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

<i>TorchTrainer</i>	TorchTrainer for using single GPU or multi CPUs on a single node
---------------------	--

## Module Contents

```
class dicee.trainer.torch_trainer.TorchTrainer (args, callbacks)  
    Bases: dicee.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

---

<i>TorchDDPTrainer</i>	A Trainer based on torch.nn.parallel.DistributedDataParallel
<i>NodeTrainer</i>	

---

### Functions

---

<i>make_iterable_verbose</i> (→ Iterable)
---

---

## Module Contents

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

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

Bases: *dicee.abstracts.AbstractTrainer*

A Trainer based on torch.nn.parallel.DistributedDataParallel

Arguments

**entity\_idxs**

mapping.

**relation\_idxs**

mapping.

**form**

?

**store**

?

**label\_smoothing\_rate**

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

**Return type**

torch.utils.data.Dataset

```
fit (*args, **kwargs)
```

Train model

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

**trainer**

**local\_rank**

**global\_rank**

**optimizer**

**train\_dataset\_loader**

**loss\_func**

**callbacks**

**model**

**num\_epochs**

```
loss_history = []
```

**ctx**

**scaler**

```
extract_input_outputs (z: list)
```

```
train()
```

Training loop for DDP

## Classes

---

```
DICE_Trainer
```

```
DICE_Trainer implement
```

---

### Package Contents

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

```
DICE_Trainer implement
```

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

```
args
```

```
is_continual_training:bool
```

```
storage_path:str
```

```
evaluator:
```

```
report:dict
```

```
report
```

```
args
```

```
trainer = None
```

```
is_continual_training
```

```
storage_path
```

```
evaluator = None
```

```
form_of_labelling = None
```

```
continual_start (knowledge_graph)
```

(1) Initialize training.

(2) Load model

(3) Load trainer (3) Fit model

### Parameter

```
returns
```

- *model*
- **form\_of\_labelling** (*str*)

```

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

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 = [ $\text{dev}_1, \text{dev}_2, \dots, \text{dev}_K$ ], 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  $\theta$  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  $\beta$  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: #  $w_{twa} = \text{mean}_w + P * \beta$  #  $\text{mean}_w = (1/n) * \sum_i w_i$  (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, 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)

abstract load_queries(path)

get_queries(query_type: str, gen_num: int)

static save_queries_and_answers(path: str, data: List[Tuple[str, Tuple[collections.defaultdict]]])
    → None
    Save Queries into Disk

static load_queries_and_answers(path: str) → List[Tuple[str, Tuple[collections.defaultdict]]]
    Load Queries from Disk to Memory

```

```
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_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, form_of_labelling: str = 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) → 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,  
form_of_labelling: str = 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\_\_ = '0.1.5'

## Python Module Index

### d

    dicee, 12  
    dicee.\_\_main\_\_, 12  
    dicee.abstracts, 12  
    dicee.analyse\_experiments, 19  
    dicee.callbacks, 21  
    dicee.config, 27  
    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, 66  
    dicee.executer, 69  
    dicee.knowledge\_graph, 72  
    dicee.knowledge\_graph\_embeddings, 75  
    dicee.models, 78  
        dicee.models.adopt, 78  
        dicee.models.base\_model, 87  
        dicee.models.clifford, 96  
        dicee.models.complex, 103  
        dicee.models.dualE, 106  
        dicee.models.ensemble, 107  
        dicee.models.function\_space, 108  
        dicee.models.literal, 111  
        dicee.models.octonion, 113  
        dicee.models.pykeen\_models, 116  
        dicee.models.quaternion, 117  
        dicee.models.real, 120  
        dicee.models.static\_funcs, 123  
        dicee.models.transformers, 123  
    dicee.query\_generator, 182  
    dicee.read\_preprocess\_save\_load\_kg, 184  
        dicee.read\_preprocess\_save\_load\_kg.preprocess,  
            184  
    dicee.read\_preprocess\_save\_load\_kg.read\_from\_disk,  
        185  
    dicee.read\_preprocess\_save\_load\_kg.save\_load\_disk,  
        185  
    dicee.read\_preprocess\_save\_load\_kg.util,  
        186  
    dicee.sanity\_checkers, 190  
    dicee.scripts, 191  
        dicee.scripts.index\_serve, 191  
        dicee.scripts.run, 193  
    dicee.static\_funcs, 193  
    dicee.static\_funcs\_training, 198

# Index

## Non-alphabetical

`__call__()` (*dicee.models.base\_model.IdentityClass method*), 96  
`__call__()` (*dicee.models.ensemble.EnsembleKGE method*), 108  
`__call__()` (*dicee.models.IdentityClass method*), 143, 157, 163  
`__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*), 74  
`__iter__()` (*dicee.models.ensemble.EnsembleKGE method*), 107  
`__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*), 36  
`__len__()` (*dicee.dataset\_classes.TriplePredictionDataset method*), 39  
`__len__()` (*dicee.knowledge\_graph.KG method*), 74  
`__len__()` (*dicee.models.ensemble.EnsembleKGE method*), 107  
`__setstate__()` (*dicee.models.ADOPT method*), 133  
`__setstate__()` (*dicee.models.adopt.ADOPT method*), 82  
`__str__()` (*dicee.KGE method*), 215  
`__str__()` (*dicee.knowledge\_graph\_embeddings.KGE method*), 75  
`__str__()` (*dicee.models.ensemble.EnsembleKGE method*), 108  
`__version__` (*in module dicee*), 224

## A

`AbstractCallback` (*class in dicee.abstracts*), 16  
`AbstractPPECallback` (*class in dicee.abstracts*), 17  
`AbstractTrainer` (*class in dicee.abstracts*), 13  
`AccumulateEpochLossCallback` (*class in dicee.callbacks*), 21  
`achieve_answer()` (*dicee.query\_generator.QueryGenerator method*), 183  
`achieve_answer()` (*dicee.QueryGenerator method*), 219  
`AConEx` (*class in dicee.models*), 152  
`AConEx` (*class in dicee.models.complex*), 104  
`AConvO` (*class in dicee.models*), 165  
`AConvO` (*class in dicee.models.octonion*), 115  
`AConvQ` (*class in dicee.models*), 159  
`AConvQ` (*class in dicee.models.quaternion*), 119  
`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*), 73  
`add_noisy_triples()` (*in module dicee.static\_funcs*), 196  
`add_noisy_triples_into_training()` (*dicee.read\_preprocess\_save\_load\_kg.read\_from\_disk.ReadFromDisk method*), 185  
`add_noisy_triples_into_training()` (*dicee.read\_preprocess\_save\_load\_kg.ReadFromDisk method*), 190  
`add_reciprocal` (*dicee.knowledge\_graph.KG attribute*), 73  
`ADOPT` (*class in dicee.models*), 131  
`ADOPT` (*class in dicee.models.adopt*), 80  
`adopt()` (*in module dicee.models.adopt*), 83  
`AllvsAll` (*class in dicee.dataset\_classes*), 35  
`alphas` (*dicee.abstracts.AbstractPPECallback attribute*), 18

```

alphas (dicee.weight_averaging.ASWA attribute), 208
analyse() (in module dicee.analyse_experiments), 20
answer_multi_hop_query() (dicee.KGE method), 217
answer_multi_hop_query() (dicee.knowledge_graph_embeddings.KGE method), 77
app (in module dicee.scripts.index_server), 192
apply_coefficients() (dicee.models.clifford.DeCaL method), 102
apply_coefficients() (dicee.models.clifford.Keci method), 98
apply_coefficients() (dicee.models.DeCaL method), 171
apply_coefficients() (dicee.models.Keci method), 167
apply_reciprocal_or_noise() (in module dicee.read_preprocess_save_load_kg.util), 188
apply_semantic_constraint (dicee.abstracts.BaseInteractiveKGE attribute), 14
apply_unit_norm (dicee.models.base_model.BaseKGE attribute), 94
apply_unit_norm (dicee.models.BaseKGE attribute), 141, 144, 150, 154, 160, 173, 177
args (dicee.DICE_Trainer attribute), 220
args (dicee.evaluation.Evaluator attribute), 59
args (dicee.evaluation.evaluator.Evaluator attribute), 50, 51
args (dicee.Evaluator attribute), 221, 222
args (dicee.evaluator.Evaluator attribute), 66, 67
args (dicee.Execute attribute), 213, 214
args (dicee.executer.Execute attribute), 70
args (dicee.models.base_model.BaseKGE attribute), 94
args (dicee.models.base_model.IdentityClass attribute), 96
args (dicee.models.BaseKGE attribute), 141, 144, 150, 154, 160, 173, 176
args (dicee.models.ensemble.EnsembleKGE attribute), 107
args (dicee.models.IdentityClass attribute), 143, 157, 163
args (dicee.models.pykeen_models.PykeenKGE attribute), 116
args (dicee.models.PykeenKGE attribute), 175
args (dicee.trainer.DICE_Trainer attribute), 206
args (dicee.trainer.dice_trainer.DICE_Trainer attribute), 201
ASWA (class in dicee.weight_averaging), 207
aswa (dicee.analyse_experiments.Experiment attribute), 20
attn (dicee.models.Block attribute), 146
attn (dicee.models.transformers.Block attribute), 128
attn_dropout (dicee.models.transformers.SelfAttention attribute), 127
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), 73
base_weights (dicee.weight_averaging.TWA attribute), 212
BaseInteractiveKGE (class in dicee.abstracts), 14
BaseInteractiveTrainKGE (class in dicee.abstracts), 18
BaseKGE (class in dicee.models), 140, 143, 149, 154, 160, 172, 176
BaseKGE (class in dicee.models.base_model), 93
BaseKGELightning (class in dicee.models), 134
BaseKGELightning (class in dicee.models.base_model), 87
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), 212
bias (dicee.models.CoKEConfig attribute), 148, 149
bias (dicee.models.real.CoKEConfig attribute), 122
bias (dicee.models.transformers.GPTConfig attribute), 129
bias (dicee.models.transformers.LayerNorm attribute), 126
Block (class in dicee.models), 146
Block (class in dicee.models.transformers), 128
block_size (dicee.config.Namespace attribute), 30
block_size (dicee.dataset_classes.MultiClassClassificationDataset attribute), 33
block_size (dicee.models.base_model.BaseKGE attribute), 95
block_size (dicee.models.BaseKGE attribute), 142, 145, 151, 155, 161, 174, 177
block_size (dicee.models.CoKEConfig attribute), 148
block_size (dicee.models.real.CoKEConfig attribute), 122
block_size (dicee.models.transformers.GPTConfig attribute), 128

```

blocks (*dicee.models.CoKE attribute*), 149  
 blocks (*dicee.models.real.CoKE attribute*), 123  
 bn\_conv1 (*dicee.models.AConvQ attribute*), 159  
 bn\_conv1 (*dicee.models.ConvQ attribute*), 159  
 bn\_conv1 (*dicee.models.quaternion.AConvQ attribute*), 120  
 bn\_conv1 (*dicee.models.quaternion.ConvQ attribute*), 119  
 bn\_conv2 (*dicee.models.AConvQ attribute*), 159  
 bn\_conv2 (*dicee.models.ConvQ attribute*), 159  
 bn\_conv2 (*dicee.models.quaternion.AConvQ attribute*), 120  
 bn\_conv2 (*dicee.models.quaternion.ConvQ attribute*), 119  
 bn\_conv2d (*dicee.models.AConEx attribute*), 152  
 bn\_conv2d (*dicee.models.AConvO attribute*), 165  
 bn\_conv2d (*dicee.models.complex.AConEx attribute*), 104  
 bn\_conv2d (*dicee.models.complex.ConEx attribute*), 104  
 bn\_conv2d (*dicee.models.ConEx attribute*), 152  
 bn\_conv2d (*dicee.models.ConvO attribute*), 165  
 bn\_conv2d (*dicee.models.octonion.AConvO attribute*), 116  
 bn\_conv2d (*dicee.models.octonion.ConvO attribute*), 115  
 BPE\_NegativeSamplingDataset (*class in dicee.dataset\_classes*), 32  
 build\_chain\_funcs () (*dicee.models.FMult2 method*), 180  
 build\_chain\_funcs () (*dicee.models.function\_space.FMult2 method*), 109  
 build\_func () (*dicee.models.FMult2 method*), 180  
 build\_func () (*dicee.models.function\_space.FMult2 method*), 109  
 build\_projection () (*dicee.weight\_averaging.TWA method*), 212  
 ByteE (*class in dicee.models.transformers*), 124  
 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*), 73  
 byte\_pair\_encoding (*dicee.models.base\_model.BaseKGE attribute*), 94  
 byte\_pair\_encoding (*dicee.models.BaseKGE attribute*), 142, 145, 151, 155, 161, 174, 177

## C

c\_attn (*dicee.models.transformers.SelfAttention attribute*), 126  
 c\_fc (*dicee.models.transformers.MLP attribute*), 127  
 c\_proj (*dicee.models.transformers.MLP attribute*), 128  
 c\_proj (*dicee.models.transformers.SelfAttention attribute*), 127  
 callbacks (*dicee.abstracts.AbstractTrainer attribute*), 13  
 callbacks (*dicee.analyse\_experiments.Experiment attribute*), 19  
 callbacks (*dicee.config.Namespace attribute*), 28  
 callbacks (*dicee.trainer.torch\_trainer\_ddp.NodeTrainer attribute*), 205  
 causal (*dicee.models.CoKEConfig attribute*), 148, 149  
 causal (*dicee.models.real.CoKEConfig attribute*), 122  
 causal (*dicee.models.transformers.GPTConfig attribute*), 129  
 causal (*dicee.models.transformers.SelfAttention attribute*), 127  
 chain\_func () (*dicee.models.FMult method*), 179  
 chain\_func () (*dicee.models.function\_space.FMult method*), 108  
 chain\_func () (*dicee.models.function\_space.GFMult method*), 109  
 chain\_func () (*dicee.models.GFMult method*), 179  
 CKeci (*class in dicee.models*), 169  
 CKeci (*class in dicee.models.clifford*), 100  
 cl\_pqr () (*dicee.models.clifford.DeCaL method*), 101  
 cl\_pqr () (*dicee.models.DeCaL method*), 170  
 cleanup () (*dicee.Execute method*), 214  
 cleanup () (*dicee.executer.Execute method*), 70  
 clifford\_multiplication () (*dicee.models.clifford.Keci method*), 98  
 clifford\_multiplication () (*dicee.models.Keci method*), 167  
 clip\_lambda (*dicee.models.ADOPT attribute*), 133  
 clip\_lambda (*dicee.models.adopt.ADOPT attribute*), 82  
 CoKE (*class in dicee.models*), 149  
 CoKE (*class in dicee.models.real*), 122  
 coke\_dropout (*dicee.models.CoKE attribute*), 149  
 coke\_dropout (*dicee.models.real.CoKE attribute*), 123  
 CoKEConfig (*class in dicee.models*), 148  
 CoKEConfig (*class in dicee.models.real*), 122  
 collate\_fn (*dicee.dataset\_classes.AllvsAll attribute*), 35  
 collate\_fn (*dicee.dataset\_classes.KvsAll attribute*), 34  
 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.OnesvsAllDataset attribute), 34
collate_fn (dicee.dataset_classes.OnesvsSample attribute), 36
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), 192
comp_func () (dicee.models.function_space.LFMult method), 111
comp_func () (dicee.models.LFMult method), 181
ComplEx (class in dicee.models), 153
ComplEx (class in dicee.models.complex), 105
compute_convergence () (in module dicee.callbacks), 24
compute_func () (dicee.models.FMult method), 179
compute_func () (dicee.models.FMult2 method), 180
compute_func () (dicee.models.function_space.FMult method), 108
compute_func () (dicee.models.function_space.FMult2 method), 109
compute_func () (dicee.models.function_space.GFMult method), 109
compute_func () (dicee.models.GFMult method), 179
compute_metrics_from_ranks () (in module dicee.evaluation), 65
compute_metrics_from_ranks () (in module dicee.evaluation.utils), 57
compute_metrics_from_ranks_simple () (in module dicee.evaluation.utils), 57
compute_mrr () (dicee.weight_averaging.ASWA static method), 208
compute_sigma_pp () (dicee.models.clifford.DeCaL method), 102
compute_sigma_pp () (dicee.models.clifford.Keci method), 97
compute_sigma_pp () (dicee.models.DeCaL method), 171
compute_sigma_pp () (dicee.models.Keci method), 166
compute_sigma_pq () (dicee.models.clifford.DeCaL method), 103
compute_sigma_pq () (dicee.models.clifford.Keci method), 98
compute_sigma_pq () (dicee.models.DeCaL method), 172
compute_sigma_pq () (dicee.models.Keci method), 167
compute_sigma_pr () (dicee.models.clifford.DeCaL method), 103
compute_sigma_pr () (dicee.models.DeCaL method), 172
compute_sigma_qq () (dicee.models.clifford.DeCaL method), 102
compute_sigma_qq () (dicee.models.clifford.Keci method), 98
compute_sigma_qq () (dicee.models.DeCaL method), 171
compute_sigma_qq () (dicee.models.Keci method), 167
compute_sigma_qr () (dicee.models.clifford.DeCaL method), 103
compute_sigma_qr () (dicee.models.DeCaL method), 172
compute_sigma_rr () (dicee.models.clifford.DeCaL method), 103
compute_sigma_rr () (dicee.models.DeCaL method), 172
compute_sigmas_multivect () (dicee.models.clifford.DeCaL method), 101
compute_sigmas_multivect () (dicee.models.DeCaL method), 170
compute_sigmas_single () (dicee.models.clifford.DeCaL method), 101
compute_sigmas_single () (dicee.models.DeCaL method), 170
ConEx (class in dicee.models), 152
ConEx (class in dicee.models.complex), 104
config (dicee.models.CoKE attribute), 149
config (dicee.models.real.CoKE attribute), 123
config (dicee.models.transformers.BytE attribute), 124
config (dicee.models.transformers.GPT attribute), 129
configs (dicee.abstracts.BaseInteractiveKGE attribute), 14
configure_optimizers () (dicee.models.base_model.BaseKGELightning method), 92
configure_optimizers () (dicee.models.BaseKGELightning method), 139
configure_optimizers () (dicee.models.transformers.GPT method), 130
construct_batch_selected_cl_multivector () (dicee.models.clifford.Keci method), 99
construct_batch_selected_cl_multivector () (dicee.models.Keci method), 168
construct_cl_multivector () (dicee.models.clifford.DeCaL method), 102
construct_cl_multivector () (dicee.models.clifford.Keci method), 98
construct_cl_multivector () (dicee.models.DeCaL method), 171
construct_cl_multivector () (dicee.models.Keci method), 168
construct_dataset () (in module dicee.dataset_classes), 32
construct_ensemble (dicee.abstracts.BaseInteractiveKGE attribute), 14
construct_graph () (dicee.query_generator.QueryGenerator method), 183
construct_graph () (dicee.QueryGenerator method), 219
construct_input_and_output () (dicee.abstracts.BaseInteractiveKGE method), 16
construct_multi_coeff () (dicee.models.function_space.LFMult method), 110
construct_multi_coeff () (dicee.models.LFMult method), 181
continual_learning (dicee.config.Namespace attribute), 30

```

continual\_start() (*dicee.DICE\_Trainer method*), 220  
 continual\_start() (*dicee.executer.ContinuousExecute method*), 72  
 continual\_start() (*dicee.trainer.DICE\_Trainer method*), 206  
 continual\_start() (*dicee.trainer.dice\_trainer.DICE\_Trainer method*), 201  
 continual\_training\_setup\_executor() (*in module dicee.static\_funcs*), 197  
 ContinuousExecute (*class in dicee.executer*), 71  
 conv2d (*dicee.models.AConEx attribute*), 152  
 conv2d (*dicee.models.AConvO attribute*), 165  
 conv2d (*dicee.models.AConvQ attribute*), 159  
 conv2d (*dicee.models.complex.AConEx attribute*), 104  
 conv2d (*dicee.models.complex.ConEx attribute*), 104  
 conv2d (*dicee.models.ConEx attribute*), 152  
 conv2d (*dicee.models.ConvO attribute*), 165  
 conv2d (*dicee.models.ConvQ attribute*), 159  
 conv2d (*dicee.models.octonion.AConvO attribute*), 115  
 conv2d (*dicee.models.octonion.ConvO attribute*), 115  
 conv2d (*dicee.models.quaternion.AConvQ attribute*), 120  
 conv2d (*dicee.models.quaternion.ConvQ attribute*), 119  
 ConvO (*class in dicee.models*), 164  
 ConvO (*class in dicee.models.octonion*), 114  
 ConvQ (*class in dicee.models*), 158  
 ConvQ (*class in dicee.models.quaternion*), 119  
 count\_triples() (*in module dicee.read\_preprocess\_save\_load\_kg.util*), 188  
 create\_and\_store\_kg() (*dicee.Execute method*), 214  
 create\_and\_store\_kg() (*dicee.executer.Execute method*), 71  
 create\_constraints() (*in module dicee.read\_preprocess\_save\_load\_kg.util*), 188  
 create\_constraints() (*in module dicee.static\_preprocess\_funcs*), 200  
 create\_experiment\_folder() (*in module dicee.static\_funcs*), 197  
 create\_random\_data() (*dicee.callbacks.PseudoLabellingCallback method*), 24  
 create\_reciprocal\_triples() (*in module dicee.read\_preprocess\_save\_load\_kg.util*), 189  
 create\_reciprocal\_triples() (*in module dicee.static\_funcs*), 194  
 create\_vector\_database() (*dicee.KGE method*), 215  
 create\_vector\_database() (*dicee.knowledge\_graph\_embeddings.KGE method*), 75  
 crop\_block\_size() (*dicee.models.transformers.GPT method*), 130  
 ctx (*dicee.trainer.torch\_trainer\_ddp.NodeTrainer attribute*), 205  
 current\_epoch (*dicee.weight\_averaging.EMA attribute*), 211  
 current\_epoch (*dicee.weight\_averaging.SWA attribute*), 209  
 current\_epoch (*dicee.weight\_averaging.SWAG attribute*), 210  
 current\_epoch (*dicee.weight\_averaging.TWA attribute*), 212  
 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*), 112  
 data\_property\_to\_idx (*dicee.dataset\_classes.LiteralDataset attribute*), 44  
 dataset\_dir (*dicee.config.Namespace attribute*), 28  
 dataset\_dir (*dicee.knowledge\_graph.KG attribute*), 72, 73  
 dataset\_sanity\_checking() (*in module dicee.read\_preprocess\_save\_load\_kg.util*), 189  
 DeCaL (*class in dicee.models*), 169  
 DeCaL (*class in dicee.models.clifford*), 100  
 decay (*dicee.weight\_averaging.EMA attribute*), 211  
 decide() (*dicee.weight\_averaging.ASWA method*), 208  
 default\_eval\_model (*dicee.callbacks.PeriodicEvalCallback attribute*), 26  
 degree (*dicee.models.function\_space.LFMult attribute*), 110  
 degree (*dicee.models.LFMult attribute*), 180  
 denormalize() (*dicee.dataset\_classes.LiteralDataset static method*), 44  
 describe() (*dicee.knowledge\_graph.KG method*), 74  
 description\_of\_input (*dicee.knowledge\_graph.KG attribute*), 74  
 deviations (*dicee.weight\_averaging.SWAG attribute*), 210  
 device (*dicee.models.literal.LiteralEmbeddings property*), 113  
 DICE\_Trainer (*class in dicee*), 219  
 DICE\_Trainer (*class in dicee.trainer*), 206  
 DICE\_Trainer (*class in dicee.trainer.dice\_trainer*), 201  
 dicee  
 module, 12  
 dicee.\_\_main\_\_

```
    module, 12
dicee.abstracts
    module, 12
dicee.analyse_experiments
    module, 19
dicee.callbacks
    module, 21
dicee.config
    module, 27
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, 66
dicee.executer
    module, 69
dicee.knowledge_graph
    module, 72
dicee.knowledge_graph_embeddings
    module, 75
dicee.models
    module, 78
dicee.models.adopt
    module, 78
dicee.models.base_model
    module, 87
dicee.models.clifford
    module, 96
dicee.models.complex
    module, 103
dicee.models.dualE
    module, 106
dicee.models.ensemble
    module, 107
dicee.models.function_space
    module, 108
dicee.models.literal
    module, 111
dicee.models.octonion
    module, 113
dicee.models.pykeen_models
    module, 116
dicee.models.quaternion
    module, 117
dicee.models.real
    module, 120
dicee.models.static_funcs
    module, 123
dicee.models.transformers
    module, 123
dicee.query_generator
    module, 182
dicee.read_preprocess_save_load_kg
    module, 184
dicee.read_preprocess_save_load_kg.preprocess
```

```

        module, 184
dicee.read_preprocess_save_load_kg.read_from_disk
        module, 185
dicee.read_preprocess_save_load_kg.save_load_disk
        module, 185
dicee.read_preprocess_save_load_kg.util
        module, 186
dicee.sanity_checkers
        module, 190
dicee.scripts
        module, 191
dicee.scripts.index_serve
        module, 191
dicee.scripts.run
        module, 193
dicee.static_funcs
        module, 193
dicee.static_funcs_training
        module, 198
dicee.static_preprocess_funcs
        module, 199
dicee.trainer
        module, 200
dicee.trainer.dice_trainer
        module, 200
dicee.trainer.model_parallelism
        module, 202
dicee.trainer.torch_trainer
        module, 203
dicee.trainer.torch_trainer_ddp
        module, 204
dicee.weight_averaging
        module, 207
discrete_points (dicee.models.FMult2 attribute), 179
discrete_points (dicee.models.function_space.FMult2 attribute), 109
dist_func (dicee.models.Pyke attribute), 148
dist_func (dicee.models.real.Pyke attribute), 121
DistMult (class in dicee.models), 147
DistMult (class in dicee.models.real), 120
distributed (dicee.Execute attribute), 213
distributed (dicee.executer.Execute attribute), 70
domain_constraints_per_rel (dicee.evaluation.Evaluator attribute), 59
domain_constraints_per_rel (dicee.evaluation.evaluator.Evaluator attribute), 51
domain_constraints_per_rel (dicee.Evaluator attribute), 222
domain_constraints_per_rel (dicee.evaluator.Evaluator attribute), 67
download_file () (in module dicee.static_funcs), 197
download_files_from_url () (in module dicee.static_funcs), 197
download_pretrained_model () (in module dicee.static_funcs), 197
dropout (dicee.models.CoKEConfig attribute), 148
dropout (dicee.models.literal.LiteralEmbeddings attribute), 112
dropout (dicee.models.real.CoKEConfig attribute), 122
dropout (dicee.models.transformers.GPTConfig attribute), 129
dropout (dicee.models.transformers.MLP attribute), 128
dropout (dicee.models.transformers.SelfAttention attribute), 127
DualE (class in dicee.models), 181
DualE (class in dicee.models.dualE), 106
dummy_eval () (dicee.evaluation.Evaluator method), 61
dummy_eval () (dicee.evaluation.evaluator.Evaluator method), 52
dummy_eval () (dicee.Evaluator method), 224
dummy_eval () (dicee.evaluator.Evaluator method), 69
dummy_id (dicee.knowledge_graph.KG attribute), 74
during_training (dicee.evaluation.Evaluator attribute), 59, 60
during_training (dicee.evaluation.evaluator.Evaluator attribute), 50, 51
during_training (dicee.Evaluator attribute), 221, 222
during_training (dicee.evaluator.Evaluator attribute), 67

```

## E

ee\_vocab (*dicee.evaluation.Evaluator attribute*), 59

ee\_vocab (*dicee.evaluation.evaluator.Evaluator* attribute), 50  
 ee\_vocab (*dicee.Evaluator* attribute), 221, 222  
 ee\_vocab (*dicee.evaluator.Evaluator* attribute), 66, 67  
 efficient\_zero\_grad() (*in module dicee.evaluation.utils*), 58  
 efficient\_zero\_grad() (*in module dicee.static\_funcs\_training*), 199  
 EMA (*class in dicee.weight\_averaging*), 210  
 ema (*dicee.config.Namespace* attribute), 30  
 ema\_c\_epochs (*dicee.weight\_averaging.EMA* attribute), 211  
 ema\_model (*dicee.weight\_averaging.EMA* attribute), 211  
 ema\_start\_epoch (*dicee.weight\_averaging.EMA* attribute), 211  
 ema\_update() (*dicee.weight\_averaging.EMA static method*), 211  
 embedding\_dim (*dicee.analyse\_experiments.Experiment* attribute), 20  
 embedding\_dim (*dicee.config.Namespace* attribute), 28  
 embedding\_dim (*dicee.models.base\_model.BaseKGE* attribute), 94  
 embedding\_dim (*dicee.models.BaseKGE* attribute), 141, 144, 150, 154, 160, 173, 177  
 embedding\_dim (*dicee.models.literal.LiteralEmbeddings* attribute), 112  
 embedding\_dims (*dicee.models.literal.LiteralEmbeddings* attribute), 112  
 enable\_log (*in module dicee.static\_preprocess\_funcs*), 200  
 enc (*dicee.knowledge\_graph.KG* attribute), 74  
 end() (*dicee.Execute* method), 214  
 end() (*dicee.executer.Execute* method), 71  
 EnsembleKGE (*class in dicee.models.ensemble*), 107  
 ent2id (*dicee.query\_generator.QueryGenerator* attribute), 183  
 ent2id (*dicee.QueryGenerator* attribute), 219  
 ent\_in (*dicee.query\_generator.QueryGenerator* attribute), 183  
 ent\_in (*dicee.QueryGenerator* attribute), 219  
 ent\_out (*dicee.query\_generator.QueryGenerator* attribute), 183  
 ent\_out (*dicee.QueryGenerator* attribute), 219  
 entities\_str (*dicee.knowledge\_graph.KG* property), 74  
 entity\_embeddings (*dicee.models.AConvQ* attribute), 159  
 entity\_embeddings (*dicee.models.clifford.DeCaL* attribute), 100  
 entity\_embeddings (*dicee.models.ConvQ* attribute), 159  
 entity\_embeddings (*dicee.models.DeCaL* attribute), 169  
 entity\_embeddings (*dicee.models.DualE* attribute), 182  
 entity\_embeddings (*dicee.models.dualE.DualE* attribute), 106  
 entity\_embeddings (*dicee.models.FMult* attribute), 178  
 entity\_embeddings (*dicee.models.FMult2* attribute), 179  
 entity\_embeddings (*dicee.models.function\_space.FMult* attribute), 108  
 entity\_embeddings (*dicee.models.function\_space.FMult2* attribute), 109  
 entity\_embeddings (*dicee.models.function\_space.GFMult* attribute), 109  
 entity\_embeddings (*dicee.models.function\_space.LFMult* attribute), 110  
 entity\_embeddings (*dicee.models.function\_space.LFMult1* attribute), 110  
 entity\_embeddings (*dicee.models.GFMult* attribute), 179  
 entity\_embeddings (*dicee.models.LFMult* attribute), 180  
 entity\_embeddings (*dicee.models.LFMult1* attribute), 180  
 entity\_embeddings (*dicee.models.literal.LiteralEmbeddings* attribute), 112  
 entity\_embeddings (*dicee.models.pykeen\_models.PykeenKGE* attribute), 116  
 entity\_embeddings (*dicee.models.PykeenKGE* attribute), 175  
 entity\_embeddings (*dicee.models.quaternion.AConvQ* attribute), 120  
 entity\_embeddings (*dicee.models.quaternion.ConvQ* attribute), 119  
 entity\_to\_idx (*dicee.dataset\_classes.LiteralDataset* attribute), 43, 44  
 entity\_to\_idx (*dicee.knowledge\_graph.KG* attribute), 73  
 entity\_to\_idx (*dicee.scripts.index\_serve.NeuralSearcher* attribute), 192  
 epoch\_count (*dicee.abstracts.AbstractPPECallback* attribute), 18  
 epoch\_count (*dicee.weight\_averaging.ASWA* attribute), 208  
 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  
 er\_vocab (*dicee.evaluation.evaluator.Evaluator* attribute), 50  
 er\_vocab (*dicee.Evaluator* attribute), 221, 222  
 er\_vocab (*dicee.evaluator.Evaluator* attribute), 66, 67  
 estimate\_mfu() (*dicee.models.transformers.GPT* method), 130  
 estimate\_q() (*in module dicee.callbacks*), 24  
 Eval (*class in dicee.callbacks*), 24  
 eval() (*dicee.evaluation.Evaluator* method), 60  
 eval() (*dicee.evaluation.evaluator.Evaluator* method), 51

```

eval() (dicee.Evaluator method), 222
eval() (dicee.evaluator.Evaluator method), 67
eval() (dicee.models.ensemble.EnsembleKGE method), 107
eval_at_epochs (dicee.config.Namespace attribute), 31
eval_epochs (dicee.callbacks.PeriodicEvalCallback attribute), 26
eval_every_n_epochs (dicee.config.Namespace attribute), 30
eval_lp_performance() (dicee.KGE method), 215
eval_lp_performance() (dicee.knowledge_graph_embeddings.KGE method), 75
eval_model (dicee.config.Namespace attribute), 29
eval_model (dicee.knowledge_graph.KG attribute), 73
eval_rank_of_head_and_tail_byte_pair_encoded_entity() (dicee.evaluation.Evaluator method), 60
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), 222
eval_rank_of_head_and_tail_byte_pair_encoded_entity() (dicee.evaluator.Evaluator method), 68
eval_rank_of_head_and_tail_entity() (dicee.evaluation.Evaluator method), 60
eval_rank_of_head_and_tail_entity() (dicee.evaluation.evaluator.Evaluator method), 51
eval_rank_of_head_and_tail_entity() (dicee.Evaluator method), 222
eval_rank_of_head_and_tail_entity() (dicee.evaluator.Evaluator method), 67
eval_with_bpe_vs_all() (dicee.evaluation.Evaluator method), 60
eval_with_bpe_vs_all() (dicee.evaluation.evaluator.Evaluator method), 51
eval_with_bpe_vs_all() (dicee.Evaluator method), 222
eval_with_bpe_vs_all() (dicee.evaluator.Evaluator method), 68
eval_with_byte() (dicee.evaluation.Evaluator method), 60
eval_with_byte() (dicee.evaluation.evaluator.Evaluator method), 51
eval_with_byte() (dicee.Evaluator method), 222
eval_with_byte() (dicee.evaluator.Evaluator method), 68
eval_with_data() (dicee.evaluation.Evaluator method), 61
eval_with_data() (dicee.evaluation.evaluator.Evaluator method), 52
eval_with_data() (dicee.Evaluator method), 224
eval_with_data() (dicee.evaluator.Evaluator method), 69
eval_with_vs_all() (dicee.evaluation.Evaluator method), 60
eval_with_vs_all() (dicee.evaluation.evaluator.Evaluator method), 51
eval_with_vs_all() (dicee.Evaluator method), 223
eval_with_vs_all() (dicee.evaluator.Evaluator method), 68
evaluate() (in module dicee.static_funcs), 197
evaluate_bpe_lp() (in module dicee.evaluation), 63
evaluate_bpe_lp() (in module dicee.evaluation.link_prediction), 55
evaluate_bpe_lp() (in module dicee.static_funcs_training), 198
evaluate_ensemble_link_prediction_performance() (in module dicee.eval_static_funcs), 47
evaluate_ensemble_link_prediction_performance() (in module dicee.evaluation), 64
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), 62
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), 62
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), 62
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), 62
evaluate_link_prediction_performance_with_reciprocals() (in module dicee.evaluation.link_prediction), 53
evaluate_literal_prediction() (in module dicee.eval_static_funcs), 46
evaluate_literal_prediction() (in module dicee.evaluation), 64
evaluate_literal_prediction() (in module dicee.evaluation.literal_prediction), 56
evaluate_lp() (dicee.evaluation.Evaluator method), 61
evaluate_lp() (dicee.evaluation.evaluator.Evaluator method), 52
evaluate_lp() (dicee.Evaluator method), 223
evaluate_lp() (dicee.evaluator.Evaluator method), 69
evaluate_lp() (in module dicee.evaluation), 63
evaluate_lp() (in module dicee.evaluation.link_prediction), 54
evaluate_lp() (in module dicee.static_funcs_training), 198
evaluate_lp_bpe_k_vs_all() (dicee.evaluation.Evaluator method), 61
evaluate_lp_bpe_k_vs_all() (dicee.evaluation.evaluator.Evaluator method), 52
evaluate_lp_bpe_k_vs_all() (dicee.Evaluator method), 223
evaluate_lp_bpe_k_vs_all() (dicee.evaluator.Evaluator method), 68
evaluate_lp_bpe_k_vs_all() (in module dicee.eval_static_funcs), 46

```

evaluate\_lp\_bpe\_k\_vs\_all() (*in module dicee.evaluation*), 63  
 evaluate\_lp\_bpe\_k\_vs\_all() (*in module dicee.evaluation.link\_prediction*), 55  
 evaluate\_lp\_k\_vs\_all() (*dicee.evaluation.Evaluator method*), 60  
 evaluate\_lp\_k\_vs\_all() (*dicee.evaluation.evaluator.Evaluator method*), 51  
 evaluate\_lp\_k\_vs\_all() (*dicee.Evaluator method*), 223  
 evaluate\_lp\_k\_vs\_all() (*dicee.evaluator.Evaluator method*), 68  
 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*), 223  
 evaluate\_lp\_with\_byte() (*dicee.evaluator.Evaluator method*), 68  
 Evaluator (*class in dicee*), 221  
 Evaluator (*class in dicee.evaluation*), 59  
 Evaluator (*class in dicee.evaluation.evaluator*), 50  
 Evaluator (*class in dicee.evaluator*), 66  
 evaluator (*dicee.DICE\_Trainer attribute*), 220  
 evaluator (*dicee.Execute attribute*), 213, 214  
 evaluator (*dicee.executer.Execute attribute*), 70  
 evaluator (*dicee.trainer.DICE\_Trainer attribute*), 206  
 evaluator (*dicee.trainer.dice\_trainer.DICE\_Trainer attribute*), 201  
 every\_x\_epoch (*dicee.callbacks.KGESaveCallback attribute*), 23  
 example\_input\_array (*dicee.models.ensemble.EnsembleKGE property*), 107  
 Execute (*class in dicee*), 213  
 Execute (*class in dicee.executer*), 70  
 exists() (*dicee.knowledge\_graph.KG method*), 74  
 Experiment (*class in dicee.analyse\_experiments*), 19  
 experiment\_dir (*dicee.callbacks.LRScheduler attribute*), 27  
 experiment\_dir (*dicee.callbacks.PeriodicEvalCallback attribute*), 26  
 explicit (*dicee.models.QMult attribute*), 158  
 explicit (*dicee.models.quaternion.QMult attribute*), 118  
 exponential\_function() (*in module dicee.static\_funcs*), 197  
 extract\_input\_outputs() (*dicee.trainer.torch\_trainer\_ddp.NodeTrainer method*), 205  
 extract\_input\_outputs() (*in module dicee.trainer.model\_parallelism*), 203  
 extract\_input\_outputs\_set\_device() (*dicee.trainer.torch\_trainer.TorchTrainer method*), 204

## F

f (*dicee.callbacks.KronE attribute*), 25  
 fc (*dicee.models.literal.LiteralEmbeddings attribute*), 112  
 fc1 (*dicee.models.AConEx attribute*), 152  
 fc1 (*dicee.models.ACovO attribute*), 165  
 fc1 (*dicee.models.ACovQ attribute*), 159  
 fc1 (*dicee.models.complex.AConEx attribute*), 104  
 fc1 (*dicee.models.complex.ConEx attribute*), 104  
 fc1 (*dicee.models.ConEx attribute*), 152  
 fc1 (*dicee.models.ConvO attribute*), 165  
 fc1 (*dicee.models.ConvQ attribute*), 159  
 fc1 (*dicee.models.octonion.ACovO attribute*), 116  
 fc1 (*dicee.models.octonion.ConvO attribute*), 115  
 fc1 (*dicee.models.quaternion.ACovQ attribute*), 120  
 fc1 (*dicee.models.quaternion.ConvQ attribute*), 119  
 fc\_num\_input (*dicee.models.AConEx attribute*), 152  
 fc\_num\_input (*dicee.models.ACovO attribute*), 165  
 fc\_num\_input (*dicee.models.ACovQ attribute*), 159  
 fc\_num\_input (*dicee.models.complex.AConEx attribute*), 104  
 fc\_num\_input (*dicee.models.complex.ConEx attribute*), 104  
 fc\_num\_input (*dicee.models.ConEx attribute*), 152  
 fc\_num\_input (*dicee.models.ConvO attribute*), 165  
 fc\_num\_input (*dicee.models.ConvQ attribute*), 159  
 fc\_num\_input (*dicee.models.octonion.ACovO attribute*), 115  
 fc\_num\_input (*dicee.models.octonion.ConvO attribute*), 115  
 fc\_num\_input (*dicee.models.quaternion.ACovQ attribute*), 120  
 fc\_num\_input (*dicee.models.quaternion.ConvQ attribute*), 119  
 fc\_out (*dicee.models.literal.LiteralEmbeddings attribute*), 112  
 feature\_map\_dropout (*dicee.models.AConEx attribute*), 152  
 feature\_map\_dropout (*dicee.models.ACovO attribute*), 165  
 feature\_map\_dropout (*dicee.models.ACovQ attribute*), 159  
 feature\_map\_dropout (*dicee.models.complex.AConEx attribute*), 105  
 feature\_map\_dropout (*dicee.models.complex.ConEx attribute*), 104

feature\_map\_dropout (*dicee.models.ConEx* attribute), 152  
 feature\_map\_dropout (*dicee.models.ConvO* attribute), 165  
 feature\_map\_dropout (*dicee.models.ConvQ* attribute), 159  
 feature\_map\_dropout (*dicee.models.octonion.AConvO* attribute), 116  
 feature\_map\_dropout (*dicee.models.octonion.ConvO* attribute), 115  
 feature\_map\_dropout (*dicee.models.quaternion.AConvQ* attribute), 120  
 feature\_map\_dropout (*dicee.models.quaternion.ConvQ* attribute), 119  
 feature\_map\_dropout\_rate (*dicee.config.Namespace* attribute), 30  
 feature\_map\_dropout\_rate (*dicee.models.base\_model.BaseKGE* attribute), 94  
 feature\_map\_dropout\_rate (*dicee.models.BaseKGE* attribute), 141, 144, 150, 155, 161, 173, 177  
 fetch\_worker () (*in module dicee.read\_preprocess\_save\_load\_kg.util*), 188  
 fill\_query () (*dicee.query\_generator.QueryGenerator* method), 183  
 fill\_query () (*dicee.QueryGenerator* method), 219  
 find\_good\_batch\_size () (*in module dicee.trainer.model\_parallelism*), 203  
 find\_missing\_triples () (*dicee.KGE* method), 218  
 find\_missing\_triples () (*dicee.knowledge\_graph\_embeddings.KGE* method), 77  
 fit () (*dicee.trainer.model\_parallelism.TensorParallel* method), 203  
 fit () (*dicee.trainer.torch\_trainer\_ddp.TorchDDPTrainer* method), 205  
 fit () (*dicee.trainer.torch\_trainer.TorchTrainer* method), 204  
 flash (*dicee.models.transformers.SelfAttention* attribute), 127  
 FMult (*class in dicee.models*), 178  
 FMult (*class in dicee.models.function\_space*), 108  
 FMult2 (*class in dicee.models*), 179  
 FMult2 (*class in dicee.models.function\_space*), 109  
 form\_of\_labelling (*dicee.DICE\_Trainer* attribute), 220  
 form\_of\_labelling (*dicee.trainer.DICE\_Trainer* attribute), 206  
 form\_of\_labelling (*dicee.trainer.dice\_trainer.DICE\_Trainer* attribute), 201  
 forward () (*dicee.models.base\_model.BaseKGE* method), 95  
 forward () (*dicee.models.base\_model.IdentityClass* static method), 96  
 forward () (*dicee.models.BaseKGE* method), 142, 145, 151, 155, 161, 174, 178  
 forward () (*dicee.models.Block* method), 147  
 forward () (*dicee.models.IdentityClass* static method), 143, 157, 163  
 forward () (*dicee.models.literal.LiteralEmbeddings* method), 113  
 forward () (*dicee.models.transformers.Block* method), 128  
 forward () (*dicee.models.transformers.BytE* method), 124  
 forward () (*dicee.models.transformers.GPT* method), 130  
 forward () (*dicee.models.transformers.LayerNorm* method), 126  
 forward () (*dicee.models.transformers.MLP* method), 128  
 forward () (*dicee.models.transformers.SelfAttention* method), 127  
 forward\_backward\_update () (*dicee.trainer.torch\_trainer.TorchTrainer* method), 204  
 forward\_backward\_update\_loss () (*in module dicee.trainer.model\_parallelism*), 203  
 forward\_byte\_pair\_encoded\_k\_vs\_all () (*dicee.models.base\_model.BaseKGE* method), 95  
 forward\_byte\_pair\_encoded\_k\_vs\_all () (*dicee.models.BaseKGE* method), 142, 145, 151, 155, 161, 174, 177  
 forward\_byte\_pair\_encoded\_triple () (*dicee.models.base\_model.BaseKGE* method), 95  
 forward\_byte\_pair\_encoded\_triple () (*dicee.models.BaseKGE* method), 142, 145, 151, 155, 161, 174, 177  
 forward\_k\_vs\_all () (*dicee.models.AConEx* method), 152  
 forward\_k\_vs\_all () (*dicee.models.AConvO* method), 165  
 forward\_k\_vs\_all () (*dicee.models.AConvQ* method), 160  
 forward\_k\_vs\_all () (*dicee.models.base\_model.BaseKGE* method), 95  
 forward\_k\_vs\_all () (*dicee.models.BaseKGE* method), 142, 145, 151, 156, 162, 175, 178  
 forward\_k\_vs\_all () (*dicee.models.clifford.DeCaL* method), 101  
 forward\_k\_vs\_all () (*dicee.models.clifford.Keci* method), 99  
 forward\_k\_vs\_all () (*dicee.models.CoKE* method), 149  
 forward\_k\_vs\_all () (*dicee.models.ComplEx* method), 154  
 forward\_k\_vs\_all () (*dicee.models.complex.AConEx* method), 105  
 forward\_k\_vs\_all () (*dicee.models.complex.ComplEx* method), 106  
 forward\_k\_vs\_all () (*dicee.models.complex.ConEx* method), 104  
 forward\_k\_vs\_all () (*dicee.models.ConEx* method), 152  
 forward\_k\_vs\_all () (*dicee.models.ConvO* method), 165  
 forward\_k\_vs\_all () (*dicee.models.ConvQ* method), 159  
 forward\_k\_vs\_all () (*dicee.models.DeCaL* method), 170  
 forward\_k\_vs\_all () (*dicee.models.DistMult* method), 147  
 forward\_k\_vs\_all () (*dicee.models.DualE* method), 182  
 forward\_k\_vs\_all () (*dicee.models.dualE.DualE* method), 107  
 forward\_k\_vs\_all () (*dicee.models.Keci* method), 168  
 forward\_k\_vs\_all () (*dicee.models.octonion.AConvO* method), 116  
 forward\_k\_vs\_all () (*dicee.models.octonion.ConvO* method), 115  
 forward\_k\_vs\_all () (*dicee.models.octonion.OMult* method), 114

```

forward_k_vs_all() (dicee.models.OMult method), 164
forward_k_vs_all() (dicee.models.pykeen_models.PykeenKGE method), 116
forward_k_vs_all() (dicee.models.PykeenKGE method), 175
forward_k_vs_all() (dicee.models.QMult method), 158
forward_k_vs_all() (dicee.models.quaternion.AConvQ method), 120
forward_k_vs_all() (dicee.models.quaternion.ConvQ method), 119
forward_k_vs_all() (dicee.models.quaternion.QMult method), 119
forward_k_vs_all() (dicee.models.real.CoKE method), 123
forward_k_vs_all() (dicee.models.real.DistMult method), 121
forward_k_vs_all() (dicee.models.real.Shallom method), 121
forward_k_vs_all() (dicee.models.real.TransE method), 121
forward_k_vs_all() (dicee.models.Shallom method), 147
forward_k_vs_all() (dicee.models.TransE method), 147
forward_k_vs_sample() (dicee.models.AConEx method), 153
forward_k_vs_sample() (dicee.models.base_model.BaseKGE method), 95
forward_k_vs_sample() (dicee.models.BaseKGE method), 142, 145, 151, 156, 162, 175, 178
forward_k_vs_sample() (dicee.models.clifford.Keci method), 99
forward_k_vs_sample() (dicee.models.CoKE method), 149
forward_k_vs_sample() (dicee.models.ComplEx method), 154
forward_k_vs_sample() (dicee.models.complex.AConEx method), 105
forward_k_vs_sample() (dicee.models.complex.ComplEx method), 106
forward_k_vs_sample() (dicee.models.complex.ConEx method), 104
forward_k_vs_sample() (dicee.models.ConEx method), 152
forward_k_vs_sample() (dicee.models.DistMult method), 147
forward_k_vs_sample() (dicee.models.Keci method), 168
forward_k_vs_sample() (dicee.models.pykeen_models.PykeenKGE method), 117
forward_k_vs_sample() (dicee.models.PykeenKGE method), 176
forward_k_vs_sample() (dicee.models.QMult method), 158
forward_k_vs_sample() (dicee.models.quaternion.QMult method), 119
forward_k_vs_sample() (dicee.models.real.CoKE method), 123
forward_k_vs_sample() (dicee.models.real.DistMult method), 121
forward_k_vs_with_explicit() (dicee.models.clifford.Keci method), 99
forward_k_vs_with_explicit() (dicee.models.Keci method), 168
forward_triples() (dicee.models.AConEx method), 153
forward_triples() (dicee.models.AConvO method), 165
forward_triples() (dicee.models.AConvQ method), 159
forward_triples() (dicee.models.base_model.BaseKGE method), 95
forward_triples() (dicee.models.BaseKGE method), 142, 145, 151, 156, 162, 174, 178
forward_triples() (dicee.models.clifford.DeCaL method), 101
forward_triples() (dicee.models.clifford.Keci method), 99
forward_triples() (dicee.models.complex.AConEx method), 105
forward_triples() (dicee.models.complex.ConEx method), 104
forward_triples() (dicee.models.ConEx method), 152
forward_triples() (dicee.models.ConvO method), 165
forward_triples() (dicee.models.ConvQ method), 159
forward_triples() (dicee.models.DeCaL method), 170
forward_triples() (dicee.models.DualE method), 182
forward_triples() (dicee.models.dualE.DualE method), 106
forward_triples() (dicee.models.FMult method), 179
forward_triples() (dicee.models.FMult2 method), 180
forward_triples() (dicee.models.function_space.FMult method), 108
forward_triples() (dicee.models.function_space.FMult2 method), 110
forward_triples() (dicee.models.function_space.GFMult method), 109
forward_triples() (dicee.models.function_space.LFMult method), 110
forward_triples() (dicee.models.function_space.LFMult1 method), 110
forward_triples() (dicee.models.GFMult method), 179
forward_triples() (dicee.models.Keci method), 169
forward_triples() (dicee.models.LFMult method), 180
forward_triples() (dicee.models.LFMult1 method), 180
forward_triples() (dicee.models.octonion.AConvO method), 116
forward_triples() (dicee.models.octonion.ConvO method), 115
forward_triples() (dicee.models.Pyke method), 148
forward_triples() (dicee.models.pykeen_models.PykeenKGE method), 117
forward_triples() (dicee.models.PykeenKGE method), 176
forward_triples() (dicee.models.quaternion.AConvQ method), 120
forward_triples() (dicee.models.quaternion.ConvQ method), 119
forward_triples() (dicee.models.real.Pyke method), 121
forward_triples() (dicee.models.real.Shallom method), 121

```

```

forward_triples() (dicee.models.Shallom method), 147
freeze_entity_embeddings (dicee.models.literal.LiteralEmbeddings attribute), 112
frequency (dicee.callbacks.Perturb attribute), 26
from_pretrained() (dicee.models.transformers.GPT class method), 130
from_pretrained_model_write_embeddings_into_csv() (in module dicee.static_funcs), 197
full_storage_path (dicee.analyse_experiments.Experiment attribute), 20
func_triple_to_bpe_representation (dicee.evaluation.Evaluator attribute), 59
func_triple_to_bpe_representation (dicee.evaluation.evaluator.Evaluator attribute), 50
func_triple_to_bpe_representation (dicee.Evaluator attribute), 222
func_triple_to_bpe_representation (dicee.evaluator.Evaluator attribute), 67
func_triple_to_bpe_representation() (dicee.knowledge_graph.KG method), 74
function() (dicee.models.FMult2 method), 180
function() (dicee.models.function_space.FMult2 method), 109

```

## G

```

gamma (dicee.models.FMult attribute), 179
gamma (dicee.models.function_space.FMult attribute), 108
gate_residual (dicee.models.literal.LiteralEmbeddings attribute), 112
gated_residual_proj (dicee.models.literal.LiteralEmbeddings attribute), 112
gelu (dicee.models.transformers.MLP attribute), 127
gen_test (dicee.query_generator.QueryGenerator attribute), 183
gen_test (dicee.QueryGenerator attribute), 218
gen_valid (dicee.query_generator.QueryGenerator attribute), 183
gen_valid (dicee.QueryGenerator attribute), 218
generate() (dicee.KGE method), 215
generate() (dicee.knowledge_graph_embeddings.KGE method), 75
generate() (dicee.models.transformers.ByE method), 125
generate_queries() (dicee.query_generator.QueryGenerator method), 183
generate_queries() (dicee.QueryGenerator method), 219
get_aswa_state_dict() (dicee.weight_averaging.ASWA method), 208
get_bpe_head_and_relation_representation() (dicee.models.base_model.BaseKGE method), 95
get_bpe_head_and_relation_representation() (dicee.models.BaseKGE method), 142, 146, 151, 156, 162, 175, 178
get_bpe_token_representation() (dicee.absracts.BaseInteractiveKGE method), 15
get_callbacks() (in module dicee.trainer.dice_trainer), 201
get_default_arguments() (in module dicee.analyse_experiments), 19
get_default_arguments() (in module dicee.scripts.index_serve), 192
get_default_arguments() (in module dicee.scripts.run), 193
get_ee_vocab() (in module dicee.read_preprocess_save_load_kg.util), 188
get_ee_vocab() (in module dicee.static_funcs), 195
get_ee_vocab() (in module dicee.static_preprocess_funcs), 200
get_embeddings() (dicee.models.base_model.BaseKGE method), 95
get_embeddings() (dicee.models.BaseKGE method), 143, 146, 151, 156, 162, 175, 178
get_embeddings() (dicee.models.ensemble.EnsembleKGE method), 108
get_embeddings() (dicee.models.real.Shallom method), 121
get_embeddings() (dicee.models.Shallom method), 147
get_entity_embeddings() (dicee.absracts.BaseInteractiveKGE method), 16
get_entity_index() (dicee.absracts.BaseInteractiveKGE method), 15
get_er_vocab() (in module dicee.read_preprocess_save_load_kg.util), 188
get_er_vocab() (in module dicee.static_funcs), 194
get_er_vocab() (in module dicee.static_preprocess_funcs), 200
get_eval_report() (dicee.absracts.BaseInteractiveKGE method), 15
get_head_relation_representation() (dicee.models.base_model.BaseKGE method), 95
get_head_relation_representation() (dicee.models.BaseKGE method), 142, 145, 151, 156, 162, 175, 178
get_kronecker_triple_representation() (dicee.callbacks.KronE method), 25
get_mean_and_var() (dicee.weight_averaging.SWAG method), 210
get_num_params() (dicee.models.transformers.GPT method), 129
get_padded_bpe_triple_representation() (dicee.absracts.BaseInteractiveKGE method), 15
get_queries() (dicee.query_generator.QueryGenerator method), 184
get_queries() (dicee.QueryGenerator method), 219
get_re_vocab() (in module dicee.read_preprocess_save_load_kg.util), 188
get_re_vocab() (in module dicee.static_funcs), 195
get_re_vocab() (in module dicee.static_preprocess_funcs), 200
get_relation_embeddings() (dicee.absracts.BaseInteractiveKGE method), 16
get_relation_index() (dicee.absracts.BaseInteractiveKGE method), 15
get_sentence_representation() (dicee.models.base_model.BaseKGE method), 95
get_sentence_representation() (dicee.models.BaseKGE method), 142, 146, 151, 156, 162, 175, 178
get_transductive_entity_embeddings() (dicee.KGE method), 215

```

get\_transductive\_entity\_embeddings() (*dicee.knowledge\_graph\_embeddings.KGE method*), 75  
 get\_triple\_representation() (*dicee.models.base\_model.BaseKGE method*), 95  
 get\_triple\_representation() (*dicee.models.BaseKGE method*), 142, 145, 151, 156, 162, 175, 178  
 GFMult (*class in dicee.models*), 179  
 GFMult (*class in dicee.models.function\_space*), 109  
 global\_rank (*dicee.abstracts.AbstractTrainer attribute*), 13  
 global\_rank (*dicee.trainer.torch\_trainer\_ddp.NodeTrainer attribute*), 205  
 GPT (*class in dicee.models.transformers*), 129  
 GPTConfig (*class in dicee.models.transformers*), 128  
 gpus (*dicee.config.Namespace attribute*), 28  
 gradient\_accumulation\_steps (*dicee.config.Namespace attribute*), 29  
 ground\_queries() (*dicee.query\_generator.QueryGenerator method*), 183  
 ground\_queries() (*dicee.QueryGenerator method*), 219  
 gsma\_n (*dicee.weight\_averaging.SWAG attribute*), 210

## H

hidden\_dim (*dicee.models.literal.LiteralEmbeddings attribute*), 112  
 hidden\_dropout (*dicee.models.base\_model.BaseKGE attribute*), 94  
 hidden\_dropout (*dicee.models.BaseKGE attribute*), 142, 145, 150, 155, 161, 174, 177  
 hidden\_dropout\_rate (*dicee.config.Namespace attribute*), 30  
 hidden\_dropout\_rate (*dicee.models.base\_model.BaseKGE attribute*), 94  
 hidden\_dropout\_rate (*dicee.models.BaseKGE attribute*), 141, 144, 150, 155, 161, 173, 177  
 hidden\_normalizer (*dicee.models.base\_model.BaseKGE attribute*), 94  
 hidden\_normalizer (*dicee.models.BaseKGE attribute*), 141, 145, 150, 155, 161, 174, 177

## I

IdentityClass (*class in dicee.models*), 143, 156, 162  
 IdentityClass (*class in dicee.models.base\_model*), 95  
 idx\_entity\_to\_bpe\_shaped (*dicee.knowledge\_graph.KG attribute*), 74  
 index() (*in module dicee.scripts.index\_serve*), 192  
 index\_triple() (*dicee.abstracts.BaseInteractiveKGE method*), 15  
 init\_dataloader() (*dicee.DICE\_Trainer method*), 220  
 init\_dataloader() (*dicee.trainer.DICE\_Trainer method*), 207  
 init\_dataloader() (*dicee.trainer.dice\_trainer.DICE\_Trainer method*), 202  
 init\_dataset() (*dicee.DICE\_Trainer method*), 220  
 init\_dataset() (*dicee.trainer.DICE\_Trainer method*), 207  
 init\_dataset() (*dicee.trainer.dice\_trainer.DICE\_Trainer method*), 202  
 init\_param (*dicee.config.Namespace attribute*), 29  
 init\_params\_with\_sanity\_checking() (*dicee.models.base\_model.BaseKGE method*), 95  
 init\_params\_with\_sanity\_checking() (*dicee.models.BaseKGE method*), 142, 145, 151, 155, 161, 174, 178  
 initial\_eval\_setting (*dicee.weight\_averaging.ASWA attribute*), 208  
 initialize\_or\_load\_model() (*dicee.DICE\_Trainer method*), 220  
 initialize\_or\_load\_model() (*dicee.trainer.DICE\_Trainer method*), 207  
 initialize\_or\_load\_model() (*dicee.trainer.dice\_trainer.DICE\_Trainer method*), 202  
 initialize\_trainer() (*dicee.DICE\_Trainer method*), 220  
 initialize\_trainer() (*dicee.trainer.DICE\_Trainer method*), 206  
 initialize\_trainer() (*dicee.trainer.dice\_trainer.DICE\_Trainer method*), 202  
 initialize\_trainer() (*in module dicee.trainer.dice\_trainer*), 201  
 input\_dp\_ent\_real (*dicee.models.base\_model.BaseKGE attribute*), 94  
 input\_dp\_ent\_real (*dicee.models.BaseKGE attribute*), 142, 145, 150, 155, 161, 174, 177  
 input\_dp\_rel\_real (*dicee.models.base\_model.BaseKGE attribute*), 94  
 input\_dp\_rel\_real (*dicee.models.BaseKGE attribute*), 142, 145, 150, 155, 161, 174, 177  
 input\_dropout\_rate (*dicee.config.Namespace attribute*), 30  
 input\_dropout\_rate (*dicee.models.base\_model.BaseKGE attribute*), 94  
 input\_dropout\_rate (*dicee.models.BaseKGE attribute*), 141, 144, 150, 155, 161, 173, 177  
 InteractiveQueryDecomposition (*class in dicee.abstracts*), 16  
 initialize\_model() (*in module dicee.static\_funcs*), 196  
 is\_continual\_training (*dicee.DICE\_Trainer attribute*), 220  
 is\_continual\_training (*dicee.evaluation.Evaluator attribute*), 59  
 is\_continual\_training (*dicee.evaluation.evaluator.Evaluator attribute*), 50  
 is\_continual\_training (*dicee.Evaluator attribute*), 222  
 is\_continual\_training (*dicee.evaluator.Evaluator attribute*), 67  
 is\_continual\_training (*dicee.Execute attribute*), 214  
 is\_continual\_training (*dicee.executer.Execute attribute*), 70  
 is\_continual\_training (*dicee.trainer.DICE\_Trainer attribute*), 206  
 is\_continual\_training (*dicee.trainer.dice\_trainer.DICE\_Trainer attribute*), 201  
 is\_global\_zero (*dicee.abstracts.AbstractTrainer attribute*), 13

`is_rank_zero()` (*dicee.Execute method*), 214  
`is_rank_zero()` (*dicee.executer.Execute method*), 70  
`is_seen()` (*dicee.abstracts.BaseInteractiveKGE method*), 15  
`is_sparql_endpoint_alive()` (*in module dicee.sanity\_checkers*), 191

## K

`k` (*dicee.models.FMult attribute*), 178  
`k` (*dicee.models.FMult2 attribute*), 179  
`k` (*dicee.models.function\_space.FMult attribute*), 108  
`k` (*dicee.models.function\_space.FMult2 attribute*), 109  
`k` (*dicee.models.function\_space.GFMult attribute*), 109  
`k` (*dicee.models.GFMult attribute*), 179  
`k_fold_cross_validation()` (*dicee.DICE\_Trainer method*), 221  
`k_fold_cross_validation()` (*dicee.trainer.DICE\_Trainer method*), 207  
`k_fold_cross_validation()` (*dicee.trainer.dice\_trainer.DICE\_Trainer method*), 202  
`k_vs_all_score()` (*dicee.models.clifford.Keci method*), 99  
`k_vs_all_score()` (*dicee.models.ComplEx static method*), 153  
`k_vs_all_score()` (*dicee.models.complex.ComplEx static method*), 106  
`k_vs_all_score()` (*dicee.models.DistMult method*), 147  
`k_vs_all_score()` (*dicee.models.Keci method*), 168  
`k_vs_all_score()` (*dicee.models.octonion.OMult method*), 114  
`k_vs_all_score()` (*dicee.models.OMult method*), 164  
`k_vs_all_score()` (*dicee.models.QMult method*), 158  
`k_vs_all_score()` (*dicee.models.quaternion.QMult method*), 119  
`k_vs_all_score()` (*dicee.models.real.DistMult method*), 121  
`Keci` (*class in dicee.models*), 166  
`Keci` (*class in dicee.models.clifford*), 97  
`kernel_size` (*dicee.config.Namespace attribute*), 30  
`kernel_size` (*dicee.models.base\_model.BaseKGE attribute*), 94  
`kernel_size` (*dicee.models.BaseKGE attribute*), 141, 144, 150, 155, 161, 173, 177  
`KG` (*class in dicee.knowledge\_graph*), 72  
`kg` (*dicee.callbacks.PseudoLabellingCallback attribute*), 24  
`kg` (*dicee.read\_preprocess\_save\_load\_kg.LoadSaveToDisk attribute*), 190  
`kg` (*dicee.read\_preprocess\_save\_load\_kg.PreprocessKG attribute*), 189  
`kg` (*dicee.read\_preprocess\_save\_load\_kg.preprocess.PreprocessKG attribute*), 184  
`kg` (*dicee.read\_preprocess\_save\_load\_kg.read\_from\_disk.ReadFromDisk attribute*), 185  
`kg` (*dicee.read\_preprocess\_save\_load\_kg.ReadFromDisk attribute*), 190  
`kg` (*dicee.read\_preprocess\_save\_load\_kg.save\_load\_disk.LoadSaveToDisk attribute*), 185  
`KGE` (*class in dicee*), 215  
`KGE` (*class in dicee.knowledge\_graph\_embeddings*), 75  
`KGESaveCallback` (*class in dicee.callbacks*), 22  
`knowledge_graph` (*dicee.Execute attribute*), 213, 214  
`knowledge_graph` (*dicee.executer.Execute attribute*), 70  
`KronE` (*class in dicee.callbacks*), 25  
`KvsAll` (*class in dicee.dataset\_classes*), 34  
`kvsall_score()` (*dicee.models.DualE method*), 182  
`kvsall_score()` (*dicee.models.dualE.DualE method*), 106  
`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*), 34  
`label_smoothing_rate` (*dicee.dataset\_classes.KvsSampleDataset attribute*), 38  
`label_smoothing_rate` (*dicee.dataset\_classes.OnevsSample attribute*), 36  
`label_smoothing_rate` (*dicee.dataset\_classes.TriplePredictionDataset attribute*), 39  
`labels` (*dicee.dataset\_classes.NegSampleDataset attribute*), 38  
`layer_norm` (*dicee.models.literal.LiteralEmbeddings attribute*), 113  
`LayerNorm` (*class in dicee.models.transformers*), 126  
`learning_rate` (*dicee.models.base\_model.BaseKGE attribute*), 94  
`learning_rate` (*dicee.models.BaseKGE attribute*), 141, 144, 150, 154, 160, 173, 177  
`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*), 180  
`LFMult` (*class in dicee.models.function\_space*), 110  
`LFMult1` (*class in dicee.models*), 180

LFMult1 (*class in dicee.models.function\_space*), 110  
 linear() (*dicee.models.function\_space.LFMult method*), 110  
 linear() (*dicee.models.LFMult method*), 181  
 list2tuple() (*dicee.query\_generator.QueryGenerator method*), 183  
 list2tuple() (*dicee.QueryGenerator method*), 219  
 LiteralDataset (*class in dicee.dataset\_classes*), 43  
 LiteralEmbeddings (*class in dicee.models.literal*), 111  
 lm\_head (*dicee.models.transformers.ByE attribute*), 124  
 lm\_head (*dicee.models.transformers.GPT attribute*), 129  
 ln\_1 (*dicee.models.Block attribute*), 146  
 ln\_1 (*dicee.models.transformers.Block attribute*), 128  
 ln\_2 (*dicee.models.Block attribute*), 147  
 ln\_2 (*dicee.models.transformers.Block attribute*), 128  
 ln\_f (*dicee.models.CoKE attribute*), 149  
 ln\_f (*dicee.models.real.CoKE attribute*), 123  
 load() (*dicee.read\_preprocess\_save\_load\_kg.LoadSaveToDisk method*), 190  
 load() (*dicee.read\_preprocess\_save\_load\_kg.save\_load\_disk.LoadSaveToDisk method*), 185  
 load\_and\_validate\_literal\_data() (*dicee.dataset\_classes.LiteralDataset static method*), 44  
 load\_from\_memmap() (*dicee.Execute method*), 214  
 load\_from\_memmap() (*dicee.executer.Execute method*), 71  
 load\_json() (*in module dicee.static\_funcs*), 197  
 load\_model() (*in module dicee.static\_funcs*), 196  
 load\_model\_ensemble() (*in module dicee.static\_funcs*), 196  
 load\_numpy() (*in module dicee.static\_funcs*), 197  
 load\_numpy\_ndarray() (*in module dicee.read\_preprocess\_save\_load\_kg.util*), 189  
 load\_pickle() (*in module dicee.read\_preprocess\_save\_load\_kg.util*), 189  
 load\_pickle() (*in module dicee.static\_funcs*), 195  
 load\_queries() (*dicee.query\_generator.QueryGenerator method*), 184  
 load\_queries() (*dicee.QueryGenerator method*), 219  
 load\_queries\_and\_answers() (*dicee.query\_generator.QueryGenerator static method*), 184  
 load\_queries\_and\_answers() (*dicee.QueryGenerator static method*), 219  
 load\_state\_dict() (*dicee.models.ensemble.EnsembleKGE method*), 108  
 load\_term\_mapping() (*in module dicee.static\_funcs*), 195  
 load\_term\_mapping() (*in module dicee.trainer.dice\_trainer*), 200  
 load\_with\_pandas() (*in module dicee.read\_preprocess\_save\_load\_kg.util*), 189  
 loader\_backend (*dicee.dataset\_classes.LiteralDataset attribute*), 44  
 LoadSaveToDisk (*class in dicee.read\_preprocess\_save\_load\_kg*), 190  
 LoadSaveToDisk (*class in dicee.read\_preprocess\_save\_load\_kg.save\_load\_disk*), 185  
 local\_rank (*dicee.abstracts.AbstractTrainer attribute*), 13  
 local\_rank (*dicee.Execute attribute*), 213  
 local\_rank (*dicee.executer.Execute attribute*), 70  
 local\_rank (*dicee.trainer.torch\_trainer\_ddp.NodeTrainer attribute*), 205  
 loss (*dicee.models.base\_model.BaseKGE attribute*), 94  
 loss (*dicee.models.BaseKGE attribute*), 141, 144, 150, 155, 161, 174, 177  
 loss\_func (*dicee.trainer.torch\_trainer\_ddp.NodeTrainer attribute*), 205  
 loss\_function (*dicee.trainer.torch\_trainer.TorchTrainer attribute*), 203  
 loss\_function() (*dicee.models.base\_model.BaseKGELightning method*), 89  
 loss\_function() (*dicee.models.BaseKGELightning method*), 136  
 loss\_function() (*dicee.models.transformers.ByE method*), 124  
 loss\_history (*dicee.models.base\_model.BaseKGE attribute*), 94  
 loss\_history (*dicee.models.BaseKGE attribute*), 142, 145, 151, 155, 161, 174, 177  
 loss\_history (*dicee.models.pykeen\_models.PykeenKGE attribute*), 116  
 loss\_history (*dicee.models.PykeenKGE attribute*), 175  
 loss\_history (*dicee.trainer.torch\_trainer\_ddp.NodeTrainer attribute*), 205  
 lr (*dicee.analyse\_experiments.Experiment attribute*), 20  
 lr (*dicee.config.Namespace attribute*), 28  
 lr\_init (*dicee.weight\_averaging.SWA attribute*), 209  
 lr\_init (*dicee.weight\_averaging.SWAG attribute*), 210  
 lr\_init (*dicee.weight\_averaging.TWA attribute*), 212  
 lr\_lambda (*dicee.callbacks.LRScheduler attribute*), 27  
 LRScheduler (*class in dicee.callbacks*), 26

## M

m (*dicee.models.function\_space.LFMult attribute*), 110  
 m (*dicee.models.LFMult attribute*), 180  
 main() (*in module dicee.scripts.index\_serve*), 193  
 main() (*in module dicee.scripts.run*), 193

make\_iterable\_verbose() (in module dicee.evaluation), 65  
make\_iterable\_verbose() (in module dicee.evaluation.utils), 57  
make\_iterable\_verbose() (in module dicee.static\_funcs\_training), 199  
make\_iterable\_verbose() (in module dicee.trainer.torch\_trainer\_ddp), 205  
mapping\_from\_first\_two\_cols\_to\_third() (in module dicee.static\_preprocess\_funcs), 200  
margin (dicee.models.Pyke attribute), 148  
margin (dicee.models.real.Pyke attribute), 121  
margin (dicee.models.real.TransE attribute), 121  
margin (dicee.models.TransE attribute), 147  
mask\_emb (dicee.models.CoKE attribute), 149  
mask\_emb (dicee.models.real.CoKE attribute), 123  
max\_ans\_num (dicee.query\_generator.QueryGenerator attribute), 183  
max\_ans\_num (dicee.QueryGenerator attribute), 219  
max\_epochs (dicee.callbacks.KGESaveCallback attribute), 23  
max\_epochs (dicee.callbacks.PeriodicEvalCallback attribute), 26  
max\_epochs (dicee.weight\_averaging.EMA attribute), 211  
max\_epochs (dicee.weight\_averaging.SWA attribute), 209  
max\_epochs (dicee.weight\_averaging.SWAG attribute), 210  
max\_epochs (dicee.weight\_averaging.TWA attribute), 212  
max\_length\_subword\_tokens (dicee.knowledge\_graph.KG attribute), 74  
max\_length\_subword\_tokens (dicee.models.base\_model.BaseKGE attribute), 94  
max\_length\_subword\_tokens (dicee.models.BaseKGE attribute), 142, 145, 151, 155, 161, 174, 177  
max\_num\_models (dicee.weight\_averaging.SWAG attribute), 210  
max\_num\_of\_classes (dicee.dataset\_classes.KvsSampleDataset attribute), 38  
mean (dicee.weight\_averaging.SWAG attribute), 210  
mem\_of\_model() (dicee.models.base\_model.BaseKGELightning method), 88  
mem\_of\_model() (dicee.models.BaseKGELightning method), 135  
mem\_of\_model() (dicee.models.ensemble.EnsembleKGE method), 108  
method (dicee.callbacks.Perturb attribute), 26  
MLP (class in dicee.models.transformers), 127  
mlp (dicee.models.Block attribute), 147  
mlp (dicee.models.transformers.Block attribute), 128  
mode (dicee.query\_generator.QueryGenerator attribute), 183  
mode (dicee.QueryGenerator attribute), 219  
model (dicee.config.Namespace attribute), 28  
model (dicee.models.pykeen\_models.PykeenKGE attribute), 116  
model (dicee.models.PykeenKGE attribute), 175  
model (dicee.trainer.torch\_trainer\_ddp.NodeTrainer attribute), 205  
model (dicee.trainer.torch\_trainer.TorchTrainer attribute), 204  
model\_kwarg (dicee.models.pykeen\_models.PykeenKGE attribute), 116  
model\_kwarg (dicee.models.PykeenKGE attribute), 175  
model\_name (dicee.analyse\_experiments.Experiment attribute), 19  
MODEL\_REGISTRY (in module dicee.static\_funcs), 194  
module  
    dicee, 12  
    dicee.\_\_main\_\_, 12  
    dicee.abstracts, 12  
    dicee.analyse\_experiments, 19  
    dicee.callbacks, 21  
    dicee.config, 27  
    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, 66  
    dicee.executer, 69  
    dicee.knowledge\_graph, 72  
    dicee.knowledge\_graph\_embeddings, 75  
    dicee.models, 78  
    dicee.models.adopt, 78  
    dicee.models.base\_model, 87  
    dicee.models.clifford, 96  
    dicee.models.complex, 103  
    dicee.models.dualE, 106

```

dicee.models.ensemble, 107
dicee.models.function_space, 108
dicee.models.literal, 111
dicee.models.octonion, 113
dicee.models.pykeen_models, 116
dicee.models.quaternion, 117
dicee.models.real, 120
dicee.models.static_funcs, 123
dicee.models.transformers, 123
dicee.query_generator, 182
dicee.read_preprocess_save_load_kg, 184
dicee.read_preprocess_save_load_kg.preprocess, 184
dicee.read_preprocess_save_load_kg.read_from_disk, 185
dicee.read_preprocess_save_load_kg.save_load_disk, 185
dicee.read_preprocess_save_load_kg.util, 186
dicee.sanity_checkers, 190
dicee.scripts, 191
dicee.scripts.index_serve, 191
dicee.scripts.run, 193
dicee.static_funcs, 193
dicee.static_funcs_training, 198
dicee.static_preprocess_funcs, 199
dicee.trainer, 200
dicee.trainer.dice_trainer, 200
dicee.trainer.model_parallelism, 202
dicee.trainer.torch_trainer, 203
dicee.trainer.torch_trainer_ddp, 204
dicee.weight_averaging, 207
modules() (dicee.models.ensemble.EnsembleKGE method), 107
moving_average() (dicee.weight_averaging.SWA static method), 209
MultiClassClassificationDataset (class in dicee.dataset_classes), 33
MultiLabelDataset (class in dicee.dataset_classes), 32

```

## N

```

n (dicee.models.FMult2 attribute), 179
n (dicee.models.function_space.FMult2 attribute), 109
n_embd (dicee.models.CoKEConfig attribute), 148
n_embd (dicee.models.real.CoKEConfig attribute), 122
n_embd (dicee.models.transformers.GPTConfig attribute), 129
n_embd (dicee.models.transformers.SelfAttention attribute), 127
n_epochs_eval_model (dicee.callbacks.PeriodicEvalCallback attribute), 26
n_epochs_eval_model (dicee.config.Namespace attribute), 31
n_head (dicee.models.CoKEConfig attribute), 148
n_head (dicee.models.real.CoKEConfig attribute), 122
n_head (dicee.models.transformers.GPTConfig attribute), 129
n_head (dicee.models.transformers.SelfAttention attribute), 127
n_layer (dicee.models.CoKEConfig attribute), 148
n_layer (dicee.models.real.CoKEConfig attribute), 122
n_layer (dicee.models.transformers.GPTConfig attribute), 129
n_layers (dicee.models.FMult2 attribute), 179
n_layers (dicee.models.function_space.FMult2 attribute), 109
name (dicee.abtracts.BaseInteractiveKGE property), 15
name (dicee.models.AConEx attribute), 152
name (dicee.models.AConvO attribute), 165
name (dicee.models.ACOnvQ attribute), 159
name (dicee.models.CKeci attribute), 169
name (dicee.models.clifford.CKeci attribute), 100
name (dicee.models.clifford.DeCaL attribute), 100
name (dicee.models.clifford.Keci attribute), 97
name (dicee.models.CoKE attribute), 149
name (dicee.models.ComplEx attribute), 153
name (dicee.models.complex.AConEx attribute), 104
name (dicee.models.complex.ComplEx attribute), 105
name (dicee.models.complex.ConEx attribute), 104
name (dicee.models.ConEx attribute), 152
name (dicee.models.ConvO attribute), 165
name (dicee.models.ConvQ attribute), 159

```

name (*dicee.models.DeCaL attribute*), 169  
 name (*dicee.models.DistMult attribute*), 147  
 name (*dicee.models.DualE attribute*), 181  
 name (*dicee.models.dualE.DualE attribute*), 106  
 name (*dicee.models.ensemble.EnsembleKGE attribute*), 107  
 name (*dicee.models.FMulti attribute*), 178  
 name (*dicee.models.FMulti2 attribute*), 179  
 name (*dicee.models.function\_space.FMulti attribute*), 108  
 name (*dicee.models.function\_space.FMulti2 attribute*), 109  
 name (*dicee.models.function\_space.GFMult attribute*), 109  
 name (*dicee.models.function\_space.LFMult attribute*), 110  
 name (*dicee.models.function\_space.LFMult1 attribute*), 110  
 name (*dicee.models.GFMult attribute*), 179  
 name (*dicee.models.Keci attribute*), 166  
 name (*dicee.models.LFMult attribute*), 180  
 name (*dicee.models.LFMult1 attribute*), 180  
 name (*dicee.models.octonion.AConvO attribute*), 115  
 name (*dicee.models.octonion.ConvO attribute*), 115  
 name (*dicee.models.octonion.OMult attribute*), 114  
 name (*dicee.models.OMult attribute*), 164  
 name (*dicee.models.Pyke attribute*), 148  
 name (*dicee.models.pykeen\_models.PykeenKGE attribute*), 116  
 name (*dicee.models.PykeenKGE attribute*), 175  
 name (*dicee.models.QMult attribute*), 158  
 name (*dicee.models.quaternion.AConvQ attribute*), 120  
 name (*dicee.models.quaternion.ConvQ attribute*), 119  
 name (*dicee.models.quaternion.QMult attribute*), 118  
 name (*dicee.models.real.CoKE attribute*), 122  
 name (*dicee.models.real.DistMult attribute*), 120  
 name (*dicee.models.real.Pyke attribute*), 121  
 name (*dicee.models.real.Shallom attribute*), 121  
 name (*dicee.models.real.TransE attribute*), 121  
 name (*dicee.models.Shallom attribute*), 147  
 name (*dicee.models.TransE attribute*), 147  
 name (*dicee.models.transformers.BytE attribute*), 124  
 named\_children () (*dicee.models.ensemble.EnsembleKGE method*), 107  
 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*), 37  
 neg\_sample\_ratio (*dicee.dataset\_classes.CVDataModule attribute*), 40  
 neg\_sample\_ratio (*dicee.dataset\_classes.NegSampleDataset attribute*), 38  
 neg\_sample\_ratio (*dicee.dataset\_classes.OnesVsSample attribute*), 36  
 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*), 192  
 NeuralSearcher (*class in dicee.scripts.index\_serve*), 192  
 NodeTrainer (*class in dicee.trainer.torch\_trainer\_ddp*), 205  
 norm\_fc1 (*dicee.models.AConEx attribute*), 152  
 norm\_fc1 (*dicee.models.AConvO attribute*), 165  
 norm\_fc1 (*dicee.models.complex.AConEx attribute*), 104  
 norm\_fc1 (*dicee.models.complex.ConEx attribute*), 104  
 norm\_fc1 (*dicee.models.ConEx attribute*), 152  
 norm\_fc1 (*dicee.models.ConvO attribute*), 165  
 norm\_fc1 (*dicee.models.octonion.AConvO attribute*), 116  
 norm\_fc1 (*dicee.models.octonion.ConvO attribute*), 115  
 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*), 94  
 normalize\_head\_entity\_embeddings (*dicee.models.BaseKGE attribute*), 141, 145, 150, 155, 161, 174, 177  
 normalize\_relation\_embeddings (*dicee.models.base\_model.BaseKGE attribute*), 94  
 normalize\_relation\_embeddings (*dicee.models.BaseKGE attribute*), 141, 145, 150, 155, 161, 174, 177  
 normalize\_tail\_entity\_embeddings (*dicee.models.base\_model.BaseKGE attribute*), 94  
 normalize\_tail\_entity\_embeddings (*dicee.models.BaseKGE attribute*), 141, 145, 150, 155, 161, 174, 177

normalizer\_class (*dicee.models.base\_model.BaseKGE* attribute), 94  
 normalizer\_class (*dicee.models.BaseKGE* attribute), 141, 145, 150, 155, 161, 174, 177  
 num\_bpe\_entities (*dicee.dataset\_classes.BPE\_NegativeSamplingDataset* attribute), 32  
 num\_bpe\_entities (*dicee.knowledge\_graph.KG* attribute), 74  
 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), 182  
 num\_ent (*dicee.models.dualE.DualE* attribute), 106  
 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.Onesample* attribute), 36  
 num\_entities (*dicee.dataset\_classes.TriplePredictionDataset* attribute), 39  
 num\_entities (*dicee.evaluation.Evaluator* attribute), 59  
 num\_entities (*dicee.evaluation.evaluator.Evaluator* attribute), 50  
 num\_entities (*dicee.Evaluator* attribute), 221, 222  
 num\_entities (*dicee.evaluator.Evaluator* attribute), 66, 67  
 num\_entities (*dicee.knowledge\_graph.KG* attribute), 72, 73  
 num\_entities (*dicee.models.base\_model.BaseKGE* attribute), 94  
 num\_entities (*dicee.models.BaseKGE* attribute), 141, 144, 150, 154, 160, 173, 177  
 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), 205  
 num\_epochs (*dicee.weight\_averaging.ASWA* attribute), 208  
 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), 112  
 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), 94  
 num\_of\_output\_channels (*dicee.models.BaseKGE* attribute), 141, 144, 150, 155, 161, 174, 177  
 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.Onesample* attribute), 36  
 num\_relations (*dicee.dataset\_classes.TriplePredictionDataset* attribute), 39  
 num\_relations (*dicee.evaluation.Evaluator* attribute), 59  
 num\_relations (*dicee.evaluation.evaluator.Evaluator* attribute), 50  
 num\_relations (*dicee.Evaluator* attribute), 221, 222  
 num\_relations (*dicee.evaluator.Evaluator* attribute), 66, 67  
 num\_relations (*dicee.knowledge\_graph.KG* attribute), 73  
 num\_relations (*dicee.models.base\_model.BaseKGE* attribute), 94  
 num\_relations (*dicee.models.BaseKGE* attribute), 141, 144, 150, 154, 160, 173, 177  
 num\_sample (*dicee.models.FMult* attribute), 178  
 num\_sample (*dicee.models.function\_space.FMult* attribute), 108  
 num\_sample (*dicee.models.function\_space.GFMult* attribute), 109  
 num\_sample (*dicee.models.GFMult* attribute), 179  
 num\_samples (*dicee.weight\_averaging.TWA* attribute), 212  
 num\_tokens (*dicee.knowledge\_graph.KG* attribute), 74  
 num\_tokens (*dicee.models.base\_model.BaseKGE* attribute), 94  
 num\_tokens (*dicee.models.BaseKGE* attribute), 141, 144, 150, 154, 160, 173, 177  
 num\_workers (*dicee.dataset\_classes.CVDataModule* attribute), 40  
 numpy\_data\_type\_changer () (*in module dicee.static\_funcs*), 196

## O

octonion\_mul () (*in module dicee.models*), 163  
 octonion\_mul () (*in module dicee.models.octonion*), 113  
 octonion\_mul\_norm () (*in module dicee.models*), 163  
 octonion\_mul\_norm () (*in module dicee.models.octonion*), 113  
 octonion\_normalizer () (*dicee.models.AConvO static method*), 165  
 octonion\_normalizer () (*dicee.models.ConvO static method*), 165  
 octonion\_normalizer () (*dicee.models.octonion.AConvO static method*), 116  
 octonion\_normalizer () (*dicee.models.octonion.ConvO static method*), 115

octonion\_normalizer() (*dicee.models.octonion.OMult static method*), 114  
 octonion\_normalizer() (*dicee.models.OMult static method*), 164  
 OMult (*class in dicee.models*), 163  
 OMult (*class in dicee.models.octonion*), 113  
 on\_epoch\_end() (*dicee.callbacks.KGESaveCallback method*), 23  
 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*), 24  
 on\_fit\_end() (*dicee.callbacks.KGESaveCallback method*), 23  
 on\_fit\_end() (*dicee.callbacks.LRScheduler method*), 27  
 on\_fit\_end() (*dicee.callbacks.PeriodicEvalCallback method*), 26  
 on\_fit\_end() (*dicee.callbacks.PrintCallback method*), 22  
 on\_fit\_end() (*dicee.weight\_averaging.ASWA method*), 208  
 on\_fit\_end() (*dicee.weight\_averaging.EMA method*), 211  
 on\_fit\_end() (*dicee.weight\_averaging.SWA method*), 209  
 on\_fit\_end() (*dicee.weight\_averaging.SWAG method*), 210  
 on\_fit\_end() (*dicee.weight\_averaging.TWA method*), 212  
 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*), 25  
 on\_fit\_start() (*dicee.callbacks.PrintCallback method*), 22  
 on\_init\_end() (*dicee.abstracts.AbstractCallback method*), 16  
 on\_init\_start() (*dicee.abstracts.AbstractCallback method*), 16  
 on\_train\_batch\_end() (*dicee.abstracts.AbstractCallback method*), 17  
 on\_train\_batch\_end() (*dicee.abstracts.AbstractTrainer method*), 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*), 26  
 on\_train\_epoch\_end() (*dicee.callbacks.PrintCallback method*), 22  
 on\_train\_epoch\_end() (*dicee.models.base\_model.BaseKGELighting method*), 89  
 on\_train\_epoch\_end() (*dicee.models.BaseKGELighting method*), 136  
 on\_train\_epoch\_end() (*dicee.weight\_averaging.ASWA method*), 208  
 on\_train\_epoch\_end() (*dicee.weight\_averaging.EMA method*), 211  
 on\_train\_epoch\_end() (*dicee.weight\_averaging.SWA method*), 209  
 on\_train\_epoch\_end() (*dicee.weight\_averaging.SWAG method*), 210  
 on\_train\_epoch\_end() (*dicee.weight\_averaging.TWA method*), 212  
 on\_train\_epoch\_start() (*dicee.abstracts.AbstractTrainer method*), 13  
 on\_train\_epoch\_start() (*dicee.weight\_averaging.EMA method*), 211  
 on\_train\_epoch\_start() (*dicee.weight\_averaging.SWA method*), 209  
 on\_train\_epoch\_start() (*dicee.weight\_averaging.SWAG method*), 210  
 on\_train\_epoch\_start() (*dicee.weight\_averaging.TWA method*), 212  
 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*), 205  
 optimizer (*dicee.trainer.torch\_trainer.TorchTrainer attribute*), 203  
 optimizer\_name (*dicee.models.base\_model.BaseKGE attribute*), 94  
 optimizer\_name (*dicee.models.BaseKGE attribute*), 141, 144, 150, 155, 161, 173, 177  
 ordered\_bpe\_entities (*dicee.dataset\_classes.BPE\_NegativeSamplingDataset attribute*), 32  
 ordered\_bpe\_entities (*dicee.knowledge\_graph.KG attribute*), 74  
 ordered\_shaped\_bpe\_tokens (*dicee.knowledge\_graph.KG attribute*), 73

# P

p (*dicee.config.Namespace attribute*), 30  
p (*dicee.models.clifford.DeCaL attribute*), 100  
p (*dicee.models.clifford.Keci attribute*), 97  
p (*dicee.models.DeCaL attribute*), 170  
p (*dicee.models.Keci attribute*), 166  
p (*dicee.weight\_averaging.TWA attribute*), 212  
padding (*dicee.knowledge\_graph.KG attribute*), 74  
pandas\_dataframe\_indexer () (in module *dicee.read\_preprocess\_save\_load\_kg.util*), 187  
param\_init (*dicee.models.base\_model.BaseKGE attribute*), 94  
param\_init (*dicee.models.BaseKGE attribute*), 141, 145, 150, 155, 161, 174, 177  
parameters () (*dicee.abstracts.BaseInteractiveKGE method*), 16  
parameters () (*dicee.models.ensemble.EnsembleKGE method*), 107  
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*), 207  
path\_dataset\_folder (*dicee.analyse\_experiments.Experiment attribute*), 20  
path\_for\_deserialization (*dicee.knowledge\_graph.KG attribute*), 73  
path\_for\_serialization (*dicee.knowledge\_graph.KG attribute*), 73  
path\_single\_kg (*dicee.config.Namespace attribute*), 28  
path\_single\_kg (*dicee.knowledge\_graph.KG attribute*), 73  
path\_to\_store\_single\_run (*dicee.config.Namespace attribute*), 28  
PeriodicEvalCallback (*class in dicee.callbacks*), 26  
Perturb (*class in dicee.callbacks*), 25  
polars\_dataframe\_indexer () (in module *dicee.read\_preprocess\_save\_load\_kg.util*), 186  
poly\_NN () (*dicee.models.function\_space.LFMult method*), 110  
poly\_NN () (*dicee.models.LFMult method*), 181  
polynomial () (*dicee.models.function\_space.LFMult method*), 111  
polynomial () (*dicee.models.LFMult method*), 181  
pop () (*dicee.models.function\_space.LFMult method*), 111  
pop () (*dicee.models.LFMult method*), 181  
pos\_emb (*dicee.models.CoKE attribute*), 149  
pos\_emb (*dicee.models.real.CoKE attribute*), 123  
pq (*dicee.analyse\_experiments.Experiment attribute*), 20  
predict () (*dicee.KGE method*), 216  
predict () (*dicee.knowledge\_graph\_embeddings.KGE method*), 76  
predict\_dataloader () (*dicee.models.base\_model.BaseKGELightning method*), 91  
predict\_dataloader () (*dicee.models.BaseKGELightning method*), 138  
predict\_literals () (*dicee.KGE method*), 218  
predict\_literals () (*dicee.knowledge\_graph\_embeddings.KGE method*), 78  
predict\_missing\_head\_entity () (*dicee.KGE method*), 215  
predict\_missing\_head\_entity () (*dicee.knowledge\_graph\_embeddings.KGE method*), 75  
predict\_missing\_relations () (*dicee.KGE method*), 216  
predict\_missing\_relations () (*dicee.knowledge\_graph\_embeddings.KGE method*), 75  
predict\_missing\_tail\_entity () (*dicee.KGE method*), 216  
predict\_missing\_tail\_entity () (*dicee.knowledge\_graph\_embeddings.KGE method*), 76  
predict\_topk () (*dicee.KGE method*), 216  
predict\_topk () (*dicee.knowledge\_graph\_embeddings.KGE method*), 76  
prepare\_data () (*dicee.dataset\_classes.CVDataModule method*), 42  
preprocess\_with\_byte\_pair\_encoding () (*dicee.read\_preprocess\_save\_load\_kg.PreprocessKG method*), 189  
preprocess\_with\_byte\_pair\_encoding () (*dicee.read\_preprocess\_save\_load\_kg.preprocess.PreprocessKG method*), 184  
preprocess\_with\_byte\_pair\_encoding\_with\_padding () (*dicee.read\_preprocess\_save\_load\_kg.PreprocessKG method*), 190  
preprocess\_with\_byte\_pair\_encoding\_with\_padding () (*dicee.read\_preprocess\_save\_load\_kg.preprocess.PreprocessKG method*), 184  
preprocess\_with\_pandas () (*dicee.read\_preprocess\_save\_load\_kg.PreprocessKG method*), 190  
preprocess\_with\_pandas () (*dicee.read\_preprocess\_save\_load\_kg.preprocess.PreprocessKG method*), 184  
preprocess\_with\_polars () (*dicee.read\_preprocess\_save\_load\_kg.PreprocessKG method*), 190  
preprocess\_with\_polars () (*dicee.read\_preprocess\_save\_load\_kg.preprocess.PreprocessKG method*), 184  
preprocesses\_input\_args () (in module *dicee.static\_preprocess\_funcs*), 200  
PreprocessKG (*class in dicee.read\_preprocess\_save\_load\_kg*), 189  
PreprocessKG (*class in dicee.read\_preprocess\_save\_load\_kg.preprocess*), 184  
PrintCallback (*class in dicee.callbacks*), 21  
process (*dicee.trainer.torch\_trainer.TorchTrainer attribute*), 204  
PseudoLabellingCallback (*class in dicee.callbacks*), 23  
Pyke (*class in dicee.models*), 148  
Pyke (*class in dicee.models.real*), 121  
pykeen\_model\_kwarg (*dicee.config.Namespace attribute*), 30

`PykeenKGE` (*class in dicee.models*), 175

`PykeenKGE` (*class in dicee.models.pykeen\_models*), 116

## Q

`q` (*dicee.config.Namespace attribute*), 30

`q` (*dicee.models.clifford.DeCaL attribute*), 101

`q` (*dicee.models.clifford.Keci attribute*), 97

`q` (*dicee.models.DeCaL attribute*), 170

`q` (*dicee.models.Keci attribute*), 166

`qdant_client` (*dicee.scripts.index\_serve.NeuralSearcher attribute*), 192

`QMult` (*class in dicee.models*), 157

`QMult` (*class in dicee.models.quaternion*), 117

`quaternion_mul()` (*in module dicee.models*), 154

`quaternion_mul()` (*in module dicee.models.static\_funcs*), 123

`quaternion_mul_with_unit_norm()` (*in module dicee.models*), 157

`quaternion_mul_with_unit_norm()` (*in module dicee.models.quaternion*), 117

`quaternion_multiplication_followed_by_inner_product()` (*dicee.models.QMult method*), 158

`quaternion_multiplication_followed_by_inner_product()` (*dicee.models.quaternion.QMult method*), 118

`quaternion_normalizer()` (*dicee.models.QMult static method*), 158

`quaternion_normalizer()` (*dicee.models.quaternion.QMult static method*), 118

`queries` (*dicee.scripts.index\_serve.StringListRequest attribute*), 192

`query_name_to_struct` (*dicee.query\_generator.QueryGenerator attribute*), 183

`query_name_to_struct` (*dicee.QueryGenerator attribute*), 219

`QueryGenerator` (*class in dicee*), 218

`QueryGenerator` (*class in dicee.query\_generator*), 183

## R

`r` (*dicee.models.clifford.DeCaL attribute*), 101

`r` (*dicee.models.clifford.Keci attribute*), 97

`r` (*dicee.models.DeCaL attribute*), 170

`r` (*dicee.models.Keci attribute*), 166

`random_seed` (*dicee.config.Namespace attribute*), 29

`range_constraints_per_rel` (*dicee.evaluation.Evaluator attribute*), 59

`range_constraints_per_rel` (*dicee.evaluation.evaluator.Evaluator attribute*), 51

`range_constraints_per_rel` (*dicee.Evaluator attribute*), 222

`range_constraints_per_rel` (*dicee.evaluator.Evaluator attribute*), 67

`rank` (*dicee.Execute attribute*), 213

`rank` (*dicee.executer.Execute attribute*), 70

`ratio` (*dicee.callbacks.Perturb attribute*), 26

`raw_test_set` (*dicee.knowledge\_graph.KG attribute*), 74

`raw_train_set` (*dicee.knowledge\_graph.KG attribute*), 73

`raw_valid_set` (*dicee.knowledge\_graph.KG attribute*), 73

`re` (*dicee.models.clifford.DeCaL attribute*), 101

`re` (*dicee.models.DeCaL attribute*), 170

`re_vocab` (*dicee.evaluation.Evaluator attribute*), 59

`re_vocab` (*dicee.evaluation.evaluator.Evaluator attribute*), 50

`re_vocab` (*dicee.Evaluator attribute*), 221

`re_vocab` (*dicee.evaluator.Evaluator attribute*), 66, 67

`read_from_disk()` (*in module dicee.read\_preprocess\_save\_load\_kg.util*), 188

`read_from_triple_store_with_pandas()` (*in module dicee.read\_preprocess\_save\_load\_kg.util*), 188

`read_from_triple_store_with_polars()` (*in module dicee.read\_preprocess\_save\_load\_kg.util*), 188

`read_only_few` (*dicee.config.Namespace attribute*), 29

`read_only_few` (*dicee.knowledge\_graph.KG attribute*), 73

`read_or_load_kg()` (*in module dicee.static\_funcs*), 196

`read_with_pandas()` (*in module dicee.read\_preprocess\_save\_load\_kg.util*), 188

`read_with_polars()` (*in module dicee.read\_preprocess\_save\_load\_kg.util*), 188

`ReadFromDisk` (*class in dicee.read\_preprocess\_save\_load\_kg*), 190

`ReadFromDisk` (*class in dicee.read\_preprocess\_save\_load\_kg.read\_from\_disk*), 185

`reducer` (*dicee.scripts.index\_serve.StringListRequest attribute*), 192

`reg_lambda` (*dicee.weight\_averaging.TWA attribute*), 212

`rel2id` (*dicee.query\_generator.QueryGenerator attribute*), 183

`rel2id` (*dicee.QueryGenerator attribute*), 219

`relation_embeddings` (*dicee.models.AConvQ attribute*), 159

`relation_embeddings` (*dicee.models.clifford.DeCaL attribute*), 100

`relation_embeddings` (*dicee.models.ConvQ attribute*), 159

`relation_embeddings` (*dicee.models.DeCaL attribute*), 170

`relation_embeddings` (*dicee.models.DualE attribute*), 182

relation\_embeddings (*dicee.models.dualE.DualE* attribute), 106  
 relation\_embeddings (*dicee.models.FMult* attribute), 178  
 relation\_embeddings (*dicee.models.FMult2* attribute), 180  
 relation\_embeddings (*dicee.models.function\_space.FMult* attribute), 108  
 relation\_embeddings (*dicee.models.function\_space.FMult2* attribute), 109  
 relation\_embeddings (*dicee.models.function\_space.GFMult* attribute), 109  
 relation\_embeddings (*dicee.models.function\_space.LFMult* attribute), 110  
 relation\_embeddings (*dicee.models.function\_space.LFMultI* attribute), 110  
 relation\_embeddings (*dicee.models.GFMult* attribute), 179  
 relation\_embeddings (*dicee.models.LFMult* attribute), 180  
 relation\_embeddings (*dicee.models.LFMultI* attribute), 180  
 relation\_embeddings (*dicee.models.pykeen\_models.PykeenKGE* attribute), 116  
 relation\_embeddings (*dicee.models.PykeenKGE* attribute), 175  
 relation\_embeddings (*dicee.models.quaternion.AConvQ* attribute), 120  
 relation\_embeddings (*dicee.models.quaternion.ConvQ* attribute), 119  
 relation\_to\_idx (*dicee.knowledge\_graph.KG* attribute), 73  
 relations\_str (*dicee.knowledge\_graph.KG* property), 74  
 reload\_dataset () (in module *dicee.dataset\_classes*), 32  
 report (*dicee.DICE\_Trainer* attribute), 220  
 report (*dicee.evaluation.Evaluator* attribute), 59  
 report (*dicee.evaluation.evaluator.Evaluator* attribute), 50, 51  
 report (*dicee.Evaluator* attribute), 221, 222  
 report (*dicee.evaluator.Evaluator* attribute), 66, 67  
 report (*dicee.Execute* attribute), 213, 214  
 report (*dicee.executer.Execute* attribute), 70  
 report (*dicee.trainer.DICE\_Trainer* attribute), 206  
 report (*dicee.trainer.dice\_trainer.DICE\_Trainer* attribute), 201  
 reports (*dicee.callbacks.Eval* attribute), 24  
 reports (*dicee.callbacks.PeriodicEvalCallback* attribute), 26  
 requires\_grad\_for\_interactions (*dicee.models.CKeci* attribute), 169  
 requires\_grad\_for\_interactions (*dicee.models.clifford.CKeci* attribute), 100  
 requires\_grad\_for\_interactions (*dicee.models.clifford.Keci* attribute), 97  
 requires\_grad\_for\_interactions (*dicee.models.Keci* attribute), 166  
 resid\_dropout (*dicee.models.transformers.SelfAttention* attribute), 127  
 residual\_convolution () (*dicee.models.AConEx* method), 152  
 residual\_convolution () (*dicee.models.AConvO* method), 165  
 residual\_convolution () (*dicee.models.AConvQ* method), 159  
 residual\_convolution () (*dicee.models.complex.AConEx* method), 105  
 residual\_convolution () (*dicee.models.complex.ConEx* method), 104  
 residual\_convolution () (*dicee.models.ConEx* method), 152  
 residual\_convolution () (*dicee.models.ConvO* method), 165  
 residual\_convolution () (*dicee.models.ConvQ* method), 159  
 residual\_convolution () (*dicee.models.octonion.AConvO* method), 116  
 residual\_convolution () (*dicee.models.octonion.ConvO* method), 115  
 residual\_convolution () (*dicee.models.quaternion.AConvQ* method), 120  
 residual\_convolution () (*dicee.models.quaternion.ConvQ* method), 119  
 retrieve\_embedding () (*dicee.scripts.index\_serve.NeuralSearcher* method), 192  
 retrieve\_embeddings () (in module *dicee.scripts.index\_serve*), 192  
 return\_multi\_hop\_query\_results () (*dicee.KGE* method), 217  
 return\_multi\_hop\_query\_results () (*dicee.knowledge\_graph\_embeddings.KGE* method), 77  
 root () (in module *dicee.scripts.index\_serve*), 192  
 roots (*dicee.models.FMult* attribute), 179  
 roots (*dicee.models.function\_space.FMult* attribute), 108  
 roots (*dicee.models.function\_space.GFMult* attribute), 109  
 roots (*dicee.models.GFMult* attribute), 179  
 runtime (*dicee.analyse\_experiments.Experiment* attribute), 20

## S

sample () (*dicee.weight\_averaging.SWAG* method), 210  
 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), 29  
 sample\_triples\_ratio (*dicee.knowledge\_graph.KG* attribute), 73  
 sample\_weights () (*dicee.weight\_averaging.TWA* method), 212  
 sampling\_ratio (*dicee.dataset\_classes.LiteralDataset* attribute), 43, 44  
 sanity\_check\_callback\_args () (in module *dicee.sanity\_checkers*), 191

sanity\_checking\_with\_arguments() (*in module dicee.sanity\_checkers*), 191  
 save() (*dicee.abstracts.BaseInteractiveKGE method*), 15  
 save() (*dicee.read\_preprocess\_save\_load\_kg.LoadSaveToDisk method*), 190  
 save() (*dicee.read\_preprocess\_save\_load\_kg.save\_load\_disk.LoadSaveToDisk method*), 185  
 save\_checkpoint() (*dicee.abstracts.AbstractTrainer static method*), 14  
 save\_checkpoint\_model() (*in module dicee.static\_funcs*), 196  
 save\_embeddings() (*in module dicee.static\_funcs*), 197  
 save\_embeddings\_as\_csv(*dicee.config.Namespace attribute*), 28  
 save\_every\_n\_epochs(*dicee.config.Namespace attribute*), 30  
 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*), 189  
 save\_numpy\_ndarray() (*in module dicee.static\_funcs*), 196  
 save\_pickle() (*in module dicee.read\_preprocess\_save\_load\_kg.util*), 189  
 save\_pickle() (*in module dicee.static\_funcs*), 195  
 save\_queries() (*dicee.query\_generator.QueryGenerator method*), 184  
 save\_queries() (*dicee.QueryGenerator method*), 219  
 save\_queries\_and\_answers() (*dicee.query\_generator.QueryGenerator static method*), 184  
 save\_queries\_and\_answers() (*dicee.QueryGenerator static method*), 219  
 save\_trained\_model() (*dicee.Execute method*), 214  
 save\_trained\_model() (*dicee.executer.Execute method*), 71  
 scalar\_batch\_NN() (*dicee.models.function\_space.LFMult method*), 110  
 scalar\_batch\_NN() (*dicee.models.LFMult method*), 181  
 scaler(*dicee.callbacks.Perturb attribute*), 26  
 scaler(*dicee.trainer.torch\_trainer\_ddp.NodeTrainer attribute*), 205  
 scheduler(*dicee.callbacks.LRScheduler attribute*), 27  
 score() (*dicee.models.clifford.Keci method*), 99  
 score() (*dicee.models.CoKE method*), 149  
 score() (*dicee.models.ComplEx static method*), 153  
 score() (*dicee.models.complex.ComplEx static method*), 105  
 score() (*dicee.models.DistMult method*), 147  
 score() (*dicee.models.Keci method*), 168  
 score() (*dicee.models.octonion.OMult method*), 114  
 score() (*dicee.models.OMult method*), 164  
 score() (*dicee.models.QMult method*), 158  
 score() (*dicee.models.quaternion.QMult method*), 119  
 score() (*dicee.models.real.CoKE method*), 123  
 score() (*dicee.models.real.DistMult method*), 121  
 score() (*dicee.models.real.TransE method*), 121  
 score() (*dicee.models.TransE method*), 147  
 score\_func(*dicee.models.FMult2 attribute*), 179  
 score\_func(*dicee.models.function\_space.FMult2 attribute*), 109  
 scoring\_technique (*dicee.analyse\_experiments.Experiment attribute*), 20  
 scoring\_technique (*dicee.config.Namespace attribute*), 29  
 search() (*dicee.scripts.index\_serve.NeuralSearcher method*), 192  
 search\_embeddings() (*in module dicee.scripts.index\_serve*), 192  
 search\_embeddings\_batch() (*in module dicee.scripts.index\_serve*), 192  
 seed(*dicee.query\_generator.QueryGenerator attribute*), 183  
 seed(*dicee.QueryGenerator attribute*), 218  
 select\_model() (*in module dicee.static\_funcs*), 196  
 selected\_optimizer(*dicee.models.base\_model.BaseKGE attribute*), 94  
 selected\_optimizer(*dicee.models.BaseKGE attribute*), 141, 144, 150, 155, 161, 174, 177  
 SelfAttention (*class in dicee.models.transformers*), 126  
 separator(*dicee.config.Namespace attribute*), 29  
 separator(*dicee.knowledge\_graph.KG attribute*), 73  
 sequential\_vocabulary\_construction() (*dicee.read\_preprocess\_save\_load\_kg.PreprocessKG method*), 190  
 sequential\_vocabulary\_construction() (*dicee.read\_preprocess\_save\_load\_kg.preprocess.PreprocessKG method*), 184  
 serve() (*in module dicee.scripts.index\_serve*), 193  
 set\_global\_seed() (*dicee.query\_generator.QueryGenerator method*), 183  
 set\_global\_seed() (*dicee.QueryGenerator method*), 219  
 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*), 214  
 setup\_executor() (*dicee.executer.Execute method*), 70  
 Shallom (*class in dicee.models*), 147  
 Shallom (*class in dicee.models.real*), 121

shallom (*dicee.models.real.Shallom* attribute), 121  
 shallom (*dicee.models.Shallom* attribute), 147  
 single\_hop\_query\_answering() (*dicee.KGE* method), 217  
 single\_hop\_query\_answering() (*dicee.knowledge\_graph\_embeddings.KGE* method), 77  
 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), 73  
 sq\_mean (*dicee.weight\_averaging.SWAG* attribute), 210  
 start () (*dicee.DICE\_Trainer* method), 220  
 start () (*dicee.Execute* method), 215  
 start () (*dicee.executer.Execute* method), 71  
 start () (*dicee.read\_preprocess\_save\_load\_kg.PreprocessKG* method), 189  
 start () (*dicee.read\_preprocess\_save\_load\_kg.preprocess.PreprocessKG* method), 184  
 start () (*dicee.read\_preprocess\_save\_load\_kg.read\_from\_disk.ReadFromDisk* method), 185  
 start () (*dicee.read\_preprocess\_save\_load\_kg.ReadFromDisk* method), 190  
 start () (*dicee.trainer.DICE\_Trainer* method), 207  
 start () (*dicee.trainer.dice\_trainer.DICE\_Trainer* method), 202  
 start\_time (*dicee.callbacks.PrintCallback* attribute), 22  
 start\_time (*dicee.Execute* attribute), 214  
 start\_time (*dicee.executer.Execute* attribute), 70  
 state\_dict () (*dicee.models.ensemble.EnsembleKGE* method), 108  
 step () (*dicee.models.ADOPT* method), 133  
 step () (*dicee.models.adopt.ADOPT* method), 82  
 step () (*dicee.models.ensemble.EnsembleKGE* method), 108  
 step\_count (*dicee.callbacks.LRScheduler* attribute), 27  
 storage\_path (*dicee.config.Namespace* attribute), 28  
 storage\_path (*dicee.DICE\_Trainer* attribute), 220  
 storage\_path (*dicee.trainer.DICE\_Trainer* attribute), 206  
 storage\_path (*dicee.trainer.dice\_trainer.DICE\_Trainer* attribute), 201  
 store () (*in module dicee.static\_funcs*), 196  
 store\_ensemble () (*dicee.abstracts.AbstractPPECallback* method), 18  
 strategy (*dicee.abstracts.AbstractTrainer* attribute), 13  
 StringListRequest (*class in dicee.scripts.index\_serve*), 192  
 SWA (*class in dicee.weight\_averaging*), 208  
 swa (*dicee.config.Namespace* attribute), 30  
 swa\_c\_epochs (*dicee.config.Namespace* attribute), 31  
 swa\_c\_epochs (*dicee.weight\_averaging.SWA* attribute), 209  
 swa\_c\_epochs (*dicee.weight\_averaging.SWAG* attribute), 210  
 swa\_lr (*dicee.weight\_averaging.SWA* attribute), 209  
 swa\_lr (*dicee.weight\_averaging.SWAG* attribute), 210  
 swa\_model (*dicee.weight\_averaging.SWA* attribute), 209  
 swa\_n (*dicee.weight\_averaging.SWA* attribute), 209  
 swa\_start\_epoch (*dicee.config.Namespace* attribute), 31  
 swa\_start\_epoch (*dicee.weight\_averaging.SWA* attribute), 209  
 swa\_start\_epoch (*dicee.weight\_averaging.SWAG* attribute), 210  
 SWAG (*class in dicee.weight\_averaging*), 209  
 swag (*dicee.config.Namespace* attribute), 30

## T

T () (*dicee.models.DualE* method), 182  
 T () (*dicee.models.dualE.DualE* method), 107  
 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), 74  
 temperature (*dicee.models.transformers.BytE* attribute), 124  
 tensor\_t\_norm () (*dicee.abstracts.InteractiveQueryDecomposition* method), 16  
 TensorParallel (*class in dicee.trainer.model\_parallelism*), 203  
 test\_dataloader () (*dicee.models.base\_model.BaseKGELighting* method), 90  
 test\_dataloader () (*dicee.models.BaseKGELighting* method), 137  
 test\_epoch\_end () (*dicee.models.base\_model.BaseKGELighting* method), 89  
 test\_epoch\_end () (*dicee.models.BaseKGELighting* method), 137  
 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), 183  
test\_path (*dicee.QueryGenerator* attribute), 218  
test\_set (*dicee.knowledge\_graph.KG* attribute), 73, 74  
timeit () (in module *dicee.read\_preprocess\_save\_load\_kg.util*), 188  
timeit () (in module *dicee.static\_funcs*), 195  
timeit () (in module *dicee.static\_preprocess\_funcs*), 200  
to () (*dicee.KGE* method), 215  
to () (*dicee.knowledge\_graph\_embeddings.KGE* method), 75  
to () (*dicee.models.ensemble.EnsembleKGE* method), 107  
to\_df () (*dicee.analyse\_experiments.Experiment* method), 20  
topk (*dicee.models.transformers.BytE* attribute), 124  
topk (*dicee.scripts.index\_serve.NeuralSearcher* attribute), 192  
torch\_ordered\_shaped\_bpe\_entities (*dicee.dataset\_classes.MultiLabelDataset* attribute), 33  
TorchDDPTrainer (*class* in *dicee.trainer.torch\_trainer\_ddp*), 205  
TorchTrainer (*class* in *dicee.trainer.torch\_trainer*), 203  
total\_epochs (*dicee.callbacks.LRScheduler* attribute), 27  
total\_steps (*dicee.callbacks.LRScheduler* attribute), 27  
train () (*dicee.abstracts.BaseInteractiveTrainKGE* method), 18  
train () (*dicee.trainer.torch\_trainer\_ddp.NodeTrainer* method), 206  
train\_data (*dicee.dataset\_classes.AllvsAll* attribute), 35  
train\_data (*dicee.dataset\_classes.KvsAll* attribute), 34  
train\_data (*dicee.dataset\_classes.KvsSampleDataset* attribute), 37  
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), 91  
train\_dataloader () (*dicee.models.BaseKGELightning* method), 138  
train\_dataloaders (*dicee.trainer.torch\_trainer.TorchTrainer* attribute), 204  
train\_dataset\_loader (*dicee.trainer.torch\_trainer\_ddp.NodeTrainer* attribute), 205  
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), 18  
train\_mode (*dicee.models.ensemble.EnsembleKGE* attribute), 107  
train\_mrr (*dicee.analyse\_experiments.Experiment* attribute), 20  
train\_path (*dicee.query\_generator.QueryGenerator* attribute), 183  
train\_path (*dicee.QueryGenerator* attribute), 218  
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), 73, 74  
train\_set\_idx (*dicee.dataset\_classes.CVDataModule* attribute), 39  
train\_set\_target (*dicee.knowledge\_graph.KG* attribute), 74  
train\_target (*dicee.dataset\_classes.AllvsAll* attribute), 35  
train\_target (*dicee.dataset\_classes.KvsAll* attribute), 34  
train\_target (*dicee.dataset\_classes.KvsSampleDataset* attribute), 37  
train\_target\_indices (*dicee.knowledge\_graph.KG* attribute), 74  
train\_triples (*dicee.dataset\_classes.NegSampleDataset* attribute), 38  
trained\_triples () (*dicee.abstracts.BaseInteractiveTrainKGE* method), 18  
trained\_model (*dicee.Execute* attribute), 213, 214  
trained\_model (*dicee.executer.Execute* attribute), 70  
trainer (*dicee.config.Namespace* attribute), 29  
trainer (*dicee.DICE\_Trainer* attribute), 220  
trainer (*dicee.Execute* attribute), 213, 214  
trainer (*dicee.executer.Execute* attribute), 70  
trainer (*dicee.trainer.DICE\_Trainer* attribute), 206  
trainer (*dicee.trainer.dice\_trainer.DICE\_Trainer* attribute), 201  
trainer (*dicee.trainer.torch\_trainer\_ddp.NodeTrainer* attribute), 205  
training\_step (*dicee.trainer.torch\_trainer.TorchTrainer* attribute), 204  
training\_step () (*dicee.models.base\_model.BaseKGELightning* method), 88  
training\_step () (*dicee.models.BaseKGELightning* method), 135

training\_step() (*dicee.models.transformers.BytE method*), 125  
training\_step\_outputs (*dicee.models.base\_model.BaseKGELightning attribute*), 88  
training\_step\_outputs (*dicee.models.BaseKGELightning attribute*), 135  
training\_technique (*dicee.knowledge\_graph.KG attribute*), 73  
TransE (*class in dicee.models*), 147  
TransE (*class in dicee.models.real*), 121  
transfer\_batch\_to\_device () (*dicee.dataset\_classes.CVDataModule method*), 41  
transformer (*dicee.models.transformers.BytE attribute*), 124  
transformer (*dicee.models.transformers.GPT attribute*), 129  
trapezoid() (*dicee.models.FMult2 method*), 180  
trapezoid() (*dicee.models.function\_space.FMult2 method*), 109  
tri\_score() (*dicee.models.function\_space.LFMult method*), 111  
tri\_score() (*dicee.models.function\_space.LFMult1 method*), 110  
tri\_score() (*dicee.models.LFM method*), 181  
tri\_score() (*dicee.models.LFMult1 method*), 180  
triple\_score() (*dicee.KGE method*), 217  
triple\_score() (*dicee.knowledge\_graph\_embeddings.KGE method*), 76  
TriplePredictionDataset (*class in dicee.dataset\_classes*), 38  
tuple2list () (*dicee.query\_generator.QueryGenerator method*), 183  
tuple2list () (*dicee.QueryGenerator method*), 219  
TWA (*class in dicee.weight\_averaging*), 211  
twa (*dicee.config.Namespace attribute*), 30  
twa\_c\_epochs (*dicee.weight\_averaging.TWA attribute*), 212  
twa\_model (*dicee.weight\_averaging.TWA attribute*), 212  
twa\_start\_epoch (*dicee.weight\_averaging.TWA attribute*), 212

## U

unlabelled\_size (*dicee.callbacks.PseudoLabellingCallback attribute*), 24  
unmap () (*dicee.query\_generator.QueryGenerator method*), 183  
unmap () (*dicee.QueryGenerator method*), 219  
unmap\_query () (*dicee.query\_generator.QueryGenerator method*), 183  
unmap\_query () (*dicee.QueryGenerator method*), 219  
update\_hits () (*in module dicee.evaluation.utils*), 58

## V

val\_aswa (*dicee.weight\_averaging.ASWA attribute*), 208  
val\_dataloader () (*dicee.models.base\_model.BaseKGELightning method*), 90  
val\_dataloader () (*dicee.models.BaseKGELightning method*), 137  
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*), 183  
val\_path (*dicee.QueryGenerator attribute*), 218  
valid\_set (*dicee.knowledge\_graph.KG attribute*), 73, 74  
validate\_knowledge\_graph () (*in module dicee.sanity\_checkers*), 191  
var\_clamp (*dicee.weight\_averaging.SWAG attribute*), 210  
vocab\_preparation () (*dicee.evaluation.Evaluator method*), 60  
vocab\_preparation () (*dicee.evaluation.evaluator.Evaluator method*), 51  
vocab\_preparation () (*dicee.Evaluator method*), 222  
vocab\_preparation () (*dicee.evaluator.Evaluator method*), 67  
vocab\_size (*dicee.models.CoKEConfig attribute*), 148  
vocab\_size (*dicee.models.real.CoKEConfig attribute*), 122  
vocab\_size (*dicee.models.transformers.GPTConfig attribute*), 128  
vocab\_to\_parquet () (*in module dicee.static\_funcs*), 197  
vtp\_score () (*dicee.models.function\_space.LFMult method*), 111  
vtp\_score () (*dicee.models.function\_space.LFMult1 method*), 110  
vtp\_score () (*dicee.models.LFM method*), 181  
vtp\_score () (*dicee.models.LFMult1 method*), 180

## W

warmup\_steps (*dicee.callbacks.LRScheduler attribute*), 27  
weight (*dicee.models.transformers.LayerNorm attribute*), 126  
weight\_decay (*dicee.config.Namespace attribute*), 29  
weight\_decay (*dicee.models.base\_model.BaseKGE attribute*), 94  
weight\_decay (*dicee.models.BaseKGE attribute*), 141, 144, 150, 155, 161, 174, 177

`weight_samples (dicee.weight_averaging.TWA attribute), 212`  
`weights (dicee.models.FMult attribute), 179`  
`weights (dicee.models.function_space.FMult attribute), 108`  
`weights (dicee.models.function_space.GFMult attribute), 109`  
`weights (dicee.models.GFMult attribute), 179`  
`world_size (dicee.Execute attribute), 213`  
`world_size (dicee.executer.Execute attribute), 70`  
`write_csv_from_parallel() (in module dicee.static_funcs), 197`  
`write_links() (dicee.query_generator.QueryGenerator method), 183`  
`write_links() (dicee.QueryGenerator method), 219`  
`write_report() (dicee.Execute method), 215`  
`write_report() (dicee.executer.Execute method), 71`

## X

`x_values (dicee.models.function_space.LFMult attribute), 110`  
`x_values (dicee.models.LFMult attribute), 180`