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# DICE Embeddings

*Release 0.1.3.2*

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

## 1 Dicee Manual

**Version:** dicee 0.3.2

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

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

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Dicee is a hardware-agnostic framework for large-scale knowledge graph embeddings.

Knowledge graph embedding research has mainly focused on learning continuous representations of knowledge graphs towards the link prediction problem. Recently developed frameworks can be effectively applied in a wide range of research-related applications. Yet, using these frameworks in real-world applications becomes more challenging as the size of the knowledge graph grows

We developed the DICE Embeddings framework (dicee) to compute embeddings for large-scale knowledge graphs in a hardware-agnostic manner. To achieve this goal, we rely on

1. **Pandas<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.

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<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
```

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```
pre_trained_kge = KGE(path=result['path_experiment_folder'])

# (3) Single-hop query answering
# Query: ?E : \exist E.hasSibling(E, F9M167)
# Question: Who are the siblings of F9M167?
# Answer: [F9M157, F9F141], as (F9M167, hasSibling, F9M157) and (F9M167, hasSibling, ↵F9F141)

predictions = pre_trained_kge.answer_multi_hop_query(query_type="1p",
                                                      query='http://www.benchmark.org/↪family#F9M167',
                                                      ('http://www.benchmark.
                                                       ↪org/family#hasSibling',)),
                                                       tnorm="min", k=3)

top_entities = [topk_entity for topk_entity, query_score in predictions]
assert "http://www.benchmark.org/family#F9F141" in top_entities
assert "http://www.benchmark.org/family#F9M157" in top_entities

# (2) Two-hop query answering
# Query: ?D : \exist E.Married(D, E) \land hasSibling(E, F9M167)
# Question: To whom a sibling of F9M167 is married to?
# Answer: [F9F158, F9M142] as (F9M157 #married F9F158) and (F9F141 #married F9M142)
predictions = pre_trained_kge.answer_multi_hop_query(query_type="2p",
                                                      query="http://www.benchmark.org/↪family#F9M167",
                                                      ("http://www.benchmark.
                                                       ↪org/family#hasSibling",
                                                       "http://www.benchmark.
                                                       ↪org/family#married")),,
                                                       tnorm="min", k=3)

top_entities = [topk_entity for topk_entity, query_score in predictions]
assert "http://www.benchmark.org/family#F9M142" in top_entities
assert "http://www.benchmark.org/family#F9F158" in top_entities

# (3) Three-hop query answering
# Query: ?T : \exist D.type(D, T) \land Married(D, E) \land hasSibling(E, F9M167)
# Question: What are the type of people who are married to a sibling of F9M167?
# (3) Answer: [Person, Male, Father] since F9M157 is [Brother Father Grandfather ↵Male] and F9M142 is [Male Grandfather Father]

predictions = pre_trained_kge.answer_multi_hop_query(query_type="3p", query="http://↪www.benchmark.org/family#F9M167",
                                                      ("http://
                                                       ↪www.benchmark.org/family#hasSibling",
                                                       "http://
                                                       ↪www.benchmark.org/family#married",
                                                       "http://
                                                       ↪www.w3.org/1999/02/22-rdf-syntax-ns#type")),,
                                                       tnorm="min", k=5)

top_entities = [topk_entity for topk_entity, query_score in predictions]
print(top_entities)
assert "http://www.benchmark.org/family#Person" in top_entities
assert "http://www.benchmark.org/family#Father" in top_entities
assert "http://www.benchmark.org/family#Male" in top_entities
```

For more, please refer to examples/multi\_hop\_query\_answering.

## 8 Predicting Missing Links

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

## 9 Downloading Pretrained Models

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

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

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

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

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<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>

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

## 13 How to cite

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

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

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```
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
```

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```

@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  $[0,1]^{\{n \text{ times } d\}}$  where n denotes the number of hops and d denotes number of entities

**t\_conorm** (`tens_1: torch.Tensor, tens_2: torch.Tensor, tconorm: str = 'min'`) → torch.Tensor

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

**class dicee.abstracts.AbstractCallback**

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

Abstract class for Callback class for knowledge graph embedding models

### Parameter

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

## Parameter

trainer:

model:

### **rtype**

None

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

Call at the beginning of the training.

## Parameter

trainer:

model:

### **rtype**

None

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

Call at the beginning of the training.

## Parameter

trainer:

model:

### **rtype**

None

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

Call at the end of each epoch during training.

## Parameter

trainer:

model:

### **rtype**

None

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

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

## Parameter

trainer:

model:

### **rtype**

None

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

Call at the end of the training.

## Parameter

trainer:

model:

### rtype

None

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

Bases: *AbstractCallback*

Abstract class for Callback class for knowledge graph embedding models

## Parameter

**num\_epochs**

**path**

**sample\_counter** = 0

**epoch\_count** = 0

**alphas** = None

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

Call at the beginning of the training.

## Parameter

trainer:

model:

### rtype

None

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

Call at the end of the training.

## Parameter

trainer:

model:

### rtype

None

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

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

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

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

```

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

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

```

### Parameters

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

## dicee.analyse\_experiments

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

### Classes

---

<i>Experiment</i>
-------------------

---

### Functions

---

<i>get_default_arguments()</i>
<i>analyse(args)</i>

---

### 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

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

### Functions

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

### Module Contents

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

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

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

Bases: `torch.utils.data.Dataset`

An abstract class representing a Dataset.

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

### Note

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

`train_set`

`ordered_bpe_entities`

`num_bpe_entities`

`neg_ratio`

`num_datapoints`

`__len__()`

`__getitem__(idx)`

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

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

Bases: `torch.utils.data.Dataset`

An abstract class representing a Dataset.

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

### Note

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

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

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

Bases: `torch.utils.data.Dataset`

Dataset for the 1vsALL training strategy

#### Parameters

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

#### Return type

`torch.utils.data.Dataset`

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

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

Bases: `torch.utils.data.Dataset`

Dataset for the 1vsALL training strategy

#### Parameters

- **train\_set\_idx** – Indexed triples for the training.
- **entity\_idxs** – mapping.
- **relation\_idxs** – mapping.
- **form** – ?
- **num\_workers** – int for <https://pytorch.org/docs/stable/data.html#torch.utils.data.DataLoader>

**Return type**

torch.utils.data.Dataset

**train\_data**

**target\_dim**

**collate\_fn = None**

**\_\_len\_\_()**

**\_\_getitem\_\_(idx)**

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

Bases: torch.utils.data.Dataset

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

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

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

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

y:labels are represented in torch.float16

**train\_set\_idx**

Indexed triples for the training.

**entity\_idxs**

mapping.

**relation\_idxs**

mapping.

**form**

?

**store**

?

**label\_smoothing\_rate**

collate\_fn: batch:List[torch.IntTensor] Returns ----- torch.utils.data.Dataset

**label\_smoothing\_rate**

**neg\_sample\_ratio**

**train\_set**

**length**

**num\_entities**

**num\_relations**

**\_\_len\_\_()**

**\_\_getitem\_\_(idx)**

**collate\_fn**(batch: List[torch.Tensor])

**class** dicee.dataset\_classes.**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_.</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_i</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(→ Optional[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.

## Module Contents

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

Evaluate link prediction performance with head and tail prediction.

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

### Parameters

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

#### Returns

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

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

Evaluate link prediction with reciprocal relations.

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

#### Parameters

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

#### Returns

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

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

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

#### Parameters

- **model** – KGE model wrapper with BPE support.
- **within\_entities** – List of entities to evaluate within.
- **triples** – Test triples as list of (head, relation, tail) tuples.
- **er\_vocab** – Mapping (entity, relation) -> list of valid tail entities.
- **re\_vocab** – Mapping (relation, entity) -> list of valid head entities.

#### Returns

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

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

Evaluate link prediction with BPE encoding and reciprocals.

#### Parameters

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

#### Returns

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

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

Evaluate BPE link prediction with KvsAll scoring.

#### Parameters

- **model** – The KGE model wrapper.
- **triples** – List of string triples.
- **er\_vocab** – Entity-relation vocabulary for filtering.
- **batch\_size** – Batch size for processing.
- **func\_triple\_to\_bpe\_representation** – Function to convert triples to BPE.
- **str\_to\_bpe\_entity\_to\_idx** – Mapping from string entities to BPE indices.

#### Returns

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

#### Raises

**ValueError** – If batch\_size is not provided.

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

Evaluate trained literal prediction model on a test file.

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

#### Parameters

- **kge\_model** – Trained KGE model with literal prediction capability.
- **eval\_file\_path** – Path to the evaluation file containing test literals.
- **store\_lit\_preds** – If True, stores predictions to CSV file.
- **eval\_literals** – If True, evaluates and prints error metrics.
- **loader\_backend** – Backend for loading dataset ('pandas' or 'rdflib').
- **return\_attr\_error\_metrics** – If True, returns the metrics DataFrame.

#### Returns

DataFrame with per-attribute MAE and RMSE if return\_attr\_error\_metrics is True, otherwise None.

#### Raises

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

#### Example

```
>>> from dicee import KGE  
>>> from dicee.evaluation import evaluate_literal_prediction  
>>> model = KGE(path="pretrained_model")  
>>> metrics = evaluate_literal_prediction(
```

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```
...     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.

### Attributes

`VALID_SCORING_TECHNIQUES`

### Classes

`Evaluator`

Evaluator class for KGE models in various downstream tasks.

### Module Contents

`dicee.evaluation.evaluator.VALID_SCORING_TECHNIQUES`

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

Evaluator class for KGE models in various downstream tasks.

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

`er_vocab`

Entity-relation to tail vocabulary for filtered ranking.

`re_vocab`

Relation-entity (tail) to head vocabulary.

`ee_vocab`

Entity-entity to relation vocabulary.

`num_entities`

Total number of entities in the knowledge graph.

`num_relations`

Total number of relations in the knowledge graph.

**args**  
 Configuration arguments.

**report**  
 Dictionary storing evaluation results.

**during\_training**  
 Whether evaluation is happening during training.

## Example

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

**re\_vocab**: Dict | None = None  
**er\_vocab**: Dict | None = None  
**ee\_vocab**: Dict | None = None  
**func\_triple\_to\_bpe\_representation** = None

**is\_continual\_training** = False  
**num\_entities**: int | None = None  
**num\_relations**: int | None = None  
**domain\_constraints\_per\_rel** = None  
**range\_constraints\_per\_rel** = None

**args**

**report**: Dict  
**during\_training** = False

**vocab\_preparation**(dataset) → None

Prepare vocabularies from the dataset for evaluation.

Resolves any future objects and saves vocabularies to disk.

### Parameters

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

**eval**(dataset, trained\_model, form\_of\_labelling: str, during\_training: bool = False) → Dict | None

Evaluate the trained model on the dataset.

### Parameters

- **dataset** – Knowledge graph dataset (KG instance).
- **trained\_model** – The trained KGE model.
- **form\_of\_labelling** – Type of labelling ('EntityPrediction' or 'RelationPrediction').
- **during\_training** – Whether evaluation is during training.

### Returns

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

`eval_rank_of_head_and_tail_entity`(\**, train\_set, valid\_set=None, test\_set=None, trained\_model)*  
→ None

Evaluate with negative sampling scoring.

`eval_rank_of_head_and_tail_byte_pair_encoded_entity`(\**, train\_set=None, valid\_set=None,  
test\_set=None, ordered\_bpe\_entities, trained\_model)* → None

Evaluate with BPE-encoded entities and negative sampling.

`eval_with_byte`(\**, raw\_train\_set, raw\_valid\_set=None, raw\_test\_set=None, trained\_model,  
form\_of\_labelling)* → None

Evaluate BytE model with generation.

`eval_with_bpe_vs_all`(\**, raw\_train\_set, raw\_valid\_set=None, raw\_test\_set=None, trained\_model,  
form\_of\_labelling)* → None

Evaluate with BPE and KvsAll scoring.

`eval_with_vs_all`(\**, train\_set, valid\_set=None, test\_set=None, trained\_model, form\_of\_labelling)*  
→ None

Evaluate with KvsAll or 1vsAll scoring.

`evaluate_lp_k_vs_all`(*model, triple\_idx, info: str | None = None,  
form\_of\_labelling: str | None = None*) → Dict[str, float]

Filtered link prediction evaluation with KvsAll scoring.

### Parameters

- **model** – The trained model to evaluate.
- **triple\_idx** – Integer-indexed test triples.
- **info** – Description to print.
- **form\_of\_labelling** – ‘EntityPrediction’ or ‘RelationPrediction’.

### Returns

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

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

Evaluate ByteE model with text generation.

### Parameters

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

### Returns

Dictionary with placeholder metrics (-1 values).

`evaluate_lp_bpe_k_vs_all`(*model, triples: List[List[str]], info: str | None = None,  
form\_of\_labelling: str | None = None*) → Dict[str, float]

Evaluate BPE model with KvsAll scoring.

### Parameters

- **model** – BPE-enabled model.
- **triples** – String triples.

- **info** – Description to print.
- **form\_of\_labelling** – Type of labelling.

#### Returns

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

**evaluate\_lp** (*model*, *triple\_idx*, *info*: str) → Dict[str, float]

Evaluate link prediction with negative sampling.

#### Parameters

- **model** – The model to evaluate.
- **triple\_idx** – Integer-indexed triples.
- **info** – Description to print.

#### Returns

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

**dummy\_eval** (*trained\_model*, *form\_of\_labelling*: str) → None

Run evaluation from saved data (for continual training).

#### Parameters

- **trained\_model** – The trained model.
- **form\_of\_labelling** – Type of labelling.

**eval\_with\_data** (*dataset*, *trained\_model*, *triple\_idx*: numpy.ndarray, *form\_of\_labelling*: str)  
→ Dict[str, float]

Evaluate a trained model on a given dataset.

#### Parameters

- **dataset** – Knowledge graph dataset.
- **trained\_model** – The trained model.
- **triple\_idx** – Integer-indexed triples to evaluate.
- **form\_of\_labelling** – Type of labelling.

#### Returns

Dictionary with evaluation metrics.

#### Raises

**ValueError** – If scoring technique is invalid.

## dicee.evaluation.link\_prediction

Link prediction evaluation functions.

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

## Functions

<code>evaluate_link_prediction_performance</code> (→ Dict[str, float])	Evaluate link prediction performance with head and tail prediction.
<code>evaluate_link_prediction_performance_with_</code>	Evaluate link prediction with reciprocal relations.

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

## Module Contents

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

Evaluate link prediction performance with head and tail prediction.

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

### Parameters

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

### Returns

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

`dicee.evaluation.link_prediction.`

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

Evaluate link prediction with reciprocal relations.

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

### Parameters

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

### Returns

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

`dicee.evaluation.link_prediction.`

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

Evaluate link prediction with BPE encoding and reciprocals.

### Parameters

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

### Returns

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

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

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

### Parameters

- **model** – KGE model wrapper with BPE support.
- **within\_entities** – List of entities to evaluate within.
- **triples** – Test triples as list of (head, relation, tail) tuples.
- **er\_vocab** – Mapping (entity, relation) -> list of valid tail entities.
- **re\_vocab** – Mapping (relation, entity) -> list of valid head entities.

### Returns

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

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

Evaluate link prediction with batched processing.

Memory-efficient evaluation using chunked entity scoring.

### Parameters

- **model** – The KGE model to evaluate.
- **triple\_idx** – Integer-indexed triples as numpy array.
- **num\_entities** – Total number of entities.
- **er\_vocab** – Mapping (head\_idx, rel\_idx) -> list of tail indices.
- **re\_vocab** – Mapping (rel\_idx, tail\_idx) -> list of head indices.
- **info** – Description to print.
- **batch\_size** – Batch size for triple processing.
- **chunk\_size** – Chunk size for entity scoring.

### Returns

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

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

Evaluate link prediction with BPE-encoded entities.

### Parameters

- **model** – The KGE model to evaluate.
- **triple\_idx** – List of BPE-encoded triple tuples.
- **all\_bpe\_shaped\_entities** – All entities with BPE representations.
- **er\_vocab** – Mapping for tail filtering.
- **re\_vocab** – Mapping for head filtering.

- **info** – Description to print.

### Returns

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

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

Evaluate BPE link prediction with KvsAll scoring.

### Parameters

- **model** – The KGE model wrapper.
- **triples** – List of string triples.
- **er\_vocab** – Entity-relation vocabulary for filtering.
- **batch\_size** – Batch size for processing.
- **func\_triple\_to\_bpe\_representation** – Function to convert triples to BPE.
- **str\_to\_bpe\_entity\_to\_idx** – Mapping from string entities to BPE indices.

### Returns

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

### Raises

**ValueError** – If batch\_size is not provided.

## dicee.evaluation.literal\_prediction

Literal prediction evaluation functions.

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

### Functions

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

### Module Contents

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

Evaluate trained literal prediction model on a test file.

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

### Parameters

- **kge\_model** – Trained KGE model with literal prediction capability.
- **eval\_file\_path** – Path to the evaluation file containing test literals.

- **store\_lit\_preds** – If True, stores predictions to CSV file.
- **eval\_literals** – If True, evaluates and prints error metrics.
- **loader\_backend** – Backend for loading dataset ('pandas' or 'rdflib').
- **return\_attr\_error\_metrics** – If True, returns the metrics DataFrame.

#### Returns

DataFrame with per-attribute MAE and RMSE if return\_attr\_error\_metrics is True, otherwise None.

#### Raises

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

#### Example

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

## dicee.evaluation.utils

Utility functions for evaluation module.

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

#### Attributes

---

<i>DEFAULT_HITS_RANGE</i>
<i>ALL_HITS_RANGE</i>

---

#### Functions

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

## Module Contents

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

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

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

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

### Parameters

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

### Returns

The original iterable or a tqdm-wrapped version.

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

Compute standard link prediction metrics from ranks.

### Parameters

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

### Returns

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

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

Compute link prediction metrics without scaling factor.

### Parameters

- **ranks** – List of ranks for each prediction.
- **num\_triples** – Total number of triples evaluated.
- **hits\_dict** – Dictionary mapping hit levels to lists of hits.

### Returns

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

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

Update hits dictionary based on rank.

### Parameters

- **hits** – Dictionary to update in-place.
- **rank** – The rank to check against hit levels.

- **hits\_range** – List of hit levels to check (default: ALL\_HITS\_RANGE).

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

Create an initialized hits dictionary.

#### Parameters

**hits\_range** – List of hit levels to initialize (default: ALL\_HITS\_RANGE).

#### Returns

Dictionary with empty lists for each hit level.

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

Efficiently zero gradients using parameter.grad = None.

This is more efficient than optimizer.zero\_grad() as it avoids memory operations.

See: [https://pytorch.org/tutorials/recipes/recipes/tuning\\_guide.html](https://pytorch.org/tutorials/recipes/recipes/tuning_guide.html)

#### Parameters

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

## Attributes

---

<code>DEFAULT_HITS_RANGE</code>
<code>ALL_HITS_RANGE</code>

---

## 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_ij</code>	Evaluate link prediction with BPE encoding and reciprocals.
<code>evaluate_lp(→ Dict[str, float])</code>	Evaluate link prediction with batched processing.
<code>evaluate_lp_bpe_k_vs_all(→ Dict[str, float])</code>	Evaluate BPE link prediction with KvsAll scoring.
<code>evaluate_bpe_lp(→ Dict[str, float])</code>	Evaluate link prediction with BPE-encoded entities.
<code>evaluate_literal_prediction(→ Operational[pandas.DataFrame])</code>	Evaluate trained literal prediction model on a test file.
<code>evaluate_ensemble_link_prediction_performanc</code>	Evaluate link prediction performance of an ensemble of KGE models.
<code>compute_metrics_from_ranks(→ Dict[str, float])</code>	Compute standard link prediction metrics from ranks.
<code>compute_metrics_from_ranks_simple(→ Dict[str, float])</code>	Compute link prediction metrics without scaling factor.

---

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<code>make_iterable_verbose</code> (→ Iterable)	Wrap an iterable with tqdm progress bar if verbose is True.
<code>update_hits</code> (→ None)	Update hits dictionary based on rank.
<code>create_hits_dict</code> (→ Dict[int, List[float]])	Create an initialized hits dictionary.

## Package Contents

**class** dicee.evaluation.**Evaluator**(*args*, *is\_continual\_training*: bool = False)

Evaluator class for KGE models in various downstream tasks.

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

**er\_vocab**

Entity-relation to tail vocabulary for filtered ranking.

**re\_vocab**

Relation-entity (tail) to head vocabulary.

**ee\_vocab**

Entity-entity to relation vocabulary.

**num\_entities**

Total number of entities in the knowledge graph.

**num\_relations**

Total number of relations in the knowledge graph.

**args**

Configuration arguments.

**report**

Dictionary storing evaluation results.

**during\_training**

Whether evaluation is happening during training.

## Example

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

**re\_vocab**: Dict | None = None

**er\_vocab**: Dict | None = None

**ee\_vocab**: Dict | None = None

**func\_triple\_to\_bpe\_representation** = None

**is\_continual\_training** = False

**num\_entities**: int | None = None

```

num_relations: int | None = None
domain_constraints_per_rel = None
range_constraints_per_rel = None
args
report: Dict
during_training = False
vocab_preparation(dataset) → None
    Prepare vocabularies from the dataset for evaluation.
    Resolves any future objects and saves vocabularies to disk.

Parameters
    dataset – Knowledge graph dataset with vocabulary attributes.

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

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

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

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

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

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

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

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

evaluate_lp_k_vs_all(model, triple_idx, info: str | None = None,
    form_of_labelling: str | None = None) → Dict[str, float]
    Filtered link prediction evaluation with KvsAll scoring.

```

#### **Parameters**

- **model** – The trained model to evaluate.

- **triple\_idx** – Integer-indexed test triples.
- **info** – Description to print.
- **form\_of\_labelling** – ‘EntityPrediction’ or ‘RelationPrediction’.

#### Returns

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

**evaluate\_lp\_with\_byte** (*model*, *triples*: *List[List[str]]*, *info*: *str* | *None* = *None*) → *Dict[str, float]*

Evaluate BytE model with text generation.

#### Parameters

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

#### Returns

Dictionary with placeholder metrics (-1 values).

**evaluate\_lp\_bpe\_k\_vs\_all** (*model*, *triples*: *List[List[str]]*, *info*: *str* | *None* = *None*, *form\_of\_labelling*: *str* | *None* = *None*) → *Dict[str, float]*

Evaluate BPE model with KvsAll scoring.

#### Parameters

- **model** – BPE-enabled model.
- **triples** – String triples.
- **info** – Description to print.
- **form\_of\_labelling** – Type of labelling.

#### Returns

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

**evaluate\_lp** (*model*, *triple\_idx*, *info*: *str*) → *Dict[str, float]*

Evaluate link prediction with negative sampling.

#### Parameters

- **model** – The model to evaluate.
- **triple\_idx** – Integer-indexed triples.
- **info** – Description to print.

#### Returns

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

**dummy\_eval** (*trained\_model*, *form\_of\_labelling*: *str*) → *None*

Run evaluation from saved data (for continual training).

#### Parameters

- **trained\_model** – The trained model.
- **form\_of\_labelling** – Type of labelling.

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

→ Dict[str, float]

Evaluate a trained model on a given dataset.

#### Parameters

- **dataset** – Knowledge graph dataset.
- **trained\_model** – The trained model.
- **triple\_idx** – Integer-indexed triples to evaluate.
- **form\_of\_labelling** – Type of labelling.

#### Returns

Dictionary with evaluation metrics.

#### Raises

**ValueError** – If scoring technique is invalid.

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

Evaluate link prediction performance with head and tail prediction.

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

#### Parameters

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

#### Returns

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

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

Evaluate link prediction with reciprocal relations.

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

#### Parameters

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

#### Returns

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

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

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

#### Parameters

- **model** – KGE model wrapper with BPE support.
- **within\_entities** – List of entities to evaluate within.

- **triples** – Test triples as list of (head, relation, tail) tuples.
- **er\_vocab** – Mapping (entity, relation) -> list of valid tail entities.
- **re\_vocab** – Mapping (relation, entity) -> list of valid head entities.

#### Returns

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

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

Evaluate link prediction with BPE encoding and reciprocals.

#### Parameters

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

#### Returns

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

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

Evaluate link prediction with batched processing.

Memory-efficient evaluation using chunked entity scoring.

#### Parameters

- **model** – The KGE model to evaluate.
- **triple\_idx** – Integer-indexed triples as numpy array.
- **num\_entities** – Total number of entities.
- **er\_vocab** – Mapping (head\_idx, rel\_idx) -> list of tail indices.
- **re\_vocab** – Mapping (rel\_idx, tail\_idx) -> list of head indices.
- **info** – Description to print.
- **batch\_size** – Batch size for triple processing.
- **chunk\_size** – Chunk size for entity scoring.

#### Returns

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

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

Evaluate BPE link prediction with KvsAll scoring.

#### Parameters

- **model** – The KGE model wrapper.
- **triples** – List of string triples.
- **er\_vocab** – Entity-relation vocabulary for filtering.

- **batch\_size** – Batch size for processing.
- **func\_triple\_to\_bpe\_representation** – Function to convert triples to BPE.
- **str\_to\_bpe\_entity\_to\_idx** – Mapping from string entities to BPE indices.

#### Returns

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

#### Raises

**ValueError** – If batch\_size is not provided.

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

Evaluate link prediction with BPE-encoded entities.

#### Parameters

- **model** – The KGE model to evaluate.
- **triple\_idx** – List of BPE-encoded triple tuples.
- **all\_bpe\_shaped\_entities** – All entities with BPE representations.
- **er\_vocab** – Mapping for tail filtering.
- **re\_vocab** – Mapping for head filtering.
- **info** – Description to print.

#### Returns

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

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

Evaluate trained literal prediction model on a test file.

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

#### Parameters

- **kge\_model** – Trained KGE model with literal prediction capability.
- **eval\_file\_path** – Path to the evaluation file containing test literals.
- **store\_lit\_preds** – If True, stores predictions to CSV file.
- **eval\_literals** – If True, evaluates and prints error metrics.
- **loader\_backend** – Backend for loading dataset ('pandas' or 'rdflib').
- **return\_attr\_error\_metrics** – If True, returns the metrics DataFrame.

#### Returns

DataFrame with per-attribute MAE and RMSE if return\_attr\_error\_metrics is True, otherwise None.

#### Raises

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

## Example

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

dicee.evaluation.**evaluate\_ensemble\_link\_prediction\_performance**(models: List, triples,  
er\_vocab: Dict[Tuple, List], weights: List[float] | None = None, batch\_size: int = 512,  
weighted\_averaging: bool = True, normalize\_scores: bool = True) → Dict[str, float]

Evaluate link prediction performance of an ensemble of KGE models.

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

### Parameters

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

### Returns

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

### Raises

**AssertionError** – If weighted\_averaging is True but weights are not provided or have wrong length.

## Example

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

dicee.evaluation.**compute\_metrics\_from\_ranks**(ranks: List[int], num\_triples: int,  
hits\_dict: Dict[int, List[float]], scale\_factor: int = 1) → Dict[str, float]

Compute standard link prediction metrics from ranks.

## Parameters

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

## Returns

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

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

Compute link prediction metrics without scaling factor.

## Parameters

- **ranks** – List of ranks for each prediction.
- **num\_triples** – Total number of triples evaluated.
- **hits\_dict** – Dictionary mapping hit levels to lists of hits.

## Returns

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

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

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

## Parameters

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

## Returns

The original iterable or a tqdm-wrapped version.

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

Update hits dictionary based on rank.

## Parameters

- **hits** – Dictionary to update in-place.
- **rank** – The rank to check against hit levels.
- **hits\_range** – List of hit levels to check (default: ALL\_HITS\_RANGE).

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

Create an initialized hits dictionary.

## Parameters

**hits\_range** – List of hit levels to initialize (default: ALL\_HITS\_RANGE).

## Returns

Dictionary with empty lists for each hit level.

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

## dicee.evaluator

Evaluator module for knowledge graph embedding models.

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

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

## Classes

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

## Module Contents

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

Evaluator class for KGE models in various downstream tasks.

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

**er\_vocab**

Entity-relation to tail vocabulary for filtered ranking.

**re\_vocab**

Relation-entity (tail) to head vocabulary.

**ee\_vocab**

Entity-entity to relation vocabulary.

**num\_entities**

Total number of entities in the knowledge graph.

**num\_relations**

Total number of relations in the knowledge graph.

**args**

Configuration arguments.

**report**

Dictionary storing evaluation results.

**during\_training**

Whether evaluation is happening during training.

## Example

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

```

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

```

**vocab\_preparation**(*dataset*) → None

Prepare vocabularies from the dataset for evaluation.

Resolves any future objects and saves vocabularies to disk.

#### Parameters

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

**eval**(*dataset, trained\_model, form\_of\_labelling: str, during\_training: bool = False*) → Dict | None

Evaluate the trained model on the dataset.

#### Parameters

- **dataset** – Knowledge graph dataset (KG instance).
- **trained\_model** – The trained KGE model.
- **form\_of\_labelling** – Type of labelling ('EntityPrediction' or 'RelationPrediction').
- **during\_training** – Whether evaluation is during training.

#### Returns

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

**eval\_rank\_of\_head\_and\_tail\_entity**(\**, train\_set, valid\_set=None, test\_set=None, trained\_model*)  
→ None

Evaluate with negative sampling scoring.

**eval\_rank\_of\_head\_and\_tail\_byte\_pair\_encoded\_entity**(\**, train\_set=None, valid\_set=None, test\_set=None, ordered\_bpe\_entities, trained\_model*) → None

Evaluate with BPE-encoded entities and negative sampling.

**eval\_with\_byte**(\**, raw\_train\_set, raw\_valid\_set=None, raw\_test\_set=None, trained\_model, form\_of\_labelling*) → None

Evaluate 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 = None,  
form_of_labelling: str | None = None) → Dict[str, float]
```

Filtered link prediction evaluation with KvsAll scoring.

#### Parameters

- **model** – The trained model to evaluate.
- **triple\_idx** – Integer-indexed test triples.
- **info** – Description to print.
- **form\_of\_labelling** – ‘EntityPrediction’ or ‘RelationPrediction’.

#### Returns

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

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

Evaluate BytE model with text generation.

#### Parameters

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

#### Returns

Dictionary with placeholder metrics (-1 values).

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

Evaluate BPE model with KvsAll scoring.

#### Parameters

- **model** – BPE-enabled model.
- **triples** – String triples.
- **info** – Description to print.
- **form\_of\_labelling** – Type of labelling.

#### Returns

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

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

Evaluate link prediction with negative sampling.

#### Parameters

- **model** – The model to evaluate.
- **triple\_idx** – Integer-indexed triples.
- **info** – Description to print.

### Returns

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

**dummy\_eval** (*trained\_model*, *form\_of\_labelling*: str) → None

Run evaluation from saved data (for continual training).

### Parameters

- **trained\_model** – The trained model.
- **form\_of\_labelling** – Type of labelling.

**eval\_with\_data** (*dataset*, *trained\_model*, *triple\_idx*: numpy.ndarray, *form\_of\_labelling*: str)

→ Dict[str, float]

Evaluate a trained model on a given dataset.

### Parameters

- **dataset** – Knowledge graph dataset.
- **trained\_model** – The trained model.
- **triple\_idx** – Integer-indexed triples to evaluate.
- **form\_of\_labelling** – Type of labelling.

### Returns

Dictionary with evaluation metrics.

### Raises

**ValueError** – If scoring technique is invalid.

## dicee.executor

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.executor.**Execute** (*args*, *continuous\_training*: bool = False)

Executor class for training, retraining and evaluating KGE models.

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

### **args**

Processed input arguments.

### **distributed**

Whether distributed training is enabled.

```

rank
    Process rank in distributed training.

world_size
    Total number of processes.

local_rank
    Local GPU rank.

trainer
    Training handler instance.

trained_model
    The trained model after training completes.

knowledge_graph
    The loaded knowledge graph.

report
    Dictionary storing training metrics and results.

evaluator
    Model evaluation handler.

distributed

args

is_continual_training = False

trainer: dicee.trainer.DICE_Trainer | None = None

trained_model = None

knowledge_graph: dicee.knowledge_graph.KG | None = None

report: Dict

evaluator: dicee.evaluator.Evaluator | None = None

start_time: float | None = None

is_rank_zero() → bool

cleanup()

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

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

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

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

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

```

```
save_trained_model() → None
    Save a knowledge graph embedding model
        (1) Send model to eval mode and cpu.
        (2) Store the memory footprint of the model.
        (3) Save the model into disk.
        (4) Update the stats of KG again ?
```

### Parameter

**rtype**

None

```
end(form_of_labelling: str) → dict
    End training
        (1) Store trained model.
        (2) Report runtimes.
        (3) Eval model if required.
```

### Parameter

**rtype**

A dict containing information about the training and/or evaluation

```
write_report() → None
    Report training related information in a report.json file
start() → dict
    Start training
        # (1) Loading the Data # (2) Create an evaluator object. # (3) Create a trainer object. # (4) Start the training
```

### Parameter

**rtype**

A dict containing information about the training and/or evaluation

```
class dicee.executer.ContinuousExecute(args)
Bases: Execute
A subclass of Execute Class for retraining
    (1) Loading & Preprocessing & Serializing input data.
    (2) Training & Validation & Testing
    (3) Storing all necessary info
```

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

```
continual_start() → dict
    Start Continual Training
        (1) Initialize training.
        (2) Start continual training.
        (3) Save trained model.
```

## Parameter

### rtype

A dict containing information about the training and/or evaluation

## dicee.knowledge\_graph

Knowledge Graph module for data loading and preprocessing.

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

## Classes

---

*KG*

Knowledge Graph container and processor.

---

### Module Contents

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

Knowledge Graph container and processor.

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

#### **dataset\_dir**

Path to directory containing train/valid/test files.

#### **num\_entities**

Total number of unique entities.

#### **num\_relations**

Total number of unique relations.

#### **train\_set**

Indexed training triples as numpy array.

#### **valid\_set**

Indexed validation triples (optional).

#### **test\_set**

Indexed test triples (optional).

```
entity_to_idx
    Mapping from entity strings to indices.

relation_to_idx
    Mapping from relation strings to indices.

dataset_dir = None

sparql_endpoint = None

path_single_kg = None

byte_pair_encoding = False

ordered_shaped_bpe_tokens = None

add_noise_rate = None

num_entities: int | None = None

num_relations: int | None = None

path_for_deserialization = None

add_reciprocal = None

eval_model = None

read_only_few = None

sample_triples_ratio = None

path_for_serialization = None

entity_to_idx = None

relation_to_idx = None

backend = 'pandas'

training_technique = None

separator = None

raw_train_set = None

raw_valid_set = None

raw_test_set = None

train_set = None

valid_set = None

test_set = None

idx_entity_to_bpe_shaped: Dict

enc

num_tokens
```

```

num_bpe_entities: int | None = None
padding = False
dummy_id
max_length_subword_tokens: int | None = None
train_set_target = None
target_dim: int | None = None
train_target_indices = None
ordered_bpe_entities = None
description_of_input = None
describe() → None
    Generate a description string of the dataset statistics.
property entities_str: List[str]
    Get list of all entity strings.
property relations_str: List[str]
    Get list of all relation strings.
exists(h: str, r: str, t: str) → bool
    Check if a triple exists in the training set.

```

#### Parameters

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

#### Returns

True if the triple exists, False otherwise.

```

__iter__() → Iterator[Tuple[str, str, str]]
    Iterate over training triples as string tuples.
__len__() → int
    Return number of triples in the raw training set.
func_triple_to_bpe_representation(triple: List[str])

```

## dicee.knowledge\_graph\_embeddings

### Classes

*KGE*

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

## Module Contents

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

Bases: dicee.abtracts.BaseInteractiveKGE, dicee.abtracts.InteractiveQueryDecomposition, dicee.abtracts.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  $f(e,r,x) > \text{confidence}$ .  
 at\_most: int  
 Stop after finding at\_most missing triples  
 $\{(e,r,x) \mid f(e,r,x) > \text{confidence} \text{ and } (e,r,x)$   
 otin G  
**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

<code>adopt(params, grads, exp_avgs, exp_avg_sqs, state_steps)</code>	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:  $\text{step}^{**0.25}$  (default, gradually increases clipping threshold) - lambda step: 1.0 (constant clipping) - None (no clipping) Default: lambda step:  $\text{step}^{**0.25}$
- **weight\_decay** (*float, optional*) – Weight decay coefficient (L2 penalty). Default: 0.0
- **decouple** (*bool, optional*) – If True, uses decoupled weight decay (AdamW-style), applying weight decay directly to parameters. If False, adds weight decay to gradients (L2 regularization). Default: False
- **foreach** (*bool, optional*) – If True, uses the faster foreach implementation for multi-tensor operations. Default: None (auto-select)
- **maximize** (*bool, optional*) – If True, maximizes parameters instead of minimizing. Useful for reinforcement learning. Default: False
- **capturable** (*bool, optional*) – If True, the optimizer is safe to capture in a CUDA graph. Requires learning rate as Tensor. Default: False
- **differentiable** (*bool, optional*) – If True, the optimization step can be differentiated. Useful for meta-learning. Default: False
- **fused** (*bool, optional*) – If True, uses fused kernel implementation (currently not supported). Default: None

#### Raises

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

#### Example

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

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

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

#### Note

- For most use cases, the default hyperparameters work well
- Consider using decouple=True for better generalization (similar to AdamW)

- The clip\_lambda function helps stabilize training in early steps

## `clip_lambda`

### `__setstate__(state)`

Restore optimizer state from a checkpoint.

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

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

#### Parameters

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

#### Note

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

## `step(closure=None)`

Perform a single optimization step.

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

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

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

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

#### Parameters

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

#### Returns

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

**Return type**  
Optional[Tensor]

### Example

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

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

### Note

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

```
dicee.models.adopt.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:**

- $\theta$ : parameters
- $g$ : gradients
- $m$ : first moment (momentum of normalized gradients)
- $v$ : second moment (variance of raw gradients)
- $\alpha$ : learning rate
- $\beta_1, \beta_2$ : exponential decay rates
- $\epsilon$ : numerical stability constant
- `clip()`: gradient clipping function based on step

### Automatic mode selection:

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

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

**param params**  
Parameters to optimize.

**type params**  
`List[Tensor]`

**param grads**  
Gradients for each parameter.

**type grads**  
`List[Tensor]`

**param exp\_avgs**  
First moment estimates (momentum).

**type exp\_avgs**  
`List[Tensor]`

**param exp\_avg\_sqs**  
Second moment estimates (variance).

**type exp\_avg\_sqs**  
`List[Tensor]`

**param state\_steps**  
Step counters (must be singleton tensors).

**type state\_steps**  
`List[Tensor]`

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

```

type foreach
    Optional[bool]

param capturable
    If True, ensure CUDA graph capture safety.

type capturable
    bool

param differentiable
    If True, allow gradients through optimization step.

type differentiable
    bool

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

type fused
    Optional[bool]

param grad_scale
    Gradient scaler for AMP training.

type grad_scale
    Optional[Tensor]

param found_inf
    Flag for inf/nan detection in AMP.

type found_inf
    Optional[Tensor]

param has_complex
    Whether any parameters are complex-valued.

type has_complex
    bool

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

type beta1
    float

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

type beta2
    float

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

type lr
    Union[float, Tensor]

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

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

```

```

param weight_decay
    Weight decay coefficient (L2 penalty).

type weight_decay
    float

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

type decouple
    bool

param eps
    Small constant for numerical stability in normalization.

type eps
    float

param maximize
    If True, maximize objective instead of minimize.

type maximize
    bool

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

raises RuntimeError
    If state_steps contains non-tensor elements.

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

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

```

## Example

```

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

```

 **Note**

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

## See also

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

## dicee.models.base\_model

### Classes

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

### Module Contents

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

Bases: `lightning.LightningModule`

Base class for all neural network modules.

Your models should also subclass this class.

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

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

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

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

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

### Note

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

### Variables

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

`training_step_outputs = []`

`mem_of_model() → Dict`

Size of model in MB and number of params

`training_step(batch, batch_idx=None)`

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

### Parameters

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

### Returns

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

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

Example:

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

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

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

(continues on next page)

```
# 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()`

### 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 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** ( $B \times 2 \times T$ )

```

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.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

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

### Module Contents

```

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

```

```

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

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

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

```

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

### Note

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

## Variables

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

```

name = 'Keci'

p
q
r

requires_grad_for_interactions = True

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

```

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

e2e1, e2e2, e2e3, e3e1, e3e2, e3e3

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

```

compute_sigma_qq(hq, rq)
    Compute sigma_{qq} = sum_{j=1}^{p+q-1} sum_{k=j+1}^{p+q} (h_j r_k - h_k r_j) e_j e_k sigma_{q}
    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-1} sum_{k=i+1}^p (h_i r_k - h_k r_i) e_i e_k
    (5) sigma_qq = sum_{j=1}^{p+q-1} sum_{k=j+1}^{p+q} (h_j r_k - h_k r_j) e_j e_k
    (6) sigma_pq = sum_{i=1}^p sum_{j=p+1}^{p+q} (h_i r_j - h_j r_i) e_i e_j

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

```

## Parameter

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

### returns

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

**forward\_k\_vs\_with\_explicit** (x: torch.Tensor)

**k\_vs\_all\_score** (bpe\_head\_ent\_emb, bpe\_rel\_ent\_emb, E)

**forward\_k\_vs\_all** (x: torch.Tensor) → torch.FloatTensor

Kvsall training

- (1) Retrieve real-valued embedding vectors for heads and relations  $\mathbb{R}^d$ .
- (2) Construct head entity and relation embeddings according to  $C_{p,q}(\mathbb{R}^d)$ .
- (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  $C_{p,q}(\mathbb{R}^d)$

## 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:

$$\sigma_0 t = \sigma_0 \cdot t_0 = s0 + s1 - s2s3, s4ands5$$

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

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

For same bases vectors interaction we have

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

For different base vector interactions, we have

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

**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>)

### Module Contents

```
class dicee.models.dualE(args)  
Bases: dicee.models.base_model.BaseKGE  
Dual Quaternion Knowledge Graph Embeddings (https://ojs.aaai.org/index.php/AAAI/article/download/16850/16657)  
name = 'DualE'  
entity_embeddings  
relation_embeddings  
num_ent = None  
kvsall_score(e_1_h, e_2_h, e_3_h, e_4_h, e_5_h, e_6_h, e_7_h, e_8_h, e_1_t, e_2_t, e_3_t, e_4_t,  
e_5_t, e_6_t, e_7_t, e_8_t, r_1, r_2, r_3, r_4, r_5, r_6, r_7, r_8) → torch.tensor  
KvsAll scoring function
```

#### Input

x: torch.LongTensor with (n, ) shape

#### Output

torch.FloatTensor with (n) shape

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

Negative Sampling forward pass:

## Input

x: torch.LongTensor with (n, ) shape

## Output

torch.FloatTensor with (n) shape

**forward\_k\_vs\_all** (x)

KvsAll forward pass

## Input

x: torch.LongTensor with (n, ) shape

## Output

torch.FloatTensor with (n) shape

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

Transpose function

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

## dicee.models.ensemble

### Classes

---

*EnsembleKGE*

---

### Module Contents

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

    name
    train_mode = True
    args
    named_children()
    property example_input_array
    parameters()
    modules()
    __iter__()
    __len__()
    eval()
    to(device)
```

```

state_dict ()
    Return the state dict of the ensemble.

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

mem_of_model ()

__call__ (x_batch)

step ()

get_embeddings ()

__str__ ()

```

## dicee.models.function\_space

### Classes

<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. score = <hor, t>

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

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

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

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

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

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

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

## dicee.models.literal

### Classes

*LiteralEmbeddings*

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

### Module Contents

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

Bases: `torch.nn.Module`

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

**num\_of\_data\_properties**

Number of data properties (attributes).

**Type**

`int`

**embedding\_dims**

Dimension of the embeddings.

**Type**

`int`

**entity\_embeddings**

Pre-trained entity embeddings.

**Type**

`torch.tensor`

**dropout**

Dropout rate for regularization.

**Type**

`float`

**gate\_residual**

Whether to use gated residual connections.

**Type**

`bool`

**freeze\_entity\_embeddings**

Whether to freeze the entity embeddings during training.

**Type**

`bool`

**embedding\_dim**

**num\_of\_data\_properties**

**hidden\_dim**

**gate\_residual = True**

**freeze\_entity\_embeddings = True**

**entity\_embeddings**

**data\_property\_embeddings**

**fc**

**fc\_out**

**dropout**

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

#### Parameters

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

#### Returns

scalar predictions.

#### Return type

*Tensor*

**property device**

## dicee.models.octonion

### Classes

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

### Functions

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

### Module Contents

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

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

Bases: *dicee.models.base\_model.BaseKGE*

Base class for all neural network modules.

Your models should also subclass this class.

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

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

class Model(nn.Module):
```

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```

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

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

```

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

### Note

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

### Variables

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

```

name = 'OMult'

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

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

k_vs_all_score(bpe_head_ent_emb, bpe_rel_ent_emb, E)

forward_k_vs_all(x)

```

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

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

Bases: `dicee.models.base_model.BaseKGE`

Base class for all neural network modules.

Your models should also subclass this class.

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

```

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

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

```

(continues on next page)

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

Submodules assigned in this way will be registered, and will 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)

abstractmethod forward_k_vs_sample(x: torch.LongTensor, target_entity_idx)

```

## dicee.models.quaternion

### Classes

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

### Functions

---

*quaternion\_mul\_with\_unit\_norm*(\**, Q\_1, Q\_2*)

---

### Module Contents

*dicee.models.quaternion.quaternion\_mul\_with\_unit\_norm*(\**, Q\_1, Q\_2*)

**class** *dicee.models.quaternion.QM*ult(*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>quaternion_mul</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>ByteE</code>	Base class for all neural network modules.
<code>LayerNorm</code>	LayerNorm but with an optional bias. PyTorch doesn't support simply bias=False
<code>SelfAttention</code>	Base class for all neural network modules.
<code>MLP</code>	Base class for all neural network modules.
<code>Block</code>	Base class for all neural network modules.
<code>GPTConfig</code>	
<code>GPT</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 41 – 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))
```

### Note

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

## clip\_lambda

### \_\_setstate\_\_(state)

Restore optimizer state from a checkpoint.

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

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

#### Parameters

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

### Note

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

## step(closure=None)

Perform a single optimization step.

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

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

2. For each parameter group:
  - Collects parameters with gradients and their associated state
  - Extracts hyperparameters (betas, learning rate, etc.)
  - Calls the functional adopt() API to perform the actual update
3. Returns the loss value if a closure was provided

The functional API (adopt()) handles three execution modes:

- Single-tensor: Updates one parameter at a time (default, JIT-compatible)
- Multi-tensor (foreach): Batches operations for better performance
- Fused: Uses fused CUDA kernels (not yet implemented)

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

#### Parameters

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

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

Default: None

#### Returns

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

#### Return type

Optional[Tensor]

#### Example

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

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

#### Note

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

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

Bases: lightning.LightningModule

Base class for all neural network modules.

Your models should also subclass this class.

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

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

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

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```
    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
}
```

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```

    "strict": True,
    # If using the `LearningRateMonitor` callback to monitor the
    # learning rate progress, this keyword can be used to specify
    # a custom logged name
    "name": None,
}

```

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

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

### Note

Some things to know:

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

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

Bases: `BaseKGELightning`

Base class for all neural network modules.

Your models should also subclass this class.

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

```

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

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

    def forward(self, x):

```

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```
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 x 2 x T)

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

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

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

### Note

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

## Variables

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

```
args = None

__call__(x)

static forward(x)

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

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

Bases: `dicee.models.base_model.BaseKGE`

Base class for all neural network modules.

Your models should also subclass this class.

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

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


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

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

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

### Note

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

### Variables

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

```
name = 'QMult'

explicit = True

quaternion_multiplication_followed_by_inner_product (h, r, t)
```

### Parameters

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

### Returns

Triple scores.

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

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

Absolute value of a quaternion

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

L2 norm of quaternion vector:

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

### Parameters

`x` – The vector.

### Returns

The normalized vector.

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

```
k_vs_all_score (bpe_head_ent_emb, bpe_rel_ent_emb, E)
```

### Parameters

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

```
forward_k_vs_all (x)
```

### Parameters

`x`

```

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

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

entity_embeddings
relation_embeddings
conv2d
fc_num_input
fc1
bn_conv1
bn_conv2
feature_map_dropout
residual_convolution(Q_1, Q_2)
forward_triples(indexed_triple: torch.Tensor) → torch.Tensor

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

class dicee.models.AConvQ(args)
Bases: dicee.models.base_model.BaseKGE
Additive Convolutional Quaternion Knowledge Graph Embeddings
name = 'AConvQ'

entity_embeddings
relation_embeddings
conv2d
fc_num_input
fc1
bn_conv1
bn_conv2

```

```

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

Parameters
    x

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

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

Base class for all neural network modules.

Your models should also subclass this class.

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

```

```

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

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

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

```

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

### **Note**

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

### **Variables**

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

```

args

embedding_dim = None

num_entities = None

num_relations = None

```

```

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

Parameters
  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)
```

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

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

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

### Note

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

### Variables

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

```
args = None

__call__(x)

static forward(x)

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

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

`class dicee.models.OMult(args)`

Bases: `dicee.models.base_model.BaseKGE`

Base class for all neural network modules.

Your models should also subclass this class.

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

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

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

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

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

### Note

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

### Variables

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

```
name = 'OMult'

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

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

k_vs_all_score(bpe_head_ent_emb, bpe_rel_ent_emb, E)
```

`forward_k_vs_all(x)`

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

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

Base class for all neural network modules.

Your models should also subclass this class.

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

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

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

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

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

### Note

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

## Variables

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

```
name = 'ConvO'

conv2d

fc_num_input

fc1

bn_conv2d

norm_fc1

feature_map_dropout

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

residual_convolution(O_1, O_2)

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

## Parameters

`x`

`forward_k_vs_all(x: torch.Tensor)`

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

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

Bases: `dicee.models.base_model.BaseKGE`

Additive Convolutional Octonion Knowledge Graph Embeddings

`name = 'AConvO'`

`conv2d`

`fc_num_input`

`fc1`

`bn_conv2d`

`norm_fc1`

`feature_map_dropout`

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

`residual_convolution(O_1, O_2)`

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

## Parameters

`x`

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

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

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

Bases: *dicee.models.base\_model.BaseKGE*

Base class for all neural network modules.

Your models should also subclass this class.

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

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

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

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

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

### Note

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

### Variables

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

```
name = 'Keci'
```

```
p
```

```
q
```

```
r
```

```
requires_grad_for_interactions = True
```

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

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

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

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

```

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

```

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

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

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

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

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

Compute `sigma_qq = sum_{j=1}^{p+q-1} sum_{k=j+1}^{p+q} (h_j r_k - h_k r_j) e_j e_k` sigma\_qq captures the interactions between along q bases For instance, let q e\_1, e\_2, e\_3, we compute interactions between e\_1 e\_2, e\_1 e\_3 , and e\_2 e\_3 This can be implemented with a nested two for loops

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

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

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

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

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

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

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

**compute\_sigma\_pq(\*, hp, hq, rp, rq)**

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

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

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

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

`print(sigma_pq.shape)`

**apply\_coefficients(hp, hq, rp, rq)**

Multiplying a base vector with its scalar coefficient

**clifford\_multiplication(h0, hp, hq, r0, rp, rq)**

Compute our CL multiplication

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

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

`eq j`

`h r = sigma_0 + sigma_p + sigma_q + sigma_pp + sigma_qq + sigma_pq` where

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

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

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

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

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

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

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

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

### Parameter

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

#### returns

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

**forward\_k\_vs\_with\_explicit** (*x*: torch.Tensor)

**k\_vs\_all\_score** (*bpe\_head\_ent\_emb*, *bpe\_rel\_ent\_emb*, *E*)

**forward\_k\_vs\_all** (*x*: torch.Tensor)  $\rightarrow$  torch.FloatTensor

Kvsall training

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

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

**construct\_batch\_selected\_cl\_multivector** (*x*: torch.FloatTensor, *r*: int, *p*: int, *q*: int)  
 $\rightarrow$  tuple[torch.FloatTensor, torch.FloatTensor, torch.FloatTensor]

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

### Parameter

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

#### returns

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

**forward\_k\_vs\_sample** (*x*: torch.LongTensor, *target\_entity\_idx*: torch.LongTensor)  $\rightarrow$  torch.FloatTensor

### Parameter

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

*target\_entity\_idx*: torch.LongTensor with (n, k ) shape k denotes the selected number of examples.

#### rtype

torch.FloatTensor with (n, k) shape

```

score(h, r, t)
forward_triples(x: torch.Tensor) → torch.FloatTensor

```

## Parameter

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

### **rtype**

*torch.FloatTensor* with (n) shape

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

Bases: *Keci*

Without learning dimension scaling

```
name = 'CKeci'
```

```
requires_grad_for_interactions = False
```

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

Bases: *dicee.models.base\_model.BaseKGE*

Base class for all neural network modules.

Your models should also subclass this class.

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

```

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

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

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

```

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

### **Note**

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

## Variables

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

```
name = 'DeCaL'
```

```

entity_embeddings
relation_embeddings

p



q



r



re



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


```

### Parameter

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

#### **rtype**

*torch.FloatTensor* with (n) shape

**c1\_pqr** (*a*: *torch.tensor*) → *torch.tensor*

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

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

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

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

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

and return:

$$\sigma_0 t = \sigma_0 \cdot t_0 = s0 + s1 - s2s3, s4ands5$$

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

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

For same bases vectors interaction we have

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

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)

abstractmethod forward_k_vs_sample (x: torch.LongTensor, target_entity_idx)

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

Base class for all neural network modules.

Your models should also subclass this class.

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

```

```

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

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

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

```

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

### Note

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

### Variables

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

```

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

```

#### Parameters

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

```

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

    Parameters
    -----
    init_params_with_sanity_checking()

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

    Parameters
    • x
    • y_idx
    • ordered_bpe_entities

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

    Parameters
    x

    forward_k_vs_all(*args, **kwargs)

    forward_k_vs_sample(*args, **kwargs)

    get_triple_representation(idx_hrt)

    get_head_relation_representation(indexed_triple)

    get_sentence_representation(x: torch.LongTensor)

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

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

    Parameters
    x (B x 2 x T)

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

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

    Learning Knowledge Neural Graphs

    name = 'FMult'

    entity_embeddings

    relation_embeddings

    k

```

```

num_sample = 50
gamma
roots
weights

compute_func (weights: torch.FloatTensor, x) → torch.FloatTensor
chain_func (weights, x: torch.FloatTensor)
forward_triples (idx_triple: torch.Tensor) → torch.Tensor

Parameters
x

class dicee.models.GFMult (args)
Bases: dicee.models.base_model.BaseKGE
Learning Knowledge Neural Graphs
name = 'GFMult'

entity_embeddings
relation_embeddings

k
num_sample = 250
roots
weights

compute_func (weights: torch.FloatTensor, x) → torch.FloatTensor
chain_func (weights, x: torch.FloatTensor)
forward_triples (idx_triple: torch.Tensor) → torch.Tensor

Parameters
x

class dicee.models.FMult2 (args)
Bases: dicee.models.base_model.BaseKGE
Learning Knowledge Neural Graphs
name = 'FMult2'

n_layers = 3
k
n = 50
score_func = 'compositional'
discrete_points

```

```

entity_embeddings
relation_embeddings
build_func (Vec)
build_chain_funcs (list_Vec)
compute_func (W, b, x) → torch.FloatTensor
function (list_W, list_b)
trapezoid (list_W, list_b)
forward_triples (idx_triple: torch.Tensor) → torch.Tensor

```

**Parameters**

**x**

```
class dicee.models.LFMult1 (args)
```

Bases: *dicee.models.base\_model.BaseKGE*

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

```

name = 'LFMult1'

entity_embeddings
relation_embeddings
forward_triples (idx_triple)

```

**Parameters**

**x**

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

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

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

Bases: *dicee.models.base\_model.BaseKGE*

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

```

name = 'LFMult'

entity_embeddings
relation_embeddings
degree
m
x_values

```

```

forward_triples (idx_triple)

Parameters
    x

construct_multi_coeff (x)

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

linear (x, w, b)

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

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

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

comp_func ( $h, r, t$ )
    this part implement the function composition scoring techniques: i.e. score = <hor, t>

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

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

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

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

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

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

```

```

name = 'DualE'

entity_embeddings

relation_embeddings

num_ent = None

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

```

### **Input**

x: torch.LongTensor with (n, ) shape

### **Output**

torch.FloatTensor with (n) shape

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

Negative Sampling forward pass:

### **Input**

x: torch.LongTensor with (n, ) shape

### **Output**

torch.FloatTensor with (n) shape

```
forward_k_vs_all(x)
```

KvsAll forward pass

### **Input**

x: torch.LongTensor with (n, ) shape

### **Output**

torch.FloatTensor with (n) shape

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

Transpose function

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

## **dicee.query\_generator**

### **Classes**

---

*QueryGenerator*

---

## Module Contents

```
class dicee.query_generator.QueryGenerator (train_path: str, val_path: str, test_path: str,
    ent2id: Dict = None, rel2id: Dict = None, seed: int = 1, gen_valid: bool = False,
    gen_test: bool = True)

    train_path
    val_path
    test_path
    gen_valid = False
    gen_test = True
    seed = 1
    max_ans_num = 1000000.0
    mode
    ent2id = None
    rel2id: Dict = None
    ent_in: Dict
    ent_out: Dict
    query_name_to_struct
    list2tuple (list_data)
    tuple2list (x: List | Tuple) → List | Tuple
        Convert a nested tuple to a nested list.
    set_global_seed (seed: int)
        Set seed
    construct_graph (paths: List[str]) → Tuple[Dict, Dict]
        Construct graph from triples Returns dicts with incoming and outgoing edges
    fill_query (query_structure: List[str | List], ent_in: Dict, ent_out: Dict, answer: int) → bool
        Private method for fill_query logic.
    achieve_answer (query: List[str | List], ent_in: Dict, ent_out: Dict) → set
        Private method for achieve_answer logic. @TODO: Document the code
    write_links (ent_out, small_ent_out)
    ground_queries (query_structure: List[str | List], ent_in: Dict, ent_out: Dict, small_ent_in: Dict,
        small_ent_out: Dict, gen_num: int, query_name: str)
        Generating queries and achieving answers
    unmap (query_type, queries, tp_answers, fp_answers, fn_answers)
    unmap_query (query_structure, query, id2ent, id2rel)
```

```

generate_queries (query_struct: List, gen_num: int, query_type: str)
    Passing incoming and outgoing edges to ground queries depending on mode [train valid or text] and getting
    queries and answers in return @ TODO: create a class for each single query struct

save_queries (query_type: str, gen_num: int, save_path: str)

abstractmethod load_queries (path)

get_queries (query_type: str, gen_num: int)

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

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

```

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

### Submodules

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

### Classes

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

### Module Contents

```

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

    kg

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

```

### Parameter

<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)	Add reciprocal triples if conditions are met
<code>timeit</code> (func)	
<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

<i>PreprocessKG</i>	Preprocess the data in memory
<i>LoadSaveToDisk</i>	
<i>ReadFromDisk</i>	Read the data from disk into memory

### Package Contents

```

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

    kg

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

```

#### Parameter

<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)

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

---

<b>is_sparql_endpoint_alive([sparql_endpoint])</b>	
<b>validate_knowledge_graph(args)</b>	Validating the source of knowledge graph
<b>sanity_checking_with_arguments(args)</b>	
<b>sanity_check_callback_args(args)</b>	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_server.root()

async dicee.scripts.index_server.search_embeddings(q: str)

async dicee.scripts.index_server.retrieve_embeddings(q: str)

class dicee.scripts.index_server.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

<code>MODEL_REGISTRY</code>
-----------------------------

### Functions

<code>create_reciprocal_triples(→ pandas.DataFrame)</code>	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.

continues on next page

Table 55 – continued from previous page

<code>get_ee_vocab</code> (→ Dict[Tuple[int, int], List[int]])	Build entity-entity to relation vocabulary.
<code>timeit</code> (→ Callable)	Decorator to measure and print execution time and memory usage.
<code>save_pickle</code> (→ None)	Save data to a pickle file.
<code>load_pickle</code> (→ object)	Load data from a pickle file.
<code>load_term_mapping</code> (→ Union[dict, pandas.DataFrame])	Load term-to-index mapping from pickle or CSV file.
<code>select_model</code> (args[, is_continual_training, storage_path])	
<code>load_model</code> (→ Tuple[object, Tuple[dict, dict]])	Load weights and initialize pytorch module from namespace arguments
<code>load_model_ensemble</code> (...)	Construct Ensemble Of weights and initialize pytorch module from namespace arguments
<code>save_numpy_ndarray</code> (* , data, file_path)	
<code>numpy_data_type_changer</code> (→ numpy.ndarray)	Detect most efficient data type for a given triples
<code>save_checkpoint_model</code> (→ None)	Store Pytorch model into disk
<code>store</code> (→ None)	
<code>add_noisy_triples</code> (→ pandas.DataFrame)	Add randomly constructed triples
<code>read_or_load_kg</code> (args, cls)	
<code>initialize_model</code> (...)	Initialize a knowledge graph embedding model.
<code>load_json</code> (→ Dict)	Load JSON file into a dictionary.
<code>save_embeddings</code> (→ None)	Save embeddings to a CSV file.
<code>vocab_to_parquet</code> (vocab_to_idx, name, ...)	
<code>create_experiment_folder</code> (→ str)	Create a timestamped experiment folder.
<code>continual_training_setup_executor</code> (→ None)	
<code>exponential_function</code> (→ torch.FloatTensor)	
<code>load_numpy</code> (→ numpy.ndarray)	
<code>evaluate</code> (entity_to_idx, scores, easy_answers, hard_answers)	# @TODO: CD: Renamed this function
<code>download_file</code> (url[, destination_folder])	
<code>download_files_from_url</code> (→ None)	
<code>download_pretrained_model</code> (→ str)	
<code>write_csv_from_model_parallel</code> (path)	Create
<code>from_pretrained_model_write_embeddings_int</code> (None)	

## Module Contents

```
dicee.static_funcs.MODEL_REGISTRY: Dict[str, Tuple[Type, str]]  
  
dicee.static_funcs.create_reciprocal_triples(df: pandas.DataFrame) → pandas.DataFrame  
Add inverse triples to a DataFrame.  
For each triple (s, p, o), creates an inverse triple (o, p_inverse, s).
```

### Parameters

`df` – DataFrame with ‘subject’, ‘relation’, and ‘object’ columns.

### Returns

DataFrame with original and inverse triples concatenated.

```
dicee.static_funcs.get_er_vocab(data: numpy.ndarray, file_path: str | None = None)  
→ Dict[Tuple[int, int], List[int]]
```

Build entity-relation to tail vocabulary.

### Parameters

- **data** – Array of triples with shape (n, 3) where columns are (head, relation, tail).
- **file\_path** – Optional path to save the vocabulary as pickle.

### Returns

Dictionary mapping (head, relation) pairs to list of tail entities.

```
dicee.static_funcs.get_re_vocab(data: numpy.ndarray, file_path: str | None = None)
    → Dict[Tuple[int, int], List[int]]
```

Build relation-entity (tail) to head vocabulary.

### Parameters

- **data** – Array of triples with shape (n, 3) where columns are (head, relation, tail).
- **file\_path** – Optional path to save the vocabulary as pickle.

### Returns

Dictionary mapping (relation, tail) pairs to list of head entities.

```
dicee.static_funcs.get_ee_vocab(data: numpy.ndarray, file_path: str | None = None)
    → Dict[Tuple[int, int], List[int]]
```

Build entity-entity to relation vocabulary.

### Parameters

- **data** – Array of triples with shape (n, 3) where columns are (head, relation, tail).
- **file\_path** – Optional path to save the vocabulary as pickle.

### Returns

Dictionary mapping (head, tail) pairs to list of relations.

```
dicee.static_funcs.timeit(func: Callable) → Callable
```

Decorator to measure and print execution time and memory usage.

### Parameters

**func** – Function to be timed.

### Returns

Wrapped function that prints timing information.

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

Save data to a pickle file.

Note: Consider using more portable formats (JSON, Parquet) for new code.

### Parameters

- **data** – Object to serialize. If None, nothing is saved.
- **file\_path** – Path where the pickle file will be saved.

```
dicee.static_funcs.load_pickle(file_path: str) → object
```

Load data from a pickle file.

Note: Consider using more portable formats (JSON, Parquet) for new code.

### Parameters

**file\_path** – Path to the pickle file.

### Returns

Deserialized object from the pickle file.

```
dicee.static_funcs.load_term_mapping(file_path: str) → dict | polars.DataFrame
```

Load term-to-index mapping from pickle or CSV file.

Attempts to load from pickle first, falls back to CSV if not found.

#### Parameters

**file\_path** – Base path without extension.

#### Returns

Dictionary or Polars DataFrame containing the mapping.

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

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

Load weights and initialize pytorch module from namespace arguments

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

Construct Ensemble Of weights and initialize pytorch module from namespace arguments

- (1) Detect models under given path
- (2) Accumulate parameters of detected models
- (3) Normalize parameters
- (4) Insert (3) into model.

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

```
dicee.static_funcs.numpy_data_type_changer(train_set: numpy.ndarray, num: int)  
→ numpy.ndarray
```

Detect most efficient data type for a given triples :param train\_set: :param num: :return:

```
dicee.static_funcs.save_checkpoint_model(model, path: str) → None
```

Store Pytorch model into disk

```
dicee.static_funcs.store(trained_model, model_name: str = 'model', full_storage_path: str = None,  
                        save_embeddings_as_csv=False) → None
```

```
dicee.static_funcs.add_noisy_triples(train_set: pandas.DataFrame, add_noise_rate: float)  
→ pandas.DataFrame
```

Add randomly constructed triples :param train\_set: :param add\_noise\_rate: :return:

```
dicee.static_funcs.read_or_load_kg(args, cls)
```

```
dicee.static_funcs.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 = 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

---

`enable_log`

---

### Functions

---

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

---

### Module Contents

```
dicee.static_preprocess_funcs.enable_log = False
```

```
dicee.static_preprocess_funcs.timeit(func)
```

```
dicee.static_preprocess_funcs.preprocesses_input_args(args)
```

Sanity Checking in input arguments

```
dicee.static_preprocess_funcs.create_constraints(triples: numpy.ndarray)  
→ Tuple[dict, dict, dict, dict]
```

(1) Extract domains and ranges of relations

(2) Store a mapping from relations to entities that are outside of the domain and range. Create constraints entities based on the range of relations :param triples: :return:

```
dicee.static_preprocess_funcs.get_er_vocab(data)
```

```
dicee.static_preprocess_funcs.get_re_vocab(data)
```

```
dicee.static_preprocess_funcs.get_ee_vocab(data)
```

```
dicee.static_preprocess_funcs.mapping_from_first_two_cols_to_third(train_set_idx)
```

## dicee.trainer

### Submodules

#### dicee.trainer.dice\_trainer

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

#### DICE\_Trainer

DICE\_Trainer implement

### Functions

```
load_term_mapping(→ polars.DataFrame)
```

Load term-to-index mapping from CSV file.

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

Initialize the appropriate trainer based on configuration.

```
get_callbacks(→ 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

---

*TorchDDPTrainer*  
*NodeTrainer*

---

A Trainer based on torch.nn.parallel.DistributedDataParallel

### Functions

---

*make\_iterable\_verbose*(→ Iterable)

---

### Module Contents

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

```

class dicee.trainer.torch_trainer_ddp.TorchDDPTrainer(args, callbacks)
Bases: dicee.abstracts.AbstractTrainer

A Trainer based on torch.nn.parallel.DistributedDataParallel

Arguments

entity_idxs
    mapping.

relation_idxs
    mapping.

form
    ?

store
    ?

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

Return type
    torch.utils.data.Dataset

fit(*args, **kwargs)
    Train model

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

trainer
local_rank
global_rank
optimizer
train_dataset_loader
loss_func
callbacks
model
num_epochs

loss_history = []

ctx
scaler
extract_input_outputs(z: list)
train()
    Training loop for DDP

```

## Classes

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: #  $\theta_{\text{swa}} \leftarrow (1 - \alpha) * \theta_{\text{swa}} + \alpha * \theta_1$  #  $\alpha = 1 / (n + 1)$ , 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 (sq_mean - mean2) # - D = [dev_1, dev_2, ..., dev_K], deviations from mean (low-rank approx) # - K = number of collected models

    # Sampling step: # 1. theta_diag = mean + scale * std  $\odot \epsilon$ , where  $\epsilon \sim N(0, I)$  # 2. theta_lowrank = theta_diag + (D z) / sqrt(K-1), where z ~  $N(0, I_K)$  # Final sample = theta_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: #  $\theta_{\text{ema}} \leftarrow (1 - \alpha) * \theta_{\text{ema}} + \alpha * \theta$  #  $\alpha = 1 - \text{decay}$ , 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:  $w_{twa} = mean_w + P * beta$  #  $mean_w = (1/n) * \sum_i w_i$  (SWA baseline)
    #  $beta \leftarrow (1 - \eta * \lambda) * beta - \eta * P^T * g$  #  $g$  = 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

---

*Execute*

---

Executor class for training, retraining and evaluating KGE models.

---

continues on next page

Table 69 – continued from previous page

<i>KGE</i>	Knowledge Graph Embedding Class for interactive usage of pre-trained models
<i>QueryGenerator</i>	
<i>DICE_Trainer</i>	DICE_Trainer implement
<i>Evaluator</i>	Evaluator class for KGE models in various downstream tasks.

## 14.4 Package Contents

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

Executor class for training, retraining and evaluating KGE models.

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

**args**

Processed input arguments.

**distributed**

Whether distributed training is enabled.

**rank**

Process rank in distributed training.

**world\_size**

Total number of processes.

**local\_rank**

Local GPU rank.

**trainer**

Training handler instance.

**trained\_model**

The trained model after training completes.

**knowledge\_graph**

The loaded knowledge graph.

**report**

Dictionary storing training metrics and results.

**evaluator**

Model evaluation handler.

**distributed**

**args**

**is\_continual\_training** = *False*

**trainer**: *dicee.trainer.DICE\_Trainer* | *None* = *None*

**trained\_model** = *None*

**knowledge\_graph**: *dicee.knowledge\_graph.KG* | *None* = *None*

```

report: Dict
evaluator: dicee.evaluator.Evaluator | None = None
start_time: float | None = None
is_rank_zero() → bool
cleanup()
setup_executor() → None
    Set up storage directories for the experiment.
    Creates or reuses experiment directories based on configuration. Saves the configuration to a JSON file.
create_and_store_kg() → None
    Create knowledge graph and store as memory-mapped file.
    Only executed on rank 0 in distributed training. Skips if memmap already exists.
load_from_memmap() → None
    Load knowledge graph from memory-mapped file.
save_trained_model() → None
    Save a knowledge graph embedding model
    (1) Send model to eval mode and cpu.
    (2) Store the memory footprint of the model.
    (3) Save the model into disk.
    (4) Update the stats of KG again ?

```

## Parameter

### **rtype**

None

```

end(form_of_labelling: str) → dict
    End training
    (1) Store trained model.
    (2) Report runtimes.
    (3) Eval model if required.

```

## Parameter

### **rtype**

A dict containing information about the training and/or evaluation

```

write_report() → None
    Report training related information in a report.json file
start() → dict
    Start training
    # (1) Loading the Data # (2) Create an evaluator object. # (3) Create a trainer object. # (4) Start the training

```

## Parameter

### rtype

A dict containing information about the training and/or evaluation

```
class dicee.KGE(path=None, url=None, construct_ensemble=False, model_name=None)
Bases: dicee.abstracts.BaseInteractiveKGE, dicee.abstracts.
InteractiveQueryDecomposition, dicee.abstracts.BaseInteractiveTrainKGE
Knowledge Graph Embedding Class for interactive usage of pre-trained models
__str__()
to(device: str) → None
get_transductive_entity_embeddings(indices: torch.LongTensor | List[str], as_pytorch=False,
as_numpy=False, as_list=True) → torch.FloatTensor | numpy.ndarray | List[float]
create_vector_database(collection_name: str, distance: str, location: str = 'localhost',
port: int = 6333)
generate(h='', r='')
eval_lp_performance(dataset=List[Tuple[str, str, str]], filtered=True)
predict_missing_head_entity(relation: List[str] | str, tail_entity: List[str] | str, within=None,
batch_size=2, topk=1, return_indices=False) → Tuple
Given a relation and a tail entity, return top k ranked head entity.
argmax_{e in E} f(e,r,t), where r in R, t in E.
```

## Parameter

relation: Union[List[str], str]

String representation of selected relations.

tail\_entity: Union[List[str], str]

String representation of selected entities.

k: int

Highest ranked k entities.

## Returns: Tuple

Highest K scores and entities

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

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

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

## Parameter

head\_entity: List[str]

String representation of selected entities.

tail\_entity: List[str]

String representation of selected entities.

k: int

Highest ranked k entities.

### Returns: Tuple

Highest K scores and entities

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

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

argmax\_{e in E} f(h,r,e), where h in E and r in R.

### Parameter

head\_entity: List[str]

String representation of selected entities.

tail\_entity: List[str]

String representation of selected entities.

### Returns: Tuple

scores

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

### Parameters

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

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

Predict missing item in a given triple.

### Returns

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

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

Predict triple score

## Parameter

head\_entity: List[str]  
String representation of selected entities.  
relation: List[str]  
String representation of selected relations.  
tail\_entity: List[str]  
String representation of selected entities.  
logits: bool  
If logits is True, unnormalized score returned

## Returns: Tuple

pytorch tensor of triple score

```
return_multi_hop_query_results(aggregated_query_for_all_entities, k: int, only_scores)
single_hop_query_answering(query: tuple, only_scores: bool = True, k: int = None)
answer_multi_hop_query(query_type: str = None, query: Tuple[str | Tuple[str, str], Ellipsis] = None,
queries: List[Tuple[str | Tuple[str, str], Ellipsis]] = None, tnorm: str = 'prod',
neg_norm: str = 'standard', lambda_: float = 0.0, k: int = 10, only_scores=False)
→ List[Tuple[str, torch.Tensor]]
# @TODO: Refactoring is needed # @TODO: Score computation for each query type should be done in a static function
```

Find an answer set for EPFO queries including negation and disjunction

## Parameter

query\_type: str The type of the query, e.g., “2p”.  
query: Union[str, Tuple[str, Tuple[str, Tuple[str, str]]]] The query itself, either a string or a nested tuple.  
queries: List of Tuple[Union[str, Tuple[str, str]], ...]  
tnorm: str The t-norm operator.  
neg\_norm: str The negation norm.  
**lambda\_**: float lambda parameter for sugeno and yager negation norms  
k: int The top-k substitutions for intermediate variables.

## returns

- *List[Tuple[str, torch.Tensor]]*
- *Entities and corresponding scores sorted in the descening order of scores*

```
find_missing_triples(confidence: float, entities: List[str] = None, relations: List[str] = None,
topk: int = 10, at_most: int = sys.maxsize) → Set
```

Find missing triples

Iterative over a set of entities E and a set of relation R :

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

Return (e,r,x)  
 otin G and f(e,r,x) > confidence  
 confidence: float  
 A threshold for an output of a sigmoid function given a triple.  
 topk: int  
 Highest ranked k item to select triples with f(e,r,x) > confidence .  
 at\_most: int  
 Stop after finding at\_most missing triples  
 $\{(e,r,x) \mid f(e,r,x) > \text{confidence}\}$  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*

```
class dicee.QueryGenerator(train_path, val_path: str, test_path: str, ent2id: Dict = None,
                           rel2id: Dict = None, seed: int = 1, gen_valid: bool = False, gen_test: bool = True)

  train_path
  val_path
  test_path
  gen_valid = False
  gen_test = True
  seed = 1
  max_ans_num = 1000000.0
  mode
  ent2id = None
  rel2id: Dict = None
  ent_in: Dict
```

```

ent_out: Dict
query_name_to_struct
list2tuple(list_data)
tuple2list(x: List | Tuple) → List | Tuple
    Convert a nested tuple to a nested list.

set_global_seed(seed: int)
    Set seed

construct_graph(paths: List[str]) → Tuple[Dict, Dict]
    Construct graph from triples Returns dicts with incoming and outgoing edges

fill_query(query_structure: List[str | List], ent_in: Dict, ent_out: Dict, answer: int) → bool
    Private method for fill_query logic.

achieve_answer(query: List[str | List], ent_in: Dict, ent_out: Dict) → set
    Private method for achieve_answer logic. @TODO: Document the code

write_links(ent_out, small_ent_out)

ground_queries(query_structure: List[str | List], ent_in: Dict, ent_out: Dict, small_ent_in: Dict,
    small_ent_out: Dict, gen_num: int, query_name: str)
    Generating queries and achieving answers

unmap(query_type, queries, tp_answers, fp_answers, fn_answers)

unmap_query(query_structure, query, id2ent, id2rel)

generate_queries(query_struct: List, gen_num: int, query_type: str)
    Passing incoming and outgoing edges to ground queries depending on mode [train valid or text] and getting
    queries and answers in return @ TODO: create a class for each single query struct

save_queries(query_type: str, gen_num: int, save_path: str)

abstractmethod load_queries(path)

get_queries(query_type: str, gen_num: int)

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

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

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

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

    args
    is_continual_training:bool
    storage_path:str

```

```

evaluator:
report:dict

report

args

trainer = None

is_continual_training

storage_path

evaluator = None

form_of_labelling = None

continual_start (knowledge_graph)

```

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

### Parameter

#### **returns**

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

```

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

```

```
initialize_or_load_model ()
```

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

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

```

start (knowledge_graph: dicee.knowledge_graph.KG | numpy.memmap)
    → Tuple[dicee.models.base_model.BaseKGE, str]

```

Start the training

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

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

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

Perform K-fold Cross-Validation

1. Obtain K train and test splits.

2. **For each split,**

2.1 initialize trainer and model 2.2. Train model with configuration provided in args. 2.3. Compute the mean reciprocal rank (MRR) score of the model on the test respective split.

3. Report the mean and average MRR .

#### Parameters

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

#### Returns

model

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

Evaluator class for KGE models in various downstream tasks.

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

##### **er\_vocab**

Entity-relation to tail vocabulary for filtered ranking.

##### **re\_vocab**

Relation-entity (tail) to head vocabulary.

##### **ee\_vocab**

Entity-entity to relation vocabulary.

##### **num\_entities**

Total number of entities in the knowledge graph.

##### **num\_relations**

Total number of relations in the knowledge graph.

##### **args**

Configuration arguments.

##### **report**

Dictionary storing evaluation results.

##### **during\_training**

Whether evaluation is happening during training.

### Example

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

```
re_vocab: Dict | None = None
er_vocab: Dict | None = None
ee_vocab: Dict | None = None
func_triple_to_bpe_representation = None
is_continual_training = False
```

```

num_entities: int | None = None
num_relations: int | None = None
domain_constraints_per_rel = None
range_constraints_per_rel = None
args
report: Dict
during_training = False
vocab_preparation(dataset) → None
    Prepare vocabularies from the dataset for evaluation.
    Resolves any future objects and saves vocabularies to disk.

Parameters
dataset – Knowledge graph dataset with vocabulary attributes.

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

Parameters

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

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

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

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

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

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

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

evaluate_lp_k_vs_all(model, triple_idx, info: str | None = None,
form_of_labelling: str | None = None) → Dict[str, float]
Filtered link prediction evaluation with KvsAll scoring.

Parameters

```

- **model** – The trained model to evaluate.
- **triple\_idx** – Integer-indexed test triples.
- **info** – Description to print.
- **form\_of\_labelling** – ‘EntityPrediction’ or ‘RelationPrediction’.

#### Returns

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

**evaluate\_lp\_with\_bytE** (*model*, *triples*: *List[List[str]]*, *info*: *str* | *None* = *None*) → *Dict[str, float]*

Evaluate BytE model with text generation.

#### Parameters

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

#### Returns

Dictionary with placeholder metrics (-1 values).

**evaluate\_lp\_bpe\_k\_vs\_all** (*model*, *triples*: *List[List[str]]*, *info*: *str* | *None* = *None*, *form\_of\_labelling*: *str* | *None* = *None*) → *Dict[str, float]*

Evaluate BPE model with KvsAll scoring.

#### Parameters

- **model** – BPE-enabled model.
- **triples** – String triples.
- **info** – Description to print.
- **form\_of\_labelling** – Type of labelling.

#### Returns

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

**evaluate\_lp** (*model*, *triple\_idx*, *info*: *str*) → *Dict[str, float]*

Evaluate link prediction with negative sampling.

#### Parameters

- **model** – The model to evaluate.
- **triple\_idx** – Integer-indexed triples.
- **info** – Description to print.

#### Returns

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

**dummy\_eval** (*trained\_model*, *form\_of\_labelling*: *str*) → *None*

Run evaluation from saved data (for continual training).

#### Parameters

- **trained\_model** – The trained model.
- **form\_of\_labelling** – Type of labelling.

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

Evaluate a trained model on a given dataset.

#### Parameters

- **dataset** – Knowledge graph dataset.
- **trained\_model** – The trained model.
- **triple\_idx** – Integer-indexed triples to evaluate.
- **form\_of\_labelling** – Type of labelling.

#### Returns

Dictionary with evaluation metrics.

#### Raises

**ValueError** – If scoring technique is invalid.

```
dicee.__version__ = '0.3.2'
```

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