
DICE Embeddings

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Contents:

| | |
|--|------------|
| 1 Dicee Manual | 2 |
| 2 Installation | 3 |
| 2.1 Installation from Source | 3 |
| 3 Download Knowledge Graphs | 3 |
| 4 Knowledge Graph Embedding Models | 3 |
| 5 How to Train | 3 |
| 6 Creating an Embedding Vector Database | 5 |
| 6.1 Learning Embeddings | 5 |
| 6.2 Loading Embeddings into Qdrant Vector Database | 6 |
| 6.3 Launching Webservice | 6 |
| 7 Answering Complex Queries | 6 |
| 8 Predicting Missing Links | 8 |
| 9 Downloading Pretrained Models | 8 |
| 10 How to Deploy | 8 |
| 11 Docker | 8 |
| 12 Coverage Report | 8 |
| 13 How to cite | 10 |
| 14 dicee | 12 |
| 14.1 Submodules | 12 |
| 14.2 Attributes | 183 |
| 14.3 Classes | 184 |
| 14.4 Functions | 185 |
| 14.5 Package Contents | 186 |
| Python Module Index | 232 |

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

1 Dicee Manual

Version: dicee 0.2.0

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

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

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

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

1. **Pandas³ & Co.** to use parallelism at preprocessing a large knowledge graph,
2. **PyTorch⁴ & Co.** to learn knowledge graph embeddings via multi-CPUs, GPUs, TPUs or computing cluster, and
3. **Huggingface⁵** to ease the deployment of pre-trained models.

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

Why PyTorch⁷ & Co. ? PyTorch is one of the most popular machine learning frameworks available at the time of writing. PytorchLightning facilitates scaling the training procedure of PyTorch without boilerplate. In our framework, we combine PyTorch⁸ & PytorchLightning⁹. Users can choose the trainer class (e.g., DDP by Pytorch) to train large knowledge graph embedding models with billions of parameters. PytorchLightning allows us to use state-of-the-art model parallelism techniques (e.g. Fully Sharded Training, FairScale, or DeepSpeed) without extra effort. With our framework, practitioners can directly use PytorchLightning for model parallelism to train gigantic embedding models.

Why Hugging-face Gradio¹⁰? Deploy a pre-trained embedding model without writing a single line of code.

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

² <https://github.com/Demirrr>

³ <https://pandas.pydata.org/>

⁴ <https://pytorch.org/>

⁵ <https://huggingface.co/>

⁶ <https://pandas.pydata.org/>

⁷ <https://pytorch.org/>

⁸ <https://pytorch.org/>

⁹ <https://www.pytorchlightning.ai/>

¹⁰ <https://huggingface.co/gradio>

2 Installation

2.1 Installation from Source

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

or

```
pip install dicee
```

3 Download Knowledge Graphs

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

To test the Installation

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

4 Knowledge Graph Embedding Models

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

For more, please refer to examples.

5 How to Train

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

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

where the data is in the following form

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

A KGE model can also be trained from the command line

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

dicee automatically detects available GPUs and trains a model with distributed data 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/¹¹

10 How to Deploy

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

11 Docker

To build the Docker image:

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

To test the Docker image:

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

12 Coverage Report

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

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

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

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

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| | | | | |
|---|------------------|------------------|-------------------|---|
| <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 Moussalle, Diego and Ngomo, Axel-Cyrille Ngonga},
  booktitle={2021 IEEE 15th International Conference on Semantic Computing (ICSC)},
  pages={179--182},
  year={2021},
  organization={IEEE}
```

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

14 dicee

14.1 Submodules

dicee.__main__

dicee.abstracts

Classes

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

Module Contents

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

Abstract class for Trainer class for knowledge graph embedding models

Parameter

args
[str] ?

callbacks: list
?

```
attributes  
callbacks  
is_global_zero = True  
global_rank = 0  
local_rank = 0  
strategy = None  
on_fit_start(*args, **kwargs)
```

A function to call callbacks before the training starts.

Parameter

args

kwargs

rtype

None

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

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

Parameter

args

kwargs

rtype

None

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

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

Parameter

args

kwargs

rtype

None

```
on_train_epoch_end(*args, **kwargs)
```

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

Parameter

args

kwargs

rtype

None

```
on_train_batch_end(*args, **kwargs)
```

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

Parameter

args

kwargs

rtype

None

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

A static function to save a model into disk

Parameter

full_path : str

model:

rtype

None

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

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

Parameter

```
path_of_pretrained_model_dir  
[str] ?
```

```
construct_ensemble: boolean  
?
```

model_name: str apply_semantic_constraint : boolean

```
construct_ensemble = False
```

```
apply_semantic_constraint = False
```

configs

```
get_eval_report() → dict
```

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

Parameters

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

Return type

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

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

Parameters

triples

set_model_train_mode() → None
Setting the model into training mode

Parameter

set_model_eval_mode() → None
Setting the model into eval mode

Parameter

property name
sample_entity(n: int) → List[str]
sample_relation(n: int) → List[str]
is_seen(entity: str = None, relation: str = None) → bool
save() → None
get_entity_index(x: str)
get_relation_index(x: str)
index_triple(head_entity: List[str], relation: List[str], tail_entity: List[str])
→ Tuple[torch.LongTensor, torch.LongTensor, torch.LongTensor]
Index Triple

Parameter

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

Returns: Tuple

pytorch tensor of triple score

add_new_entity_embeddings(entity_name: str = None, embeddings: torch.FloatTensor = None)
get_entity_embeddings(items: List[str])
Return embedding of an entity given its string representation

Parameter

items:
entities

get_relation_embeddings(items: List[str])
Return embedding of a relation given its string representation

Parameter

items:

relations

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

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

parameters ()

class dicee.abstracts.**InteractiveQueryDecomposition**

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

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

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

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

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

class dicee.abstracts.**AbstractCallback**

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

Abstract class for Callback class for knowledge graph embedding models

Parameter

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

Parameter

trainer:

model:

rtype

None

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

Call at the beginning of the training.

Parameter

trainer:

model:

rtype

None

on_fit_start (*trainer*, *model*)

Call at the beginning of the training.

Parameter

trainer:

model:

rtype

None

on_train_epoch_end(*trainer, model*)

Call at the end of each epoch during training.

Parameter

trainer:

model:

rtype

None

on_train_batch_end(**args, **kwargs*)

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

Parameter

trainer:

model:

rtype

None

on_fit_end(**args, **kwargs*)

Call at the end of the training.

Parameter

trainer:

model:

rtype

None

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

Bases: *AbstractCallback*

Abstract class for Callback class for knowledge graph embedding models

Parameter

num_epochs

path

sample_counter = 0

```

epoch_count = 0
alphas = None

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

```

Parameter

trainer:

model:

rtype

None

```

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

```

Parameter

trainer:

model:

rtype

None

```
store_ensemble(param_ensemble) → None
```

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

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

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

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

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

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

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

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

Trains the Literal Embeddings model using literal data.

Parameters

- **train_file_path** (*str*) – Path to the training data file.
- **num_epochs** (*int*) – Number of training epochs.
- **lit_lr** (*float*) – Learning rate for the literal model.
- **norm_type** (*str*) – Normalization type to use ('z-norm', 'min-max', or None).
- **batch_size** (*int*) – Batch size for training.
- **sampling_ratio** (*float*) – Ratio of training triples to use.

- **loader_backend** (*str*) – Backend for loading the dataset ('pandas' or 'rdflib').
- **freeze_entity_embeddings** (*bool*) – If True, freeze the entity embeddings during training.
- **gate_residual** (*bool*) – If True, use gate residual connections in the model.
- **device** (*str*) – Device to use for training ('cuda' or 'cpu'). If None, will use available GPU or CPU.
- **shuffle_data** (*bool*) – If True, shuffle the dataset before training.

dicee.analyse_experiments

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

Classes

Experiment

Functions

get_default_arguments()
analyse(args)

Module Contents

```
dicee.analyse_experiments.get_default_arguments()

class dicee.analyse_experiments.Experiment

    model_name = []
    callbacks = []
    embedding_dim = []
    num_params = []
    num_epochs = []
    batch_size = []
    lr = []
    byte_pair_encoding = []
    aswa = []
    path_dataset_folder = []
```

```
full_storage_path = []

pq = []

train_mrr = []

train_h1 = []

train_h3 = []

train_h10 = []

val_mrr = []

val_h1 = []

val_h3 = []

val_h10 = []

test_mrr = []

test_h1 = []

test_h3 = []

test_h10 = []

runtime = []

normalization = []

scoring_technique = []

save_experiment(x)

to_df()

dicee.analyse_experiments.analyse(args)
```

dicee.callbacks

Classes

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

Functions

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

Module Contents

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

Bases: `dicee.abstracts.AbstractCallback`

Abstract class for Callback class for knowledge graph embedding models

Parameter

`path`

`on_fit_end(trainer, model) → None`

Store epoch loss

Parameter

trainer:

model:

`rtype`

None

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

Parameter

start_time

on_fit_start (*trainer, pl_module*)

Call at the beginning of the training.

Parameter

trainer:

model:

rtype

None

on_fit_end (*trainer, pl_module*)

Call at the end of the training.

Parameter

trainer:

model:

rtype

None

on_train_batch_end (**args, **kwargs*)

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

Parameter

trainer:

model:

rtype

None

on_train_epoch_end (**args, **kwargs*)

Call at the end of each epoch during training.

Parameter

trainer:

model:

rtype

None

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

Bases: *dicee.abstracts.AbstractCallback*

Abstract class for Callback class for knowledge graph embedding models

Parameter

every_x_epoch

max_epochs

epoch_counter = 0

path

on_train_batch_end(*args, **kwargs)

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

Parameter

trainer:

model:

rtype

None

on_fit_start(*trainer*, *pl_module*)

Call at the beginning of the training.

Parameter

trainer:

model:

rtype

None

on_train_epoch_end(*args, **kwargs)

Call at the end of each epoch during training.

Parameter

trainer:

model:

rtype

None

on_fit_end(*args, **kwargs)

Call at the end of the training.

Parameter

trainer:

model:

rtype

None

on_epoch_end(model, trainer, **kwargs)

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

Bases: dicee.abstracts.AbstractCallback

Abstract class for Callback class for knowledge graph embedding models

Parameter

data_module

kg

num_of_epochs = 0

unlabelled_size

batch_size

create_random_data()

on_epoch_end(trainer, model)

dicee.callbacks.estimate_q(eps)

estimate rate of convergence q from sequence esp

dicee.callbacks.compute_convergence(seq, i)

class dicee.callbacks.ASWA(num_epochs, path)

Bases: dicee.abstracts.AbstractCallback

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

path

num_epochs

initial_eval_setting = None

epoch_count = 0

alphas = []

val_aswa = -1

on_fit_end(trainer, model)

Call at the end of the training.

Parameter

trainer:

model:

rtype

None

```
static compute_mrr(trainer, model) → float  
  
get_aswa_state_dict(model)  
  
decide(running_model_state_dict, ensemble_state_dict, val_running_model,  
        mrr_updated_ensemble_model)
```

Perform Hard Update, software or rejection

Parameters

- running_model_state_dict
- ensemble_state_dict
- val_running_model
- mrr_updated_ensemble_model

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

Call at the end of each epoch during training.

Parameter

trainer:

model:

rtype

None

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

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

Abstract class for Callback class for knowledge graph embedding models

Parameter

path

reports = []

epoch_ratio = None

epoch_counter = 0

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

Call at the beginning of the training.

Parameter

trainer:

model:

rtype

None

on_fit_end(*trainer, model*)

Call at the end of the training.

Parameter

trainer:

model:

rtype

None

on_train_epoch_end(*trainer, model*)

Call at the end of each epoch during training.

Parameter

trainer:

model:

rtype

None

on_train_batch_end(*args, **kwargs)

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

Parameter

trainer:

model:

rtype

None

class dicee.callbacks.Krone

Bases: *dicee.abstracts.AbstractCallback*

Abstract class for Callback class for knowledge graph embedding models

Parameter

f = None

static batch_kronecker_product(*a, b*)

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

```

class dicee.callbacks.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 callbacks.

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.

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.

```

dicee.config

Classes

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

Module Contents

```

class dicee.config.Namespace(**kwargs)
Bases: argparse.Namespace

Simple object for storing attributes.

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

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

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

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

```

```

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

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

sparql_endpoint = None
    An endpoint of a triple store.

model: str = 'Keci'
    KGE model

optim: str = 'Adam'
    Optimizer

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

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

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

lr: float = 0.1
    Learning rate

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

gpus = None
    Number GPUs to be used during training

callbacks
    10}

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

        Type
            { "last_percent_to_consider"

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

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

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

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

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

weight_decay: float = 0.0
    Weight decay for all trainable params

```

```

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

init_param: str = None
    xavier_normal or None

gradient_accumulation_steps: int = 0
    Not tested e

num_folds_for_cv: int = 0
    Number of folds for CV

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

Type
    Evaluate trained model choices

save_model_at_every_epoch: int = None
    Not tested

label_smoothing_rate: float = 0.0

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

random_seed: int = 0
    Random Seed

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

read_only_few: int = None
    Read only first few triples

pykeen_model_kwargs
    Additional keyword arguments for pykeen models

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

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

p: int = 0
    P parameter of Clifford Embeddings

q: int = 1
    Q parameter of Clifford Embeddings

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

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

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

```

```

byte_pair_encoding: bool = False
    Byte pair encoding

    Type
        WIP

adaptive_swa: bool = False
    Adaptive stochastic weight averaging

swa: bool = False
    Stochastic weight averaging

block_size: int = None
    block size of LLM

continual_learning = None
    Path of a pretrained model size of LLM

auto_batch_finding = False
    A flag for using auto batch finding

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

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

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

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

adaptive_lr
    "cca"}'

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

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

__iter__()

dicee.dataset_classes

```

Classes

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

Functions

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

Module Contents

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

Reload the files from disk to construct the Pytorch dataset

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

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

Bases: torch.utils.data.Dataset

An abstract class representing a Dataset.

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

Note

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

```
train_set
ordered_bpe_entities
num_bpe_entities
neg_ratio
num_datapoints
__len__()
__getitem__(idx)
collate_fn(batch_shaped_bpe_triples: List[Tuple[torch.Tensor, torch.Tensor]])  

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

Bases: `torch.utils.data.Dataset`

An abstract class representing a `Dataset`.

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

Note

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

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

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

Bases: torch.utils.data.Dataset

Dataset for the 1vsALL training strategy

Parameters

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

Return type

torch.utils.data.Dataset

train_data

block_size = 8

num_of_data_points

collate_fn = None

__len__()

__getitem__(idx)

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

Bases: torch.utils.data.Dataset

Dataset for the 1vsALL training strategy

Parameters

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

Return type

torch.utils.data.Dataset

train_data

target_dim

collate_fn = None

__len__()

__getitem__(idx)

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

Bases: torch.utils.data.Dataset

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

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

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

Note

TODO

train_set_idx

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

entity_idxs

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

relation_idxs

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

self : torch.utils.data.Dataset

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

```
train_data = None
```

```
train_target = None
```

```
label_smoothing_rate
```

```
collate_fn = None
```

```
__len__()
```

```
__getitem__(idx)
```

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

Bases: torch.utils.data.Dataset

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

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

orall $y_i = 1$ s.t. $(h, r) \in E$ 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.CVDataModule(train_set_idx: numpy.ndarray, num_entities,
                                         num_relations, neg_sample_ratio, batch_size, num_workers)

```

Bases: pytorch_lightning.LightningDataModule

Create a Dataset for cross validation

Parameters

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

Return type

?

```

train_set_idx
num_entities
num_relations
neg_sample_ratio
batch_size
num_workers

```

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

An iterable or collection of iterables specifying training samples.

For more information about multiple dataloaders, see this section.

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

For data processing use the following pattern:

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

However, the above are only necessary for distributed processing.

⚠ Warning

do not assign state in `prepare_data`

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

ℹ Note

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

`setup(*args, **kwargs)`

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

Parameters

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

Example:

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

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

        # don't do this
        self.something = else

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

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

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

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

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

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

Note

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

Parameters

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

Returns

A reference to the data on the new device.

Example:

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

See also

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

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

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

⚠ Warning

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

Example:

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

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

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

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

Example:

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

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

This is called before requesting the dataloaders:

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

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

Bases: `torch.utils.data.Dataset`

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

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

`train_file_path`

Path to the training data file.

Type

str

`normalization`

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

Type

str

`normalization_params`

Parameters used for normalization.

Type

dict

`sampling_ratio`

Fraction of the training set to use for ablations.

Type

float

`entity_to_idx`

Mapping of entities to their indices.

Type

dict

`num_entities`

Total number of entities.

Type

int

`data_property_to_idx`

Mapping of data properties to their indices.

Type

dict

`num_data_properties`

Total number of data properties.

Type

int

`loader_backend`

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

Type

str

```

train_file_path
loader_backend = 'pandas'
normalization_type = 'z-norm'
normalization_params
sampling_ratio = None
entity_to_idx = None
num_entities
__getitem__(index)
__len__()

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

```

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

Returns

DataFrame containing the loaded and validated data.

Return type

pd.DataFrame

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

Denormalizes the predictions based on the normalization type.

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

Returns

Denormalized predictions.

Return type

np.ndarray

dicee.eval_static_funcs

Functions

| | |
|--|---|
| evaluate_link_prediction_performance(→ Dict) | |
| evaluate_link_prediction_performance_with_... | |
| evaluate_link_prediction_performance_with_j | |
| evaluate_link_prediction_performance_with_j ...) | |
| evaluate_lp_bpe_k_vs_all(model, triples[, er_vocab, ...]) | Evaluates the trained literal prediction model on a test file. |
| evaluate_literal_prediction(kge_model[, ...]) | Evaluates link prediction performance of an ensemble of KGE models. |
| evaluate_ensemble_link_prediction_performa... | |

Module Contents

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

Parameters

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

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

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

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

Parameters

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

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

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

Evaluates the trained literal prediction model on a test file.

Parameters

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

Returns

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

Return type

pd.DataFrame

Raises

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

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

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

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

Parameters

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

Returns

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

dicee.evaluator

Classes

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

Module Contents

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

Evaluator class to evaluate KGE models in various downstream tasks

Arguments

```
re_vocab = None  
er_vocab = None  
ee_vocab = None  
func_triple_to_bpe_representation = None  
is_continual_training = None  
num_entities = None  
num_relations = None  
args  
report
```

```

during_training = False
vocab_preparation(dataset) → None
    A function to wait future objects for the attributes of executor

Return type
    None

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

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

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

eval_with_byte(*raw_train_set, raw_valid_set=None, raw_test_set=None, trained_model,
    form_of_labelling) → None
    Evaluate model after reciprocal triples are added

eval_with_bpe_vs_all(*raw_train_set, raw_valid_set=None, raw_test_set=None, trained_model,
    form_of_labelling) → None
    Evaluate model after reciprocal triples are added

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

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

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

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

Parameters

- model
- triples (List of lists)
- info
- form_of_labelling

evaluate_lp(model, triple_idx, info: str)

dummy_eval(trained_model, form_of_labelling: str)

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

```

dicee.executer

Classes

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

Module Contents

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

A class for Training, Retraining and Evaluation a model.

(1) Loading & Preprocessing & Serializing input data.

(2) Training & Validation & Testing

(3) Storing all necessary info

distributed

args

```
is_continual_training = False
```

```
trainer = None
```

```
trained_model = None
```

```
knowledge_graph = None
```

report

```
evaluator = None
```

```
start_time = None
```

```
is_rank_zero() → bool
```

```
cleanup()
```

```
setup_executor() → None
```

```
create_and_store_kg()
```

```
load_from_memmap()
```

```
save_trained_model() → None
```

Save a knowledge graph embedding model

(1) Send model to eval mode and cpu.

(2) Store the memory footprint of the model.

(3) Save the model into disk.

(4) Update the stats of KG again ?

Parameter

rtype

None

```
end(form_of_labelling: str) → dict
```

End training

(1) Store trained model.

(2) Report runtimes.

(3) Eval model if required.

Parameter

rtype

A dict containing information about the training and/or evaluation

`write_report()` → None

Report training related information in a report.json file

`start()` → dict

Start training

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

Parameter

rtype

A dict containing information about the training and/or evaluation

`class dicee.executer.ContinuousExecute(args)`

Bases: `Execute`

A subclass of Execute Class for retraining

(1) Loading & Preprocessing & Serializing input data.

(2) Training & Validation & Testing

(3) Storing all necessary info

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

`continual_start()` → dict

Start Continual Training

(1) Initialize training.

(2) Start continual training.

(3) Save trained model.

Parameter

rtype

A dict containing information about the training and/or evaluation

`dicee.knowledge_graph`

Classes

| | |
|-----------------|-----------------|
| <code>KG</code> | Knowledge Graph |
|-----------------|-----------------|

Module Contents

```

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

Knowledge Graph

dataset_dir = None

sparql_endpoint = None

path_single_kg = None

byte_pair_encoding = False

ordered_shaped_bpe_tokens = None

add_noise_rate = None

num_entities = None

num_relations = None

path_for_deserialization = None

add_reciprocal = None

eval_model = None

read_only_few = None

sample_triples_ratio = None

path_for_serialization = None

entity_to_idx = None

relation_to_idx = None

backend = 'pandas'

training_technique = None

idx_entity_to_bpe_shaped

enc

num_tokens

num_bpe_entities = None

padding = False

dummy_id

max_length_subword_tokens = None

train_set_target = None

```

```

target_dim = None
train_target_indices = None
ordered_bpe_entities = None
separator = None
description_of_input = None
describe() → None
property entities_str: List
property relations_str: List
exists(h: str, r: str, t: str)
__iter__()
__len__()
func_triple_to_bpe_representation(triple: List[str])

```

dicee.knowledge_graph_embeddings

Classes

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

Module Contents

```

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

```

Parameter

relation: Union[List[str], str]

String representation of selected relations.

tail_entity: Union[List[str], str]

String representation of selected entities.

k: int

Highest ranked k entities.

Returns: Tuple

Highest K scores and entities

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

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

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

Parameter

head_entity: List[str]

String representation of selected entities.

tail_entity: List[str]

String representation of selected entities.

k: int

Highest ranked k entities.

Returns: Tuple

Highest K scores and entities

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

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

$\text{argmax}_{\{e \text{ in } E\}} f(h, r, e)$, 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]], ...]

t_norm: str The t-norm operator.

neg_norm: str The negation norm.

lambda_: float lambda parameter for sugeno and yager negation norms

k: int The top-k substitutions for intermediate variables.

returns

- *List[Tuple[str, torch.Tensor]]*

- *Entities and corresponding scores sorted in the descending order of scores*

find_missing_triples (confidence: float, entities: List[str] = None, relations: List[str] = None, topk: int = 10, at_most: int = sys.maxsize) → Set

Find missing triples

Iterative over a set of entities E and a set of relation R :

orall e in E and orall r in R f(e,r,x)

Return (e,r,x)

otin G and f(e,r,x) > confidence

confidence: float

A threshold for an output of a sigmoid function given a triple.

topk: int

Highest ranked k item to select triples with f(e,r,x) > confidence .

at_most: int

Stop after finding at_most missing triples

{(e,r,x) | f(e,r,x) > confidence land (e,r,x)}

otin G

deploy (share: bool = False, top_k: int = 10)

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

Predicts literal values for given entities and attributes.

Parameters

- **entity** (*Union[List[str], str]*) – Entity or list of entities to predict literals for.

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

Returns

Predictions for the given entities and attributes.

Return type

numpy ndarray

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

Module Contents

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

Bases: `torch.optim.optimizer.Optimizer`

ADOPT Optimizer.

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

The algorithm performs the following key operations: 1. Normalizes gradients by the square root of the second moment estimate 2. Applies optional gradient clipping based on the training step 3. Updates parameters using

momentum-smoothed normalized gradients 4. Supports decoupled weight decay (AdamW-style) or L2 regularization

Mathematical formulation:

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

$$v_t = \beta_2 * v_{t-1} + (1 - \beta_2) * g_t^2$$

$$\theta_t = \theta_{t-1} - \alpha * m_t$$

where:

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

Reference:

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

Parameters

- **params** (*ParamsT*) – Iterable of parameters to optimize or dicts defining parameter groups.
- **lr** (*float or Tensor, optional*) – Learning rate. Can be a float or 1-element Tensor. Default: 1e-3
- **betas** (*Tuple[float, float], optional*) – Coefficients (β_1, β_2) for computing running averages of gradient and its square. β_1 controls momentum, β_2 controls variance. Default: (0.9, 0.9999)
- **eps** (*float, optional*) – Term added to denominator to improve numerical stability. Default: 1e-6
- **clip_lambda** (*Callable[[int], float], optional*) – Function that takes the step number and returns the gradient clipping threshold. Common choices: - lambda step: $step^{**0.25}$ (default, gradually increases clipping threshold) - lambda step: 1.0 (constant clipping) - None (no clipping) Default: lambda step: $step^{**0.25}$
- **weight_decay** (*float, optional*) – Weight decay coefficient (L2 penalty). Default: 0.0
- **decouple** (*bool, optional*) – If True, uses decoupled weight decay (AdamW-style), applying weight decay directly to parameters. If False, adds weight decay to gradients (L2 regularization). Default: False
- **foreach** (*bool, optional*) – If True, uses the faster foreach implementation for multi-tensor operations. Default: None (auto-select)
- **maximize** (*bool, optional*) – If True, maximizes parameters instead of minimizing. Useful for reinforcement learning. Default: False
- **capturable** (*bool, optional*) – If True, the optimizer is safe to capture in a CUDA graph. Requires learning rate as Tensor. Default: False
- **differentiable** (*bool, optional*) – If True, the optimization step can be differentiated. Useful for meta-learning. Default: False
- **fused** (*bool, optional*) – If True, uses fused kernel implementation (currently not supported). Default: None

Raises

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

Example

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

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

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

Note

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

clip_lambda

__setstate__(state)

Restore optimizer state from a checkpoint.

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

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

Parameters

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

Note

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

`step` (*closure=None*)

Perform a single optimization step.

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

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

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

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

Parameters

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

Returns

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

Return type

`Optional[Tensor]`

Example

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

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

Note

- Call `zero_grad()` before computing gradients for the next step

- CUDA graph capture is checked for safety when capturable=True
- The method is thread-safe for different parameter groups

```
dicee.models.adopt( 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_t^2
```

where:

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

Automatic mode selection:

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

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

| | |
|-------------------------|--|
| <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. |

Module Contents

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

Bases: `lightning.LightningModule`

Base class for all neural network modules.

Your models should also subclass this class.

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

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

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

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

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

Note

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

Variables

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

`training_step_outputs` = []

`mem_of_model()` → Dict

Size of model in MB and number of params

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

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

Parameters

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

Returns

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

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

Example:

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

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

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

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

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

Note

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

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

Parameters

- `yhat_batch`

- `y_batch`

`on_train_epoch_end(*args, **kwargs)`

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

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

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

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

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

`test_epoch_end(outputs: List[Any])`

`test_dataloader() → None`

An iterable or collection of iterables specifying test samples.

For more information about multiple dataloaders, see this section.

For data processing use the following pattern:

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

However, the above are only necessary for distributed processing.

⚠ Warning

do not assign state in `prepare_data`

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

ℹ Note

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

Note

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

`val_dataloader() → None`

An iterable or collection of iterables specifying validation samples.

For more information about multiple dataloaders, see this section.

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

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

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

Note

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

Note

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

`predict_dataloader() → None`

An iterable or collection of iterables specifying prediction samples.

For more information about multiple dataloaders, see this section.

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

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

Note

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

Returns

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

`train_dataloader() → None`

An iterable or collection of iterables specifying training samples.

For more information about multiple dataloaders, see this section.

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

For data processing use the following pattern:

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

However, the above are only necessary for distributed processing.

Warning

do not assign state in `prepare_data`

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

Note

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

`configure_optimizers(parameters=None)`

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

Returns

Any of these 6 options.

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

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

```

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

```

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

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

Note

Some things to know:

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

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

Bases: `BaseKGELightning`

Base class for all neural network modules.

Your models should also subclass this class.

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

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

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

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

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

Note

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

Variables

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

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

```

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

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

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

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

Bases: torch.nn.Module

Base class for all neural network modules.

Your models should also subclass this class.

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

```

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

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

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

```

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

Note

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

Variables

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

```

args = None

__call__(x)

static forward(x)

```

dicee.models.clifford

Classes

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

Module Contents

```

class dicee.models.clifford.Keci(args)
Bases: dicee.models.base_model.BaseKGE

```

Base class for all neural network modules.

Your models should also subclass this class.

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

```

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

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_q + sigma_pq where
(1) sigma_0 = h_0 r_0 + sum_{i=1}^p (h_0 r_i) e_i - sum_{j=p+1}^{p+q} (h_j r_j) e_j
(2) sigma_p = sum_{i=1}^p (h_0 r_i + h_i r_0) e_i
(3) sigma_q = sum_{j=p+1}^{p+q} (h_0 r_j + h_j r_0) e_j
(4) sigma_pp = sum_{i=1}^{p-1} sum_{k=i+1}^p (h_i r_k - h_k r_i) e_i e_k
(5) sigma_qq = sum_{j=1}^{p+q-1} sum_{k=j+1}^{p+q} (h_j r_k - h_k r_j) e_j e_k
(6) sigma_pq = sum_{i=1}^p sum_{j=p+1}^{p+q} (h_i r_j - h_j r_i) e_i e_j

```

construct_cl_multivector (x: `torch.FloatTensor`, r: int, p: int, q: int)
 \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*) → *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`

`c1_pqr (a: torch.tensor) → torch.tensor`

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

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

`compute_sigmas_single (list_h_emb, list_r_emb, list_t_emb)`

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

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

and return:

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

compute_sigmas_multivect (*list_h_emb*, *list_r_emb*)

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

For same bases vectors interaction we have

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

For different base vector interactions, we have

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

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

Kvsall training

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

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

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

Multiplying a base vector with its scalar coefficient

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

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

Parameter

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

returns

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

compute_sigma_pp (*hp, rp*)

Compute .. math:

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

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

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

```

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

```

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

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

e2e1, e2e2, e2e3, e3e1, e3e2, e3e3

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

```
compute_sigma_qq(hq, rq)
```

Compute

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

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

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

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

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

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

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

e2e1, e2e2, e2e3, e3e1, e3e2, e3e3

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

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

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

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

Compute

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

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

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

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

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

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

Compute

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

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

```

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

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


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


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

```

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)

```

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

```

name = 'LFMult1'

entity_embeddings

relation_embeddings

forward_triples (idx_triple)

```

Parameters

x

```

tri_score (h, r, t)

vtp_score (h, r, t)

```

```

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

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

name = 'LFMult'

entity_embeddings

relation_embeddings

degree

m

x_values

forward_triples (idx_triple)

Parameters

x

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

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

tri_score (coeff_h, coeff_r, coeff_t)
this part implements the trilinear scoring techniques:
score( $h, r, t$ ) =  $\int_0^1 h(x)r(x)t(x) dx = \sum_{i,j,k=0}^{d-1} \frac{a_i b_j c_k}{(1+i+j+k)\%d}$ 
1. generate the range for i,j and k from [0 d-1]
2. perform  $\frac{a_i b_j c_k}{(1+i+j+k)\%d}$  in parallel for every batch
3. take the sum over each batch

vtp_score (h, r, t)
this part implements the vector triple product scoring techniques:
score( $h, r, t$ ) =  $\int_0^1 h(x)r(x)t(x) dx = \sum_{i,j,k=0}^{d-1} \frac{a_i c_j b_k - b_i c_j a_k}{((1+i+j)\%d)(1+k)}$ 
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 implements the function composition scoring techniques: i.e. score = <hor, t>

```

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

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

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

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

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

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

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

dicee.models.literal

Classes

LiteralEmbeddings

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

Module Contents

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

Bases: torch.nn.Module

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

num_of_data_properties

Number of data properties (attributes).

Type

int

embedding_dims

Dimension of the embeddings.

Type

int

entity_embeddings

Pre-trained entity embeddings.

Type

torch.tensor

dropout

Dropout rate for regularization.

Type

float

gate_residual

Whether to use gated residual connections.

```

Type
    bool

freeze_entity_embeddings
    Whether to freeze the entity embeddings during training.

Type
    bool

embedding_dim

num_of_data_properties

hidden_dim

gate_residual = True

freeze_entity_embeddings = True

entity_embeddings

data_property_embeddings

fc

fc_out

dropout

gated_residual_proj

layer_norm

forward(entity_idx, attr_idx)

```

Parameters

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

Returns

scalar predictions.

Return type

Tensor

property device

dicee.models.octonion

Classes

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

Functions

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

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

Module Contents

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

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

Bases: `dicee.models.base_model.BaseKGE`

Base class for all neural network modules.

Your models should also subclass this class.

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

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

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

Note

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

Variables

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

```
name = 'OMult'  
  
static octonion_normalizer(emb_rel_e0, emb_rel_e1, emb_rel_e2, emb_rel_e3, emb_rel_e4,  
                           emb_rel_e5, emb_rel_e6, emb_rel_e7)
```

```

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

k_vs_all_score(bpe_head_ent_emb, bpe_rel_ent_emb, E)

forward_k_vs_all(x)

```

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

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

Bases: *dicee.models.base_model.BaseKGE*

Base class for all neural network modules.

Your models should also subclass this class.

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

```

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

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

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

```

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

Note

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

Variables

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

```

name = 'ConvO'

conv2d

fc_num_input

fc1

bn_conv2d

norm_fc1

```

```

feature_map_dropout

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

residual_convolution(O_1, O_2)

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

Parameters
    x

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

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

conv2d

fc_num_input

fc1

bn_conv2d

norm_fc1

feature_map_dropout

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

residual_convolution(O_1, O_2)

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

Parameters
    x

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

[dicee.models.pykeen_models](#)

Classes

PykeenKGE

A class for using knowledge graph embedding models implemented in Pykeen

Module Contents

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

A class for using knowledge graph embedding models implemented in Pykeen

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

model_kwarg
name
model
loss_history = []
args
entity_embeddings = None
relation_embeddings = None
forward_k_vs_all(x: torch.LongTensor)
# => Explicit version by this we can apply bn and dropout
# (1) Retrieve embeddings of heads and relations + apply Dropout & Normalization if given. h, r = self.get_head_relation_representation(x) # (2) Reshape (1). if self.last_dim > 0:
    h = h.reshape(len(x), self.embedding_dim, self.last_dim) r = r.reshape(len(x), self.embedding_dim, self.last_dim)
# (3) Reshape all entities. if self.last_dim > 0:
    t = self.entity_embeddings.weight.reshape(self.num_entities, self.embedding_dim, self.last_dim)

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

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

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

dicee.models.quaternion

Classes

| | |
|---------------------|--|
| <code>QMult</code> | Base class for all neural network modules. |
| <code>ConvQ</code> | Convolutional Quaternion Knowledge Graph Embeddings |
| <code>AConvQ</code> | Additive Convolutional Quaternion Knowledge Graph Embeddings |

Functions

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

Module Contents

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

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

Bases: `dicee.models.base_model.BaseKGE`

Base class for all neural network modules.

Your models should also subclass this class.

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

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

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

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

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

Note

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

Variables

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

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

Parameters

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

Returns

Triple scores.

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

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

Absolute value of a quaternion

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

L2 norm of quaternion vector:

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

Parameters

`x` – The vector.

Returns

The normalized vector.

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

`k_vs_all_score(bpe_head_ent_emb, bpe_rel_ent_emb, E)`

Parameters

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

`forward_k_vs_all(x)`

Parameters

`x`

`forward_k_vs_sample(x, target_entity_idx)`

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

```

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

Convolutional Quaternion Knowledge Graph Embeddings

name = 'ConvQ'

entity_embeddings

relation_embeddings

conv2d

fc_num_input

fc1

bn_conv1

bn_conv2

feature_map_dropout

residual_convolution(Q_1, Q_2) → torch.Tensor

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

Parameters

x

forward_k_vs_all(x: torch.Tensor)

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

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

Additive Convolutional Quaternion Knowledge Graph Embeddings

name = 'AConvQ'

entity_embeddings

relation_embeddings

conv2d

fc_num_input

fc1

bn_conv1

bn_conv2

feature_map_dropout

residual_convolution(Q_1, Q_2)

```

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

Parameters

x

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

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

dicee.models.real

Classes

| | |
|-------------------|--|
| <i>DistMult</i> | Embedding Entities and Relations for Learning and Inference in Knowledge Bases |
| <i>TransE</i> | Translating Embeddings for Modeling |
| <i>Shallow</i> | A shallow neural model for relation prediction (https://arxiv.org/abs/2101.09090) |
| <i>Pyke</i> | A Physical Embedding Model for Knowledge Graphs |
| <i>CoKEConfig</i> | Configuration for the CoKE (Contextualized Knowledge Graph Embedding) model. |
| <i>CoKE</i> | Contextualized Knowledge Graph Embedding (CoKE) model. |

Module Contents

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

Bases: *dicee.models.base_model.BaseKGE*

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

```
name = 'DistMult'
```

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

Parameters

- emb_h
- emb_r
- emb_E

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

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

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

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

Bases: *dicee.models.base_model.BaseKGE*

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

```

name = 'TransE'

margin = 4

score(head_ent_emb, rel_ent_emb, tail_ent_emb)

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

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

shallom

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

forward_k_vs_all(x) → torch.FloatTensor

forward_triples(x) → torch.FloatTensor

Parameters
x

Returns

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

dist_func

margin = 1.0

forward_triples(x: torch.LongTensor)

Parameters
x

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

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

vocab_size
Total vocabulary size (num_entities + num_relations)

n_layer
Number of transformer layers

n_head
Number of attention heads per layer

n_embd
Embedding dimension (set to match model embedding_dim)

```

```

dropout
    Dropout rate applied throughout the model

bias
    Whether to use bias in linear layers

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

block_size: int = 3

vocab_size: int = None

n_layer: int = 6

n_head: int = 8

n_embd: int = None

dropout: float = 0.3

bias: bool = True

causal: bool = False

```

class dicee.models.real.**CoKE**(*args, config: CoKEConfig = CoKEConfig()*)

Bases: *dicee.models.base_model.BaseKGE*

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

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

The model creates a sequence [head_emb, relation_emb, mask_emb], adds positional embeddings, and processes it through transformer layers to predict the tail entity.

```

name = 'CoKE'

config

pos_emb

mask_emb

blocks

ln_f

coke_dropout

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

```

dicee.models.static_funcs

Functions

```
quaternion_mul(→ Tuple[torch.Tensor, torch.Tensor, ...]) → Perform quaternion multiplication
```

Module Contents

```
dicee.models.static_funcs.quaternion_mul(*, Q_1, Q_2)
    → Tuple[torch.Tensor, torch.Tensor, torch.Tensor, torch.Tensor]
    Perform quaternion multiplication :param Q_1: :param Q_2: :return:
```

dicee.models.transformers

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

Classes

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

Module Contents

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

Bases: *dicee.models.base_model.BaseKGE*

Base class for all neural network modules.

Your models should also subclass this class.

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

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

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

(continues on next page)

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

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

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

Note

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

Variables

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

```
name = 'Byte'
config
temperature = 0.5
topk = 2
transformer
lm_head
loss_function(yhat_batch, y_batch)
```

Parameters

- `yhat_batch`
- `y_batch`

`forward(x: torch.LongTensor)`

Parameters

`x` (B by T tensor)

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

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

`training_step(batch, batch_idx=None)`

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

Parameters

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

Returns

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

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

Example:

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

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

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

Note

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

```
class dicee.models.transformers.LayerNorm(ndim, bias)  
Bases: torch.nn.Module  
LayerNorm but with an optional bias. PyTorch doesn't support simply bias=False  
weight  
bias  
forward(input)
```

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

Bases: torch.nn.Module

Base class for all neural network modules.

Your models should also subclass this class.

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

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

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

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

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

Note

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

Variables

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

```
c_attn
c_proj
attn_dropout
resid_dropout
n_head
n_embd
dropout
causal
flash = True
forward(x)
```

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

Bases: `torch.nn.Module`

Base class for all neural network modules.

Your models should also subclass this class.

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

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

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

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

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

Note

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

Variables

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

`c_fc`

`gelu`

`c_proj`

`dropout`

`forward(x)`

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

Bases: `torch.nn.Module`

Base class for all neural network modules.

Your models should also subclass this class.

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

```

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

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

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

```

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

Note

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

Variables

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

```

ln_1

attn

ln_2

mlp

forward(x)

class dicee.models.transformers.GPTConfig

block_size: int = 1024
vocab_size: int = 50304
n_layer: int = 12
n_head: int = 12
n_embd: int = 768
dropout: float = 0.0
bias: bool = False
causal: bool = True

```

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

Bases: `torch.nn.Module`

Base class for all neural network modules.

Your models should also subclass this class.

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

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

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

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

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

Note

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

Variables

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

`config`

`transformer`

`lm_head`

`get_num_params` (`non_embedding=True`)

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

`forward` (`idx, targets=None`)

`crop_block_size` (`block_size`)

`classmethod from_pretrained` (`model_type, override_args=None`)

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

`estimate_mfu` (`fwdbwd_per_iter, dt`)

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

Classes

| | |
|-------------------------|--|
| <i>ADOPT</i> | ADOPT Optimizer. |
| <i>BaseKGELightning</i> | Base class for all neural network modules. |
| <i>BaseKGE</i> | Base class for all neural network modules. |
| <i>IdentityClass</i> | Base class for all neural network modules. |
| <i>BaseKGE</i> | Base class for all neural network modules. |
| <i>Block</i> | Base class for all neural network modules. |
| <i>DistMult</i> | Embedding Entities and Relations for Learning and Inference in Knowledge Bases |
| <i>TransE</i> | Translating Embeddings for Modeling |
| <i>Shallow</i> | A shallow neural model for relation prediction (https://arxiv.org/abs/2101.09090) |
| <i>Pyke</i> | A Physical Embedding Model for Knowledge Graphs |
| <i>CoKEConfig</i> | Configuration for the CoKE (Contextualized Knowledge Graph Embedding) model. |
| <i>CoKE</i> | Contextualized Knowledge Graph Embedding (CoKE) model. |
| <i>BaseKGE</i> | Base class for all neural network modules. |
| <i>ConEx</i> | Convolutional ComplEx Knowledge Graph Embeddings |
| <i>AConEx</i> | Additive Convolutional ComplEx Knowledge Graph Embeddings |
| <i>ComplEx</i> | Base class for all neural network modules. |
| <i>BaseKGE</i> | Base class for all neural network modules. |
| <i>IdentityClass</i> | Base class for all neural network modules. |
| <i>QMult</i> | Base class for all neural network modules. |
| <i>ConvQ</i> | Convolutional Quaternion Knowledge Graph Embeddings |
| <i>AConvQ</i> | Additive Convolutional Quaternion Knowledge Graph Embeddings |
| <i>BaseKGE</i> | Base class for all neural network modules. |
| <i>IdentityClass</i> | Base class for all neural network modules. |
| <i>OMult</i> | Base class for all neural network modules. |
| <i>ConvO</i> | Base class for all neural network modules. |
| <i>AConvO</i> | Additive Convolutional Octonion Knowledge Graph Embeddings |
| <i>Keci</i> | Base class for all neural network modules. |
| <i>CKeci</i> | Without learning dimension scaling |
| <i>DeCaL</i> | Base class for all neural network modules. |
| <i>BaseKGE</i> | Base class for all neural network modules. |
| <i>PykeenKGE</i> | A class for using knowledge graph embedding models implemented in Pykeen |
| <i>BaseKGE</i> | Base class for all neural network modules. |
| <i>FMult</i> | Learning Knowledge Neural Graphs |
| <i>GFMult</i> | Learning Knowledge Neural Graphs |
| <i>FMult2</i> | Learning Knowledge Neural Graphs |
| <i>LFMult1</i> | Embedding with trigonometric functions. We represent all entities and relations in the complex number space as: |
| <i>LFMult</i> | Embedding with polynomial functions. We represent all entities and relations in the polynomial space as: |

continues on next page

Table 1 – continued from previous page

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

Functions

| | |
|--|-----------------------------------|
| <i>quaternion_mul</i> (→ Tuple[torch.Tensor, torch.Tensor, ...]) <i>quaternion_mul_with_unit_norm</i> (*, Q_1, Q_2) | Perform quaternion multiplication |
| <i>octonion_mul</i> (*, O_1, O_2) | |
| <i>octonion_mul_norm</i> (*, O_1, O_2) | |

Package Contents

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

Bases: `torch.optim.optimizer.Optimizer`

ADOPT Optimizer.

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

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

Mathematical formulation:

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

where:

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

Reference:

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

Parameters

- **params** (*ParamsT*) – Iterable of parameters to optimize or dicts defining parameter groups.
- **lr** (*float or Tensor, optional*) – Learning rate. Can be a float or 1-element Tensor. Default: 1e-3
- **betas** (*Tuple[float, float], optional*) – Coefficients (β_1, β_2) for computing running averages of gradient and its square. β_1 controls momentum, β_2 controls variance. Default: (0.9, 0.9999)
- **eps** (*float, optional*) – Term added to denominator to improve numerical stability. Default: 1e-6
- **clip_lambda** (*Callable[[int], float], optional*) – Function that takes the step number and returns the gradient clipping threshold. Common choices: - lambda step: $\text{step}^{**0.25}$ (default, gradually increases clipping threshold) - lambda step: 1.0 (constant clipping) - None (no clipping) Default: lambda step: $\text{step}^{**0.25}$
- **weight_decay** (*float, optional*) – Weight decay coefficient (L2 penalty). Default: 0.0
- **decouple** (*bool, optional*) – If True, uses decoupled weight decay (AdamW-style), applying weight decay directly to parameters. If False, adds weight decay to gradients (L2 regularization). Default: False
- **foreach** (*bool, optional*) – If True, uses the faster foreach implementation for multi-tensor operations. Default: None (auto-select)
- **maximize** (*bool, optional*) – If True, maximizes parameters instead of minimizing. Useful for reinforcement learning. Default: False
- **capturable** (*bool, optional*) – If True, the optimizer is safe to capture in a CUDA graph. Requires learning rate as Tensor. Default: False
- **differentiable** (*bool, optional*) – If True, the optimization step can be differentiated. Useful for meta-learning. Default: False
- **fused** (*bool, optional*) – If True, uses fused kernel implementation (currently not supported). Default: None

Raises

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

Example

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

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

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

Note

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

`clip_lambda`

`__setstate__(state)`

Restore optimizer state from a checkpoint.

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

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

Parameters

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

Note

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

`step(closure=None)`

Perform a single optimization step.

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

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

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

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

Parameters

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

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

Default: None

Returns

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

Return type

Optional[Tensor]

Example

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

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

Note

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

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

Bases: lightning.LightningModule

Base class for all neural network modules.

Your models should also subclass this class.

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

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

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

(continues on next page)

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

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

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

Note

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

Variables

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

`training_step_outputs` = []

`mem_of_model()` → Dict

Size of model in MB and number of params

`training_step` (batch, batch_idx=None)

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

Parameters

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

Returns

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

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

Example:

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

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

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

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

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

Note

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

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

Parameters

- `yhat_batch`
- `y_batch`

`on_train_epoch_end(*args, **kwargs)`

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

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

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

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

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

`test_epoch_end(outputs: List[Any])`

`test_dataloader() → None`

An iterable or collection of iterables specifying test samples.

For more information about multiple dataloaders, see this section.

For data processing use the following pattern:

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

However, the above are only necessary for distributed processing.

⚠ Warning

do not assign state in `prepare_data`

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

ℹ Note

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

ℹ Note

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

`val_dataloader() → None`

An iterable or collection of iterables specifying validation samples.

For more information about multiple dataloaders, see this section.

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

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

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

Note

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

Note

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

`predict_dataloader() → None`

An iterable or collection of iterables specifying prediction samples.

For more information about multiple dataloaders, see this section.

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

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

Note

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

Returns

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

`train_dataloader() → None`

An iterable or collection of iterables specifying training samples.

For more information about multiple dataloaders, see this section.

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

For data processing use the following pattern:

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

However, the above are only necessary for distributed processing.

Warning

do not assign state in `prepare_data`

- `fit()`

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

Note

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

`configure_optimizers(parameters=None)`

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

Returns

Any of these 6 options.

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

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

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

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

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

Note

Some things to know:

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

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

Bases: `BaseKG``Lightning`

Base class for all neural network modules.

Your models should also subclass this class.

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

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

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

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

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

Note

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

Variables

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

```
args  
  
embedding_dim = None  
  
num_entities = None  
  
num_relations = None  
  
num_tokens = None  
  
learning_rate = None  
  
apply_unit_norm = None  
  
input_dropout_rate = None  
  
hidden_dropout_rate = None  
  
optimizer_name = None  
  
feature_map_dropout_rate = None  
  
kernel_size = None  
  
num_of_output_channels = None  
  
weight_decay = None  
  
loss  
  
selected_optimizer = None  
  
normalizer_class = None  
  
normalize_head_entity_embeddings  
  
normalize_relation_embeddings  
  
normalize_tail_entity_embeddings  
  
hidden_normalizer  
  
param_init  
  
input_dp_ent_real  
  
input_dp_rel_real  
  
hidden_dropout  
  
loss_history = []  
  
byte_pair_encoding
```

```

max_length_subword_tokens
block_size

forward_byte_pair_encoded_k_vs_all (x: torch.LongTensor)

Parameters
  x (B 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)

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

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

Note

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

Variables

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

```
args = None

__call__(x)

static forward(x)

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

Bases: `BaseKGELightning`

Base class for all neural network modules.

Your models should also subclass this class.

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

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

class Model(nn.Module):
```

(continues on next page)

```

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

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

```

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

Note

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

Variables

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

```

args

embedding_dim = None

num_entities = None

num_relations = None

num_tokens = None

learning_rate = None

apply_unit_norm = None

input_dropout_rate = None

hidden_dropout_rate = None

optimizer_name = None

feature_map_dropout_rate = None

kernel_size = None

num_of_output_channels = None

weight_decay = None

loss

selected_optimizer = None

normalizer_class = None

normalize_head_entity_embeddings

```

```

normalize_relation_embeddings
normalize_tail_entity_embeddings
hidden_normalizer
param_init
input_dp_ent_real
input_dp_rel_real
hidden_dropout
loss_history = []
byte_pair_encoding
max_length_subword_tokens
block_size
forward_byte_pair_encoded_k_vs_all(x: torch.LongTensor)

Parameters
    x (B x 2 x T)

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

Parameters
-----
init_params_with_sanity_checking()

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

Parameters
    • x
    • y_idx
    • ordered_bpe_entities

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

Parameters
    x

forward_k_vs_all(*args, **kwargs)

forward_k_vs_sample(*args, **kwargs)

get_triple_representation(idx_hrt)

get_head_relation_representation(indexed_triple)

```

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

Parameters

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

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

→ Tuple[torch.FloatTensor, torch.FloatTensor]

Parameters

x (B x 2 x T)

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

```
class dicee.models.Block(config)
```

Bases: torch.nn.Module

Base class for all neural network modules.

Your models should also subclass this class.

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

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

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

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

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

Note

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

Variables

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

`ln_1`

`attn`

```

ln_2

mlp

forward(x)

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

name = 'DistMult'

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

Parameters

- emb_h
- emb_r
- emb_E

forward_k_vs_all(x: torch.LongTensor)

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

score(h, r, t)

class dicee.models.TransE(args)
Bases: dicee.models.base_model.BaseKGE
Translating Embeddings for Modeling Multi-relational Data https://proceedings.neurips.cc/paper/2013/file/1cecc7a77928ca8133fa24680a88d2f9-Paper.pdf

name = 'TransE'

margin = 4

score(head_ent_emb, rel_ent_emb, tail_ent_emb)

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

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

shallow

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

forward_k_vs_all(x) → torch.FloatTensor

forward_triples(x) → torch.FloatTensor

Parameters
x

Returns

```

```

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

    A Physical Embedding Model for Knowledge Graphs

    name = 'Pyke'

    dist_func

    margin = 1.0

    forward_triples(x: torch.LongTensor)
```

Parameters

x

```

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

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

    vocab_size
        Total vocabulary size (num_entities + num_relations)

    n_layer
        Number of transformer layers

    n_head
        Number of attention heads per layer

    n_embd
        Embedding dimension (set to match model embedding_dim)

    dropout
        Dropout rate applied throughout the model

    bias
        Whether to use bias in linear layers

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

    block_size: int = 3

    vocab_size: int = None

    n_layer: int = 6

    n_head: int = 8

    n_embd: int = None

    dropout: float = 0.3

    bias: bool = True

    causal: bool = False
```

```
class dicee.models.CoKE(args, config: CoKEConfig = CoKEConfig())
```

Bases: *dicee.models.base_model.BaseKGE*

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

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

The model creates a sequence [head_emb, relation_emb, mask_emb], adds positional embeddings, and processes it through transformer layers to predict the tail entity.

```
name = 'CoKE'
```

```
config
```

```
pos_emb
```

```
mask_emb
```

```
blocks
```

```
ln_f
```

```
coke_dropout
```

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

```
score(emb_h, emb_r, emb_t)
```

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

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

Bases: *BaseKGLightning*

Base class for all neural network modules.

Your models should also subclass this class.

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

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

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

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

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

Note

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

Variables

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

```
args

embedding_dim = None

num_entities = None

num_relations = None

num_tokens = None

learning_rate = None

apply_unit_norm = None

input_dropout_rate = None

hidden_dropout_rate = None

optimizer_name = None

feature_map_dropout_rate = None

kernel_size = None

num_of_output_channels = None

weight_decay = None

loss

selected_optimizer = None

normalizer_class = None

normalize_head_entity_embeddings

normalize_relation_embeddings

normalize_tail_entity_embeddings

hidden_normalizer

param_init

input_dp_ent_real

input_dp_rel_real

hidden_dropout

loss_history = []
```

```

byte_pair_encoding
max_length_subword_tokens
block_size

forward_byte_pair_encoded_k_vs_all(x: torch.LongTensor) → torch.FloatTensor

    Parameters
        x (B × 2 × T)
    forward_byte_pair_encoded_triple(x: Tuple[torch.LongTensor, torch.LongTensor]) → torch.FloatTensor
        byte pair encoded neural link predictors

    Parameters
    -----
    init_params_with_sanity_checking()

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

    Parameters
        • x
        • y_idx
        • ordered_bpe_entities

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

    Parameters
        x
    forward_k_vs_all(*args, **kwargs)
    forward_k_vs_sample(*args, **kwargs)
    get_triple_representation(idx_hrt)
    get_head_relation_representation(indexed_triple)
    get_sentence_representation(x: torch.LongTensor) → torch.FloatTensor

    Parameters
        • (b (x shape))
        • 3
        • t)
    get_bpe_head_and_relation_representation(x: torch.LongTensor) → Tuple[torch.FloatTensor, torch.FloatTensor]

    Parameters
        x (B × 2 × T)
    get_embeddings() → Tuple[numpy.ndarray, numpy.ndarray]

```

```

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

    Convolutional ComplEx Knowledge Graph Embeddings

    name = 'ConEx'

    conv2d

    fc_num_input

    fc1

    norm_fc1

    bn_conv2d

    feature_map_dropout

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

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

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

    Parameters
    x

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

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

    Additive Convolutional ComplEx Knowledge Graph Embeddings

    name = 'AConEx'

    conv2d

    fc_num_input

    fc1

    norm_fc1

    bn_conv2d

    feature_map_dropout

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

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

```

```

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

Parameters
    x

```

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

```

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

```

Base class for all neural network modules.

Your models should also subclass this class.

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

```

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

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

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

```

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

Note

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

Variables

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

```

name = 'ComplEx'

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

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

```

Parameters

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

```

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

dicee.models.quaternion_mul(*Q_1, Q_2)
    → Tuple[torch.Tensor, torch.Tensor, torch.Tensor, torch.Tensor]
Perform quaternion multiplication :param Q_1: :param Q_2: :return:

class dicee.models.BaseKGE(args: dict)
Bases: 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 sub-modules as regular attributes:

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

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

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

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

Note

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

Variables

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

```
name = 'QMult'

explicit = True

quaternion_multiplication_followed_by_inner_product(h, r, t)
```

Parameters

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

Returns

Triple scores.

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

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

Absolute value of a quaternion

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

L2 norm of quaternion vector:

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

Parameters

`x` – The vector.

Returns

The normalized vector.

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

`k_vs_all_score(bpe_head_ent_emb, bpe_rel_ent_emb, E)`

Parameters

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

`forward_k_vs_all(x)`

Parameters

`x`

`forward_k_vs_sample(x, target_entity_idx)`

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

```

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

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

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

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

entity_embeddings
relation_embeddings
conv2d
fc_num_input
fc1
bn_conv1
bn_conv2
feature_map_dropout
residual_convolution(Q_1, Q_2)

```

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

Parameters

x

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

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

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

Bases: *BaseKGLightning*

Base class for all neural network modules.

Your models should also subclass this class.

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

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

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

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

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

Note

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

Variables

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

`args`

`embedding_dim` = None

`num_entities` = None

`num_relations` = None

`num_tokens` = None

`learning_rate` = None

```

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

Parameters
  x (B x 2 x T)

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

Parameters
-----
init_params_with_sanity_checking()

```

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

Parameters

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

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

Parameters

x

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

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

```
get_triple_representation(idx_hrt)
```

```
get_head_relation_representation(indexed_triple)
```

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

Parameters

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

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

Parameters

x (B x 2 x T)

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

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

Bases: torch.nn.Module

Base class for all neural network modules.

Your models should also subclass this class.

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

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

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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.octonion_mul(*, O_1, O_2)

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

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

Bases: `dicee.models.base_model.BaseKGE`

Base class for all neural network modules.

Your models should also subclass this class.

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

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

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

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

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

Note

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

Variables

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

`name = 'OMult'`

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

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

`k_vs_all_score(bpe_head_ent_emb, bpe_rel_ent_emb, E)`

`forward_k_vs_all(x)`

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

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

Bases: `dicee.models.base_model.BaseKGE`

Base class for all neural network modules.

Your models should also subclass this class.

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

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

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

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

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

Note

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

Variables

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

```
name = 'ConvO'

conv2d

fc_num_input

fc1

bn_conv2d

norm_fc1

feature_map_dropout

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

residual_convolution(O_1, O_2)

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

Parameters

`x`

`forward_k_vs_all(x: torch.Tensor)`

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

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

Bases: `dicee.models.base_model.BaseKGE`

Additive Convolutional Octonion Knowledge Graph Embeddings

`name = 'AConvO'`

`conv2d`

`fc_num_input`

`fc1`

`bn_conv2d`

`norm_fc1`

`feature_map_dropout`

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

`residual_convolution(O_1, O_2)`

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

Parameters

`x`

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

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

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

Bases: *dicee.models.base_model.BaseKGE*

Base class for all neural network modules.

Your models should also subclass this class.

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

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

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

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

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

i Note

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

Variables

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

```
name = 'Keci'
```

```
p
```

```
q
```

```
r
```

```
requires_grad_for_interactions = True
```

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

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

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

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

```

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

```

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

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

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

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

compute_sigma_qq(hq, rq)

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

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

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

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

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

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

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

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

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

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

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

for j in range(q):

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

`print(sigma_pq.shape)`

apply_coefficients(hp, hq, rp, rq)

Multiplying a base vector with its scalar coefficient

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

Compute our CL multiplication

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

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

`eq j`

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

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

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

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

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

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

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

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

Parameter

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

returns

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

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

k_vs_all_score (*bpe_head_ent_emb*, *bpe_rel_ent_emb*, *E*)

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

Kvsall training

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

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

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

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

Parameter

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

returns

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

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

Parameter

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

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

rtype

torch.FloatTensor with (n, k) shape

```

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

```

Parameter

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

rtype

torch.FloatTensor with (n) shape

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

Bases: *Keci*

Without learning dimension scaling

```
name = 'CKeci'
```

```
requires_grad_for_interactions = False
```

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

Bases: *dicee.models.base_model.BaseKGE*

Base class for all neural network modules.

Your models should also subclass this class.

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

```

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

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

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

```

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

Note

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

Variables

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

```
name = 'DeCaL'
```

```

entity_embeddings
relation_embeddings

p



q



r



re



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


```

Parameter

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

rtype

torch.FloatTensor with (n) shape

c1_pqr (*a*: *torch.tensor*) → *torch.tensor*

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

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

compute_sigmas_single (*list_h_emb*, *list_r_emb*, *list_t_emb*)

here we compute all the sums with no others vectors interaction taken with the scalar product with t, that is,

$$s0 = h_0 r_0 t_0 s1 = \sum_{i=1}^p h_i r_i t_0 s2 = \sum_{j=p+1}^{p+q} h_j r_j t_0 s3 = \sum_{i=1}^q (h_0 r_i t_i + h_i r_0 t_i) s4 = \sum_{i=p+1}^{p+q} (h_0 r_i t_i + h_i r_0 t_i) s5 = \sum_{i=p+q+1}^{p+q+r} (h_0 r_i t_i + h_i r_0 t_i)$$

and return:

$$\sigma_0 t = \sigma_0 \cdot t_0 = s0 + s1 - s2s3, s4 and s5$$

compute_sigmas_multivect (*list_h_emb*, *list_r_emb*)

Here we compute and return all the sums with vectors interaction for the same and different bases.

For same bases vectors interaction we have

$$\sigma_{pp} = \sum_{i=1}^{p-1} \sum_{i'=i+1}^p (h_i r_{i'} - h_{i'} r_i) \text{ (modelsthe interactions between } e_i \text{ and } e'_{i'} \text{ for } 1 \leq i, i' \leq p) \sigma_{qq} = \sum_{j=p+1}^{p+q-1} \sum_{j'=j+1}^{p+q} (h_j r_{j'} - h_{j'} r_j) \text{ (interactionsn between } e_i \text{ and } e_j \text{ for } 1 \leq i \leq p \text{ and } p+1 \leq j \leq p+q)$$

For different base vector interactions, we have

$$\sigma_{pq} = \sum_{i=1}^p \sum_{j=p+1}^{p+q} (h_i r_j - h_j r_i) \text{ (interactionsn between } e_i \text{ and } e_j \text{ for } 1 \leq i \leq p \text{ and } p+1 \leq j \leq p+q) \sigma_{pr} = \sum_{i=1}^p \sum_{j=p+1}^{p+q} (h_i r_j - h_j r_i) \text{ (interactionsn between } e_i \text{ and } e_j \text{ for } 1 \leq i \leq p \text{ and } p+1 \leq j \leq p+q)$$

forward_k_vs_all (*x*: *torch.Tensor*) → *torch.FloatTensor*
 Kvsall training
 (1) Retrieve real-valued embedding vectors for heads and relations
 (2) Construct head entity and relation embeddings according to $\text{Cl}_{\{p,q,r\}}(\mathbb{R}^d)$.
 (3) Perform Cl multiplication
 (4) Inner product of (3) and all entity embeddings

forward_k_vs_with_explicit and this funcitons are identical Parameter ——— *x*: *torch.LongTensor* with (n,) shape :*dtype*: *torch.FloatTensor* with (n, |E|) shape

apply_coefficients (*h0, hp, hq, hk, r0, rp, rq, rk*)

Multiplying a base vector with its scalar coefficient

construct_cl_multivector (*x*: *torch.FloatTensor*, *re*: int, *p*: int, *q*: int, *r*: int)
 → tuple[*torch.FloatTensor*, *torch.FloatTensor*, *torch.FloatTensor*]

Construct a batch of multivectors $\text{Cl}_{\{p,q,r\}}(\mathbb{R}^d)$

Parameter

x: *torch.FloatTensor* with (n,d) shape

returns

- **a0** (*torch.FloatTensor*)
- **ap** (*torch.FloatTensor*)
- **aq** (*torch.FloatTensor*)
- **ar** (*torch.FloatTensor*)

compute_sigma_pp (*hp, rp*)

Compute .. math:

$$\sigma_{pp} = \sum_{i=1}^{p-1} \sum_{i'=i+1}^p (x_i y_{i'} - x_{i'} y_i)$$

σ_{pp} captures the interactions between along p bases For instance, let p e_1, e_2, e_3, we compute interactions between e_1 e_2, e_1 e_3 , and e_2 e_3 This can be implemented with a nested two for loops

results = [] for i in range(p - 1):

```
for k in range(i + 1, p):
    results.append(hp[:, :, i] * rp[:, :, k] - hp[:, :, k] * rp[:, :, i])
sigma_pp = torch.stack(results, dim=2) assert sigma_pp.shape == (b, r, int((p * (p - 1)) / 2))
```

Yet, this computation would be quite inefficient. Instead, we compute interactions along all p, e.g., e1e1, e1e2, e1e3,

e2e1, e2e2, e2e3, e3e1, e3e2, e3e3

Then select the triangular matrix without diagonals: e1e2, e1e3, e2e3.

compute_sigma_qq (*hq, rq*)

Compute

$$\sigma_{q,q}^* = \sum_{j=p+1}^{p+q-1} \sum_{j'=j+1}^{p+q} (x_j y_{j'} - x_{j'} y_j) \quad \text{Eq.16}$$

`sigma_{q}` captures the interactions between along q bases For instance, let q e_1, e_2, e_3, we compute interactions between e_1 e_2, e_1 e_3 , and e_2 e_3 This can be implemented with a nested two for loops

results = [] for j in range(q - 1):

for k in range(j + 1, q):

results.append(hq[:, :, j] * rq[:, :, k] - hq[:, :, k] * rq[:, :, j])

sigma_qq = torch.stack(results, dim=2) assert sigma_qq.shape == (b, r, int((q * (q - 1)) / 2))

Yet, this computation would be quite inefficient. Instead, we compute interactions along all p, e.g., e1e1, e1e2, e1e3,

e2e1, e2e2, e2e3, e3e1, e3e2, e3e3

Then select the triangular matrix without diagonals: e1e2, e1e3, e2e3.

compute_sigma_rr(hk, rk)

$$\sigma_{r,r}^* = \sum_{k=p+q+1}^{p+q+r-1} \sum_{k'=k+1}^p (x_k y_{k'} - x_{k'} y_k)$$

compute_sigma_pq(* hp, hq, rp, rq)

Compute

$$\sum_{i=1}^p \sum_{j=p+1}^{p+q} (h_i r_j - h_j r_i) e_i e_j$$

results = [] sigma_pq = torch.zeros(b, r, p, q) for i in range(p):

for j in range(q):

sigma_pq[:, :, i, j] = hp[:, :, i] * rq[:, :, j] - hq[:, :, j] * rp[:, :, i]

print(sigma_pq.shape)

compute_sigma_pr(* hp, hk, rp, rk)

Compute

$$\sum_{i=1}^p \sum_{j=p+1}^{p+q} (h_i r_j - h_j r_i) e_i e_j$$

results = [] sigma_pq = torch.zeros(b, r, p, q) for i in range(p):

for j in range(q):

sigma_pq[:, :, i, j] = hp[:, :, i] * rq[:, :, j] - hq[:, :, j] * rp[:, :, i]

print(sigma_pq.shape)

compute_sigma_qr(* hq, hk, rq, rk)

$$\sum_{i=1}^p \sum_{j=p+1}^{p+q} (h_i r_j - h_j r_i) e_i e_j$$

results = [] sigma_pq = torch.zeros(b, r, p, q) for i in range(p):

for j in range(q):

sigma_pq[:, :, i, j] = hp[:, :, i] * rq[:, :, j] - hq[:, :, j] * rp[:, :, i]

print(sigma_pq.shape)

```
class dicee.models.BaseKGE(args: dict)
```

Bases: `BaseKGELightning`

Base class for all neural network modules.

Your models should also subclass this class.

Modules can also contain other Modules, allowing them to be nested in a tree structure. You can assign the sub-modules as regular attributes:

```
import torch.nn as nn
import torch.nn.functional as F

class Model(nn.Module):
    def __init__(self) -> None:
        super().__init__()
        self.conv1 = nn.Conv2d(1, 20, 5)
        self.conv2 = nn.Conv2d(20, 20, 5)

    def forward(self, x):
        x = F.relu(self.conv1(x))
        return F.relu(self.conv2(x))
```

Submodules assigned in this way will be registered, and will also have their parameters converted when you call `to()`, etc.

Note

As per the example above, an `__init__()` call to the parent class must be made before assignment on the child.

Variables

`training` (`bool`) – Boolean represents whether this module is in training or evaluation mode.

`args`

```
embedding_dim = None
num_entities = None
num_relations = None
num_tokens = None
learning_rate = None
apply_unit_norm = None
input_dropout_rate = None
hidden_dropout_rate = None
optimizer_name = None
feature_map_dropout_rate = None
```

```

kernel_size = None
num_of_output_channels = None
weight_decay = None
loss
selected_optimizer = None
normalizer_class = None
normalize_head_entity_embeddings
normalize_relation_embeddings
normalize_tail_entity_embeddings
hidden_normalizer
param_init
input_dp_ent_real
input_dp_rel_real
hidden_dropout
loss_history = []
byte_pair_encoding
max_length_subword_tokens
block_size
forward_byte_pair_encoded_k_vs_all(x: torch.LongTensor)

Parameters
  x (B x 2 x T)

forward_byte_pair_encoded_triple(x: Tuple[torch.LongTensor, torch.LongTensor])
  byte pair encoded neural link predictors

Parameters
-----
init_params_with_sanity_checking()

forward(x: torch.LongTensor | Tuple[torch.LongTensor, torch.LongTensor],
      y_idx: torch.LongTensor = None)

Parameters
  • x
  • y_idx
  • ordered_bpe_entities

```

```
forward_triples (x: torch.LongTensor) → torch.Tensor
```

Parameters

x

```
forward_k_vs_all (*args, **kwargs)
```

```
forward_k_vs_sample (*args, **kwargs)
```

```
get_triple_representation (idx_hrt)
```

```
get_head_relation_representation (indexed_triple)
```

```
get_sentence_representation (x: torch.LongTensor)
```

Parameters

- (b (x shape)

- 3

- t)

```
get_bpe_head_and_relation_representation (x: torch.LongTensor)
```

→ Tuple[torch.FloatTensor, torch.FloatTensor]

Parameters

x (B x 2 x T)

```
get_embeddings () → Tuple[numpy.ndarray, numpy.ndarray]
```

```
class dicee.models.PykeenKGE (args: dict)
```

Bases: dicee.models.base_model.BaseKGE

A class for using knowledge graph embedding models implemented in Pykeen

Notes: Pykeen_DistMult: C Pykeen_ComplEx: Pykeen_QuatE: Pykeen_MuRE: Pykeen_CP: Pykeen_HolE: Pykeen_HolE: Pykeen_HolE: Pykeen_TransD: Pykeen_TransE: Pykeen_TransF: Pykeen_TransH: Pykeen_TransR:

model_kwargs

name

model

loss_history = []

args

entity_embeddings = None

relation_embeddings = None

```
forward_k_vs_all (x: torch.LongTensor)
```

=> Explicit version by this we can apply bn and dropout

(1) Retrieve embeddings of heads and relations + apply Dropout & Normalization if given. h, r = self.get_head_relation_representation(x) # (2) Reshape (1). if self.last_dim > 0:

h = h.reshape(len(x), self.embedding_dim, self.last_dim) r = r.reshape(len(x), self.embedding_dim, self.last_dim)

(3) Reshape all entities. if self.last_dim > 0:

```

t = self.entity_embeddings.weight.reshape(self.num_entities, self.embedding_dim, self.last_dim)

else:
    t = self.entity_embeddings.weight

# (4) Call the score_t from interactions to generate triple scores. return self.interaction.score_t(h=h, r=r,
all_entities=t, slice_size=1)

forward_triples (x: torch.LongTensor) → torch.FloatTensor
# => Explicit version by this we can apply bn and dropout
# (1) Retrieve embeddings of heads, relations and tails and apply Dropout & Normalization if given. h, r, t =
self.get_triple_representation(x) # (2) Reshape (1). if self.last_dim > 0:
    h = h.reshape(len(x), self.embedding_dim, self.last_dim) r = r.reshape(len(x), self.embedding_dim,
    self.last_dim) t = t.reshape(len(x), self.embedding_dim, self.last_dim)
# (3) Compute the triple score return self.interaction.score(h=h, r=r, t=t, slice_size=None, slice_dim=0)

abstract forward_k_vs_sample (x: torch.LongTensor, target_entity_idx)

class dicee.models.BaseKGE (args: dict)
Bases: BaseKGELightning

Base class for all neural network modules.

Your models should also subclass this class.

Modules can also contain other Modules, allowing them to be nested in a tree structure. You can assign the sub-
modules as regular attributes:

```

```

import torch.nn as nn
import torch.nn.functional as F

class Model(nn.Module):
    def __init__(self) -> None:
        super().__init__()
        self.conv1 = nn.Conv2d(1, 20, 5)
        self.conv2 = nn.Conv2d(20, 20, 5)

    def forward(self, x):
        x = F.relu(self.conv1(x))
        return F.relu(self.conv2(x))

```

Submodules assigned in this way will be registered, and will also have their parameters converted when you call `to()`, etc.

Note

As per the example above, an `__init__()` call to the parent class must be made before assignment on the child.

Variables

`training (bool)` – Boolean represents whether this module is in training or evaluation mode.

```

args
embedding_dim = None
num_entities = None
num_relations = None
num_tokens = None
learning_rate = None
apply_unit_norm = None
input_dropout_rate = None
hidden_dropout_rate = None
optimizer_name = None
feature_map_dropout_rate = None
kernel_size = None
num_of_output_channels = None
weight_decay = None
loss
selected_optimizer = None
normalizer_class = None
normalize_head_entity_embeddings
normalize_relation_embeddings
normalize_tail_entity_embeddings
hidden_normalizer
param_init
input_dp_ent_real
input_dp_rel_real
hidden_dropout
loss_history = []
byte_pair_encoding
max_length_subword_tokens
block_size
forward_byte_pair_encoded_k_vs_all (x: torch.LongTensor)

```

Parameters

x ($B \times 2 \times T$)

```

forward_byte_pair_encoded_triple(x: Tuple[torch.LongTensor, torch.LongTensor])
    byte pair encoded neural link predictors

    Parameters
    -----
    init_params_with_sanity_checking()

forward(x: torch.LongTensor | Tuple[torch.LongTensor, torch.LongTensor],
        y_idx: torch.LongTensor = None)

    Parameters
    *
    * x
    * y_idx
    * ordered_bpe_entities

forward_triples(x: torch.LongTensor) → torch.Tensor

    Parameters
    x

forward_k_vs_all(*args, **kwargs)

forward_k_vs_sample(*args, **kwargs)

get_triple_representation(idx_hrt)
get_head_relation_representation(indexed_triple)
get_sentence_representation(x: torch.LongTensor)

    Parameters
    *
    * (b (x shape)
    * 3
    * t)

get_bpe_head_and_relation_representation(x: torch.LongTensor)
    → Tuple[torch.FloatTensor, torch.FloatTensor]

    Parameters
    x (B x 2 x T)
get_embeddings() → Tuple[numpy.ndarray, numpy.ndarray]

class dicee.models.FMult(args)
    Bases: dicee.models.base_model.BaseKGE

    Learning Knowledge Neural Graphs

    name = 'FMult'

    entity_embeddings

    relation_embeddings

    k

```

```

num_sample = 50
gamma
roots
weights

compute_func (weights: torch.FloatTensor, x) → torch.FloatTensor
chain_func (weights, x: torch.FloatTensor)
forward_triples (idx_triple: torch.Tensor) → torch.Tensor

Parameters
x

class dicee.models.GFMult (args)
Bases: dicee.models.base_model.BaseKGE
Learning Knowledge Neural Graphs
name = 'GFMult'
entity_embeddings
relation_embeddings
k
num_sample = 250
roots
weights

compute_func (weights: torch.FloatTensor, x) → torch.FloatTensor
chain_func (weights, x: torch.FloatTensor)
forward_triples (idx_triple: torch.Tensor) → torch.Tensor

Parameters
x

class dicee.models.FMult2 (args)
Bases: dicee.models.base_model.BaseKGE
Learning Knowledge Neural Graphs
name = 'FMult2'
n_layers = 3
k
n = 50
score_func = 'compositional'
discrete_points

```

```

entity_embeddings
relation_embeddings
build_func(Vec)
build_chain_funcs(list_Vec)
compute_func(W, b, x) → torch.FloatTensor
function(list_W, list_b)
trapezoid(list_W, list_b)
forward_triples(idx_triple: torch.Tensor) → torch.Tensor

```

Parameters

x

```
class dicee.models.LFMult1(args)
```

Bases: *dicee.models.base_model.BaseKGE*

Embedding with trigonometric functions. We represent all entities and relations in the complex number space as: $f(x) = \sum_{k=0}^d \{k=0\}^k w_k e^{ikx}$. and use the three different scoring function as in the paper to evaluate the score

```

name = 'LFMult1'

entity_embeddings
relation_embeddings
forward_triples(idx_triple)

```

Parameters

x

tri_score(*h, r, t*)

vtp_score(*h, r, t*)

```
class dicee.models.LFMult(args)
```

Bases: *dicee.models.base_model.BaseKGE*

Embedding with polynomial functions. We represent all entities and relations in the polynomial space as: $f(x) = \sum_{i=0}^d a_i x^i$ and use the three different scoring function as in the paper to evaluate the score. We also consider combining with Neural Networks.

```

name = 'LFMult'

entity_embeddings
relation_embeddings
degree
m
x_values

```

```

forward_triples (idx_triple)

Parameters
    x

construct_multi_coeff (x)

poly_NN (x, coefh, coefr, coeft)
    Constructing a 2 layers NN to represent the embeddings. h = sigma( $wh^T x + bh$ ), r = sigma( $wr^T x + br$ ), t = sigma( $wt^T x + bt$ )

linear (x, w, b)

scalar_batch_NN (a, b, c)
    element wise multiplication between a,b and c: Inputs : a, b, c =====> torch.tensor of size batch_size x m x d Output : a tensor of size batch_size x d

tri_score (coeff_h, coeff_r, coeff_t)
    this part implement the trilinear scoring techniques:
    score( $h, r, t$ ) =  $\int_{\{0\}} \{1\} h(x)r(x)t(x) dx = \sum_{\{i,j,k=0\}}^{d-1} \frac{a_i * b_j * c_k}{(1+(i+j+k)\%d)}$ 
    1. generate the range for i,j and k from [0 d-1]
    2. perform  $\frac{a_i * b_j * c_k}{(1+(i+j+k)\%d)}$  in parallel for every batch
    3. take the sum over each batch

vtp_score ( $h, r, t$ )
    this part implement the vector triple product scoring techniques:
    score( $h, r, t$ ) =  $\int_{\{0\}} \{1\} h(x)r(x)t(x) dx = \sum_{\{i,j,k=0\}}^{d-1} \frac{a_i * c_j * b_k - b_i * c_j * a_k}{((1+(i+j)\%d)(1+k))}$ 
    1. generate the range for i,j and k from [0 d-1]
    2. Compute the first and second terms of the sum
    3. Multiply with then denominator and take the sum
    4. take the sum over each batch

comp_func ( $h, r, t$ )
    this part implement the function composition scoring techniques: i.e. score = <hor, t>

polynomial (coeff, x, degree)
    This function takes a matrix tensor of coefficients (coeff), a tensor vector of points x and range of integer [0,1,...d] and return a vector tensor ( $coeff[0][0] + coeff[0][1]x + ... + coeff[0][d]x^d$ )

coeff[1][0] + coeff[1][1]x +...+ coeff[1][d]x^d

pop (coeff, x, degree)
    This function allow us to evaluate the composition of two polynomials without for loops :) it takes a matrix tensor of coefficients (coeff), a matrix tensor of points x and range of integer [0,1,...d]
    and return a tensor ( $coeff[0][0] + coeff[0][1]x + ... + coeff[0][d]x^d$ )

coeff[1][0] + coeff[1][1]x +...+ coeff[1][d]x^d

class dicee.models.Duale (args)
Bases: dicee.models.base_model.BaseKGE

Dual Quaternion Knowledge Graph Embeddings (https://ojs.aaai.org/index.php/AAAI/article/download/16850/16657)

```

```

name = 'DualE'

entity_embeddings

relation_embeddings

num_ent = None

kvsall_score(e_1_h, e_2_h, e_3_h, e_4_h, e_5_h, e_6_h, e_7_h, e_8_h, e_1_t, e_2_t, e_3_t, e_4_t,
    e_5_t, e_6_t, e_7_t, e_8_t, r_1, r_2, r_3, r_4, r_5, r_6, r_7, r_8) → torch.tensor
    KvsAll scoring function

```

Input

x: torch.LongTensor with (n,) shape

Output

torch.FloatTensor with (n) shape

```
forward_triples(idx_triple: torch.tensor) → torch.tensor
```

Negative Sampling forward pass:

Input

x: torch.LongTensor with (n,) shape

Output

torch.FloatTensor with (n) shape

```
forward_k_vs_all(x)
```

KvsAll forward pass

Input

x: torch.LongTensor with (n,) shape

Output

torch.FloatTensor with (n) shape

```
T(x: torch.tensor) → torch.tensor
```

Transpose function

Input: Tensor with shape (nxm) Output: Tensor with shape (mxn)

dicee.query_generator

Classes

QueryGenerator

Module Contents

```
class dicee.query_generator.QueryGenerator (train_path: str, val_path: str, test_path: str,
    ent2id: Dict = None, rel2id: Dict = None, seed: int = 1, gen_valid: bool = False,
    gen_test: bool = True)

    train_path
    val_path
    test_path
    gen_valid = False
    gen_test = True
    seed = 1
    max_ans_num = 1000000.0
    mode
    ent2id = None
    rel2id: Dict = None
    ent_in: Dict
    ent_out: Dict
    query_name_to_struct
    list2tuple (list_data)
    tuple2list (x: List | Tuple) → List | Tuple
        Convert a nested tuple to a nested list.
    set_global_seed (seed: int)
        Set seed
    construct_graph (paths: List[str]) → Tuple[Dict, Dict]
        Construct graph from triples Returns dicts with incoming and outgoing edges
    fill_query (query_structure: List[str | List], ent_in: Dict, ent_out: Dict, answer: int) → bool
        Private method for fill_query logic.
    achieve_answer (query: List[str | List], ent_in: Dict, ent_out: Dict) → set
        Private method for achieve_answer logic. @TODO: Document the code
    write_links (ent_out, small_ent_out)
    ground_queries (query_structure: List[str | List], ent_in: Dict, ent_out: Dict, small_ent_in: Dict,
        small_ent_out: Dict, gen_num: int, query_name: str)
        Generating queries and achieving answers
    unmap (query_type, queries, tp_answers, fp_answers, fn_answers)
    unmap_query (query_structure, query, id2ent, id2rel)
```

```

generate_queries (query_struct: List, gen_num: int, query_type: str)
    Passing incoming and outgoing edges to ground queries depending on mode [train valid or text] and getting
    queries and answers in return @ TODO: create a class for each single query struct

save_queries (query_type: str, gen_num: int, save_path: str)

abstract load_queries (path)

get_queries (query_type: str, gen_num: int)

static save_queries_and_answers (path: str, data: List[Tuple[str, Tuple[collections.defaultdict]]])
    → None
    Save Queries into Disk

static load_queries_and_answers (path: str) → List[Tuple[str, Tuple[collections.defaultdict]]]
    Load Queries from Disk to Memory

```

dicee.read_preprocess_save_load_kg

Submodules

dicee.read_preprocess_save_load_kg.preprocess

Classes

| | |
|---------------------|-------------------------------|
| <i>PreprocessKG</i> | Preprocess the data in memory |
|---------------------|-------------------------------|

Module Contents

```

class dicee.read_preprocess_save_load_kg.preprocess.PreprocessKG (kg)
    Preprocess the data in memory

    kg

    start () → None
        Preprocess train, valid and test datasets stored in knowledge graph instance

```

Parameter

| | |
|--|--|
| rtype | |
| None | |
| | |
| preprocess_with_byte_pair_encoding() | |
| preprocess_with_byte_pair_encoding_with_padding() → None | |
| Preprocess with byte pair encoding and add padding | |
| preprocess_with_pandas() → None | |
| Preprocess with pandas: add reciprocal triples, construct vocabulary, and index datasets | |
| preprocess_with_polars() → None | |
| Preprocess with polars: add reciprocal triples and create indexed datasets | |

```
sequential_vocabulary_construction() → None  
    (1) Read input data into memory  
    (2) Remove triples with a condition  
    (3) Serialize vocabularies in a pandas dataframe where  
        => the index is integer and => a single column is string (e.g. URI)
```

dicee.read_preprocess_save_load_kg.read_from_disk

Classes

| | |
|---------------------|-------------------------------------|
| <i>ReadFromDisk</i> | Read the data from disk into memory |
|---------------------|-------------------------------------|

Module Contents

```
class dicee.read_preprocess_save_load_kg.read_from_disk.ReadFromDisk(kg)  
    Read the data from disk into memory  
  
kg  
  
start() → None  
    Read a knowledge graph from disk into memory  
    Data will be available at the train_set, test_set, valid_set attributes.
```

Parameter

None

rtype
None

```
add_noisy_triples_into_training()
```

dicee.read_preprocess_save_load_kg.save_load_disk

Classes

| |
|-----------------------|
| <i>LoadSaveToDisk</i> |
|-----------------------|

Module Contents

```
class dicee.read_preprocess_save_load_kg.save_load_disk.LoadSaveToDisk(kg)  
  
kg  
  
save()  
  
load()
```

dicee.read_preprocess_save_load_kg.util

Functions

| | |
|---|--|
| <code>polars_dataframe_indexer</code> (→ polars.DataFrame) | Replaces 'subject', 'relation', and 'object' columns in the input Polars DataFrame with their corresponding index values |
| <code>pandas_dataframe_indexer</code> (→ pandas.DataFrame) | Replaces 'subject', 'relation', and 'object' columns in the input Pandas DataFrame with their corresponding index values |
| <code>apply_reciprocal_or_noise</code> (add_reciprocal, eval_model) <code>timeit</code> (func) | Add reciprocal triples if conditions are met |
| <code>read_with_polars</code> (→ polars.DataFrame) | Load and Preprocess via Polars |
| <code>read_with_pandas</code> (data_path[, read_only_few, ...]) | Load and Preprocess via Pandas |
| <code>read_from_disk</code> (→ Tuple[polars.DataFrame, pandas.DataFrame]) | |
| <code>count_triples</code> (→ int) | Returns the total number of triples in the triple store. |
| <code>fetch_worker</code> (endpoint, offsets, chunk_size, ...) | Worker process: fetch assigned chunks and save to disk with per-worker tqdm. |
| <code>read_from_triple_store_with_polars</code> (endpoint[, ...]) | Main function to read all triples in parallel, save as Parquet, and load into Polars dataframe. |
| <code>read_from_triple_store_with_pandas</code> ([endpoint]) | Read triples from triple store into pandas dataframe |
| <code>get_er_vocab</code> (data[, file_path]) | |
| <code>get_re_vocab</code> (data[, file_path]) | |
| <code>get_ee_vocab</code> (data[, file_path]) | |
| <code>create_constraints</code> (triples[, file_path]) | |
| <code>load_with_pandas</code> (→ None) | Deserialize data |
| <code>save_numpy_ndarray</code> (* data, file_path) | |
| <code>load_numpy_ndarray</code> (* file_path) | |
| <code>save_pickle</code> (* data[, file_path]) | |
| <code>load_pickle</code> (*[, file_path]) | |
| <code>create_reciprocal_triples</code> (x) | Add inverse triples into dask dataframe |
| <code>dataset_sanity_checking</code> (→ None) | |

Module Contents

```
dicee.read_preprocess_save_load_kg.util.polars_dataframe_indexer(  
    df_polars: polars.DataFrame, idx_entity: polars.DataFrame, idx_relation: polars.DataFrame)  
    → polars.DataFrame  
Replaces 'subject', 'relation', and 'object' columns in the input Polars DataFrame with their corresponding index values from the entity and relation index DataFrames.
```

This function processes the DataFrame in three main steps: 1. Replace the ‘relation’ values with the corresponding index from *idx_relation*. 2. Replace the ‘subject’ values with the corresponding index from *idx_entity*. 3. Replace the ‘object’ values with the corresponding index from *idx_entity*.

Parameters:

df_polars

[polars.DataFrame] The input Polars DataFrame containing columns: ‘subject’, ‘relation’, and ‘object’.

idx_entity

[polars.DataFrame] A Polars DataFrame that contains the mapping between entity names and their corresponding indices. Must have columns: ‘entity’ and ‘index’.

idx_relation

[polars.DataFrame] A Polars DataFrame that contains the mapping between relation names and their corresponding indices. Must have columns: ‘relation’ and ‘index’.

Returns:

polars.DataFrame

A DataFrame with the ‘subject’, ‘relation’, and ‘object’ columns replaced by their corresponding indices.

Example Usage:

```
>>> df_polars = pl.DataFrame({
    "subject": ["Alice", "Bob", "Charlie"],
    "relation": ["knows", "works_with", "lives_in"],
    "object": ["Dave", "Eve", "Frank"]
})
>>> idx_entity = pl.DataFrame({
    "entity": ["Alice", "Bob", "Charlie", "Dave", "Eve", "Frank"],
    "index": [0, 1, 2, 3, 4, 5]
})
>>> idx_relation = pl.DataFrame({
    "relation": ["knows", "works_with", "lives_in"],
    "index": [0, 1, 2]
})
>>> polars_dataframe_indexer(df_polars, idx_entity, idx_relation)
```

Steps:

1. Join the input DataFrame *df_polars* on the ‘relation’ column with *idx_relation* to replace the relations with their indices.
2. Join on ‘subject’ to replace it with the corresponding entity index using a left join on *idx_entity*.
3. Join on ‘object’ to replace it with the corresponding entity index using a left join on *idx_entity*.
4. Select only the ‘subject’, ‘relation’, and ‘object’ columns to return the final result.

```
dicee.read_preprocess_save_load_kg.util.pandas_dataframe_indexer(
    df_pandas: pandas.DataFrame, idx_entity: pandas.DataFrame, idx_relation: pandas.DataFrame)
    → pandas.DataFrame
```

Replaces ‘subject’, ‘relation’, and ‘object’ columns in the input Pandas DataFrame with their corresponding index values from the entity and relation index DataFrames.

Parameters:

df_pandas

[pd.DataFrame] The input Pandas DataFrame containing columns: ‘subject’, ‘relation’, and ‘object’.

idx_entity

[pd.DataFrame] A Pandas DataFrame that contains the mapping between entity names and their corresponding indices. Must have columns: ‘entity’ and ‘index’.

idx_relation

[pd.DataFrame] A Pandas DataFrame that contains the mapping between relation names and their corresponding indices. Must have columns: ‘relation’ and ‘index’.

Returns:

pd.DataFrame

A DataFrame with the ‘subject’, ‘relation’, and ‘object’ columns replaced by their corresponding indices.

```
dicee.read_preprocess_save_load_kg.util.apply_reciprocal_or_noise(add_reciprocal: bool,  
eval_model: str, df: object = None, info: str = None)
```

Add reciprocal triples if conditions are met

```
dicee.read_preprocess_save_load_kg.util.timeit(func)
```

```
dicee.read_preprocess_save_load_kg.util.read_with_polars(data_path,  
read_only_few: int = None, sample_triples_ratio: float = None, separator: str = None)  
→ polars.DataFrame
```

Load and Preprocess via Polars

```
dicee.read_preprocess_save_load_kg.util.read_with_pandas(data_path,  
read_only_few: int = None, sample_triples_ratio: float = None, separator: str = None)
```

Load and Preprocess via Pandas

```
dicee.read_preprocess_save_load_kg.util.read_from_disk(data_path: str,  
read_only_few: int = None, sample_triples_ratio: float = None, backend: str = None,  
separator: str = None) → Tuple[polars.DataFrame, pandas.DataFrame]
```

```
dicee.read_preprocess_save_load_kg.util.count_triples(endpoint: str) → int
```

Returns the total number of triples in the triple store.

```
dicee.read_preprocess_save_load_kg.util.fetch_worker(endpoint: str, offsets: list[int],  
chunk_size: int, output_dir: str, worker_id: int)
```

Worker process: fetch assigned chunks and save to disk with per-worker tqdm.

```
dicee.read_preprocess_save_load_kg.util.read_from_triple_store_with_polars(  
endpoint: str, chunk_size: int = 500000, output_dir: str = 'triples_parquet')
```

Main function to read all triples in parallel, save as Parquet, and load into Polars dataframe.

```
dicee.read_preprocess_save_load_kg.util.read_from_triple_store_with_pandas(  
endpoint: str = None)
```

Read triples from triple store into pandas dataframe

```
dicee.read_preprocess_save_load_kg.util.get_er_vocab(data, file_path: str = None)
```

```
dicee.read_preprocess_save_load_kg.util.get_re_vocab(data, file_path: str = None)
```

```
dicee.read_preprocess_save_load_kg.util.get_ee_vocab(data, file_path: str = None)
```

```
dicee.read_preprocess_save_load_kg.util.create_constraints(triples, file_path: str = None)
```

(1) Extract domains and ranges of relations

(2) Store a mapping from relations to entities that are outside of the domain and range. Create constrained entities based on the range of relations :param triples: :return: Tuple[dict, dict]

```
dicee.read_preprocess_save_load_kg.util.load_with_pandas(self) → None
```

Deserialize data

```
dicee.read_preprocess_save_load_kg.util.save_numpy_ndarray(*, data: numpy.ndarray, file_path: str)
```

```
dicee.read_preprocess_save_load_kg.util.load_numpy_ndarray(*, file_path: str)
```

```
dicee.read_preprocess_save_load_kg.util.save_pickle(*, data: object, file_path=str)
```

```
dicee.read_preprocess_save_load_kg.util.load_pickle(*, file_path=str)
```

```
dicee.read_preprocess_save_load_kg.util.create_recipriocal_triples(x)
```

Add inverse triples into dask dataframe :param x: :return:

```
dicee.read_preprocess_save_load_kg.util.dataset_sanity_checking( train_set: numpy.ndarray, num_entities: int, num_relations: int) → None
```

Parameters

- `train_set`
- `num_entities`
- `num_relations`

Returns

Classes

| | |
|-----------------------------|-------------------------------------|
| <code>PreprocessKG</code> | Preprocess the data in memory |
| <code>LoadSaveToDisk</code> | |
| <code>ReadFromDisk</code> | Read the data from disk into memory |

Package Contents

```
class dicee.read_preprocess_save_load_kg.PreprocessKG(kg)
```

Preprocess the data in memory

`kg`

`start()` → None

Preprocess train, valid and test datasets stored in knowledge graph instance

Parameter

`rtype`

None

```

preprocess_with_byte_pair_encoding()
preprocess_with_byte_pair_encoding_with_padding() → None
    Preprocess with byte pair encoding and add padding

preprocess_with_pandas() → None
    Preprocess with pandas: add reciprocal triples, construct vocabulary, and index datasets

preprocess_with_polars() → None
    Preprocess with polars: add reciprocal triples and create indexed datasets

sequential_vocabulary_construction() → None
    (1) Read input data into memory
    (2) Remove triples with a condition
    (3) Serialize vocabularies in a pandas dataframe where
        => the index is integer and => a single column is string (e.g. URI)

class dicee.read_preprocess_save_load_kg.LoadSaveToDisk(kg)

    kg
    save()
    load()

class dicee.read_preprocess_save_load_kg.ReadFromDisk(kg)
    Read the data from disk into memory
    kg
    start() → None
        Read a knowledge graph from disk into memory
        Data will be available at the train_set, test_set, valid_set attributes.

```

Parameter

None

rtype

None

add_noisy_triples_into_training()

dicee.sanity_checkers

Functions

is_sparql_endpoint_alive([sparql_endpoint])

validate_knowledge_graph(args)
sanity_checking_with_arguments(args)

Validating the source of knowledge graph

sanity_check_callback_args(args) Perform sanity checks on callback-related arguments.

Module Contents

`dicee.sanity_checkers.is_sparql_endpoint_alive(sparql_endpoint: str = None)`

`dicee.sanity_checkers.validate_knowledge_graph(args)`

Validating the source of knowledge graph

`dicee.sanity_checkers.sanity_checking_with_arguments(args)`

`dicee.sanity_checkers.sanity_check_callback_args(args)`

Perform sanity checks on callback-related arguments.

`dicee.scripts`

Submodules

`dicee.scripts.index_serve`

```
$ docker pull qdrant/qdrant && docker run -p 6333:6333 -p 6334:6334 -v $(pwd)/qdrant_storage:/qdrant/storage:z  
qdrant/qdrant $ dicee_vector_db -index -serve -path CountryEmbeddings -collection "countries_vdb"
```

Attributes

`app`

`neural_searcher`

Classes

`NeuralSearcher`

`StringListRequest`

Functions

```
get_default_arguments()  
  
index(args)  
  
root()  
  
search_embeddings(q)  
  
retrieve_embeddings(q)  
  
search_embeddings_batch(request)  
  
serve(args)  
  
main()
```

Module Contents

```
dicee.scripts.index_serve.get_default_arguments()  
  
dicee.scripts.index_serve.index(args)  
  
dicee.scripts.index_serve.app  
  
dicee.scripts.index_serve.neural_searcher = None  
  
class dicee.scripts.index_serve.NeuralSearcher(args)  
  
    collection_name  
  
    entity_to_idx = None  
  
    qdrant_client  
  
    topk = 5  
  
    retrieve_embedding(entity: str = None, entities: List[str] = None) → List  
  
    search(entity: str)  
  
async dicee.scripts.index_serve.root()  
  
async dicee.scripts.index_serve.search_embeddings(q: str)  
  
async dicee.scripts.index_serve.retrieve_embeddings(q: str)  
  
class dicee.scripts.index_serve.StringListRequest  
    Bases: pydantic.BaseModel  
  
    queries: List[str]  
  
    reducer: str | None = None
```

```
async dicee.scripts.index_server.search_embeddings_batch(request: StringListRequest)  
dicee.scripts.index_server.serve(args)  
dicee.scripts.index_server.main()
```

dicee.scripts.run

Functions

| | |
|---|---|
| <code>get_default_arguments([description])</code> | Extends pytorch_lightning Trainer's arguments with ours |
| <code>main()</code> | |

Module Contents

```
dicee.scripts.run.get_default_arguments(description=None)  
    Extends pytorch_lightning Trainer's arguments with ours  
dicee.scripts.run.main()
```

dicee.static_funcs

Functions

| | |
|--|--|
| <code>create_reciprocal_triples(x)</code> | Add inverse triples into dask dataframe |
| <code>get_er_vocab(data[, file_path])</code> | |
| <code>get_re_vocab(data[, file_path])</code> | |
| <code>get_ee_vocab(data[, file_path])</code> | |
| <code>timeit(func)</code> | |
| <code>save_pickle(*[, data, file_path])</code> | |
| <code>load_pickle([file_path])</code> | |
| <code>load_term_mapping([file_path])</code> | |
| <code>select_model(args[, is_continual_training, storage_path])</code> | |
| <code>load_model(→ Tuple[object, Tuple[dict, dict]])</code> | Load weights and initialize pytorch module from namespace arguments |
| <code>load_model_ensemble(...)</code> | Construct Ensemble Of weights and initialize pytorch module from namespace arguments |
| <code>save_numpy_ndarray(*, data, file_path)</code> | |
| <code>numpy_data_type_changer(→ numpy.ndarray)</code> | Detect most efficient data type for a given triples |
| <code>save_checkpoint_model(→ None)</code> | Store Pytorch model into disk |

continues on next page

Table 2 – continued from previous page

| | |
|---|----------------------------------|
| <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> (→ Tuple[object, str]) | |
| <code>load_json</code> (→ dict) | |
| <code>save_embeddings</code> (→ None) | Save it as CSV if memory allows. |
| <code>random_prediction</code> (pre_trained_kge) | |
| <code>deploy_triple_prediction</code> (pre_trained_kge, str_subject, ...) | |
| <code>deploy_tail_entity_prediction</code> (pre_trained_kge, ...) | |
| <code>deploy_head_entity_prediction</code> (pre_trained_kge, ...) | |
| <code>deploy_relation_prediction</code> (pre_trained_kge, ...) | |
| <code>vocab_to_parquet</code> (vocab_to_idx, name, ...) | |
| <code>create_experiment_folder</code> ([folder_name]) | |
| <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, # @TODO: CD: Renamed this function hard_answers) | |
| <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.create_recipriocal_triples(x)
    Add inverse triples into dask dataframe :param x: :return:
dicee.static_funcs.get_er_vocab(data, file_path: str = None)
dicee.static_funcs.get_re_vocab(data, file_path: str = None)
dicee.static_funcs.get_ee_vocab(data, file_path: str = None)
```

```

dicee.static_funcs.timeit(func)

dicee.static_funcs.save_pickle(*args: object = None, file_path=str)

dicee.static_funcs.load_pickle(file_path=str)

dicee.static_funcs.load_term_mapping(file_path=str)

dicee.static_funcs.select_model(args: dict, is_continual_training: bool = None,
                           storage_path: str = None)

dicee.static_funcs.load_model(path_of_experiment_folder: str, model_name='model.pt', verbose=0)
    → Tuple[object, Tuple[dict, dict]]

Load weights and initialize pytorch module from namespace arguments

dicee.static_funcs.load_model_ensemble(path_of_experiment_folder: str)
    → Tuple[dicee.models.base_model.BaseKGE, Tuple[pandas.DataFrame, pandas.DataFrame]]

Construct Ensemble Of weights and initialize pytorch module from namespace arguments

(1) Detect models under given path
(2) Accumulate parameters of detected models
(3) Normalize parameters
(4) Insert (3) into model.

dicee.static_funcs.save_numpy_ndarray(*args: object, file_path: str)

dicee.static_funcs.numpy_data_type_changer(train_set: numpy.ndarray, num: int)
    → numpy.ndarray

Detect most efficient data type for a given triples :param train_set: :param num: :return:

dicee.static_funcs.save_checkpoint_model(model, path: str) → None

Store Pytorch model into disk

dicee.static_funcs.store(trained_model, model_name: str = 'model', full_storage_path: str = None,
                        save_embeddings_as_csv=False) → None

dicee.static_funcs.add_noisy_triples(train_set: pandas.DataFrame, add_noise_rate: float)
    → pandas.DataFrame

Add randomly constructed triples :param train_set: :param add_noise_rate: :return:

dicee.static_funcs.read_or_load_kg(args, cls)

dicee.static_funcs.intialize_model(args: dict, verbose=0) → Tuple[object, str]

dicee.static_funcs.load_json(p: str) → dict

dicee.static_funcs.save_embeddings(embeddings: numpy.ndarray, indexes, path: str) → None

Save it as CSV if memory allows. :param embeddings: :param indexes: :param path: :return:

dicee.static_funcs.random_prediction(pre_trained_kge)

dicee.static_funcs.deploy_triple_prediction(pre_trained_kge, str_subject, str_predicate,
                                             str_object)

dicee.static_funcs.deploy_tail_entity_prediction(pre_trained_kge, str_subject, str_predicate,
                                                 top_k)

```

```

dicee.static_funcs.deploy_head_entity_prediction(pre_trained_kge, str_object, str_predicate,
                                             top_k)

dicee.static_funcs.deploy_relation_prediction(pre_trained_kge, str_subject, str_object, top_k)

dicee.static_funcs.vocab_to_parquet(vocab_to_idx, name, path_for_serialization, print_into)

dicee.static_funcs.create_experiment_folder(folder_name='Experiments')

dicee.static_funcs.continual_training_setup_executor(executor) → None

dicee.static_funcs.exponential_function(x: numpy.ndarray, lam: float, ascending_order=True)
                         → torch.FloatTensor

dicee.static_funcs.load_numpy(path) → numpy.ndarray

dicee.static_funcs.evaluate(entity_to_idx, scores, easy_answers, hard_answers)

# @TODO: CD: Renamed this function Evaluate multi hop query answering on different query types

dicee.static_funcs.download_file(url, destination_folder='.')

dicee.static_funcs.download_files_from_url(base_url: str, destination_folder= '.') → None

```

Parameters

- **base_url** (e.g. “<https://files.dice-research.org/projects/DiceEmbeddings/KINSHIP-Keci-dim128-epoch256-KvsAll>”)
- **destination_folder** (e.g. “*KINSHIP-Keci-dim128-epoch256-KvsAll*”)

```
dicee.static_funcs.download_pretrained_model(url: str) → str
```

```
dicee.static_funcs.write_csv_from_model_parallel(path: str)
```

Create

```
dicee.static_funcs.from_pretrained_model_write_embeddings_into_csv(path: str) → None
```

dicee.static_funcs_training

Functions

`make_iterable_verbose`(→ Iterable)

`evaluate_lp`([model, triple_idx, num_entities, ...])

`evaluate_bpe_lp`(model, triple_idx, ...[, info])

`efficient_zero_grad`(model)

Module Contents

```
dicee.static_funcs_training.make_iterable_verbose(iterable_object, verbose, desc='Default',
                                                 position=None, leave=True) → Iterable
```

```

dicee.static_funcs_training.evaluate_lp(model=None, triple_idx=None, num_entities=None,
    er_vocab: Dict[Tuple, List] = None, re_vocab: Dict[Tuple, List] = None, info='Eval Starts',
    batch_size=128, chunk_size=1000)

dicee.static_funcs_training.evaluate_bpe_lp(model, triple_idx: List[Tuple],
    all_bpe_shaped_entities, er_vocab: Dict[Tuple, List], re_vocab: Dict[Tuple, List],
    info='Eval Starts')

dicee.static_funcs_training.efficient_zero_grad(model)

```

dicee.static_preprocess_funcs

Attributes

| |
|-------------------------|
| <code>enable_log</code> |
|-------------------------|

Functions

| | |
|--|------------------------------------|
| <code>timeit(func)</code> | |
| <code>preprocesses_input_args(args)</code> | Sanity Checking in input arguments |
| <code>create_constraints(→ Tuple[dict, dict, dict, dict])</code> | |
| <code>get_er_vocab(data)</code> | |
| <code>get_re_vocab(data)</code> | |
| <code>get_ee_vocab(data)</code> | |
| <code>mapping_from_first_two_cols_to_third(train_se</code> | |

Module Contents

```

dicee.static_preprocess_funcs.enable_log = False

dicee.static_preprocess_funcs.timeit(func)

dicee.static_preprocess_funcs.preprocesses_input_args(args)
    Sanity Checking in input arguments

dicee.static_preprocess_funcs.create_constraints(triples: numpy.ndarray)
    → Tuple[dict, dict, dict, dict]

    (1) Extract domains and ranges of relations

    (2) Store a mapping from relations to entities that are outside of the domain and range. Create constraints entities
        based on the range of relations :param triples: :return:

dicee.static_preprocess_funcs.get_er_vocab(data)

dicee.static_preprocess_funcs.get_re_vocab(data)

```

```
dicee.static_preprocess_funcs.get_ee_vocab(data)
dicee.static_preprocess_funcs.mapping_from_first_two_cols_to_third(train_set_idx)
```

dicee.trainer

Submodules

dicee.trainer.dice_trainer

Classes

DICE_Trainer

DICE_Trainer implement

Functions

```
load_term_mapping([file_path])
initialize_trainer(...)
get_callbacks(args)
```

Module Contents

```
dicee.trainer.dice_trainer.load_term_mapping(file_path=str)
dicee.trainer.dice_trainer.initialize_trainer(args, callbacks)
    → dicee.trainer.torch_trainer.TorchTrainer | dicee.trainer.model_parallelism.TensorParallel | dicee.trainer.torch_trainer_ddp
dicee.trainer.dice_trainer.get_callbacks(args)

class dicee.trainer.dice_trainer.DICE_Trainer(args, is_continual_training: bool, storage_path,
                                              evaluator=None)

DICE_Trainer implement
1- Pytorch Lightning trainer (https://pytorch-lightning.readthedocs.io/en/stable/common/trainer.html)
2- Multi-GPU Trainer(https://pytorch.org/docs/stable/generated/torch.nn.parallel.DistributedDataParallel.html)
3- CPU Trainer

args
is_continual_training:bool
storage_path:str
evaluator:
report:dict

report
args
trainer = None
```

```

is_continual_training
storage_path
evaluator = None
form_of_labelling = None
continual_start(knowledge_graph)

```

- (1) Initialize training.
- (2) Load model
- (3) Load trainer (3) Fit model

Parameter

returns

- *model*
- **form_of_labelling** (*str*)

initialize_trainer (*callbacks: List*)

→ lightning.Trainer | dicee.trainer.model_parallelism.TensorParallel | dicee.trainer.torch_trainer.TorchTrainer | dicee.

Initialize Trainer from input arguments

initialize_or_load_model ()

init_dataloader (*dataset: torch.utils.data.Dataset*) → torch.utils.data.DataLoader

init_dataset () → torch.utils.data.Dataset

start (*knowledge_graph: dicee.knowledge_graph.KG* | *numpy.memmap*)

→ Tuple[dicee.models.base_model.BaseKGE, str]

Start the training

- (1) Initialize Trainer
- (2) Initialize or load a pretrained KGE model

in DDP setup, we need to load the memory map of already read/index KG.

k_fold_cross_validation (*dataset*) → Tuple[dicee.models.base_model.BaseKGE, str]

Perform K-fold Cross-Validation

1. Obtain K train and test splits.
2. **For each split,**
 - 2.1 initialize trainer and model
 - 2.2. Train model with configuration provided in args.
 - 2.3. Compute the mean reciprocal rank (MRR) score of the model on the test respective split.
3. Report the mean and average MRR .

Parameters

- **self**
- **dataset**

Returns

model

dicee.trainer.model_parallelism

Classes

`TensorParallel`

Abstract class for Trainer class for knowledge graph embedding models

Functions

```
extract_input_outputs(z[, device])
find_good_batch_size(train_loader,
tp_ensemble_model)
forward_backward_update_loss(→ float)
```

Module Contents

```
dicee.trainer.model_parallelism.extract_input_outputs (z: list, device=None)
dicee.trainer.model_parallelism.find_good_batch_size (train_loader, tp_ensemble_model)
dicee.trainer.model_parallelism.forward_backward_update_loss (z: Tuple, ensemble_model)
    → float
class dicee.trainer.model_parallelism.TensorParallel (args, callbacks)
    Bases: dicee.abstracts.AbstractTrainer
    Abstract class for Trainer class for knowledge graph embedding models
```

Parameter

```
args
    [str] ?
callbacks: list
    ?
fit (*args, **kwargs)
    Train model
```

dicee.trainer.torch_trainer

Classes

`TorchTrainer`

TorchTrainer for using single GPU or multi CPUs on a single node

Module Contents

```
class dicee.trainer.torch_trainer.TorchTrainer(args, callbacks)
```

Bases: `dicee.abstracts.AbstractTrainer`

TorchTrainer for using single GPU or multi CPUs on a single node

Arguments

callbacks: list of Abstract callback instances

```
loss_function = None
```

```
optimizer = None
```

```
model = None
```

```
train_dataloaders = None
```

```
training_step = None
```

```
process
```

```
fit(*args, train_dataloaders, **kwargs) → None
```

Training starts

Arguments

kwargs:Tuple

empty dictionary

Return type

batch loss (float)

```
forward_backward_update(x_batch: torch.Tensor, y_batch: torch.Tensor) → torch.Tensor
```

Compute forward, loss, backward, and parameter update

Arguments

Return type

batch loss (float)

```
extract_input_outputs_set_device(batch: list) → Tuple
```

Construct inputs and outputs from a batch of inputs with outputs From a batch of inputs and put

Arguments

Return type

(tuple) mini-batch on select device

dicee.trainer.torch_trainer_ddp

Classes

`TorchDDPTrainer`
`NodeTrainer`

A Trainer based on torch.nn.parallel.DistributedDataParallel

Functions

`make_iterable_verbose`(\rightarrow Iterable)

Module Contents

`dicee.trainer.torch_trainer_ddp.make_iterable_verbose`(*iterable_object*, *verbose*,
desc='Default', *position=None*, *leave=True*) \rightarrow Iterable

class `dicee.trainer.torch_trainer_ddp.TorchDDPTrainer`(*args*, *callbacks*)

Bases: `dicee.abstracts.AbstractTrainer`

A Trainer based on torch.nn.parallel.DistributedDataParallel

Arguments

entity_idxs
mapping.

relation_idxs
mapping.

form
?

store
?

label_smoothing_rate

Using hard targets (0,1) drives weights to infinity. An outlier produces enormous gradients.

Return type

`torch.utils.data.Dataset`

fit(**args*, ***kwargs*)

Train model

class `dicee.trainer.torch_trainer_ddp.NodeTrainer`(*trainer*, *model*: `torch.nn.Module`,
train_dataset_loader: `torch.utils.data.DataLoader`, *callbacks*, *num_epochs*: `int`)

trainer

local_rank

global_rank

```

optimizer
train_dataset_loader
loss_func
callbacks
model
num_epochs
loss_history = []
ctx
scaler
extract_input_outputs(z: list)
train()
    Training loop for DDP

```

Classes

| | |
|---------------------|------------------------|
| <i>DICE_Trainer</i> | DICE_Trainer implement |
|---------------------|------------------------|

Package Contents

```
class dicee.trainer.DICE_Trainer(args, is_continual_training: bool, storage_path, evaluator=None)
```

DICE_Trainer implement

- 1- Pytorch Lightning trainer (<https://pytorch-lightning.readthedocs.io/en/stable/common/trainer.html>)
- 2- Multi-GPU Trainer(<https://pytorch.org/docs/stable/generated/torch.nn.parallel.DistributedDataParallel.html>)
- 3- CPU Trainer

```

args
is_continual_training:bool
storage_path:str
evaluator:
report:dict

report

args

trainer = None

is_continual_training

storage_path

evaluator = None

form_of_labelling = None

```

```
continual_start (knowledge_graph)
```

- (1) Initialize training.
- (2) Load model
- (3) Load trainer (3) Fit model

Parameter

returns

- *model*
- **form_of_labelling** (*str*)

```
initialize_trainer (callbacks: List)
```

→ lightning.Trainer | dicee.trainer.model_parallelism.TensorParallel | dicee.trainer.torch_trainer.TorchTrainer | dicee.

Initialize Trainer from input arguments

```
initialize_or_load_model ()
```

```
init_dataloader (dataset: torch.utils.data.Dataset) → torch.utils.data.DataLoader
```

```
init_dataset () → torch.utils.data.Dataset
```

```
start (knowledge_graph: dicee.knowledge_graph.KG | numpy.memmap)
```

→ Tuple[*dicee.models.base_model.BaseKGE*, *str*]

Start the training

- (1) Initialize Trainer
- (2) Initialize or load a pretrained KGE model

in DDP setup, we need to load the memory map of already read/index KG.

```
k_fold_cross_validation (dataset) → Tuple[dicee.models.base_model.BaseKGE, str]
```

Perform K-fold Cross-Validation

1. Obtain K train and test splits.
2. **For each split**,
2.1 initialize trainer and model 2.2. Train model with configuration provided in args. 2.3. Compute the mean reciprocal rank (MRR) score of the model on the test respective split.
3. Report the mean and average MRR .

Parameters

- **self**
- **dataset**

Returns

model

14.2 Attributes

```
__version__
```

14.3 Classes

| | |
|--|--|
| <i>Pyke</i> | A Physical Embedding Model for Knowledge Graphs |
| <i>DistMult</i> | Embedding Entities and Relations for Learning and Inference in Knowledge Bases |
| <i>CKeci</i> | Without learning dimension scaling |
| <i>Keci</i> | Base class for all neural network modules. |
| <i>TransE</i> | Translating Embeddings for Modeling |
| <i>DeCaL</i> | Base class for all neural network modules. |
| <i>Duale</i> | Dual Quaternion Knowledge Graph Embeddings (https://ojs.aaai.org/index.php/AAAI/article/download/16850/16657) |
| <i>ComplEx</i> | Base class for all neural network modules. |
| <i>AConEx</i> | Additive Convolutional ComplEx Knowledge Graph Embeddings |
| <i>AConvO</i> | Additive Convolutional Octonion Knowledge Graph Embeddings |
| <i>AConvQ</i> | Additive Convolutional Quaternion Knowledge Graph Embeddings |
| <i>ConvQ</i> | Convolutional Quaternion Knowledge Graph Embeddings |
| <i>ConvO</i> | Base class for all neural network modules. |
| <i>ConEx</i> | Convolutional ComplEx Knowledge Graph Embeddings |
| <i>QMult</i> | Base class for all neural network modules. |
| <i>OMult</i> | Base class for all neural network modules. |
| <i>Shallom</i> | A shallow neural model for relation prediction (https://arxiv.org/abs/2101.09090) |
| <i>LFMult</i> | Embedding with polynomial functions. We represent all entities and relations in the polynomial space as: |
| <i>CoKE</i> | Contextualized Knowledge Graph Embedding (CoKE) model. |
| <i>PykeenKGE</i> | A class for using knowledge graph embedding models implemented in Pykeen |
| <i>Byte</i> | Base class for all neural network modules. |
| <i>BaseKGE</i> | Base class for all neural network modules. |
| <i>EnsembleKGE</i> | |
| <i>DICE_Trainer</i> | DICE_Trainer implement |
| <i>KGE</i> | Knowledge Graph Embedding Class for interactive usage of pre-trained models |
| <i>BPE_NegativeSamplingDataset</i> | An abstract class representing a Dataset. |
| <i>MultiLabelDataset</i> | An abstract class representing a Dataset. |
| <i>MultiClassClassificationDataset</i> | Dataset for the 1vsALL training strategy |
| <i>OnevsAllDataset</i> | Dataset for the 1vsALL training strategy |
| <i>KvsAll</i> | Creates a dataset for KvsAll training by inheriting from torch.utils.data.Dataset. |
| <i>AllvsAll</i> | Creates a dataset for AllvsAll training by inheriting from torch.utils.data.Dataset. |
| <i>OnevsSample</i> | A custom PyTorch Dataset class for knowledge graph embeddings, which includes |
| <i>KvsSampleDataset</i> | KvsSample a Dataset: |
| <i>NegSampleDataset</i> | An abstract class representing a Dataset. |

continues on next page

Table 3 – continued from previous page

| | |
|--------------------------------|---|
| <i>TriplePredictionDataset</i> | Triple Dataset |
| <i>CVDataModule</i> | Create a Dataset for cross validation |
| <i>LiteralDataset</i> | Dataset for loading and processing literal data for training Literal Embedding model. |
| <i>QueryGenerator</i> | |

14.4 Functions

| | |
|---|--|
| <i>create_reciprocal_triples</i> (x) | Add inverse triples into dask dataframe |
| <i>get_er_vocab</i> (data[, file_path]) | |
| <i>get_re_vocab</i> (data[, file_path]) | |
| <i>get_ee_vocab</i> (data[, file_path]) | |
| <i>timeit</i> (func) | |
| <i>save_pickle</i> (*[, data, file_path]) | |
| <i>load_pickle</i> ([file_path]) | |
| <i>load_term_mapping</i> ([file_path]) | |
| <i>select_model</i> (args[, is_continual_training, storage_path]) | |
| <i>load_model</i> (→ Tuple[object, Tuple[dict, dict]]) | Load weights and initialize pytorch module from namespace arguments |
| <i>load_model_ensemble</i> (...) | Construct Ensemble Of weights and initialize pytorch module from namespace arguments |
| <i>save_numpy_ndarray</i> (*[, data, file_path]) | |
| <i>numpy_data_type_changer</i> (→ numpy.ndarray) | Detect most efficient data type for a given triples |
| <i>save_checkpoint_model</i> (→ None) | Store Pytorch model into disk |
| <i>store</i> (→ None) | |
| <i>add_noisy_triples</i> (→ pandas.DataFrame) | Add randomly constructed triples |
| <i>read_or_load_kg</i> (args, cls) | |
| <i>intialize_model</i> (→ Tuple[object, str]) | |
| <i>load_json</i> (→ dict) | |
| <i>save_embeddings</i> (→ None) | Save it as CSV if memory allows. |
| <i>random_prediction</i> (pre_trained_kge) | |
| <i>deploy_triple_prediction</i> (pre_trained_kge, str_subject, ...) | |
| <i>deploy_tail_entity_prediction</i> (pre_trained_kge, ...) | |

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Table 4 – continued from previous page

| | |
|---|---|
| <code>deploy_head_entity_prediction</code> (<code>pre_trained_kge</code> , ...) | |
| <code>deploy_relation_prediction</code> (<code>pre_trained_kge</code> , ...) | |
| <code>vocab_to_parquet</code> (<code>vocab_to_idx</code> , <code>name</code> , ...) | |
| <code>create_experiment_folder</code> ([<code>folder_name</code>]) | |
| <code>continual_training_setup_executor</code> (→ <code>None</code>) | |
| <code>exponential_function</code> (→ <code>torch.FloatTensor</code>) | |
| <code>load_numpy</code> (→ <code>numpy.ndarray</code>) | |
| <code>evaluate</code> (<code>entity_to_idx</code> , <code>scores</code> , <code>easy_answers</code> , # @TODO: CD: Renamed this function <code>hard_answers</code>) | |
| <code>download_file</code> (<code>url</code> [, <code>destination_folder</code>]) | |
| <code>download_files_from_url</code> (→ <code>None</code>) | |
| <code>download_pretrained_model</code> (→ <code>str</code>) | |
| <code>write_csv_from_model_parallel</code> (<code>path</code>) | Create |
| <code>from_pretrained_model_write_embeddings_int</code> (<code>None</code>) | |
| <code>mapping_from_first_two_cols_to_third</code> (<code>train_se</code>) | |
| <code>timeit</code> (<code>func</code>) | |
| <code>load_term_mapping</code> ([<code>file_path</code>]) | |
| <code>reload_dataset</code> (<code>path</code> , <code>form_of_labelling</code> , ...) | Reload the files from disk to construct the Pytorch dataset |
| <code>construct_dataset</code> (→ <code>torch.utils.data.Dataset</code>) | |

14.5 Package Contents

```
class dicee.Pyke(args)
    Bases: dicee.models.base_model.BaseKGE
    A Physical Embedding Model for Knowledge Graphs
    name = 'Pyke'
    dist_func
    margin = 1.0
    forward_triples(x: torch.LongTensor)
```

Parameters

`x`

```
class dicee.DistMult(args)
Bases: dicee.models.base_model.BaseKGE
Embedding Entities and Relations for Learning and Inference in Knowledge Bases https://arxiv.org/abs/1412.6575
```

```
name = 'DistMult'
k_vs_all_score(emb_h: torch.FloatTensor, emb_r: torch.FloatTensor, emb_E: torch.FloatTensor)
```

Parameters

- emb_h
- emb_r
- emb_E

```
forward_k_vs_all(x: torch.LongTensor)
```

```
forward_k_vs_sample(x: torch.LongTensor, target_entity_idx: torch.LongTensor)
```

```
score(h, r, t)
```

```
class dicee.CKeci(args)
```

Bases: *Keci*

Without learning dimension scaling

```
name = 'CKeci'
```

```
requires_grad_for_interactions = False
```

```
class dicee.Keci(args)
```

Bases: dicee.models.base_model.BaseKGE

Base class for all neural network modules.

Your models should also subclass this class.

Modules can also contain other Modules, allowing them to be nested in a tree structure. You can assign the sub-modules as regular attributes:

```
import torch.nn as nn
import torch.nn.functional as F

class Model(nn.Module):
    def __init__(self) -> None:
        super().__init__()
        self.conv1 = nn.Conv2d(1, 20, 5)
        self.conv2 = nn.Conv2d(20, 20, 5)

    def forward(self, x):
        x = F.relu(self.conv1(x))
        return F.relu(self.conv2(x))
```

Submodules assigned in this way will be registered, and will also have their parameters converted when you call `to()`, etc.

Note

As per the example above, an `__init__()` call to the parent class must be made before assignment on the child.

Variables

`training (bool)` – Boolean represents whether this module is in training or evaluation mode.

```
name = 'Keci'

p
q
r

requires_grad_for_interactions = True

compute_sigma_pp(hp, rp)
    Compute sigma_{pp} = sum_{i=1}^{p-1} sum_{k=i+1}^p (h_i r_k - h_k r_i) e_i e_k
    sigma_{pp} captures the interactions between along p bases For instance, let p e_1, e_2, e_3, we compute
    interactions between e_1 e_2, e_1 e_3 , and e_2 e_3 This can be implemented with a nested two for loops
    results = [] for i in range(p - 1):
        for k in range(i + 1, p):
            results.append(hp[:, :, i] * rp[:, :, k] - hp[:, :, k] * rp[:, :, i])
    sigma_pp = torch.stack(results, dim=2) assert sigma_pp.shape == (b, r, int((p * (p - 1)) / 2))
```

Yet, this computation would be quite inefficient. Instead, we compute interactions along all p, e.g., e1e1, e1e2, e1e3,

e2e1, e2e2, e2e3, e3e1, e3e2, e3e3

Then select the triangular matrix without diagonals: e1e2, e1e3, e2e3.

```
compute_sigma_qq(hq, rq)
    Compute sigma_{qq} = sum_{j=1}^{p+q-1} sum_{k=j+1}^{p+q} (h_j r_k - h_k r_j) e_j e_k sigma_{q}
    sigma_{qq} captures the interactions between along q bases For instance, let q e_1, e_2, e_3, we compute interactions
    between e_1 e_2, e_1 e_3 , and e_2 e_3 This can be implemented with a nested two for loops
```

results = [] for j in range(q - 1):
 for k in range(j + 1, q):
 results.append(hq[:, :, j] * rq[:, :, k] - hq[:, :, k] * rq[:, :, j])
 sigma_qq = torch.stack(results, dim=2) assert sigma_qq.shape == (b, r, int((q * (q - 1)) / 2))

Yet, this computation would be quite inefficient. Instead, we compute interactions along all p, e.g., e1e1, e1e2, e1e3,

e2e1, e2e2, e2e3, e3e1, e3e2, e3e3

Then select the triangular matrix without diagonals: e1e2, e1e3, e2e3.

```
compute_sigma_pq(*, hp, hq, rp, rq)
    sum_{i=1}^p sum_{j=p+1}^{p+q} (h_i r_j - h_j r_i) e_i e_j
    results = [] sigma_pq = torch.zeros(b, r, p, q) for i in range(p):
```

```

for j in range(q):
    sigma_pq[:, :, i, j] = hp[:, :, i] * rq[:, :, j] - hq[:, :, j] * rp[:, :, i]
    print(sigma_pq.shape)

apply_coefficients (hp, hq, rp, rq)
    Multiplying a base vector with its scalar coefficient

clifford_multiplication (h0, hp, hq, r0, rp, rq)
    Compute our CL multiplication
        h = h_0 + sum_{i=1}^p h_i e_i + sum_{j=p+1}^{p+q} h_j e_j
        r = r_0 + sum_{i=1}^p r_i e_i +
        sum_{j=p+1}^{p+q} r_j e_j
        ei ^2 = +1 for i <= p ej ^2 = -1 for p < j <= p+q ei ej = -eje1 for i
        eq j
        h r = sigma_0 + sigma_p + sigma_q + sigma_{pp} + sigma_{q} + sigma_{pq} where
        (1) sigma_0 = h_0 r_0 + sum_{i=1}^p (h_0 r_i) e_i - sum_{j=p+1}^{p+q} (h_j r_j) e_j
        (2) sigma_p = sum_{i=1}^p (h_0 r_i + h_i r_0) e_i
        (3) sigma_q = sum_{j=p+1}^{p+q} (h_0 r_j + h_j r_0) e_j
        (4) sigma_{pp} = sum_{i=1}^{p-1} sum_{k=i+1}^p (h_i r_k - h_k r_i) e_i e_k
        (5) sigma_{qq} = sum_{j=1}^{p+q-1} sum_{k=j+1}^{p+q} (h_j r_k - h_k r_j) e_j e_k
        (6) sigma_{pq} = sum_{i=1}^p sum_{j=p+1}^{p+q} (h_i r_j - h_j r_i) e_i e_j

construct_cl_multivector (x: torch.FloatTensor, r: int, p: int, q: int)
    → tuple[torch.FloatTensor, torch.FloatTensor, torch.FloatTensor]
Construct a batch of multivectors Cl_{p,q}(mathbb{R})^d

```

Parameter

x: torch.FloatTensor with (n,d) shape

returns

- **a0** (torch.FloatTensor with (n,r) shape)
- **ap** (torch.FloatTensor with (n,r,p) shape)
- **aq** (torch.FloatTensor with (n,r,q) shape)

forward_k_vs_with_explicit (x: torch.Tensor)

k_vs_all_score (bpe_head_ent_emb, bpe_rel_ent_emb, E)

forward_k_vs_all (x: torch.Tensor) → torch.FloatTensor

Kvsall training

- (1) Retrieve real-valued embedding vectors for heads and relations mathbb{R}^d .
- (2) Construct head entity and relation embeddings according to Cl_{p,q}(mathbb{R}^d) .
- (3) Perform Cl multiplication
- (4) Inner product of (3) and all entity embeddings

forward_k_vs_with_explicit and this funcitons are identical Parameter ——— x: torch.LongTensor with (n,2) shape :rtype: torch.FloatTensor with (n, |E|) shape

```
construct_batch_selected_cl_multivector(x: torch.FloatTensor, r: int, p: int, q: int)
    → tuple[torch.FloatTensor, torch.FloatTensor, torch.FloatTensor]
```

Construct a batch of batchs multivectors $\text{Cl}_{\{p,q\}}(\mathbb{R}^d)$

Parameter

x: torch.FloatTensor with (n,k, d) shape

returns

- **a0** (torch.FloatTensor with (n, k, m) shape)
- **ap** (torch.FloatTensor with (n, k, m, p) shape)
- **aq** (torch.FloatTensor with (n, k, m, q) shape)

```
forward_k_vs_sample(x: torch.LongTensor, target_entity_idx: torch.LongTensor) → torch.FloatTensor
```

Parameter

x: torch.LongTensor with (n,2) shape

target_entity_idx: torch.LongTensor with (n, k) shape k denotes the selected number of examples.

rtype

torch.FloatTensor with (n, k) shape

```
score(h, r, t)
```

```
forward_triples(x: torch.Tensor) → torch.FloatTensor
```

Parameter

x: torch.LongTensor with (n,3) shape

rtype

torch.FloatTensor with (n) shape

```
class dicee.TransE(args)
```

Bases: *dicee.models.base_model.BaseKGE*

Translating Embeddings for Modeling Multi-relational Data <https://proceedings.neurips.cc/paper/2013/file/1cecc7a77928ca8133fa24680a88d2f9-Paper.pdf>

```
name = 'TransE'
```

```
margin = 4
```

```
score(head_ent_emb, rel_ent_emb, tail_ent_emb)
```

```
forward_k_vs_all(x: torch.Tensor) → torch.FloatTensor
```

```
class dicee.DeCaL(args)
```

Bases: *dicee.models.base_model.BaseKGE*

Base class for all neural network modules.

Your models should also subclass this class.

Modules can also contain other Modules, allowing them to be nested in a tree structure. You can assign the sub-modules as regular attributes:

```

import torch.nn as nn
import torch.nn.functional as F

class Model(nn.Module):
    def __init__(self) -> None:
        super().__init__()
        self.conv1 = nn.Conv2d(1, 20, 5)
        self.conv2 = nn.Conv2d(20, 20, 5)

    def forward(self, x):
        x = F.relu(self.conv1(x))
        return F.relu(self.conv2(x))

```

Submodules assigned in this way will be registered, and will also have their parameters converted when you call `to()`, etc.

Note

As per the example above, an `__init__()` call to the parent class must be made before assignment on the child.

Variables

`training (bool)` – Boolean represents whether this module is in training or evaluation mode.

```

name = 'DeCaL'

entity_embeddings

relation_embeddings

p

q

r

re

forward_triples(x: torch.Tensor) → 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:

$$\text{sigma}_0 t = \sigma_0 \cdot t_0 = s0 + s1 - s2s3, s4 \text{ and } s5$$

compute_sigmas_multivect (*list_h_emb*, *list_r_emb*)

Here we compute and return all the sums with vectors interaction for the same and different bases.

For same bases vectors interaction we have

$$\sigma_p p = \sum_{i=1}^{p-1} \sum_{i'=i+1}^p (h_i r_{i'} - h_{i'} r_i) \text{ (models the interactions between } e_i \text{ and } e'_{i'} \text{ for } 1 \leq i, i' \leq p) \sigma_q q = \sum_{j=p+1}^{p+q-1} \sum_{j'=j+1}^{p+q} (h_j r_{j'} - h_{j'} r_j) \text{ (interactions between } e_i \text{ and } e_j \text{ for } 1 \leq i \leq p \text{ and } p+1 \leq j \leq p+q) \sigma_p r = \sum_{i=1}^p (h_i r_i - h_i r_i)$$

For different base vector interactions, we have

$$\sigma_p q = \sum_{i=1}^p \sum_{j=p+1}^{p+q} (h_i r_j - h_j r_i) \text{ (interactions between } e_i \text{ and } e_j \text{ for } 1 \leq i \leq p \text{ and } p+1 \leq j \leq p+q) \sigma_p r = \sum_{i=1}^p (h_i r_i - h_i r_i)$$

forward_k_vs_all (*x*: *torch.Tensor*) → *torch.FloatTensor*

Kvsall training

- (1) Retrieve real-valued embedding vectors for heads and relations
- (2) Construct head entity and relation embeddings according to $\text{Cl}_{\{p,q,r\}}(\mathbb{R}^d)$.
- (3) Perform Cl multiplication
- (4) Inner product of (3) and all entity embeddings

forward_k_vs_with_explicit and this funcitons are identical Parameter ——— *x*: *torch.LongTensor* with (n,) shape :rtype: *torch.FloatTensor* with (n, |E|) shape

apply_coefficients (*h0*, *hp*, *hq*, *hk*, *r0*, *rp*, *rq*, *rk*)

Multiplying a base vector with its scalar coefficient

construct_cl_multivector (*x*: *torch.FloatTensor*, *re*: int, *p*: int, *q*: int, *r*: int)

→ tuple[*torch.FloatTensor*, *torch.FloatTensor*, *torch.FloatTensor*]

Construct a batch of multivectors $\text{Cl}_{\{p,q,r\}}(\mathbb{R}^d)$

Parameter

x: *torch.FloatTensor* with (n,d) shape

returns

- **a0** (*torch.FloatTensor*)
- **ap** (*torch.FloatTensor*)
- **aq** (*torch.FloatTensor*)
- **ar** (*torch.FloatTensor*)

```
compute_sigma_pp(hp, rp)
```

Compute .. math:

$$\sigma_{p,p}^* = \sum_{i=1}^{p-1} \sum_{i'=i+1}^p (x_i y_{i'} - x_{i'} y_i)$$

$\sigma_{p,p}$ captures the interactions between along p bases For instance, let $p = 1, 2, 3$, we compute interactions between $e_1 e_2, e_1 e_3$, and $e_2 e_3$. This can be implemented with a nested two for loops

results = [] for i in range(p - 1):

```
for k in range(i + 1, p):
```

```
    results.append(hp[:, :, i] * rp[:, :, k] - hp[:, :, k] * rp[:, :, i])
```

```
sigma_pp = torch.stack(results, dim=2) assert sigma_pp.shape == (b, r, int((p * (p - 1)) / 2))
```

Yet, this computation would be quite inefficient. Instead, we compute interactions along all p, e.g., $e_1 e_1, e_1 e_2, e_1 e_3, e_2 e_1, e_2 e_2, e_2 e_3, e_3 e_1, e_3 e_2, e_3 e_3$

Then select the triangular matrix without diagonals: $e_1 e_2, e_1 e_3, e_2 e_3$.

```
compute_sigma_qq(hq, rq)
```

Compute

$$\sigma_{q,q}^* = \sum_{j=p+1}^{p+q-1} \sum_{j'=j+1}^{p+q} (x_j y_{j'} - x_{j'} y_j) Eq.16$$

$\sigma_{q,q}$ captures the interactions between along q bases For instance, let $q = 1, 2, 3$, we compute interactions between $e_1 e_2, e_1 e_3$, and $e_2 e_3$. This can be implemented with a nested two for loops

results = [] for j in range(q - 1):

```
for k in range(j + 1, q):
```

```
    results.append(hq[:, :, j] * rq[:, :, k] - hq[:, :, k] * rq[:, :, j])
```

```
sigma_qq = torch.stack(results, dim=2) assert sigma_qq.shape == (b, r, int((q * (q - 1)) / 2))
```

Yet, this computation would be quite inefficient. Instead, we compute interactions along all p, e.g., $e_1 e_1, e_1 e_2, e_1 e_3, e_2 e_1, e_2 e_2, e_2 e_3, e_3 e_1, e_3 e_2, e_3 e_3$

e2e1, e2e2, e2e3, e3e1, e3e2, e3e3

Then select the triangular matrix without diagonals: $e_1 e_2, e_1 e_3, e_2 e_3$.

```
compute_sigma_rr(hk, rk)
```

$$\sigma_{r,r}^* = \sum_{k=p+q+1}^{p+q+r-1} \sum_{k'=k+1}^p (x_k y_{k'} - x_{k'} y_k)$$

```
compute_sigma_pq(* , hp, hq, rp, rq)
```

Compute

$$\sum_{i=1}^p \sum_{j=p+1}^{p+q} (h_i r_j - h_j r_i) e_i e_j$$

results = [] sigma_pq = torch.zeros(b, r, p, q) for i in range(p):

```
for j in range(q):
```

```
    sigma_pq[:, :, i, j] = hp[:, :, i] * rq[:, :, j] - hq[:, :, j] * rp[:, :, i]
```

```

print(sigma_pq.shape)

compute_sigma_pr(*hp, hk, rp, rk)
    Compute

$$\sum_{i=1}^p \sum_{j=p+1}^{p+q} (h_i r_j - h_j r_i) e_i e_j$$

results = [] sigma_pq = torch.zeros(b, r, p, q) for i in range(p):
    for j in range(q):
        sigma_pq[:, :, i, j] = hp[:, :, i] * rq[:, :, j] - hk[:, :, 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] - hk[:, :, j] * rp[:, :, i]
    print(sigma_pq.shape)

class dicee.Duale(args)
Bases: dicee.models.base_model.BaseKGE

Dual Quaternion Knowledge Graph Embeddings (https://ojs.aaai.org/index.php/AAAI/article/download/16850/16657)
    name = 'DualE'

    entity_embeddings
    relation_embeddings
    num_ent = None

    kvsall_score(e_1_h, e_2_h, e_3_h, e_4_h, e_5_h, e_6_h, e_7_h, e_8_h, e_1_t, e_2_t, e_3_t, e_4_t,
                  e_5_t, e_6_t, e_7_t, e_8_t, r_1, r_2, r_3, r_4, r_5, r_6, r_7, r_8) → torch.tensor
        KvsAll scoring function

```

Input

x: torch.LongTensor with (n,) shape

Output

torch.FloatTensor with (n) shape

forward_triples(idx_triple: torch.tensor) → torch.tensor

Negative Sampling forward pass:

Input

x: torch.LongTensor with (n,) shape

Output

torch.FloatTensor with (n) shape

```
forward_k_vs_all(x)
```

KvsAll forward pass

Input

x: torch.LongTensor with (n,) shape

Output

torch.FloatTensor with (n) shape

```
T(x: torch.tensor) → torch.tensor
```

Transpose function

Input: Tensor with shape (nxm) Output: Tensor with shape (mxn)

```
class dicee.Complex(args)
```

Bases: dicee.models.base_model.BaseKGE

Base class for all neural network modules.

Your models should also subclass this class.

Modules can also contain other Modules, allowing them to be nested in a tree structure. You can assign the sub-modules as regular attributes:

```
import torch.nn as nn
import torch.nn.functional as F

class Model(nn.Module):
    def __init__(self) -> None:
        super().__init__()
        self.conv1 = nn.Conv2d(1, 20, 5)
        self.conv2 = nn.Conv2d(20, 20, 5)

    def forward(self, x):
        x = F.relu(self.conv1(x))
        return F.relu(self.conv2(x))
```

Submodules assigned in this way will be registered, and will also have their parameters converted when you call `to()`, etc.

Note

As per the example above, an `__init__()` call to the parent class must be made before assignment on the child.

Variables

`training (bool)` – Boolean represents whether this module is in training or evaluation mode.

```
name = 'ComplEx'

static score(head_ent_emb: torch.FloatTensor, rel_ent_emb: torch.FloatTensor,
            tail_ent_emb: torch.FloatTensor)

static k_vs_all_score(emb_h: torch.FloatTensor, emb_r: torch.FloatTensor,
                      emb_E: torch.FloatTensor)
```

Parameters

- `emb_h`
- `emb_r`
- `emb_E`

`forward_k_vs_all(x: torch.LongTensor) → torch.FloatTensor`

`forward_k_vs_sample(x: torch.LongTensor, target_entity_idx: torch.LongTensor)`

`class dicee.AConEx(args)`

Bases: `dicee.models.base_model.BaseKGE`

Additive Convolutional ComplEx Knowledge Graph Embeddings

`name = 'AConEx'`

`conv2d`

`fc_num_input`

`fc1`

`norm_fc1`

`bn_conv2d`

`feature_map_dropout`

`residual_convolution(C_1: Tuple[torch.Tensor, torch.Tensor],
 C_2: Tuple[torch.Tensor, torch.Tensor]) → torch.FloatTensor`

Compute residual score of two complex-valued embeddings. :param C_1: a tuple of two pytorch tensors that corresponds complex-valued embeddings :param C_2: a tuple of two pytorch tensors that corresponds complex-valued embeddings :return:

`forward_k_vs_all(x: torch.Tensor) → torch.FloatTensor`

`forward_triples(x: torch.Tensor) → torch.FloatTensor`

Parameters

`x`

`forward_k_vs_sample(x: torch.Tensor, target_entity_idx: torch.Tensor)`

`class dicee.ACOnvo(args: dict)`

Bases: `dicee.models.base_model.BaseKGE`

Additive Convolutional Octonion Knowledge Graph Embeddings

```

name = 'AConvO'

conv2d

fc_num_input

fc1

bn_conv2d

norm_fc1

feature_map_dropout

static octonion_normalizer(emb_rel_e0, emb_rel_e1, emb_rel_e2, emb_rel_e3, emb_rel_e4,
                           emb_rel_e5, emb_rel_e6, emb_rel_e7)

residual_convolution(O_1, O_2)

forward_triples(x: torch.Tensor) → torch.Tensor

```

Parameters

x

forward_k_vs_all(x: torch.Tensor)

Given a head entity and a relation (h,r), we compute scores for all entities. [score(h,r,x)|x in Entities] => [0.0,0.1,...,0.8], shape=> (1, |Entities|) Given a batch of head entities and relations => shape (size of batch,|Entities|)

```

class dicee.AConvQ(args)

```

Bases: *dicee.models.base_model.BaseKGE*

Additive Convolutional Quaternion Knowledge Graph Embeddings

```

name = 'AConvQ'

```

```

entity_embeddings

```

```

relation_embeddings

```

```

conv2d

```

```

fc_num_input

```

```

fc1

```

```

bn_conv1

```

```

bn_conv2

```

```

feature_map_dropout

```

```

residual_convolution(Q_1, Q_2)

```

```

forward_triples(indexed_triple: torch.Tensor) → torch.Tensor

```

Parameters

x

```

forward_k_vs_all(x: torch.Tensor)
    Given a head entity and a relation (h,r), we compute scores for all entities. [score(h,r,x)|x in Entities] => [0.0,0.1,...,0.8], shape=>(1, |Entities|) Given a batch of head entities and relations => shape (size of batch,|Entities|)

class dicee.ConvQ(args)
    Bases: dicee.models.base_model.BaseKGE
    Convolutional Quaternion Knowledge Graph Embeddings
    name = 'ConvQ'

    entity_embeddings
    relation_embeddings
    conv2d
    fc_num_input
    fc1
    bn_conv1
    bn_conv2
    feature_map_dropout
    residual_convolution(Q_1, Q_2)

    forward_triples(indexed_triple: torch.Tensor) → torch.Tensor

```

Parameters

x

```
forward_k_vs_all(x: torch.Tensor)
```

Given a head entity and a relation (h,r), we compute scores for all entities. [score(h,r,x)|x in Entities] => [0.0,0.1,...,0.8], shape=>(1, |Entities|) Given a batch of head entities and relations => shape (size of batch,|Entities|)

```

class dicee.ConvO(args: dict)
    Bases: dicee.models.base_model.BaseKGE

```

Base class for all neural network modules.

Your models should also subclass this class.

Modules can also contain other Modules, allowing them to be nested in a tree structure. You can assign the sub-modules as regular attributes:

```

import torch.nn as nn
import torch.nn.functional as F

class Model(nn.Module):
    def __init__(self) -> None:
        super().__init__()
        self.conv1 = nn.Conv2d(1, 20, 5)
        self.conv2 = nn.Conv2d(20, 20, 5)

```

(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 = 'Conv0'

conv2d

fc_num_input

fc1

bn_conv2d

norm_fc1

feature_map_dropout

static octonion_normalizer(emb_rel_e0, emb_rel_e1, emb_rel_e2, emb_rel_e3, emb_rel_e4,
                           emb_rel_e5, emb_rel_e6, emb_rel_e7)

residual_convolution(O_1, O_2)

forward_triples(x: torch.Tensor) → torch.Tensor
```

Parameters

`x`

`forward_k_vs_all(x: torch.Tensor)`

Given a head entity and a relation (h,r), we compute scores for all entities. [score(h,r,x)|x in Entities] => [0.0,0.1,...,0.8], shape=> (1, |Entities|) Given a batch of head entities and relations => shape (size of batch,|Entities|)

`class dicee.ConEx(args)`

Bases: `dicee.models.base_model.BaseKGE`

Convolutional ComplEx Knowledge Graph Embeddings

`name = 'ConEx'`

`conv2d`

`fc_num_input`

```

fc1
norm_fc1
bn_conv2d
feature_map_dropout

residual_convolution(C_1: Tuple[torch.Tensor, torch.Tensor],
C_2: Tuple[torch.Tensor, torch.Tensor]) → torch.FloatTensor

```

Compute residual score of two complex-valued embeddings. :param *C_1*: a tuple of two pytorch tensors that corresponds complex-valued embeddings :param *C_2*: a tuple of two pytorch tensors that corresponds complex-valued embeddings :return:

```

forward_k_vs_all(x: torch.Tensor) → torch.FloatTensor
forward_triples(x: torch.Tensor) → torch.FloatTensor

```

Parameters

x

```
forward_k_vs_sample(x: torch.Tensor, target_entity_idx: torch.Tensor)
```

class dicee.QMult(args)

Bases: *dicee.models.base_model.BaseKGE*

Base class for all neural network modules.

Your models should also subclass this class.

Modules can also contain other Modules, allowing them to be nested in a tree structure. You can assign the sub-modules as regular attributes:

```

import torch.nn as nn
import torch.nn.functional as F

class Model(nn.Module):
    def __init__(self) -> None:
        super().__init__()
        self.conv1 = nn.Conv2d(1, 20, 5)
        self.conv2 = nn.Conv2d(20, 20, 5)

    def forward(self, x):
        x = F.relu(self.conv1(x))
        return F.relu(self.conv2(x))

```

Submodules assigned in this way will be registered, and will also have their parameters converted when you call `to()`, etc.

Note

As per the example above, an `__init__()` call to the parent class must be made before assignment on the child.

Variables

`training` (`bool`) – Boolean represents whether this module is in training or evaluation mode.

```

name = 'QMult'
explicit = True
quaternion_multiplication_followed_by_inner_product(h, r, t)

```

Parameters

- **h** – shape: (*batch_dims, dim) The head representations.
- **r** – shape: (*batch_dims, dim) The head representations.
- **t** – shape: (*batch_dims, dim) The tail representations.

Returns

Triple scores.

```
static quaternion_normalizer(x: torch.FloatTensor) → torch.FloatTensor
```

Normalize the length of relation vectors, if the forward constraint has not been applied yet.

Absolute value of a quaternion

$$|a + bi + cj + dk| = \sqrt{a^2 + b^2 + c^2 + d^2}$$

L2 norm of quaternion vector:

$$\|x\|^2 = \sum_{i=1}^d |x_i|^2 = \sum_{i=1}^d (x_i.re^2 + x_i.im_1^2 + x_i.im_2^2 + x_i.im_3^2)$$

Parameters

x – The vector.

Returns

The normalized vector.

```
score(head_ent_emb: torch.FloatTensor, rel_ent_emb: torch.FloatTensor,
      tail_ent_emb: torch.FloatTensor)
```

```
k_vs_all_score(bpe_head_ent_emb, bpe_rel_ent_emb, E)
```

Parameters

- **bpe_head_ent_emb**
- **bpe_rel_ent_emb**
- **E**

```
forward_k_vs_all(x)
```

Parameters

x

```
forward_k_vs_sample(x, target_entity_idx)
```

Completed. Given a head entity and a relation (h,r), we compute scores for all possible triples,i.e., [score(h,r,x)|x in Entities] => [0.0,0.1,...,0.8], shape=> (1, |Entities|) Given a batch of head entities and relations => shape (size of batch,| Entities|)

```
class dicee.OMult(args)
Bases: dicee.models.base_model.BaseKGE
```

Base class for all neural network modules.

Your models should also subclass this class.

Modules can also contain other Modules, allowing them to be nested in a tree structure. You can assign the sub-modules as regular attributes:

```
import torch.nn as nn
import torch.nn.functional as F

class Model(nn.Module):
    def __init__(self) -> None:
        super().__init__()
        self.conv1 = nn.Conv2d(1, 20, 5)
        self.conv2 = nn.Conv2d(20, 20, 5)

    def forward(self, x):
        x = F.relu(self.conv1(x))
        return F.relu(self.conv2(x))
```

Submodules assigned in this way will be registered, and will also have their parameters converted when you call `to()`, etc.

Note

As per the example above, an `__init__()` call to the parent class must be made before assignment on the child.

Variables

`training(bool)` – Boolean represents whether this module is in training or evaluation mode.

```
name = 'OMult'

static octonion_normalizer(emb_rel_e0, emb_rel_e1, emb_rel_e2, emb_rel_e3, emb_rel_e4,
emb_rel_e5, emb_rel_e6, emb_rel_e7)

score(head_ent_emb: torch.FloatTensor, rel_ent_emb: torch.FloatTensor,
tail_ent_emb: torch.FloatTensor)

k_vs_all_score(bpe_head_ent_emb, bpe_rel_ent_emb, E)
```

`forward_k_vs_all(x)`

Completed. Given a head entity and a relation (h,r), we compute scores for all possible triples,i.e., [score(h,r,x)|x in Entities] => [0.0,0.1,...,0.8], shape=>(1, |Entities|) Given a batch of head entities and relations => shape (size of batch,| Entities|)

```
class dicee.Shallom(args)
```

Bases: dicee.models.base_model.BaseKGE

A shallow neural model for relation prediction (<https://arxiv.org/abs/2101.09090>)

```
name = 'Shallom'
```

```

shallom

get_embeddings() → Tuple[numpy.ndarray, None]

forward_k_vs_all(x) → torch.FloatTensor

forward_triples(x) → torch.FloatTensor

Parameters
    x

Returns

class dicee.LFMult(args)
    Bases: dicee.models.base_model.BaseKGE

    Embedding with polynomial functions. We represent all entities and relations in the polynomial space as:  $f(x) = \sum_{i=0}^{d-1} a_k x^{i \% d}$  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:
        
$$\text{score}(h, r, t) = \int_0^1 h(x)r(x)t(x) dx = \sum_{i,j,k=0}^{d-1} \frac{a_i * b_j * c_k}{(i+j+k) \% d}$$

        1. generate the range for i,j and k from [0 d-1]
        2. perform  $\frac{a_i * b_j * c_k}{(i+j+k) \% d}$  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 = $\langle h, r, t \rangle$

polynomial ($coeff, x, degree$)

This function takes a matrix tensor of coefficients ($coeff$), a tensor vector of points x and range of integer $[0,1,\dots,d]$ and return a vector tensor ($coeff[0][0] + coeff[0][1]x + \dots + coeff[0][d]x^d$,

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 $[0,1,\dots,d]$

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.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.PykeenKGE(args: dict)
Bases: dicee.models.base_model.BaseKGE

A class for using knowledge graph embedding models implemented in Pykeen

Notes: Pykeen_DistMult: C Pykeen_ComplEx: Pykeen_QuatE: Pykeen_MuRE: Pykeen_CP: Pykeen_HoLE: Pykeen_HoLE: Pykeen_HoLE: Pykeen_TransD: Pykeen_TransE: Pykeen_TransF: Pykeen_TransH: Pykeen_TransR:

model_kwargs

name
model
loss_history = []
args
entity_embeddings = None
relation_embeddings = None

forward_k_vs_all(x: torch.LongTensor)
    # => Explicit version by this we can apply bn and dropout
    # (1) Retrieve embeddings of heads and relations + apply Dropout & Normalization if given. h, r =
    self.get_head_relation_representation(x) # (2) Reshape (1). if self.last_dim > 0:
        h = h.reshape(len(x), self.embedding_dim, self.last_dim) r = r.reshape(len(x), self.embedding_dim,
        self.last_dim)
    # (3) Reshape all entities. if self.last_dim > 0:
        t = self.entity_embeddings.weight.reshape(self.num_entities, self.embedding_dim, self.last_dim)

    else:
        t = self.entity_embeddings.weight

    # (4) Call the score_t from interactions to generate triple scores. return self.interaction.score_t(h=h, r=r,
    all_entities=t, slice_size=1)

forward_triples(x: torch.LongTensor) → torch.FloatTensor
    # => Explicit version by this we can apply bn and dropout
    # (1) Retrieve embeddings of heads, relations and tails and apply Dropout & Normalization if given. h, r, t =
    self.get_triple_representation(x) # (2) Reshape (1). if self.last_dim > 0:
        h = h.reshape(len(x), self.embedding_dim, self.last_dim) r = r.reshape(len(x), self.embedding_dim,
        self.last_dim) t = t.reshape(len(x), self.embedding_dim, self.last_dim)
    # (3) Compute the triple score return self.interaction.score(h=h, r=r, t=t, slice_size=None, slice_dim=0)

abstract forward_k_vs_sample(x: torch.LongTensor, target_entity_idx)

class dicee.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  
    ...  
    opt2.step()
```

Note

When `accumulate_grad_batches > 1`, the loss returned here will be automatically normalized by `accumulate_grad_batches` internally.

```
class dicee.BaseKGE(args: dict)
```

Bases: BaseKGELightning

Base class for all neural network modules.

Your models should also subclass this class.

Modules can also contain other Modules, allowing them to be nested in a tree structure. You can assign the 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.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.create_reciprocal_triples(x)
Add inverse triples into dask dataframe :param x: :return:

dicee.get_er_vocab(data, file_path: str = None)
dicee.get_re_vocab(data, file_path: str = None)
dicee.get_ee_vocab(data, file_path: str = None)
dicee.timeit(func)
dicee.save_pickle(*, data: object = None, file_path=str)
dicee.load_pickle(file_path=str)
dicee.load_term_mapping(file_path=str)
dicee.select_model(args: dict, is_continual_training: bool = None, storage_path: str = None)
dicee.load_model(path_of_experiment_folder: str, model_name='model.pt', verbose=0)
→ Tuple[object, Tuple[dict, dict]]
Load weights and initialize pytorch module from namespace arguments
dicee.load_model_ensemble(path_of_experiment_folder: str)
→ Tuple[dicee.models.base_model.BaseKGE, Tuple[pandas.DataFrame, pandas.DataFrame]]
Construct Ensemble Of weights and initialize pytorch module from namespace arguments
(1) Detect models under given path
(2) Accumulate parameters of detected models
(3) Normalize parameters
(4) Insert (3) into model.
dicee.save_numpy_ndarray(*, data: numpy.ndarray, file_path: str)
dicee.numpy_data_type_changer(train_set: numpy.ndarray, num: int) → numpy.ndarray
Detect most efficient data type for a given triples :param train_set: :param num: :return:
dicee.save_checkpoint_model(model, path: str) → None
Store Pytorch model into disk
dicee.store(trained_model, model_name: str = 'model', full_storage_path: str = None,
save_embeddings_as_csv=False) → None
dicee.add_noisy_triples(train_set: pandas.DataFrame, add_noise_rate: float) → pandas.DataFrame
Add randomly constructed triples :param train_set: :param add_noise_rate: :return:
dicee.read_or_load_kg(args, cls)
dicee.initialize_model(args: dict, verbose=0) → Tuple[object, str]

```

```

dicee.load_json(p: str) → dict

dicee.save_embeddings(embeddings: numpy.ndarray, indexes, path: str) → None
    Save it as CSV if memory allows. :param embeddings: :param indexes: :param path: :return:

dicee.random_prediction(pre_trained_kge)

dicee.deploy_triple_prediction(pre_trained_kge, str_subject, str_predicate, str_object)

dicee.deploy_tail_entity_prediction(pre_trained_kge, str_subject, str_predicate, top_k)

dicee.deploy_head_entity_prediction(pre_trained_kge, str_object, str_predicate, top_k)

dicee.deploy_relation_prediction(pre_trained_kge, str_subject, str_object, top_k)

dicee.vocab_to_parquet(vocab_to_idx, name, path_for_serialization, print_into)

dicee.create_experiment_folder(folder_name='Experiments')

dicee.continual_training_setup_executor(executor) → None

dicee.exponential_function(x: numpy.ndarray, lam: float, ascending_order=True) → torch.FloatTensor

dicee.load_numpy(path) → numpy.ndarray

dicee.evaluate(entity_to_idx, scores, easy_answers, hard_answers)
    # @TODO: CD: Renamed this function Evaluate multi hop query answering on different query types

dicee.download_file(url, destination_folder='.')
dicee.download_files_from_url(base_url: str, destination_folder='.') → None

```

Parameters

- **base_url** (e.g. "https://files.dice-research.org/projects/DiceEmbeddings/KINSHIP-Keci-dim128-epoch256-KvsAll")
- **destination_folder** (e.g. "KINSHIP-Keci-dim128-epoch256-KvsAll")

```
dicee.download_pretrained_model(url: str) → str
```

```
dicee.write_csv_from_model_parallel(path: str)
```

Create

```
dicee.from_pretrained_model_write_embeddings_into_csv(path: str) → None
```

```
class dicee.DICE_Trainer(args, is_continual_training: bool, storage_path, evaluator=None)
```

DICE_Trainer implement

- 1- Pytorch Lightning trainer (<https://pytorch-lightning.readthedocs.io/en/stable/common/trainer.html>)
- 2- Multi-GPU Trainer(<https://pytorch.org/docs/stable/generated/torch.nn.parallel.DistributedDataParallel.html>)
- 3- CPU Trainer

```

args
is_continual_training:bool
storage_path:str
evaluator:
report:dict

```

```

report
args
trainer = None
is_continual_training
storage_path
evaluator = None
form_of_labelling = None
continual_start (knowledge_graph)

```

- (1) Initialize training.
- (2) Load model
- (3) Load trainer (3) Fit model

Parameter

returns

- *model*
- **form_of_labelling** (*str*)

initialize_trainer (*callbacks*: *List*)

→ lightning.Trainer | dicee.trainer.model_parallelism.TensorParallel | dicee.trainer.torch_trainer.TorchTrainer | dicee.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

```
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) | f(e,r,x) > confidence} and (e,r,x)
            otin G

deploy(share: bool = False, top_k: int = 10)

predict_literals(entity: List[str] | str = None, attribute: List[str] | str = None,
                    denormalize_preds: bool = True) → 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.mapping_from_first_two_cols_to_third(train_set_idx)

dicee.timeit(func)

dicee.load_term_mapping(file_path=str)

dicee.reload_dataset(path: str, form_of_labelling, scoring_technique, neg_ratio, label_smoothing_rate)
    Reload the files from disk to construct the Pytorch dataset

```

```

dicee.construct_dataset(*train_set: numpy.ndarray | list, valid_set=None, test_set=None,
                        ordered_bpe_entities=None, train_target_indices=None, target_dim: int = None, entity_to_idx: dict,
                        relation_to_idx: dict, form_of_labelling: str, scoring_technique: str, neg_ratio: int,
                        label_smoothing_rate: float, byte_pair_encoding=None, block_size: int = None)
    → torch.utils.data.Dataset

```

```

class dicee.BPE_NegativeSamplingDataset(train_set: torch.LongTensor,
                                             ordered_shaped_bpe_entities: torch.LongTensor, neg_ratio: int)

```

Bases: `torch.utils.data.Dataset`

An abstract class representing a Dataset.

All datasets that represent a map from keys to data samples should subclass it. All subclasses should overwrite `__getitem__()`, supporting fetching a data sample for a given key. Subclasses could also optionally overwrite `__len__()`, which is expected to return the size of the dataset by many Sampler implementations and the default

options of `DataLoader`. Subclasses could also optionally implement `__getitems__()`, for speedup batched samples loading. This method accepts list of indices of samples of batch and returns list of samples.

Note

`DataLoader` by default constructs an index sampler that yields integral indices. To make it work with a map-style dataset with non-integral indices/keys, a custom sampler must be provided.

```
train_set  
ordered_bpe_entities  
num_bpe_entities  
neg_ratio  
num_datapoints  
__len__()  
__getitem__(idx)  
collate_fn(batch_shaped_bpe_triples: List[Tuple[torch.Tensor, torch.Tensor]])  
  
class dicee.MultilabelDataset(train_set: torch.LongTensor, train_indices_target: torch.LongTensor, target_dim: int, torch_ordered_shaped_bpe_entities: torch.LongTensor)  
Bases: torch.utils.data.Dataset
```

An abstract class representing a Dataset.

All datasets that represent a map from keys to data samples should subclass it. All subclasses should overwrite `__getitem__()`, supporting fetching a data sample for a given key. Subclasses could also optionally overwrite `__len__()`, which is expected to return the size of the dataset by many `Sampler` implementations and the default options of `DataLoader`. Subclasses could also optionally implement `__getitems__()`, for speedup batched samples loading. This method accepts list of indices of samples of batch and returns list of samples.

Note

`DataLoader` by default constructs an index sampler that yields integral indices. To make it work with a map-style dataset with non-integral indices/keys, a custom sampler must be provided.

```
train_set  
train_indices_target  
target_dim  
num_datapoints  
torch_ordered_shaped_bpe_entities  
collate_fn = None  
__len__()  
__getitem__(idx)
```

```
class dicee.MultiClassClassificationDataset (subword_units: numpy.ndarray, block_size: int = 8)
```

Bases: `torch.utils.data.Dataset`

Dataset for the 1vsALL training strategy

Parameters

- **train_set_idx** – Indexed triples for the training.
- **entity_idxs** – mapping.
- **relation_idxs** – mapping.
- **form** – ?
- **num_workers** – int for <https://pytorch.org/docs/stable/data.html#torch.utils.data.DataLoader>

Return type

`torch.utils.data.Dataset`

train_data

block_size = 8

num_of_data_points

collate_fn = None

__len__()

__getitem__(*idx*)

```
class dicee.OnevsAllDataset (train_set_idx: numpy.ndarray, entity_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.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 a unique tuple of an entity h in E and a relation r in R that has been seed in the input graph. $y:$ denotes a multi-label vector in $[0,1]^{|\mathcal{E}|}$ is a binary label.

orall $y_i = 1$ s.t. $(h, r) \in E_i$ in KG

Note

TODO

train_set_idx

[numpy.ndarray] n by 3 array representing n triples

entity_idxs

[dictionary] string representation of an entity to its integer id

relation_idxs

[dictionary] string representation of a relation to its integer id

self : torch.utils.data.Dataset

```
>>> a = KvsAll()
>>> a
? array([0, 1, 2, 3, 4, 5, 6, 7, 8, 9])
```

```
train_data = None
```

```
train_target = None
```

```
label_smoothing_rate
```

```
collate_fn = None
```

```
__len__()
```

```
__getitem__(idx)
```

```
class dicee.AllvsAll (train_set_idx: numpy.ndarray, entity_idxs, relation_idxs, label_smoothing_rate=0.0)
```

Bases: torch.utils.data.Dataset

Creates a dataset for AllvsAll training by inheriting from torch.utils.data.Dataset.

Let D denote a dataset for AllvsAll training and be defined as $D := \{(x,y)_i\}_{i=1}^N$, where $x: (h,r)$ is a possible unique tuple of an entity h in E and a relation r in R. Hence $N = |\mathcal{E}| \times |\mathcal{R}|$ $y:$ denotes a multi-label vector in $[0,1]^{|\mathcal{E}|}$ is a binary label.

orall $y_i = 1$ s.t. $(h, r) \in E_i$ 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.OnevsSample(*train_set*: numpy.ndarray, *num_entities*, *num_relations*, *neg_sample_ratio*: int = None, *label_smoothing_rate*: float = 0.0)

Bases: torch.utils.data.Dataset

A custom PyTorch Dataset class for knowledge graph embeddings, which includes both positive and negative sampling for a given dataset for multi-class classification problem..

Parameters

- **train_set** (*np.ndarray*) – A numpy array containing triples of knowledge graph data. Each triple consists of (head_entity, relation, tail_entity).
- **num_entities** (*int*) – The number of unique entities in the knowledge graph.
- **num_relations** (*int*) – The number of unique relations in the knowledge graph.
- **neg_sample_ratio** (*int, optional*) – The number of negative samples to be generated per positive sample. Must be a positive integer and less than num_entities.
- **label_smoothing_rate** (*float, optional*) – A label smoothing rate to apply to the positive and negative labels. Defaults to 0.0.

train_data

The input data converted into a PyTorch tensor.

Type

torch.Tensor

```

num_entities
    Number of entities in the dataset.

    Type
        int

num_relations
    Number of relations in the dataset.

    Type
        int

neg_sample_ratio
    Ratio of negative samples to be drawn for each positive sample.

    Type
        int

label_smoothing_rate
    The smoothing factor applied to the labels.

    Type
        torch.Tensor

collate_fn
    A function that can be used to collate data samples into batches (set to None by default).

    Type
        function, optional

train_data

num_entities

num_relations

neg_sample_ratio = None

label_smoothing_rate

collate_fn = None

__len__()
    Returns the number of samples in the dataset.

__getitem__(idx)
    Retrieves a single data sample from the dataset at the given index.

Parameters
    idx (int) – The index of the sample to retrieve.

Returns
    A tuple consisting of:
    

- x (torch.Tensor): The head and relation part of the triple.
- y_idx (torch.Tensor): The concatenated indices of the true object (tail entity) and the indices of the negative samples.
- y_vec (torch.Tensor): A vector containing the labels for the positive and negative samples, with label smoothing applied.

```

Return type

tuple

```
class dicee.KvsSampleDataset (train_set_idx: numpy.ndarray, entity_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.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.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.CVDataModule(train_set_idx: numpy.ndarray, num_entities, num_relations, neg_sample_ratio,  

    batch_size, num_workers)
Bases: pytorch_lightning.LightningDataModule
Create a Dataset for cross validation

```

Parameters

- **train_set_idx** – Indexed triples for the training.
- **num_entities** – entity to index mapping.
- **num_relations** – relation to index mapping.
- **batch_size** – int
- **form** – ?
- **num_workers** – int for <https://pytorch.org/docs/stable/data.html#torch.utils.data.DataLoader>

Return type

?

```

train_set_idx
num_entities
num_relations
neg_sample_ratio
batch_size
num_workers

```

`train_dataloader()` → `torch.utils.data.DataLoader`

An iterable or collection of iterables specifying training samples.

For more information about multiple dataloaders, see this section.

The dataloader you return will not be reloaded unless you set `:param-ref:`~pytorch_lightning.trainer.Trainer.reload_dataloaders_every_n_epochs`` to a positive integer.

For data processing use the following pattern:

- download in `prepare_data()`
- process and split in `setup()`

However, the above are only necessary for distributed processing.

⚠ Warning

do not assign state in `prepare_data`

- `fit()`
- `prepare_data()`
- `setup()`

ℹ Note

Lightning tries to add the correct sampler for distributed and arbitrary hardware. There is no need to set it yourself.

`setup(*args, **kwargs)`

Called at the beginning of fit (train + validate), validate, test, or predict. This is a good hook when you need to build models dynamically or adjust something about them. This hook is called on every process when using DDP.

Parameters

`stage` – either 'fit', 'validate', 'test', or 'predict'

Example:

```
class LitModel(...):
    def __init__(self):
        self.ll = None

    def prepare_data(self):
        download_data()
        tokenize()

        # don't do this
        self.something = else

    def setup(self, stage):
        data = load_data(...)
        self.ll = nn.Linear(28, data.num_classes)
```

```
transfer_batch_to_device(*args, **kwargs)
```

Override this hook if your `DataLoader` returns tensors wrapped in a custom data structure.

The data types listed below (and any arbitrary nesting of them) are supported out of the box:

- `torch.Tensor` or anything that implements `.to(...)`
- list
- dict
- tuple

For anything else, you need to define how the data is moved to the target device (CPU, GPU, TPU, ...).

Note

This hook should only transfer the data and not modify it, nor should it move the data to any other device than the one passed in as argument (unless you know what you are doing). To check the current state of execution of this hook you can use `self.trainer.training/testing/validating/predicting` so that you can add different logic as per your requirement.

Parameters

- `batch` – A batch of data that needs to be transferred to a new device.
- `device` – The target device as defined in PyTorch.
- `dataloader_idx` – The index of the dataloader to which the batch belongs.

Returns

A reference to the data on the new device.

Example:

```
def transfer_batch_to_device(self, batch, device, dataloader_idx):  
    if isinstance(batch, CustomBatch):  
        # move all tensors in your custom data structure to the device  
        batch.samples = batch.samples.to(device)  
        batch.targets = batch.targets.to(device)  
    elif dataloader_idx == 0:  
        # skip device transfer for the first dataloader or anything you wish  
        pass  
    else:  
        batch = super().transfer_batch_to_device(batch, device, dataloader_  
→idx)  
    return batch
```

See also

- `move_data_to_device()`
- `apply_to_collection()`

```
prepare_data(*args, **kwargs)
```

Use this to download and prepare data. Downloading and saving data with multiple processes (distributed settings) will result in corrupted data. Lightning ensures this method is called only within a single process, so you can safely add your downloading logic within.

⚠ Warning

DO NOT set state to the model (use `setup` instead) since this is NOT called on every device

Example:

```
def prepare_data(self):
    # good
    download_data()
    tokenize()
    etc()

    # bad
    self.split = data_split
    self.some_state = some_other_state()
```

In a distributed environment, `prepare_data` can be called in two ways (using `prepare_data_per_node`)

1. Once per node. This is the default and is only called on `LOCAL_RANK=0`.
2. Once in total. Only called on `GLOBAL_RANK=0`.

Example:

```
# DEFAULT
# called once per node on LOCAL_RANK=0 of that node
class LitDataModule(LightningDataModule):
    def __init__(self):
        super().__init__()
        self.prepare_data_per_node = True

# call on GLOBAL_RANK=0 (great for shared file systems)
class LitDataModule(LightningDataModule):
    def __init__(self):
        super().__init__()
        self.prepare_data_per_node = False
```

This is called before requesting the dataloaders:

```
model.prepare_data()
initialize_distributed()
model.setup(stage)
model.train_dataloader()
model.val_dataloader()
model.test_dataloader()
model.predict_dataloader()
```

```
class dicee.LiteralDataset(file_path: str, ent_idx: dict = None, normalization_type: str = 'z-norm',
                           sampling_ratio: float = None, loader_backend: str = 'pandas')
```

Bases: `torch.utils.data.Dataset`

Dataset for loading and processing literal data for training Literal Embedding model. This dataset handles the loading, normalization, and preparation of triples for training a literal embedding model.

Extends `torch.utils.data.Dataset` for supporting PyTorch dataloaders.

`train_file_path`

Path to the training data file.

Type

str

`normalization`

Type of normalization to apply ('z-norm', 'min-max', or None).

Type

str

`normalization_params`

Parameters used for normalization.

Type

dict

`sampling_ratio`

Fraction of the training set to use for ablations.

Type

float

`entity_to_idx`

Mapping of entities to their indices.

Type

dict

`num_entities`

Total number of entities.

Type

int

`data_property_to_idx`

Mapping of data properties to their indices.

Type

dict

`num_data_properties`

Total number of data properties.

Type

int

`loader_backend`

Backend to use for loading data ('pandas' or 'rdflib').

Type

str

```

train_file_path
loader_backend = 'pandas'
normalization_type = 'z-norm'
normalization_params
sampling_ratio = None
entity_to_idx = None
num_entities
__getitem__(index)
__len__()

static load_and_validate_literal_data(file_path: str = None, loader_backend: str = 'pandas')
    → pandas.DataFrame

```

Loads and validates the literal data file. :param file_path: Path to the literal data file. :type file_path: str

Returns

DataFrame containing the loaded and validated data.

Return type

pd.DataFrame

```
static denormalize(preds_norm, attributes, normalization_params) → numpy.ndarray
```

Denormalizes the predictions based on the normalization type.

Args: preds_norm (np.ndarray): Normalized predictions to be denormalized. attributes (list): List of attributes corresponding to the predictions. normalization_params (dict): Dictionary containing normalization parameters for each attribute.

Returns

Denormalized predictions.

Return type

np.ndarray

```
class dicee.QueryGenerator(train_path, val_path: str, test_path: str, ent2id: Dict = None,
                           rel2id: Dict = None, seed: int = 1, gen_valid: bool = False, gen_test: bool = True)
```

```

train_path
val_path
test_path
gen_valid = False
gen_test = True
seed = 1
max_ans_num = 1000000.0
mode
ent2id = None

```

```

rel2id: Dict = None

ent_in: Dict

ent_out: Dict

query_name_to_struct

list2tuple(list_data)

tuple2list(x: List | Tuple) → List | Tuple
    Convert a nested tuple to a nested list.

set_global_seed(seed: int)
    Set seed

construct_graph(paths: List[str]) → Tuple[Dict, Dict]
    Construct graph from triples Returns dicts with incoming and outgoing edges

fill_query(query_structure: List[str | List], ent_in: Dict, ent_out: Dict, answer: int) → bool
    Private method for fill_query logic.

achieve_answer(query: List[str | List], ent_in: Dict, ent_out: Dict) → set
    Private method for achieve_answer logic. @TODO: Document the code

write_links(ent_out, small_ent_out)

ground_queries(query_structure: List[str | List], ent_in: Dict, ent_out: Dict, small_ent_in: Dict,
                 small_ent_out: Dict, gen_num: int, query_name: str)
    Generating queries and achieving answers

unmap(query_type, queries, tp_answers, fp_answers, fn_answers)

unmap_query(query_structure, query, id2ent, id2rel)

generate_queries(query_struct: List, gen_num: int, query_type: str)
    Passing incoming and outgoing edges to ground queries depending on mode [train valid or text] and getting
    queries and answers in return @ TODO: create a class for each single query struct

save_queries(query_type: str, gen_num: int, save_path: str)

abstract load_queries(path)

get_queries(query_type: str, gen_num: int)

static save_queries_and_answers(path: str, data: List[Tuple[str, Tuple[collections.defaultdict]]])
    → None
    Save Queries into Disk

static load_queries_and_answers(path: str) → List[Tuple[str, Tuple[collections.defaultdict]]]
    Load Queries from Disk to Memory

dicee.__version__ = '0.1.5'

```

Python Module Index

d

dicee, 12
dicee.__main__, 12
dicee.abstracts, 12
dicee.analyse_experiments, 19
dicee.callbacks, 20
dicee.config, 29
dicee.dataset_classes, 32
dicee.eval_static_funcs, 46
dicee.evaluator, 48
dicee.executer, 49
dicee.knowledge_graph, 51
dicee.knowledge_graph_embeddings, 53
dicee.models, 57
dicee.models.adopt, 57
dicee.models.base_model, 66
dicee.models.clifford, 75
dicee.models.complex, 82
dicee.models.duale, 84
dicee.models.ensemble, 85
dicee.models.function_space, 86
dicee.models.literal, 90
dicee.models.octonion, 91
dicee.models.pykeen_models, 94
dicee.models.quaternion, 96
dicee.models.real, 99
dicee.models.static_funcs, 102
dicee.models.transformers, 102
dicee.query_generator, 161
dicee.read_preprocess_save_load_kg, 163
dicee.read_preprocess_save_load_kg.preprocess,
 163
dicee.read_preprocess_save_load_kg.read_from_disk,
 164
dicee.read_preprocess_save_load_kg.save_load_disk,
 164
dicee.read_preprocess_save_load_kg.util,
 165
dicee.sanity_checkers, 169
dicee.scripts, 170
dicee.scripts.index_serve, 170
dicee.scripts.run, 172
dicee.static_funcs, 172
dicee.static_funcs_training, 175
dicee.static_preprocess_funcs, 176
dicee.trainer, 177
dicee.trainer.dice_trainer, 177
dicee.trainer.model_parallelism, 179
dicee.trainer.torch_trainer, 179
dicee.trainer.torch_trainer_ddp, 181

Index

Non-alphabetical

`__call__()` (*dicee.EnsembleKGE method*), 210
`__call__()` (*dicee.models.base_model.IdentityClass method*), 75
`__call__()` (*dicee.models.ensemble.EnsembleKGE method*), 86
`__call__()` (*dicee.models.IdentityClass method*), 122, 136, 142
`getitem__()` (*dicee.AllvsAll method*), 221
`getitem__()` (*dicee.BPE_NegativeSamplingDataset method*), 218
`getitem__()` (*dicee.dataset_classes.AllvsAll method*), 37
`getitem__()` (*dicee.dataset_classes.BPE_NegativeSamplingDataset method*), 34
`getitem__()` (*dicee.dataset_classes.KvsAll method*), 36
`getitem__()` (*dicee.dataset_classes.KvsSampleDataset method*), 39
`getitem__()` (*dicee.dataset_classes.LiteralDataset method*), 46
`getitem__()` (*dicee.dataset_classes.MultiClassClassificationDataset method*), 35
`getitem__()` (*dicee.dataset_classes.MultiLabelDataset method*), 34
`getitem__()` (*dicee.dataset_classes.NegSampleDataset method*), 40
`getitem__()` (*dicee.dataset_classes.OnevsAllDataset method*), 35
`getitem__()` (*dicee.dataset_classes.OnevsSample method*), 38
`getitem__()` (*dicee.dataset_classes.TriplePredictionDataset method*), 41
`getitem__()` (*dicee.KvsAll method*), 220
`getitem__()` (*dicee.KvsSampleDataset method*), 223
`getitem__()` (*dicee.LiteralDataset method*), 230
`getitem__()` (*dicee.MultiClassClassificationDataset method*), 219
`getitem__()` (*dicee.MultiLabelDataset method*), 218
`getitem__()` (*dicee.NegSampleDataset method*), 224
`getitem__()` (*dicee.OnevsAllDataset method*), 219
`getitem__()` (*dicee.OnevsSample method*), 222
`getitem__()` (*dicee.TriplePredictionDataset method*), 225
`iter__()` (*dicee.config.Namespace method*), 32
`iter__()` (*dicee.EnsembleKGE method*), 210
`iter__()` (*dicee.knowledge_graph.KG method*), 53
`iter__()` (*dicee.models.ensemble.EnsembleKGE method*), 86
`len__()` (*dicee.AllvsAll method*), 221
`len__()` (*dicee.BPE_NegativeSamplingDataset method*), 218
`len__()` (*dicee.dataset_classes.AllvsAll method*), 37
`len__()` (*dicee.dataset_classes.BPE_NegativeSamplingDataset method*), 34
`len__()` (*dicee.dataset_classes.KvsAll method*), 36
`len__()` (*dicee.dataset_classes.KvsSampleDataset method*), 39
`len__()` (*dicee.dataset_classes.LiteralDataset method*), 46
`len__()` (*dicee.dataset_classes.MultiClassClassificationDataset method*), 35
`len__()` (*dicee.dataset_classes.MultiLabelDataset method*), 34
`len__()` (*dicee.dataset_classes.NegSampleDataset method*), 40
`len__()` (*dicee.dataset_classes.OnevsAllDataset method*), 35
`len__()` (*dicee.dataset_classes.OnevsSample method*), 38
`len__()` (*dicee.dataset_classes.TriplePredictionDataset method*), 41
`len__()` (*dicee.EnsembleKGE method*), 210
`len__()` (*dicee.knowledge_graph.KG method*), 53
`len__()` (*dicee.KvsAll method*), 220
`len__()` (*dicee.KvsSampleDataset method*), 223
`len__()` (*dicee.LiteralDataset method*), 230
`len__()` (*dicee.models.ensemble.EnsembleKGE method*), 86
`len__()` (*dicee.MultiClassClassificationDataset method*), 219
`len__()` (*dicee.MultiLabelDataset method*), 218
`len__()` (*dicee.NegSampleDataset method*), 224
`len__()` (*dicee.OnevsAllDataset method*), 219
`len__()` (*dicee.OnevsSample method*), 222
`len__()` (*dicee.TriplePredictionDataset method*), 225
`setstate__()` (*dicee.models.ADOPT method*), 112
`setstate__()` (*dicee.models.adopt.ADOPT method*), 60
`str__()` (*dicee.EnsembleKGE method*), 211
`str__()` (*dicee.KGE method*), 214
`str__()` (*dicee.knowledge_graph_embeddings.KGE method*), 53
`str__()` (*dicee.models.ensemble.EnsembleKGE method*), 86
`version__` (*in module dicee*), 231

A

AbstractCallback (*class in dicee.abstracts*), 16
AbstractPPECallback (*class in dicee.abstracts*), 17
AbstractTrainer (*class in dicee.abstracts*), 12
AccumulateEpochLossCallback (*class in dicee.callbacks*), 21
achieve_answer () (*dicee.query_generator.QueryGenerator method*), 162
achieve_answer () (*dicee.QueryGenerator method*), 231
AConEx (*class in dicee*), 196
AConEx (*class in dicee.models*), 131
AConEx (*class in dicee.models.complex*), 83
AConvO (*class in dicee*), 196
AConvO (*class in dicee.models*), 144
AConvO (*class in dicee.models.octonion*), 94
AConvQ (*class in dicee*), 197
AConvQ (*class in dicee.models*), 138
AConvQ (*class in dicee.models.quaternion*), 98
adaptive_lr (*dicee.config.Namespace attribute*), 32
adaptive_swa (*dicee.config.Namespace attribute*), 32
add_new_entity_embeddings () (*dicee.abstracts.BaseInteractiveKGE method*), 15
add_noise_rate (*dicee.config.Namespace attribute*), 30
add_noise_rate (*dicee.knowledge_graph.KG attribute*), 52
add_noisy_triples () (*in module dicee*), 211
add_noisy_triples () (*in module dicee.static_funcs*), 174
add_noisy_triples_into_training () (*dicee.read_preprocess_save_load_kg.read_from_disk.ReadFromDisk method*), 164
add_noisy_triples_into_training () (*dicee.read_preprocess_save_load_kg.ReadFromDisk method*), 169
add_reciprocal (*dicee.knowledge_graph.KG attribute*), 52
ADOPT (*class in dicee.models*), 110
ADOPT (*class in dicee.models.adopt*), 58
adopt () (*in module dicee.models.adopt*), 62
AllvsAll (*class in dicee*), 220
AllvsAll (*class in dicee.dataset_classes*), 36
alphas (*dicee.abstracts.AbstractPPECallback attribute*), 18
alphas (*dicee.callbacks.ASWA attribute*), 24
analyse () (*in module dicee.analyse_experiments*), 20
answer_multi_hop_query () (*dicee.KGE method*), 216
answer_multi_hop_query () (*dicee.knowledge_graph_embeddings.KGE method*), 55
app (*in module dicee.scripts.index_server*), 171
apply_coefficients () (*dicee.DeCaL method*), 192
apply_coefficients () (*dicee.Keci method*), 189
apply_coefficients () (*dicee.models.clifford.DeCaL method*), 80
apply_coefficients () (*dicee.models.clifford.Keci method*), 76
apply_coefficients () (*dicee.models.DeCaL method*), 150
apply_coefficients () (*dicee.models.Keci method*), 146
apply_reciprocal_or_noise () (*in module dicee.read_preprocess_save_load_kg.util*), 167
apply_semantic_constraint (*dicee.abstracts.BaseInteractiveKGE attribute*), 14
apply_unit_norm (*dicee.BaseKGE attribute*), 208
apply_unit_norm (*dicee.models.base_model.BaseKGE attribute*), 72
apply_unit_norm (*dicee.models.BaseKGE attribute*), 120, 123, 129, 133, 139, 152, 156
args (*dicee.BaseKGE attribute*), 208
args (*dicee.DICE_Trainer attribute*), 213
args (*dicee.EnsembleKGE attribute*), 210
args (*dicee.evaluator.Evaluator attribute*), 48
args (*dicee.executor.Execute attribute*), 50
args (*dicee.models.base_model.BaseKGE attribute*), 72
args (*dicee.models.base_model.IdentityClass attribute*), 74
args (*dicee.models.BaseKGE attribute*), 120, 123, 129, 133, 139, 152, 155
args (*dicee.models.ensemble.EnsembleKGE attribute*), 86
args (*dicee.models.IdentityClass attribute*), 122, 136, 142
args (*dicee.models.pykeen_models.PykeenKGE attribute*), 95
args (*dicee.models.PykeenKGE attribute*), 154
args (*dicee.PykeenKGE attribute*), 205
args (*dicee.trainer.DICE_Trainer attribute*), 182
args (*dicee.trainer.dice_trainer.DICE_Trainer attribute*), 177
ASWA (*class in dicee.callbacks*), 24
aswa (*dicee.analyse_experiments.Experiment attribute*), 19
attn (*dicee.models.Block attribute*), 125
attn (*dicee.models.transformers.Block attribute*), 107
attn_dropout (*dicee.models.transformers.SelfAttention attribute*), 105

attributes (*dicee.abstracts.AbstractTrainer* attribute), 13
auto_batch_finding (*dicee.config.Namespace* attribute), 32

B

backend (*dicee.config.Namespace* attribute), 30
backend (*dicee.knowledge_graph.KG* attribute), 52
BaseInteractiveKGE (class in *dicee.abstracts*), 14
BaseInteractiveTrainKGE (class in *dicee.abstracts*), 18
BaseKGE (class in *dicee*), 207
BaseKGE (class in *dicee.models*), 119, 122, 128, 133, 139, 151, 155
BaseKGE (class in *dicee.models.base_model*), 71
BaseKGELightning (class in *dicee.models*), 113
BaseKGELightning (class in *dicee.models.base_model*), 66
batch_kronecker_product () (*dicee.callbacks.KronE* static method), 26
batch_size (*dicee.analyse_experiments.Experiment* attribute), 19
batch_size (*dicee.callbacks.PseudoLabellingCallback* attribute), 24
batch_size (*dicee.config.Namespace* attribute), 30
batch_size (*dicee.CVDataModule* attribute), 225
batch_size (*dicee.dataset_classes.CVDataModule* attribute), 41
batches_per_epoch (*dicee.callbacks.LRScheduler* attribute), 28
bias (*dicee.models.CoKEConfig* attribute), 127
bias (*dicee.models.real.CoKEConfig* attribute), 101
bias (*dicee.models.transformers.GPTConfig* attribute), 107
bias (*dicee.models.transformers.LayerNorm* attribute), 104
Block (class in *dicee.models*), 125
Block (class in *dicee.models.transformers*), 106
block_size (*dicee.BaseKGE* attribute), 209
block_size (*dicee.config.Namespace* attribute), 32
block_size (*dicee.dataset_classes.MultiClassClassificationDataset* attribute), 35
block_size (*dicee.models.base_model.BaseKGE* attribute), 73
block_size (*dicee.models.BaseKGE* attribute), 121, 124, 130, 134, 140, 153, 156
block_size (*dicee.models.CoKEConfig* attribute), 127
block_size (*dicee.models.real.CoKEConfig* attribute), 100, 101
block_size (*dicee.models.transformers.GPTConfig* attribute), 107
block_size (*dicee.MultiClassClassificationDataset* attribute), 219
blocks (*dicee.CoKE* attribute), 204
blocks (*dicee.models.CoKE* attribute), 128
blocks (*dicee.models.real.CoKE* attribute), 101
bn_conv1 (*dicee.AConvQ* attribute), 197
bn_conv1 (*dicee.ConvQ* attribute), 198
bn_conv1 (*dicee.models.AConvQ* attribute), 138
bn_conv1 (*dicee.models.ConvQ* attribute), 138
bn_conv1 (*dicee.models.quaternion.AConvQ* attribute), 98
bn_conv1 (*dicee.models.quaternion.ConvQ* attribute), 98
bn_conv2 (*dicee.AConvQ* attribute), 197
bn_conv2 (*dicee.ConvQ* attribute), 198
bn_conv2 (*dicee.models.AConvQ* attribute), 138
bn_conv2 (*dicee.models.ConvQ* attribute), 138
bn_conv2 (*dicee.models.quaternion.AConvQ* attribute), 98
bn_conv2 (*dicee.models.quaternion.ConvQ* attribute), 98
bn_conv2d (*dicee.AConEx* attribute), 196
bn_conv2d (*dicee.AConvO* attribute), 197
bn_conv2d (*dicee.ConEx* attribute), 200
bn_conv2d (*dicee.ConvO* attribute), 199
bn_conv2d (*dicee.models.AConEx* attribute), 131
bn_conv2d (*dicee.models.AConvO* attribute), 144
bn_conv2d (*dicee.models.complex.AConEx* attribute), 83
bn_conv2d (*dicee.models.complex.ConEx* attribute), 82
bn_conv2d (*dicee.models.ConEx* attribute), 131
bn_conv2d (*dicee.models.ConvO* attribute), 144
bn_conv2d (*dicee.models.octonion.AConvO* attribute), 94
bn_conv2d (*dicee.models.octonion.ConvO* attribute), 93
BPE_NegativeSamplingDataset (class in *dicee*), 217
BPE_NegativeSamplingDataset (class in *dicee.dataset_classes*), 33
build_chain_funcs () (*dicee.models.FMult2* method), 159
build_chain_funcs () (*dicee.models.function_space.FMult2* method), 88
build_func () (*dicee.models.FMult2* method), 159

```

build_func() (dicee.models.function_space.FMult2 method), 88
Byte (class in dicee), 205
Byte (class in dicee.models.transformers), 102
byte_pair_encoding (dicee.analyse_experiments.Experiment attribute), 19
byte_pair_encoding (dicee.BaseKGE attribute), 209
byte_pair_encoding (dicee.config.Namespace attribute), 31
byte_pair_encoding (dicee.knowledge_graph.KG attribute), 52
byte_pair_encoding (dicee.models.base_model.BaseKGE attribute), 73
byte_pair_encoding (dicee.models.BaseKGE attribute), 120, 124, 129, 134, 140, 153, 156

```

C

```

c_attn (dicee.models.transformers.SelfAttention attribute), 105
c_fc (dicee.models.transformers.MLP attribute), 106
c_proj (dicee.models.transformers.MLP attribute), 106
c_proj (dicee.models.transformers.SelfAttention attribute), 105
callbacks (dicee.abstracts.AbstractTrainer attribute), 13
callbacks (dicee.analyse_experiments.Experiment attribute), 19
callbacks (dicee.config.Namespace attribute), 30
callbacks (dicee.trainer.torch_trainer_ddp.NodeTrainer attribute), 182
causal (dicee.models.CoKEConfig attribute), 127
causal (dicee.models.real.CoKEConfig attribute), 101
causal (dicee.models.transformers.GPTConfig attribute), 107
causal (dicee.models.transformers.SelfAttention attribute), 105
chain_func() (dicee.models.FMult method), 158
chain_func() (dicee.models.function_space.FMult method), 87
chain_func() (dicee.models.function_space.GFMult method), 87
chain_func() (dicee.models.GFMult method), 158
CKeci (class in dicee), 187
CKeci (class in dicee.models), 148
CKeci (class in dicee.models.clifford), 78
cl_pqr() (dicee.DeCaL method), 191
cl_pqr() (dicee.models.clifford.DeCaL method), 79
cl_pqr() (dicee.models.DeCaL method), 149
cleanup() (dicee.executer.Execute method), 50
clifford_multiplication() (dicee.Keci method), 189
clifford_multiplication() (dicee.models.clifford.Keci method), 76
clifford_multiplication() (dicee.models.Keci method), 146
clip_lambda (dicee.models.ADOPT attribute), 112
clip_lambda (dicee.models.adopt.ADOPT attribute), 60
CoKE (class in dicee), 204
CoKE (class in dicee.models), 127
CoKE (class in dicee.models.real), 101
coke_dropout (dicee.CoKE attribute), 204
coke_dropout (dicee.models.CoKE attribute), 128
coke_dropout (dicee.models.real.CoKE attribute), 101
CoKEConfig (class in dicee.models), 127
CoKEConfig (class in dicee.models.real), 100
collate_fn (dicee.AllvsAll attribute), 221
collate_fn (dicee.dataset_classes.AllvsAll attribute), 37
collate_fn (dicee.dataset_classes.KvsAll attribute), 36
collate_fn (dicee.dataset_classes.KvsSampleDataset attribute), 39
collate_fn (dicee.dataset_classes.MultiClassClassificationDataset attribute), 35
collate_fn (dicee.dataset_classes.MultiLabelDataset attribute), 34
collate_fn (dicee.dataset_classes.OnevsAllDataset attribute), 35
collate_fn (dicee.dataset_classes.OnevsSample attribute), 38
collate_fn (dicee.KvsAll attribute), 220
collate_fn (dicee.KvsSampleDataset attribute), 223
collate_fn (dicee.MultiClassClassificationDataset attribute), 219
collate_fn (dicee.MultiLabelDataset attribute), 218
collate_fn (dicee.OnevsAllDataset attribute), 219
collate_fn (dicee.OnevsSample attribute), 222
collate_fn() (dicee.BPE_NegativeSamplingDataset method), 218
collate_fn() (dicee.dataset_classes.BPE_NegativeSamplingDataset method), 34
collate_fn() (dicee.dataset_classes.TriplePredictionDataset method), 41
collate_fn() (dicee.TriplePredictionDataset method), 225
collection_name (dicee.scripts.index_serve.NeuralSearcher attribute), 171
comp_func() (dicee.LFMult method), 204

```

```

comp_func() (dicee.models.function_space.LFMult method), 89
comp_func() (dicee.models.LFMult method), 160
ComplEx (class in dicee), 195
ComplEx (class in dicee.models), 132
ComplEx (class in dicee.models.complex), 83
compute_convergence() (in module dicee.callbacks), 24
compute_func() (dicee.models.FMult method), 158
compute_func() (dicee.models.FMul2 method), 159
compute_func() (dicee.models.function_space.FMult method), 87
compute_func() (dicee.models.function_space.FMul2 method), 88
compute_func() (dicee.models.function_space.GFMult method), 87
compute_func() (dicee.models.GFMult method), 158
compute_mrr() (dicee.callbacks.ASWA static method), 25
compute_sigma_pp() (dicee.DeCaL method), 192
compute_sigma_pp() (dicee.Keci method), 188
compute_sigma_pp() (dicee.models.clifford.DeCaL method), 80
compute_sigma_pp() (dicee.models.clifford.Keci method), 76
compute_sigma_pp() (dicee.models.DeCaL method), 150
compute_sigma_pp() (dicee.models.Keci method), 145
compute_sigma_pq() (dicee.DeCaL method), 193
compute_sigma_pq() (dicee.Keci method), 188
compute_sigma_pq() (dicee.models.clifford.DeCaL method), 81
compute_sigma_pq() (dicee.models.clifford.Keci method), 76
compute_sigma_pq() (dicee.models.DeCaL method), 151
compute_sigma_pq() (dicee.models.Keci method), 146
compute_sigma_pr() (dicee.DeCaL method), 194
compute_sigma_pr() (dicee.models.clifford.DeCaL method), 81
compute_sigma_pr() (dicee.models.DeCaL method), 151
compute_sigma_qq() (dicee.DeCaL method), 193
compute_sigma_qq() (dicee.Keci method), 188
compute_sigma_qq() (dicee.models.clifford.DeCaL method), 81
compute_sigma_qq() (dicee.models.clifford.Keci method), 76
compute_sigma_qq() (dicee.models.DeCaL method), 150
compute_sigma_qq() (dicee.models.Keci method), 146
compute_sigma_qr() (dicee.DeCaL method), 194
compute_sigma_qr() (dicee.models.clifford.DeCaL method), 82
compute_sigma_qr() (dicee.models.DeCaL method), 151
compute_sigma_rr() (dicee.DeCaL method), 193
compute_sigma_rr() (dicee.models.clifford.DeCaL method), 81
compute_sigma_rr() (dicee.models.DeCaL method), 151
compute_sigmas_multivect() (dicee.DeCaL method), 192
compute_sigmas_multivect() (dicee.models.clifford.DeCaL method), 79
compute_sigmas_multivect() (dicee.models.DeCaL method), 149
compute_sigmas_single() (dicee.DeCaL method), 191
compute_sigmas_single() (dicee.models.clifford.DeCaL method), 79
compute_sigmas_single() (dicee.models.DeCaL method), 149
ConEx (class in dicee), 199
ConEx (class in dicee.models), 130
ConEx (class in dicee.models.complex), 82
config (dicee.BytE attribute), 206
config (dicee.CoKE attribute), 204
config (dicee.models.CoKE attribute), 128
config (dicee.models.real.CoKE attribute), 101
config (dicee.models.transformers.BytE attribute), 103
config (dicee.models.transformers.GPT attribute), 108
configs (dicee.abstracts.BaseInteractiveKGE attribute), 14
configure_optimizers() (dicee.models.base_model.BaseKGELighting method), 70
configure_optimizers() (dicee.models.BaseKGELighting method), 118
configure_optimizers() (dicee.models.transformers.GPT method), 108
construct_batch_selected_cl_multivector() (dicee.Keci method), 189
construct_batch_selected_cl_multivector() (dicee.models.clifford.Keci method), 77
construct_batch_selected_cl_multivector() (dicee.models.Keci method), 147
construct_cl_multivector() (dicee.DeCaL method), 192
construct_cl_multivector() (dicee.Keci method), 189
construct_cl_multivector() (dicee.models.clifford.DeCaL method), 80
construct_cl_multivector() (dicee.models.clifford.Keci method), 77
construct_cl_multivector() (dicee.models.DeCaL method), 150
construct_cl_multivector() (dicee.models.Keci method), 147

```

construct_dataset () (*in module dicee*), 217
 construct_dataset () (*in module dicee.dataset_classes*), 33
 construct_ensemble (*dicee.abstracts.BaseInteractiveKGE attribute*), 14
 construct_graph () (*dicee.query_generator.QueryGenerator method*), 162
 construct_graph () (*dicee.QueryGenerator method*), 231
 construct_input_and_output () (*dicee.abstracts.BaseInteractiveKGE method*), 16
 construct_multi_coeff () (*dicee.LFMult method*), 203
 construct_multi_coeff () (*dicee.models.function_space.LFMult method*), 89
 construct_multi_coeff () (*dicee.models.LFMult method*), 160
 continual_learning (*dicee.config.Namespace attribute*), 32
 continual_start () (*dicee.DICE_Trainer method*), 213
 continual_start () (*dicee.executer.ContinuousExecute method*), 51
 continual_start () (*dicee.trainer.DICE_Trainer method*), 182
 continual_start () (*dicee.trainer.dice_trainer.DICE_Trainer method*), 178
 continual_training_setup_executor () (*in module dicee*), 212
 continual_training_setup_executor () (*in module dicee.static_funcs*), 175
 ContinuousExecute (*class in dicee.executer*), 51
 conv2d (*dicee.AConEx attribute*), 196
 conv2d (*dicee.AConvO attribute*), 197
 conv2d (*dicee.AConvQ attribute*), 197
 conv2d (*dicee.ConEx attribute*), 199
 conv2d (*dicee.ConvO attribute*), 199
 conv2d (*dicee.ConvQ attribute*), 198
 conv2d (*dicee.models.AConEx attribute*), 131
 conv2d (*dicee.models.AConvO attribute*), 144
 conv2d (*dicee.models.AConvQ attribute*), 138
 conv2d (*dicee.models.complex.AConEx attribute*), 83
 conv2d (*dicee.models.complex.ConEx attribute*), 82
 conv2d (*dicee.models.ConEx attribute*), 131
 conv2d (*dicee.models.ConvO attribute*), 144
 conv2d (*dicee.models.ConvQ attribute*), 138
 conv2d (*dicee.models.octonion.AConvO attribute*), 94
 conv2d (*dicee.models.octonion.ConvO attribute*), 93
 conv2d (*dicee.models.quaternion.AConvQ attribute*), 98
 conv2d (*dicee.models.quaternion.ConvQ attribute*), 98
 ConvO (*class in dicee*), 198
 ConvO (*class in dicee.models*), 143
 ConvO (*class in dicee.models.octonion*), 93
 ConvQ (*class in dicee*), 198
 ConvQ (*class in dicee.models*), 137
 ConvQ (*class in dicee.models.quaternion*), 97
 count_triples () (*in module dicee.read_preprocess_save_load_kg.util*), 167
 create_and_store_kg () (*dicee.executer.Execute method*), 50
 create_constraints () (*in module dicee.read_preprocess_save_load_kg.util*), 167
 create_constraints () (*in module dicee.static_preprocess_funcs*), 176
 create_experiment_folder () (*in module dicee*), 212
 create_experiment_folder () (*in module dicee.static_funcs*), 175
 create_random_data () (*dicee.callbacks.PseudoLabellingCallback method*), 24
 create_reciprocal_triples () (*in module dicee*), 211
 create_reciprocal_triples () (*in module dicee.read_preprocess_save_load_kg.util*), 168
 create_reciprocal_triples () (*in module dicee.static_funcs*), 173
 create_vector_database () (*dicee.KGE method*), 214
 create_vector_database () (*dicee.knowledge_graph_embeddings.KGE method*), 53
 crop_block_size () (*dicee.models.transformers.GPT method*), 108
 ctx (*dicee.trainer.torch_trainer_ddp.NodeTrainer attribute*), 182
 current_epoch (*dicee.callbacks.SWA attribute*), 29
 CVDataModule (*class in dicee*), 225
 CVDataModule (*class in dicee.dataset_classes*), 41
 cycle_length (*dicee.callbacks.LRScheduler attribute*), 28

D

data_module (*dicee.callbacks.PseudoLabellingCallback attribute*), 24
 data_property_embeddings (*dicee.models.literal.LiteralEmbeddings attribute*), 91
 data_property_to_idx (*dicee.dataset_classes.LiteralDataset attribute*), 45
 data_property_to_idx (*dicee.LiteralDataset attribute*), 229
 dataset_dir (*dicee.config.Namespace attribute*), 29
 dataset_dir (*dicee.knowledge_graph.KG attribute*), 52

```

dataset_sanity_checking() (in module dicee.read_preprocess_save_load_kg.util), 168
DeCaL (class in dicee), 190
DeCaL (class in dicee.models), 148
DeCaL (class in dicee.models.clifford), 78
decide() (dicee.callbacks.ASWA method), 25
default_eval_model (dicee.callbacks.PeriodicEvalCallback attribute), 28
degree (dicee.LFMult attribute), 203
degree (dicee.models.function_space.LFMult attribute), 89
degree (dicee.models.LFMult attribute), 159
denormalize() (dicee.dataset_classes.LiteralDataset static method), 46
denormalize() (dicee.LiteralDataset static method), 230
deploy() (dicee.KGE method), 217
deploy() (dicee.knowledge_graph_embeddings.KGE method), 56
deploy_head_entity_prediction() (in module dicee), 212
deploy_head_entity_prediction() (in module dicee.static_funcs), 174
deploy_relation_prediction() (in module dicee), 212
deploy_relation_prediction() (in module dicee.static_funcs), 175
deploy_tail_entity_prediction() (in module dicee), 212
deploy_tail_entity_prediction() (in module dicee.static_funcs), 174
deploy_triple_prediction() (in module dicee), 212
deploy_triple_prediction() (in module dicee.static_funcs), 174
describe() (dicee.knowledge_graph.KG method), 53
description_of_input (dicee.knowledge_graph.KG attribute), 53
device (dicee.models.literal.LiteralEmbeddings property), 91
DICE_Trainer (class in dicee), 212
DICE_Trainer (class in dicee.trainer), 182
DICE_Trainer (class in dicee.trainer.dice_trainer), 177
dicee
    module, 12
dicee.__main__
    module, 12
dicee.abstracts
    module, 12
dicee.analyse_experiments
    module, 19
dicee.callbacks
    module, 20
dicee.config
    module, 29
dicee.dataset_classes
    module, 32
dicee.eval_static_funcs
    module, 46
dicee.evaluator
    module, 48
dicee.executor
    module, 49
dicee.knowledge_graph
    module, 51
dicee.knowledge_graph_embeddings
    module, 53
dicee.models
    module, 57
dicee.models.adopt
    module, 57
dicee.models.base_model
    module, 66
dicee.models.clifford
    module, 75
dicee.models.complex
    module, 82
dicee.models.duale
    module, 84
dicee.models.ensemble
    module, 85
dicee.models.function_space
    module, 86
dicee.models.literal

```

```
    module, 90
dicee.models.octonion
    module, 91
dicee.models.pykeen_models
    module, 94
dicee.models.quaternion
    module, 96
dicee.models.real
    module, 99
dicee.models.static_funcs
    module, 102
dicee.models.transformers
    module, 102
dicee.query_generator
    module, 161
dicee.read_preprocess_save_load_kg
    module, 163
dicee.read_preprocess_save_load_kg.preprocess
    module, 163
dicee.read_preprocess_save_load_kg.read_from_disk
    module, 164
dicee.read_preprocess_save_load_kg.save_load_disk
    module, 164
dicee.read_preprocess_save_load_kg.util
    module, 165
dicee.sanity_checkers
    module, 169
dicee.scripts
    module, 170
dicee.scripts.index_serve
    module, 170
dicee.scripts.run
    module, 172
dicee.static_funcs
    module, 172
dicee.static_funcs_training
    module, 175
dicee.static_preprocess_funcs
    module, 176
dicee.trainer
    module, 177
dicee.trainer.dice_trainer
    module, 177
dicee.trainer.model_parallelism
    module, 179
dicee.trainer.torch_trainer
    module, 179
dicee.trainer.torch_trainer_ddp
    module, 181
discrete_points (dicee.models.FMult2 attribute), 158
discrete_points (dicee.models.function_space.FMult2 attribute), 88
dist_func (dicee.models.Pyke attribute), 127
dist_func (dicee.models.real.Pyke attribute), 100
dist_func (dicee.Pyke attribute), 186
DistMult (class in dicee), 186
DistMult (class in dicee.models), 126
DistMult (class in dicee.models.real), 99
distributed (dicee.executer.Execute attribute), 50
download_file () (in module dicee), 212
download_file () (in module dicee.static_funcs), 175
download_files_from_url () (in module dicee), 212
download_files_from_url () (in module dicee.static_funcs), 175
download_pretrained_model () (in module dicee), 212
download_pretrained_model () (in module dicee.static_funcs), 175
dropout (dicee.models.CoKEConfig attribute), 127
dropout (dicee.models.literal.LiteralEmbeddings attribute), 90, 91
dropout (dicee.models.real.CoKEConfig attribute), 100, 101
dropout (dicee.models.transformers.GPTConfig attribute), 107
```

dropout (*dicee.models.transformers.MLP* attribute), 106
dropout (*dicee.models.transformers.SelfAttention* attribute), 105
DualE (class in dicee), 194
DualE (class in dicee.models), 160
DualE (class in dicee.models.dualE), 84
dummy_eval () (*dicee.evaluator.Evaluator* method), 49
dummy_id (*dicee.knowledge_graph.KG* attribute), 52
during_training (*dicee.evaluator.Evaluator* attribute), 48

E

ee_vocab (*dicee.evaluator.Evaluator* attribute), 48
efficient_zero_grad () (in module *dicee.static_funcs_training*), 176
embedding_dim (*dicee.analyse_experiments.Experiment* attribute), 19
embedding_dim (*dicee.BaseKGE* attribute), 208
embedding_dim (*dicee.config.Namespace* attribute), 30
embedding_dim (*dicee.models.base_model.BaseKGE* attribute), 72
embedding_dim (*dicee.models.BaseKGE* attribute), 120, 123, 129, 133, 139, 152, 156
embedding_dim (*dicee.models.literal.LiteralEmbeddings* attribute), 91
embedding_dims (*dicee.models.literal.LiteralEmbeddings* attribute), 90
enable_log (in module *dicee.static_preprocess_funcs*), 176
enc (*dicee.knowledge_graph.KG* attribute), 52
end () (*dicee.executor.Execute* method), 50
EnsembleKGE (class in dicee), 210
EnsembleKGE (class in dicee.models.ensemble), 86
ent2id (*dicee.query_generator.QueryGenerator* attribute), 162
ent2id (*dicee.QueryGenerator* attribute), 230
ent_in (*dicee.query_generator.QueryGenerator* attribute), 162
ent_in (*dicee.QueryGenerator* attribute), 231
ent_out (*dicee.query_generator.QueryGenerator* attribute), 162
ent_out (*dicee.QueryGenerator* attribute), 231
entities_str (*dicee.knowledge_graph.KG* property), 53
entity_embeddings (*dicee.AConvQ* attribute), 197
entity_embeddings (*dicee.ConvQ* attribute), 198
entity_embeddings (*dicee.DeCaL* attribute), 191
entity_embeddings (*dicee.DualE* attribute), 194
entity_embeddings (*dicee.LFMult* attribute), 203
entity_embeddings (*dicee.models.AConvQ* attribute), 138
entity_embeddings (*dicee.models.clifford.DeCaL* attribute), 79
entity_embeddings (*dicee.models.ConvQ* attribute), 138
entity_embeddings (*dicee.models.DeCaL* attribute), 148
entity_embeddings (*dicee.models.DualE* attribute), 161
entity_embeddings (*dicee.models.dualE.DualE* attribute), 84
entity_embeddings (*dicee.models.FMult* attribute), 157
entity_embeddings (*dicee.models.FMult2* attribute), 158
entity_embeddings (*dicee.models.function_space.FMult* attribute), 87
entity_embeddings (*dicee.models.function_space.FMult2* attribute), 88
entity_embeddings (*dicee.models.function_space.GFMult* attribute), 87
entity_embeddings (*dicee.models.function_space.LFMult* attribute), 89
entity_embeddings (*dicee.models.function_space.LFMult1* attribute), 88
entity_embeddings (*dicee.models.GFMult* attribute), 158
entity_embeddings (*dicee.models.LFMult* attribute), 159
entity_embeddings (*dicee.models.LFMult1* attribute), 159
entity_embeddings (*dicee.models.literal.LiteralEmbeddings* attribute), 90, 91
entity_embeddings (*dicee.models.pykeen_models.PykeenKGE* attribute), 95
entity_embeddings (*dicee.models.PykeenKGE* attribute), 154
entity_embeddings (*dicee.models.quaternion.AConvQ* attribute), 98
entity_embeddings (*dicee.models.quaternion.ConvQ* attribute), 98
entity_embeddings (*dicee.PykeenKGE* attribute), 205
entity_to_idx (*dicee.dataset_classes.LiteralDataset* attribute), 45, 46
entity_to_idx (*dicee.knowledge_graph.KG* attribute), 52
entity_to_idx (*dicee.LiteralDataset* attribute), 229, 230
entity_to_idx (*dicee.scripts.index_serve.NeuralSearcher* attribute), 171
epoch_count (*dicee.abstracts.AbstractPPECallback* attribute), 17
epoch_count (*dicee.callbacks.ASWA* attribute), 24
epoch_counter (*dicee.callbacks.Eval* attribute), 25
epoch_counter (*dicee.callbacks.KGESaveCallback* attribute), 23
epoch_counter (*dicee.callbacks.PeriodicEvalCallback* attribute), 27

epoch_ratio (*dicee.callbacks.Eval* attribute), 25
 er_vocab (*dicee.evaluator.Evaluator* attribute), 48
 estimate_mfu() (*dicee.models.transformers.GPT* method), 108
 estimate_q() (*in module dicee.callbacks*), 24
 Eval (*class in dicee.callbacks*), 25
 eval() (*dicee.EnsembleKGE* method), 210
 eval() (*dicee.evaluator.Evaluator* method), 49
 eval() (*dicee.models.ensemble.EnsembleKGE* method), 86
 eval_at_epochs (*dicee.config.Namespace* attribute), 32
 eval_epochs (*dicee.callbacks.PeriodicEvalCallback* attribute), 28
 eval_every_n_epochs (*dicee.config.Namespace* attribute), 32
 eval_lp_performance() (*dicee.KGE* method), 214
 eval_lp_performance() (*dicee.knowledge_graph_embeddings.KGE* method), 53
 eval_model (*dicee.config.Namespace* attribute), 31
 eval_model (*dicee.knowledge_graph.KG* attribute), 52
 eval_rank_of_head_and_tail_byte_pair_encoded_entity() (*dicee.evaluator.Evaluator* method), 49
 eval_rank_of_head_and_tail_entity() (*dicee.evaluator.Evaluator* method), 49
 eval_with_bpe_vs_all() (*dicee.evaluator.Evaluator* method), 49
 eval_with_byte() (*dicee.evaluator.Evaluator* method), 49
 eval_with_data() (*dicee.evaluator.Evaluator* method), 49
 eval_with_vs_all() (*dicee.evaluator.Evaluator* method), 49
 evaluate() (*in module dicee*), 212
 evaluate() (*in module dicee.static_funcs*), 175
 evaluate_bpe_lp() (*in module dicee.static_funcs_training*), 176
 evaluate_ensemble_link_prediction_performance() (*in module dicee.eval_static_funcs*), 48
 evaluate_link_prediction_performance() (*in module dicee.eval_static_funcs*), 47
 evaluate_link_prediction_performance_with_bpe() (*in module dicee.eval_static_funcs*), 47
 evaluate_link_prediction_performance_with_reciprocals() (*in module dicee.eval_static_funcs*), 47
 evaluate_literal_prediction() (*in module dicee.eval_static_funcs*), 47
 evaluate_lp() (*dicee.evaluator.Evaluator* method), 49
 evaluate_lp() (*in module dicee.static_funcs_training*), 175
 evaluate_lp_bpe_k_vs_all() (*dicee.evaluator.Evaluator* method), 49
 evaluate_lp_bpe_k_vs_all() (*in module dicee.eval_static_funcs*), 47
 evaluate_lp_k_vs_all() (*dicee.evaluator.Evaluator* method), 49
 evaluate_lp_with_byte() (*dicee.evaluator.Evaluator* method), 49
 Evaluator (*class in dicee.evaluator*), 48
 evaluator (*dicee.DICE_Trainer* attribute), 213
 evaluator (*dicee.executer.Execute* attribute), 50
 evaluator (*dicee.trainer.DICE_Trainer* attribute), 182
 evaluator (*dicee.trainer.dice_trainer.DICE_Trainer* attribute), 178
 every_x_epoch (*dicee.callbacks.KGESaveCallback* attribute), 23
 example_input_array (*dicee.ensemble.EnsembleKGE* property), 210
 example_input_array (*dicee.models.ensemble.EnsembleKGE* property), 86
 Execute (*class in dicee.executer*), 50
 exists() (*dicee.knowledge_graph.KG* method), 53
 Experiment (*class in dicee.analyse_experiments*), 19
 experiment_dir (*dicee.callbacks.LRScheduler* attribute), 28
 experiment_dir (*dicee.callbacks.PeriodicEvalCallback* attribute), 27
 explicit (*dicee.models.QMult* attribute), 137
 explicit (*dicee.models.quaternion.QMult* attribute), 97
 explicit (*dicee.QMult* attribute), 201
 exponential_function() (*in module dicee*), 212
 exponential_function() (*in module dicee.static_funcs*), 175
 extract_input_outputs() (*dicee.trainer.torch_trainer_ddp.NodeTrainer* method), 182
 extract_input_outputs() (*in module dicee.trainer.model_parallelism*), 179
 extract_input_outputs_set_device() (*dicee.trainer.torch_trainer.TorchTrainer* method), 180

F

f (*dicee.callbacks.KronE* attribute), 26
 fc (*dicee.models.literal.LiteralEmbeddings* attribute), 91
 fc1 (*dicee.AConEx* attribute), 196
 fc1 (*dicee.AConvO* attribute), 197
 fc1 (*dicee.AConvQ* attribute), 197
 fc1 (*dicee.ConEx* attribute), 199
 fc1 (*dicee.ConvO* attribute), 199
 fc1 (*dicee.ConvQ* attribute), 198

fc1 (*dicee.models.AConEx attribute*), 131
 fc1 (*dicee.models.AConvO attribute*), 144
 fc1 (*dicee.models.AConvQ attribute*), 138
 fc1 (*dicee.models.complex.AConEx attribute*), 83
 fc1 (*dicee.models.complex.ConEx attribute*), 82
 fc1 (*dicee.models.ConEx attribute*), 131
 fc1 (*dicee.models.ConvO attribute*), 144
 fc1 (*dicee.models.ConvQ attribute*), 138
 fc1 (*dicee.models.octonion.AConvO attribute*), 94
 fc1 (*dicee.models.octonion.ConvO attribute*), 93
 fc1 (*dicee.models.quaternion.AConvQ attribute*), 98
 fc1 (*dicee.models.quaternion.ConvQ attribute*), 98
 fc_num_input (*dicee.AConEx attribute*), 196
 fc_num_input (*dicee.AConvO attribute*), 197
 fc_num_input (*dicee.AConvQ attribute*), 197
 fc_num_input (*dicee.ConEx attribute*), 199
 fc_num_input (*dicee.ConvO attribute*), 199
 fc_num_input (*dicee.ConvQ attribute*), 198
 fc_num_input (*dicee.models.AConEx attribute*), 131
 fc_num_input (*dicee.models.AConvO attribute*), 144
 fc_num_input (*dicee.models.AConvQ attribute*), 138
 fc_num_input (*dicee.models.complex.AConEx attribute*), 83
 fc_num_input (*dicee.models.complex.ConEx attribute*), 82
 fc_num_input (*dicee.models.ConEx attribute*), 131
 fc_num_input (*dicee.models.ConvO attribute*), 144
 fc_num_input (*dicee.models.ConvQ attribute*), 138
 fc_num_input (*dicee.models.octonion.AConvO attribute*), 94
 fc_num_input (*dicee.models.octonion.ConvO attribute*), 93
 fc_num_input (*dicee.models.quaternion.AConvQ attribute*), 98
 fc_num_input (*dicee.models.quaternion.ConvQ attribute*), 98
 fc_out (*dicee.models.literal.LiteralEmbeddings attribute*), 91
 feature_map_dropout (*dicee.AConEx attribute*), 196
 feature_map_dropout (*dicee.AConvO attribute*), 197
 feature_map_dropout (*dicee.AConvQ attribute*), 197
 feature_map_dropout (*dicee.ConEx attribute*), 200
 feature_map_dropout (*dicee.ConvO attribute*), 199
 feature_map_dropout (*dicee.ConvQ attribute*), 198
 feature_map_dropout (*dicee.models.AConEx attribute*), 131
 feature_map_dropout (*dicee.models.AConvO attribute*), 144
 feature_map_dropout (*dicee.models.AConvQ attribute*), 138
 feature_map_dropout (*dicee.models.complex.AConEx attribute*), 83
 feature_map_dropout (*dicee.models.complex.ConEx attribute*), 82
 feature_map_dropout (*dicee.models.ConEx attribute*), 131
 feature_map_dropout (*dicee.models.ConvO attribute*), 144
 feature_map_dropout (*dicee.models.ConvQ attribute*), 138
 feature_map_dropout (*dicee.models.octonion.AConvO attribute*), 94
 feature_map_dropout (*dicee.models.octonion.ConvO attribute*), 93
 feature_map_dropout (*dicee.models.quaternion.AConvQ attribute*), 98
 feature_map_dropout (*dicee.models.quaternion.ConvQ attribute*), 98
 feature_map_dropout_rate (*dicee.BaseKGE attribute*), 208
 feature_map_dropout_rate (*dicee.config.Namespace attribute*), 31
 feature_map_dropout_rate (*dicee.models.base_model.BaseKGE attribute*), 72
 feature_map_dropout_rate (*dicee.models.BaseKGE attribute*), 120, 123, 129, 134, 140, 152, 156
 fetch_worker () (*in module dicee.read_preprocess_save_load_kg.util*), 167
 fill_query () (*dicee.query_generator.QueryGenerator method*), 162
 fill_query () (*dicee.QueryGenerator method*), 231
 find_good_batch_size () (*in module dicee.trainer.model_parallelism*), 179
 find_missing_triples () (*dicee.KGE method*), 216
 find_missing_triples () (*dicee.knowledge_graph_embeddings.KGE method*), 56
 fit () (*dicee.trainer.model_parallelism.TensorParallel method*), 179
 fit () (*dicee.trainer.torch_trainer_ddp.TorchDDPTrainer method*), 181
 fit () (*dicee.trainer.torch.Trainer method*), 180
 flash (*dicee.models.transformers.SelfAttention attribute*), 105
 FMult (*class in dicee.models*), 157
 FMult (*class in dicee.models.function_space*), 87
 FMult2 (*class in dicee.models*), 158
 FMult2 (*class in dicee.models.function_space*), 87
 form_of_labelling (*dicee.DICE_Trainer attribute*), 213

```

form_of_labelling (dicee.trainer.DICE_Trainer attribute), 182
form_of_labelling (dicee.trainer.dice_trainer.DICE_Trainer attribute), 178
forward() (dicee.BaseKGE method), 209
forward() (dicee.BytE method), 206
forward() (dicee.models.base_model.BaseKGE method), 73
forward() (dicee.models.base_model.IdentityClass static method), 75
forward() (dicee.models.BaseKGE method), 121, 124, 130, 134, 140, 153, 157
forward() (dicee.models.Block method), 126
forward() (dicee.models.IdentityClass static method), 122, 136, 142
forward() (dicee.models.literal.LiteralEmbeddings method), 91
forward() (dicee.models.transformers.Block method), 107
forward() (dicee.models.transformers.BytE method), 103
forward() (dicee.models.transformers.GPT method), 108
forward() (dicee.models.transformers.LayerNorm method), 104
forward() (dicee.models.transformers.MLP method), 106
forward() (dicee.models.transformers.SelfAttention method), 105
forward_backward_update () (dicee.trainer.torch_trainer.TorchTrainer method), 180
forward_backward_update_loss () (in module dicee.trainer.model_parallelism), 179
forward_byte_pair_encoded_k_vs_all () (dicee.BaseKGE method), 209
forward_byte_pair_encoded_k_vs_all () (dicee.models.base_model.BaseKGE method), 73
forward_byte_pair_encoded_k_vs_all () (dicee.models.BaseKGE method), 121, 124, 130, 134, 140, 153, 156
forward_byte_pair_encoded_triple () (dicee.models.base_model.BaseKGE method), 73
forward_byte_pair_encoded_triple () (dicee.models.BaseKGE method), 121, 124, 130, 134, 140, 153, 156
forward_k_vs_all () (dicee.AConEx method), 196
forward_k_vs_all () (dicee.AConvO method), 197
forward_k_vs_all () (dicee.AConvQ method), 197
forward_k_vs_all () (dicee.BaseKGE method), 210
forward_k_vs_all () (dicee.CoKE method), 204
forward_k_vs_all () (dicee.ComplEx method), 196
forward_k_vs_all () (dicee.ConEx method), 200
forward_k_vs_all () (dicee.ConvO method), 199
forward_k_vs_all () (dicee.ConvQ method), 198
forward_k_vs_all () (dicee.DeCaL method), 192
forward_k_vs_all () (dicee.DistMult method), 187
forward_k_vs_all () (dicee.DualE method), 195
forward_k_vs_all () (dicee.Keci method), 189
forward_k_vs_all () (dicee.models.AConEx method), 131
forward_k_vs_all () (dicee.models.AConvO method), 144
forward_k_vs_all () (dicee.models.AConvQ method), 139
forward_k_vs_all () (dicee.models.base_model.BaseKGE method), 73
forward_k_vs_all () (dicee.models.BaseKGE method), 121, 124, 130, 135, 141, 154, 157
forward_k_vs_all () (dicee.models.clifford.DeCaL method), 80
forward_k_vs_all () (dicee.models.clifford.Keci method), 77
forward_k_vs_all () (dicee.models.CoKE method), 128
forward_k_vs_all () (dicee.models.ComplEx method), 132
forward_k_vs_all () (dicee.models.complex.AConEx method), 83
forward_k_vs_all () (dicee.models.complex.ComplEx method), 84
forward_k_vs_all () (dicee.models.complex.ConEx method), 82
forward_k_vs_all () (dicee.models.ConEx method), 131
forward_k_vs_all () (dicee.models.ConvO method), 144
forward_k_vs_all () (dicee.models.ConvQ method), 138
forward_k_vs_all () (dicee.models.DeCaL method), 149
forward_k_vs_all () (dicee.models.DistMult method), 126
forward_k_vs_all () (dicee.models.DualE method), 161
forward_k_vs_all () (dicee.models.dualE.DualE method), 85
forward_k_vs_all () (dicee.models.Keci method), 147
forward_k_vs_all () (dicee.models.octonion.AConvO method), 94
forward_k_vs_all () (dicee.models.octonion.ConvO method), 94
forward_k_vs_all () (dicee.models.octonion.OMult method), 93
forward_k_vs_all () (dicee.models.OMult method), 143
forward_k_vs_all () (dicee.models.pykeen_models.PykeenKGE method), 95
forward_k_vs_all () (dicee.models.PykeenKGE method), 154
forward_k_vs_all () (dicee.models.QMult method), 137
forward_k_vs_all () (dicee.models.quaternion.AConvQ method), 99
forward_k_vs_all () (dicee.models.quaternion.ConvQ method), 98
forward_k_vs_all () (dicee.models.quaternion.QMult method), 97
forward_k_vs_all () (dicee.models.real.CoKE method), 101

```

```

forward_k_vs_all() (dicee.models.real.DistMult method), 99
forward_k_vs_all() (dicee.models.real.Shallom method), 100
forward_k_vs_all() (dicee.models.real.TransE method), 100
forward_k_vs_all() (dicee.models.Shallom method), 126
forward_k_vs_all() (dicee.models.TransE method), 126
forward_k_vs_all() (dicee.OMult method), 202
forward_k_vs_all() (dicee.PykeenKGE method), 205
forward_k_vs_all() (dicee.QMult method), 201
forward_k_vs_all() (dicee.Shallom method), 203
forward_k_vs_all() (dicee.TransE method), 190
forward_k_vs_sample() (dicee.AConEx method), 196
forward_k_vs_sample() (dicee.BaseKGE method), 210
forward_k_vs_sample() (dicee.CoKE method), 204
forward_k_vs_sample() (dicee.ComplEx method), 196
forward_k_vs_sample() (dicee.ConEx method), 200
forward_k_vs_sample() (dicee.DistMult method), 187
forward_k_vs_sample() (dicee.Keci method), 190
forward_k_vs_sample() (dicee.models.AConEx method), 132
forward_k_vs_sample() (dicee.models.base_model.BaseKGE method), 73
forward_k_vs_sample() (dicee.models.BaseKGE method), 121, 124, 130, 135, 141, 154, 157
forward_k_vs_sample() (dicee.models.clifford.Keci method), 78
forward_k_vs_sample() (dicee.models.CoKE method), 128
forward_k_vs_sample() (dicee.models.ComplEx method), 133
forward_k_vs_sample() (dicee.models.complex.AConEx method), 83
forward_k_vs_sample() (dicee.models.complex.ComplEx method), 84
forward_k_vs_sample() (dicee.models.complex.ConEx method), 83
forward_k_vs_sample() (dicee.models.ConEx method), 131
forward_k_vs_sample() (dicee.models.DistMult method), 126
forward_k_vs_sample() (dicee.models.Keci method), 147
forward_k_vs_sample() (dicee.models.pykeen_models.PykeenKGE method), 95
forward_k_vs_sample() (dicee.models.PykeenKGE method), 155
forward_k_vs_sample() (dicee.models.QMult method), 137
forward_k_vs_sample() (dicee.models.quaternion.QMult method), 97
forward_k_vs_sample() (dicee.models.real.CoKE method), 101
forward_k_vs_sample() (dicee.models.real.DistMult method), 99
forward_k_vs_sample() (dicee.PykeenKGE method), 205
forward_k_vs_sample() (dicee.QMult method), 201
forward_k_vs_with_explicit() (dicee.Keci method), 189
forward_k_vs_with_explicit() (dicee.models.clifford.Keci method), 77
forward_k_vs_with_explicit() (dicee.models.Keci method), 147
forward_triples() (dicee.AConEx method), 196
forward_triples() (dicee.AConvO method), 197
forward_triples() (dicee.AConvQ method), 197
forward_triples() (dicee.BaseKGE method), 209
forward_triples() (dicee.ConEx method), 200
forward_triples() (dicee.ConvO method), 199
forward_triples() (dicee.ConvQ method), 198
forward_triples() (dicee.DeCaL method), 191
forward_triples() (dicee.DualE method), 194
forward_triples() (dicee.Keci method), 190
forward_triples() (dicee.LFMult method), 203
forward_triples() (dicee.models.AConEx method), 131
forward_triples() (dicee.models.AConvO method), 144
forward_triples() (dicee.models.AConvQ method), 138
forward_triples() (dicee.models.base_model.BaseKGE method), 73
forward_triples() (dicee.models.BaseKGE method), 121, 124, 130, 135, 141, 153, 157
forward_triples() (dicee.models.clifford.DeCaL method), 79
forward_triples() (dicee.models.clifford.Keci method), 78
forward_triples() (dicee.models.complex.AConEx method), 83
forward_triples() (dicee.models.complex.ConEx method), 82
forward_triples() (dicee.models.ConEx method), 131
forward_triples() (dicee.models.ConvO method), 144
forward_triples() (dicee.models.ConvQ method), 138
forward_triples() (dicee.models.DeCaL method), 149
forward_triples() (dicee.models.DualE method), 161
forward_triples() (dicee.models.dualE.DualE method), 85
forward_triples() (dicee.models.FMult method), 158
forward_triples() (dicee.models.FMult2 method), 159

```

```

forward_triples() (dicee.models.function_space.FMult method), 87
forward_triples() (dicee.models.function_space.FMult2 method), 88
forward_triples() (dicee.models.function_space.GFMult method), 87
forward_triples() (dicee.models.function_space.LFMult method), 89
forward_triples() (dicee.models.function_space.LFMult1 method), 88
forward_triples() (dicee.models.GFMult method), 158
forward_triples() (dicee.models.Keci method), 148
forward_triples() (dicee.models.LFMult method), 159
forward_triples() (dicee.models.LFMult1 method), 159
forward_triples() (dicee.models.octonion.AConvO method), 94
forward_triples() (dicee.models.octonion.ConvO method), 94
forward_triples() (dicee.models.Pyke method), 127
forward_triples() (dicee.models.pykeen_models.PykeenKGE method), 95
forward_triples() (dicee.models.PykeenKGE method), 155
forward_triples() (dicee.models.quaternion.AConvQ method), 98
forward_triples() (dicee.models.quaternion.ConvQ method), 98
forward_triples() (dicee.models.real.Pyke method), 100
forward_triples() (dicee.models.real.Shallom method), 100
forward_triples() (dicee.models.Shallom method), 126
forward_triples() (dicee.Pyke method), 186
forward_triples() (dicee.PykeenKGE method), 205
forward_triples() (dicee.Shallom method), 203
freeze_entity_embeddings (dicee.models.literal.LiteralEmbeddings attribute), 91
frequency (dicee.callbacks.Perturb attribute), 27
from_pretrained() (dicee.models.transformers.GPT class method), 108
from_pretrained_model_write_embeddings_into_csv() (in module dicee), 212
from_pretrained_model_write_embeddings_into_csv() (in module dicee.static_funcs), 175
full_storage_path (dicee.analyse_experiments.Experiment attribute), 19
func_triple_to_bpe_representation (dicee.evaluator.Evaluator attribute), 48
func_triple_to_bpe_representation() (dicee.knowledge_graph.KG method), 53
function() (dicee.models.FMult2 method), 159
function() (dicee.models.function_space.FMult2 method), 88

```

G

```

gamma (dicee.models.FMult attribute), 158
gamma (dicee.models.function_space.FMult attribute), 87
gate_residual (dicee.models.literal.LiteralEmbeddings attribute), 90, 91
gated_residual_proj (dicee.models.literal.LiteralEmbeddings attribute), 91
gelu (dicee.models.transformers.MLP attribute), 106
gen_test (dicee.query_generator.QueryGenerator attribute), 162
gen_test (dicee.QueryGenerator attribute), 230
gen_valid (dicee.query_generator.QueryGenerator attribute), 162
gen_valid (dicee.QueryGenerator attribute), 230
generate() (dicee.ByE method), 206
generate() (dicee.KGE method), 214
generate() (dicee.knowledge_graph_embeddings.KGE method), 53
generate() (dicee.models.transformers.ByE method), 103
generate_queries() (dicee.query_generator.QueryGenerator method), 162
generate_queries() (dicee.QueryGenerator method), 231
get_aswa_state_dict() (dicee.callbacks.ASWA method), 25
get_bpe_head_and_relation_representation() (dicee.BaseKGE method), 210
get_bpe_head_and_relation_representation() (dicee.models.base_model.BaseKGE method), 74
get_bpe_head_and_relation_representation() (dicee.models.BaseKGE method), 121, 125, 130, 135, 141, 154, 157
get_bpe_token_representation() (dicee.abtracts.BaseInteractiveKGE method), 14
get_callbacks() (in module dicee.trainer.dice_trainer), 177
get_default_arguments() (in module dicee.analyse_experiments), 19
get_default_arguments() (in module dicee.scripts.index_serve), 171
get_default_arguments() (in module dicee.scripts.run), 172
get_ee_vocab() (in module dicee), 211
get_ee_vocab() (in module dicee.read_preprocess_save_load_kg.util), 167
get_ee_vocab() (in module dicee.static_funcs), 173
get_ee_vocab() (in module dicee.static_preprocess_funcs), 176
get_embeddings() (dicee.BaseKGE method), 210
get_embeddings() (dicee.EnsembleKGE method), 211
get_embeddings() (dicee.models.base_model.BaseKGE method), 74
get_embeddings() (dicee.models.BaseKGE method), 121, 125, 130, 135, 141, 154, 157
get_embeddings() (dicee.models.ensemble.EnsembleKGE method), 86

```

get_embeddings() (*dicee.models.real.Shallom method*), 100
 get_embeddings() (*dicee.models.Shallom method*), 126
 get_embeddings() (*dicee.Shallom method*), 203
 get_entity_embeddings() (*dicee.abstracts.BaseInteractiveKGE method*), 15
 get_entity_index() (*dicee.abstracts.BaseInteractiveKGE method*), 15
 get_er_vocab() (*in module dicee*), 211
 get_er_vocab() (*in module dicee.read_preprocess_save_load_kg.util*), 167
 get_er_vocab() (*in module dicee.static_funcs*), 173
 get_er_vocab() (*in module dicee.static_preprocess_funcs*), 176
 get_eval_report() (*dicee.abstracts.BaseInteractiveKGE method*), 14
 get_head_relation_representation() (*dicee.BaseKGE method*), 210
 get_head_relation_representation() (*dicee.models.base_model.BaseKGE method*), 74
 get_head_relation_representation() (*dicee.models.BaseKGE method*), 121, 124, 130, 135, 141, 154, 157
 get_kronecker_triple_representation() (*dicee.callbacks.KronE method*), 26
 get_num_params() (*dicee.models.transformers.GPT method*), 108
 get_padded_bpe_triple_representation() (*dicee.abstracts.BaseInteractiveKGE method*), 14
 get_queries() (*dicee.query_generator.QueryGenerator method*), 163
 get_queries() (*dicee.QueryGenerator method*), 231
 get_re_vocab() (*in module dicee*), 211
 get_re_vocab() (*in module dicee.read_preprocess_save_load_kg.util*), 167
 get_re_vocab() (*in module dicee.static_funcs*), 173
 get_re_vocab() (*in module dicee.static_preprocess_funcs*), 176
 get_relation_embeddings() (*dicee.abstracts.BaseInteractiveKGE method*), 15
 get_relation_index() (*dicee.abstracts.BaseInteractiveKGE method*), 15
 get_sentence_representation() (*dicee.BaseKGE method*), 210
 get_sentence_representation() (*dicee.models.base_model.BaseKGE method*), 74
 get_sentence_representation() (*dicee.models.BaseKGE method*), 121, 124, 130, 135, 141, 154, 157
 get_transductive_entity_embeddings() (*dicee.KGE method*), 214
 get_transductive_entity_embeddings() (*dicee.knowledge_graph_embeddings.KGE method*), 53
 get_triple_representation() (*dicee.BaseKGE method*), 210
 get_triple_representation() (*dicee.models.base_model.BaseKGE method*), 73
 get_triple_representation() (*dicee.models.BaseKGE method*), 121, 124, 130, 135, 141, 154, 157
 GFMult (*class in dicee.models*), 158
 GFMult (*class in dicee.models.function_space*), 87
 global_rank (*dicee.abstracts.AbstractTrainer attribute*), 13
 global_rank (*dicee.trainer.torch_trainer_ddp.NodeTrainer attribute*), 181
 GPT (*class in dicee.models.transformers*), 107
 GPTConfig (*class in dicee.models.transformers*), 107
 gpus (*dicee.config.Namespace attribute*), 30
 gradient_accumulation_steps (*dicee.config.Namespace attribute*), 31
 ground_queries() (*dicee.query_generator.QueryGenerator method*), 162
 ground_queries() (*dicee.QueryGenerator method*), 231

H

hidden_dim (*dicee.models.literal.LiteralEmbeddings attribute*), 91
 hidden_dropout (*dicee.BaseKGE attribute*), 209
 hidden_dropout (*dicee.models.base_model.BaseKGE attribute*), 73
 hidden_dropout (*dicee.models.BaseKGE attribute*), 120, 124, 129, 134, 140, 153, 156
 hidden_dropout_rate (*dicee.BaseKGE attribute*), 208
 hidden_dropout_rate (*dicee.config.Namespace attribute*), 31
 hidden_dropout_rate (*dicee.models.base_model.BaseKGE attribute*), 72
 hidden_dropout_rate (*dicee.models.BaseKGE attribute*), 120, 123, 129, 134, 140, 152, 156
 hidden_normalizer (*dicee.BaseKGE attribute*), 209
 hidden_normalizer (*dicee.models.base_model.BaseKGE attribute*), 73
 hidden_normalizer (*dicee.models.BaseKGE attribute*), 120, 124, 129, 134, 140, 153, 156

I

IdentityClass (*class in dicee.models*), 121, 135, 141
 IdentityClass (*class in dicee.models.base_model*), 74
 idx_entity_to_bpe_shaped (*dicee.knowledge_graph.KG attribute*), 52
 index() (*in module dicee.scripts.index_serve*), 171
 index_triple() (*dicee.abstracts.BaseInteractiveKGE method*), 15
 init_dataloader() (*dicee.DICE_Trainer method*), 213
 init_dataloader() (*dicee.trainer.DICE_Trainer method*), 183
 init_dataloader() (*dicee.trainer.dice_trainer.DICE_Trainer method*), 178
 init_dataset() (*dicee.DICE_Trainer method*), 213
 init_dataset() (*dicee.trainer.DICE_Trainer method*), 183

```

init_dataset() (dicee.trainer.dice_trainer.DICE_Trainer method), 178
init_param (dicee.config.Namespace attribute), 31
init_params_with_sanity_checking() (dicee.BaseKGE method), 209
init_params_with_sanity_checking() (dicee.models.base_model.BaseKGE method), 73
init_params_with_sanity_checking() (dicee.models.BaseKGE method), 121, 124, 130, 134, 140, 153, 157
initial_eval_setting (dicee.callbacks.ASWA attribute), 24
initialize_or_load_model() (dicee.DICE_Trainer method), 213
initialize_or_load_model() (dicee.trainer.DICE_Trainer method), 183
initialize_or_load_model() (dicee.trainer.dice_trainer.DICE_Trainer method), 178
initialize_trainer() (dicee.DICE_Trainer method), 213
initialize_trainer() (dicee.trainer.DICE_Trainer method), 183
initialize_trainer() (dicee.trainer.dice_trainer.DICE_Trainer method), 178
initialize_trainer() (in module dicee.trainer.dice_trainer), 177
input_dp_ent_real (dicee.BaseKGE attribute), 209
input_dp_ent_real (dicee.models.base_model.BaseKGE attribute), 73
input_dp_ent_real (dicee.models.BaseKGE attribute), 120, 124, 129, 134, 140, 153, 156
input_dp_rel_real (dicee.BaseKGE attribute), 209
input_dp_rel_real (dicee.models.base_model.BaseKGE attribute), 73
input_dp_rel_real (dicee.models.BaseKGE attribute), 120, 124, 129, 134, 140, 153, 156
input_dropout_rate (dicee.BaseKGE attribute), 208
input_dropout_rate (dicee.config.Namespace attribute), 31
input_dropout_rate (dicee.models.base_model.BaseKGE attribute), 72
input_dropout_rate (dicee.models.BaseKGE attribute), 120, 123, 129, 133, 140, 152, 156
InteractiveQueryDecomposition (class in dicee.abstracts), 16
initialize_model() (in module dicee), 211
initialize_model() (in module dicee.static_funcs), 174
is_continual_training (dicee.DICE_Trainer attribute), 213
is_continual_training (dicee.evaluator.Evaluator attribute), 48
is_continual_training (dicee.executer.Execute attribute), 50
is_continual_training (dicee.trainer.DICE_Trainer attribute), 182
is_continual_training (dicee.trainer.dice_trainer.DICE_Trainer attribute), 177
is_global_zero (dicee.abstracts.AbstractTrainer attribute), 13
is_rank_zero () (dicee.executer.Execute method), 50
is_seen() (dicee.abstracts.BaseInteractiveKGE method), 15
is_sparql_endpoint_alive () (in module dicee.sanity_checkers), 170

```

K

```

k (dicee.models.FMult attribute), 157
k (dicee.models.FMult2 attribute), 158
k (dicee.models.function_space.FMult attribute), 87
k (dicee.models.function_space.FMult2 attribute), 88
k (dicee.models.function_space.GFMult attribute), 87
k (dicee.models.GFMult attribute), 158
k_fold_cross_validation() (dicee.DICE_Trainer method), 213
k_fold_cross_validation() (dicee.trainer.DICE_Trainer method), 183
k_fold_cross_validation() (dicee.trainer.dice_trainer.DICE_Trainer method), 178
k_vs_all_score() (dicee.ComplEx static method), 196
k_vs_all_score() (dicee.DistMult method), 187
k_vs_all_score() (dicee.Keci method), 189
k_vs_all_score() (dicee.models.clifford.Keci method), 77
k_vs_all_score() (dicee.models.ComplEx static method), 132
k_vs_all_score() (dicee.models.complex.ComplEx static method), 84
k_vs_all_score() (dicee.models.DistMult method), 126
k_vs_all_score() (dicee.models.Keci method), 147
k_vs_all_score() (dicee.models.octonion.OMult method), 93
k_vs_all_score() (dicee.models.OMult method), 143
k_vs_all_score() (dicee.models.QMult method), 137
k_vs_all_score() (dicee.models.quaternion.QMult method), 97
k_vs_all_score() (dicee.models.real.DistMult method), 99
k_vs_all_score() (dicee.OMult method), 202
k_vs_all_score() (dicee.QMult method), 201
Keci (class in dicee), 187
Keci (class in dicee.models), 145
Keci (class in dicee.models.clifford), 75
kernel_size (dicee.BaseKGE attribute), 208
kernel_size (dicee.config.Namespace attribute), 31
kernel_size (dicee.models.base_model.BaseKGE attribute), 72

```

kernel_size (*dicee.models.BaseKGE* attribute), 120, 123, 129, 134, 140, 152, 156
 KG (class in *dicee.knowledge_graph*), 51
 kg (*dicee.callbacks.PseudoLabellingCallback* attribute), 24
 kg (*dicee.read_preprocess_save_load_kg.LoadSaveToDisk* attribute), 169
 kg (*dicee.read_preprocess_save_load_kg.PreprocessKG* attribute), 168
 kg (*dicee.read_preprocess_save_load_kg.preprocess.PreprocessKG* attribute), 163
 kg (*dicee.read_preprocess_save_load_kg.read_from_disk.ReadFromDisk* attribute), 164
 kg (*dicee.read_preprocess_save_load_kg.ReadFromDisk* attribute), 169
 kg (*dicee.read_preprocess_save_load_kg.save_load_disk.LoadSaveToDisk* attribute), 164
 KGE (class in *dicee*), 214
 KGE (class in *dicee.knowledge_graph_embeddings*), 53
 KGESaveCallback (class in *dicee.callbacks*), 22
 knowledge_graph (*dicee.executer.Execute* attribute), 50
 KronE (class in *dicee.callbacks*), 26
 KvsAll (class in *dicee*), 219
 KvsAll (class in *dicee.dataset_classes*), 35
 kvsall_score () (*dicee.DualE* method), 194
 kvsall_score () (*dicee.models.DualE* method), 161
 kvsall_score () (*dicee.models.dualE.DualE* method), 85
 KvsSampleDataset (class in *dicee*), 223
 KvsSampleDataset (class in *dicee.dataset_classes*), 39

L

label_smoothing_rate (*dicee.AllvsAll* attribute), 221
 label_smoothing_rate (*dicee.config.Namespace* attribute), 31
 label_smoothing_rate (*dicee.dataset_classes.AllvsAll* attribute), 37
 label_smoothing_rate (*dicee.dataset_classes.KvsAll* attribute), 36
 label_smoothing_rate (*dicee.dataset_classes.KvsSampleDataset* attribute), 39
 label_smoothing_rate (*dicee.dataset_classes.OnevsSample* attribute), 38
 label_smoothing_rate (*dicee.dataset_classes.TriplePredictionDataset* attribute), 41
 label_smoothing_rate (*dicee.KvsAll* attribute), 220
 label_smoothing_rate (*dicee.KvsSampleDataset* attribute), 223
 label_smoothing_rate (*dicee.OnevsSample* attribute), 222
 label_smoothing_rate (*dicee.TriplePredictionDataset* attribute), 225
 labels (*dicee.dataset_classes.NegSampleDataset* attribute), 40
 labels (*dicee.NegSampleDataset* attribute), 224
 layer_norm (*dicee.models.literal.LiteralEmbeddings* attribute), 91
 LayerNorm (class in *dicee.models.transformers*), 104
 learning_rate (*dicee.BaseKGE* attribute), 208
 learning_rate (*dicee.models.base_model.BaseKGE* attribute), 72
 learning_rate (*dicee.models.BaseKGE* attribute), 120, 123, 129, 133, 139, 152, 156
 length (*dicee.dataset_classes.NegSampleDataset* attribute), 40
 length (*dicee.dataset_classes.TriplePredictionDataset* attribute), 41
 length (*dicee.NegSampleDataset* attribute), 224
 length (*dicee.TriplePredictionDataset* attribute), 225
 level (*dicee.callbacks.Perturb* attribute), 27
 LFMult (class in *dicee*), 203
 LFMult (class in *dicee.models*), 159
 LFMult (class in *dicee.models.function_space*), 88
 LFMult1 (class in *dicee.models*), 159
 LFMult1 (class in *dicee.models.function_space*), 88
 linear () (*dicee.LFMult* method), 203
 linear () (*dicee.models.function_space.LFMult* method), 89
 linear () (*dicee.models.LFMult* method), 160
 list2tuple () (*dicee.query_generator.QueryGenerator* method), 162
 list2tuple () (*dicee.QueryGenerator* method), 231
 LiteralDataset (class in *dicee*), 228
 LiteralDataset (class in *dicee.dataset_classes*), 44
 LiteralEmbeddings (class in *dicee.models.literal*), 90
 lm_head (*dicee.BytE* attribute), 206
 lm_head (*dicee.models.transformers.BytE* attribute), 103
 lm_head (*dicee.models.transformers.GPT* attribute), 108
 ln_1 (*dicee.models.Block* attribute), 125
 ln_1 (*dicee.models.transformers.Block* attribute), 107
 ln_2 (*dicee.models.Block* attribute), 125
 ln_2 (*dicee.models.transformers.Block* attribute), 107
 ln_f (*dicee.CoKE* attribute), 204

ln_f (*dicee.models.CoKE* attribute), 128
 ln_f (*dicee.models.real.CoKE* attribute), 101
 load() (*dicee.read_preprocess_save_load_kg.LoadSaveToDisk* method), 169
 load() (*dicee.read_preprocess_save_load_kg.save_load_disk.LoadSaveToDisk* method), 164
 load_and_validate_literal_data() (*dicee.dataset_classes.LiteralDataset* static method), 46
 load_and_validate_literal_data() (*dicee.LiteralDataset* static method), 230
 load_from_memmap() (*dicee.executer.Execute* method), 50
 load_json() (*in module dicee*), 211
 load_json() (*in module dicee.static_funcs*), 174
 load_model() (*in module dicee*), 211
 load_model() (*in module dicee.static_funcs*), 174
 load_model_ensemble() (*in module dicee*), 211
 load_model_ensemble() (*in module dicee.static_funcs*), 174
 load_numpy() (*in module dicee*), 212
 load_numpy() (*in module dicee.static_funcs*), 175
 load_numpy_ndarray() (*in module dicee.read_preprocess_save_load_kg.util*), 168
 load_pickle() (*in module dicee*), 211
 load_pickle() (*in module dicee.read_preprocess_save_load_kg.util*), 168
 load_pickle() (*in module dicee.static_funcs*), 174
 load_queries() (*dicee.query_generator.QueryGenerator* method), 163
 load_queries() (*dicee.QueryGenerator* method), 231
 load_queries_and_answers() (*dicee.query_generator.QueryGenerator* static method), 163
 load_queries_and_answers() (*dicee.QueryGenerator* static method), 231
 load_state_dict() (*dicee.EnsembleKGE* method), 210
 load_state_dict() (*dicee.models.ensemble.EnsembleKGE* method), 86
 load_term_mapping() (*in module dicee*), 211, 217
 load_term_mapping() (*in module dicee.static_funcs*), 174
 load_term_mapping() (*in module dicee.trainer.dice_trainer*), 177
 load_with_pandas() (*in module dicee.read_preprocess_save_load_kg.util*), 168
 loader_backend (*dicee.dataset_classes.LiteralDataset* attribute), 45, 46
 loader_backend (*dicee.LiteralDataset* attribute), 229, 230
 LoadSaveToDisk (*class in dicee.read_preprocess_save_load_kg*), 169
 LoadSaveToDisk (*class in dicee.read_preprocess_save_load_kg.save_load_disk*), 164
 local_rank (*dicee.abstracts.AbstractTrainer* attribute), 13
 local_rank (*dicee.trainer.torch_trainer_ddp.NodeTrainer* attribute), 181
 loss (*dicee.BaseKGE* attribute), 209
 loss (*dicee.models.base_model.BaseKGE* attribute), 72
 loss (*dicee.models.BaseKGE* attribute), 120, 123, 129, 134, 140, 153, 156
 loss_func (*dicee.trainer.torch_trainer_ddp.NodeTrainer* attribute), 182
 loss_function (*dicee.trainer.torch_trainer.TorchTrainer* attribute), 180
 loss_function() (*dicee.BytE* method), 206
 loss_function() (*dicee.models.base_model.BaseKGELighting* method), 67
 loss_function() (*dicee.models.BaseKGELighting* method), 115
 loss_function() (*dicee.models.transformers.BytE* method), 103
 loss_history (*dicee.BaseKGE* attribute), 209
 loss_history (*dicee.models.base_model.BaseKGE* attribute), 73
 loss_history (*dicee.models.BaseKGE* attribute), 120, 124, 129, 134, 140, 153, 156
 loss_history (*dicee.models.pykeen_models.PykeenKGE* attribute), 95
 loss_history (*dicee.models.PykeenKGE* attribute), 154
 loss_history (*dicee.PykeenKGE* attribute), 205
 loss_history (*dicee.trainer.torch_trainer_ddp.NodeTrainer* attribute), 182
 lr (*dicee.analyse_experiments.Experiment* attribute), 19
 lr (*dicee.config.Namespace* attribute), 30
 lr_init (*dicee.callbacks.SWA* attribute), 29
 lr_lambda (*dicee.callbacks.LRScheduler* attribute), 28
 LRScheduler (*class in dicee.callbacks*), 28

M

m (*dicee.LFMult* attribute), 203
 m (*dicee.models.function_space.LFMult* attribute), 89
 m (*dicee.models.LFMult* attribute), 159
 main() (*in module dicee.scripts.index_serve*), 172
 main() (*in module dicee.scripts.run*), 172
 make_iterable_verbose() (*in module dicee.static_funcs_training*), 175
 make_iterable_verbose() (*in module dicee.trainer.torch_trainer_ddp*), 181
 mapping_from_first_two_cols_to_third() (*in module dicee*), 217
 mapping_from_first_two_cols_to_third() (*in module dicee.static_preprocess_funcs*), 177

```

margin (dicee.models.Pyke attribute), 127
margin (dicee.models.real.Pyke attribute), 100
margin (dicee.models.real.TransE attribute), 100
margin (dicee.models.TransE attribute), 126
margin (dicee.Pyke attribute), 186
margin (dicee.TransE attribute), 190
mask_emb (dicee.CoKE attribute), 204
mask_emb (dicee.models.CoKE attribute), 128
mask_emb (dicee.models.real.CoKE attribute), 101
max_ans_num (dicee.query_generator.QueryGenerator attribute), 162
max_ans_num (dicee.QueryGenerator attribute), 230
max_epochs (dicee.callbacks.KGESaveCallback attribute), 23
max_epochs (dicee.callbacks.PeriodicEvalCallback attribute), 27
max_epochs (dicee.callbacks.SWA attribute), 29
max_length_subword_tokens (dicee.BaseKGE attribute), 209
max_length_subword_tokens (dicee.knowledge_graph.KG attribute), 52
max_length_subword_tokens (dicee.models.base_model.BaseKGE attribute), 73
max_length_subword_tokens (dicee.models.BaseKGE attribute), 120, 124, 130, 134, 140, 153, 156
max_num_of_classes (dicee.dataset_classes.KvsSampleDataset attribute), 39
max_num_of_classes (dicee.KvsSampleDataset attribute), 223
mem_of_model () (dicee.EnsembleKGE method), 210
mem_of_model () (dicee.models.base_model.BaseKGELightning method), 66
mem_of_model () (dicee.models.BaseKGELightning method), 114
mem_of_model () (dicee.models.ensemble.EnsembleKGE method), 86
method (dicee.callbacks.Perturb attribute), 27
MLP (class in dicee.models.transformers), 105
mlp (dicee.models.Block attribute), 126
mlp (dicee.models.transformers.Block attribute), 107
mode (dicee.query_generator.QueryGenerator attribute), 162
mode (dicee.QueryGenerator attribute), 230
model (dicee.config.Namespace attribute), 30
model (dicee.models.pykeen_models.PykeenKGE attribute), 95
model (dicee.models.PykeenKGE attribute), 154
model (dicee.PykeenKGE attribute), 205
model (dicee.trainer.torch_trainer_ddp.NodeTrainer attribute), 182
model (dicee.trainer.torch_trainer.TorchTrainer attribute), 180
model_kw_args (dicee.models.pykeen_models.PykeenKGE attribute), 95
model_kw_args (dicee.models.PykeenKGE attribute), 154
model_kw_args (dicee.PykeenKGE attribute), 205
model_name (dicee.analyse_experiments.Experiment attribute), 19
module
    dicee, 12
    dicee.__main__, 12
    dicee.abstracts, 12
    dicee.analyse_experiments, 19
    dicee.callbacks, 20
    dicee.config, 29
    dicee.dataset_classes, 32
    dicee.eval_static_funcs, 46
    dicee.evaluator, 48
    dicee.executer, 49
    dicee.knowledge_graph, 51
    dicee.knowledge_graph_embeddings, 53
    dicee.models, 57
    dicee.models.adopt, 57
    dicee.models.base_model, 66
    dicee.models.clifford, 75
    dicee.models.complex, 82
    dicee.models.dualE, 84
    dicee.models.ensemble, 85
    dicee.models.function_space, 86
    dicee.models.literal, 90
    dicee.models.octonion, 91
    dicee.models.pykeen_models, 94
    dicee.models.quaternion, 96
    dicee.models.real, 99
    dicee.models.static_funcs, 102
    dicee.models.transformers, 102

```

```

dicee.query_generator, 161
dicee.read_preprocess_save_load_kg, 163
dicee.read_preprocess_save_load_kg.preprocess, 163
dicee.read_preprocess_save_load_kg.read_from_disk, 164
dicee.read_preprocess_save_load_kg.save_load_disk, 164
dicee.read_preprocess_save_load_kg.util, 165
dicee.sanity_checkers, 169
dicee.scripts, 170
dicee.scripts.index_serve, 170
dicee.scripts.run, 172
dicee.static_funcs, 172
dicee.static_funcs_training, 175
dicee.static_preprocess_funcs, 176
dicee.trainer, 177
dicee.trainer.dice_trainer, 177
dicee.trainer.model_parallelism, 179
dicee.trainer.torch_trainer, 179
dicee.trainer.torch_trainer_ddp, 181
modules() (dicee.EnsembleKGE method), 210
modules() (dicee.models.ensemble.EnsembleKGE method), 86
moving_average() (dicee.callbacks.SWA static method), 29
MultiClassClassificationDataset (class in dicee), 218
MultiClassClassificationDataset (class in dicee.dataset_classes), 34
MultiLabelDataset (class in dicee), 218
MultiLabelDataset (class in dicee.dataset_classes), 34

```

N

```

n (dicee.models.FMult2 attribute), 158
n (dicee.models.function_space.FMult2 attribute), 88
n_embd (dicee.models.CoKEConfig attribute), 127
n_embd (dicee.models.real.CoKEConfig attribute), 100, 101
n_embd (dicee.models.transformers.GPTConfig attribute), 107
n_embd (dicee.models.transformers.SelfAttention attribute), 105
n_epochs_eval_model (dicee.callbacks.PeriodicEvalCallback attribute), 27
n_epochs_eval_model (dicee.config.Namespace attribute), 32
n_head (dicee.models.CoKEConfig attribute), 127
n_head (dicee.models.real.CoKEConfig attribute), 100, 101
n_head (dicee.models.transformers.GPTConfig attribute), 107
n_head (dicee.models.transformers.SelfAttention attribute), 105
n_layer (dicee.models.CoKEConfig attribute), 127
n_layer (dicee.models.real.CoKEConfig attribute), 100, 101
n_layer (dicee.models.transformers.GPTConfig attribute), 107
n_layers (dicee.models.FMult2 attribute), 158
n_layers (dicee.models.function_space.FMult2 attribute), 88
name (dicee.abstracts.BaseInteractiveKGE property), 15
name (dicee.AConEx attribute), 196
name (dicee.AConvO attribute), 196
name (dicee.AConvQ attribute), 197
name (dicee.BytE attribute), 206
name (dicee.CKeci attribute), 187
name (dicee.CoKE attribute), 204
name (dicee.ComplEx attribute), 196
name (dicee.ConEx attribute), 199
name (dicee.ConvO attribute), 199
name (dicee.ConvQ attribute), 198
name (dicee.DeCaL attribute), 191
name (dicee.DistMult attribute), 187
name (dicee.DualE attribute), 194
name (dicee.EnsembleKGE attribute), 210
name (dicee.Keci attribute), 188
name (dicee.LFMult attribute), 203
name (dicee.models.AConEx attribute), 131
name (dicee.models.AConvO attribute), 144
name (dicee.models.AConvQ attribute), 138
name (dicee.models.CKeci attribute), 148
name (dicee.models.clifford.CKeci attribute), 78
name (dicee.models.clifford.DeCaL attribute), 79

```

name (*dicee.models.clifford.Keci attribute*), 75
 name (*dicee.models.CoKE attribute*), 128
 name (*dicee.models.ComplEx attribute*), 132
 name (*dicee.models.complex.AConEx attribute*), 83
 name (*dicee.models.complex.ComplEx attribute*), 84
 name (*dicee.models.complex.ConEx attribute*), 82
 name (*dicee.models.ConEx attribute*), 131
 name (*dicee.models.ConvO attribute*), 144
 name (*dicee.models.ConvQ attribute*), 138
 name (*dicee.models.DeCaL attribute*), 148
 name (*dicee.models.DistMult attribute*), 126
 name (*dicee.models.DualE attribute*), 160
 name (*dicee.models.dualE.DualE attribute*), 84
 name (*dicee.models.ensemble.EnsembleKGE attribute*), 86
 name (*dicee.models.FMult attribute*), 157
 name (*dicee.models.FMult2 attribute*), 158
 name (*dicee.models.function_space.FMult attribute*), 87
 name (*dicee.models.function_space.FMult2 attribute*), 88
 name (*dicee.models.function_space.GFMult attribute*), 87
 name (*dicee.models.function_space.LFMult attribute*), 89
 name (*dicee.models.function_space.LFMult1 attribute*), 88
 name (*dicee.models.GFMult attribute*), 158
 name (*dicee.models.Keci attribute*), 145
 name (*dicee.models.LFMult attribute*), 159
 name (*dicee.models.LFMult1 attribute*), 159
 name (*dicee.models.octonion.AConvO attribute*), 94
 name (*dicee.models.octonion.ConvO attribute*), 93
 name (*dicee.models.octonion.OMult attribute*), 92
 name (*dicee.models.OMult attribute*), 143
 name (*dicee.models.Pyke attribute*), 127
 name (*dicee.models.pykeen_models.PykeenKGE attribute*), 95
 name (*dicee.models.PykeenKGE attribute*), 154
 name (*dicee.models.QMult attribute*), 137
 name (*dicee.models.quaternion.AConvQ attribute*), 98
 name (*dicee.models.quaternion.ConvQ attribute*), 98
 name (*dicee.models.quaternion.QMult attribute*), 97
 name (*dicee.models.real.CoKE attribute*), 101
 name (*dicee.models.real.DistMult attribute*), 99
 name (*dicee.models.real.Pyke attribute*), 100
 name (*dicee.models.real.Shallom attribute*), 100
 name (*dicee.models.real.TransE attribute*), 99
 name (*dicee.models.Shallom attribute*), 126
 name (*dicee.models.TransE attribute*), 126
 name (*dicee.models.transformers.BytE attribute*), 103
 name (*dicee.OMult attribute*), 202
 name (*dicee.Pyke attribute*), 186
 name (*dicee.PykeenKGE attribute*), 205
 name (*dicee.QMult attribute*), 201
 name (*dicee.Shallom attribute*), 202
 name (*dicee.TransE attribute*), 190
 named_children () (*dicee.EnsembleKGE method*), 210
 named_children () (*dicee.models.ensemble.EnsembleKGE method*), 86
 Namespace (*class in dicee.config*), 29
 neg_ratio (*dicee.BPE_NegativeSamplingDataset attribute*), 218
 neg_ratio (*dicee.config.Namespace attribute*), 30
 neg_ratio (*dicee.dataset_classes.BPE_NegativeSamplingDataset attribute*), 34
 neg_ratio (*dicee.dataset_classes.KvsSampleDataset attribute*), 39
 neg_ratio (*dicee.KvsSampleDataset attribute*), 223
 neg_sample_ratio (*dicee.CVDataModule attribute*), 225
 neg_sample_ratio (*dicee.dataset_classes.CVDataModule attribute*), 41
 neg_sample_ratio (*dicee.dataset_classes.NegSampleDataset attribute*), 40
 neg_sample_ratio (*dicee.dataset_classes.OnevsSample attribute*), 38
 neg_sample_ratio (*dicee.dataset_classes.TriplePredictionDataset attribute*), 41
 neg_sample_ratio (*dicee.NegSampleDataset attribute*), 224
 neg_sample_ratio (*dicee.OnevsSample attribute*), 222
 neg_sample_ratio (*dicee.TriplePredictionDataset attribute*), 225
 negnorm () (*dicee.abstracts.InteractiveQueryDecomposition method*), 16
 NegSampleDataset (*class in dicee*), 223

NegSampleDataset (*class in dicee.dataset_classes*), 39
 neural_searcher (*in module dicee.scripts.index_serve*), 171
 NeuralSearcher (*class in dicee.scripts.index_serve*), 171
 NodeTrainer (*class in dicee.trainer.torch_trainer_ddp*), 181
 norm_fc1 (*dicee.AConEx attribute*), 196
 norm_fc1 (*dicee.AConvO attribute*), 197
 norm_fc1 (*dicee.ConEx attribute*), 200
 norm_fc1 (*dicee.ConvO attribute*), 199
 norm_fc1 (*dicee.models.AConEx attribute*), 131
 norm_fc1 (*dicee.models.AConvO attribute*), 144
 norm_fc1 (*dicee.models.complex.AConEx attribute*), 83
 norm_fc1 (*dicee.models.complex.ConEx attribute*), 82
 norm_fc1 (*dicee.models.ConEx attribute*), 131
 norm_fc1 (*dicee.models.ConvO attribute*), 144
 norm_fc1 (*dicee.models.octonion.AConvO attribute*), 94
 norm_fc1 (*dicee.models.octonion.ConvO attribute*), 93
 normalization (*dicee.analyse_experiments.Experiment attribute*), 20
 normalization (*dicee.config.Namespace attribute*), 30
 normalization (*dicee.dataset_classes.LiteralDataset attribute*), 45
 normalization (*dicee.LiteralDataset attribute*), 229
 normalization_params (*dicee.dataset_classes.LiteralDataset attribute*), 45, 46
 normalization_params (*dicee.LiteralDataset attribute*), 229, 230
 normalization_type (*dicee.dataset_classes.LiteralDataset attribute*), 46
 normalization_type (*dicee.LiteralDataset attribute*), 230
 normalize_head_entity_embeddings (*dicee.BaseKGE attribute*), 209
 normalize_head_entity_embeddings (*dicee.models.base_model.BaseKGE attribute*), 73
 normalize_head_entity_embeddings (*dicee.models.BaseKGE attribute*), 120, 123, 129, 134, 140, 153, 156
 normalize_relation_embeddings (*dicee.BaseKGE attribute*), 209
 normalize_relation_embeddings (*dicee.models.base_model.BaseKGE attribute*), 73
 normalize_relation_embeddings (*dicee.models.BaseKGE attribute*), 120, 123, 129, 134, 140, 153, 156
 normalize_tail_entity_embeddings (*dicee.BaseKGE attribute*), 209
 normalize_tail_entity_embeddings (*dicee.models.base_model.BaseKGE attribute*), 73
 normalize_tail_entity_embeddings (*dicee.models.BaseKGE attribute*), 120, 124, 129, 134, 140, 153, 156
 normalizer_class (*dicee.BaseKGE attribute*), 209
 normalizer_class (*dicee.models.base_model.BaseKGE attribute*), 73
 normalizer_class (*dicee.models.BaseKGE attribute*), 120, 123, 129, 134, 140, 153, 156
 num_bpe_entities (*dicee.BPE_NegativeSamplingDataset attribute*), 218
 num_bpe_entities (*dicee.dataset_classes.BPE_NegativeSamplingDataset attribute*), 34
 num_bpe_entities (*dicee.knowledge_graph.KG attribute*), 52
 num_core (*dicee.config.Namespace attribute*), 31
 num_data_properties (*dicee.dataset_classes.LiteralDataset attribute*), 45
 num_data_properties (*dicee.LiteralDataset attribute*), 229
 num_datapoints (*dicee.BPE_NegativeSamplingDataset attribute*), 218
 num_datapoints (*dicee.dataset_classes.BPE_NegativeSamplingDataset attribute*), 34
 num_datapoints (*dicee.dataset_classes.MultiLabelDataset attribute*), 34
 num_datapoints (*dicee.MultiLabelDataset attribute*), 218
 num_ent (*dicee.DualE attribute*), 194
 num_ent (*dicee.models.DualE attribute*), 161
 num_ent (*dicee.models.dualE.DualE attribute*), 85
 num_entities (*dicee.BaseKGE attribute*), 208
 num_entities (*dicee.CVDataModule attribute*), 225
 num_entities (*dicee.dataset_classes.CVDataModule attribute*), 41
 num_entities (*dicee.dataset_classes.KvsSampleDataset attribute*), 39
 num_entities (*dicee.dataset_classes.LiteralDataset attribute*), 45, 46
 num_entities (*dicee.dataset_classes.NegSampleDataset attribute*), 40
 num_entities (*dicee.dataset_classes.OnevsSample attribute*), 37, 38
 num_entities (*dicee.dataset_classes.TriplePredictionDataset attribute*), 41
 num_entities (*dicee.evaluator.Evaluator attribute*), 48
 num_entities (*dicee.knowledge_graph.KG attribute*), 52
 num_entities (*dicee.KvsSampleDataset attribute*), 223
 num_entities (*dicee.LiteralDataset attribute*), 229, 230
 num_entities (*dicee.models.base_model.BaseKGE attribute*), 72
 num_entities (*dicee.models.BaseKGE attribute*), 120, 123, 129, 133, 139, 152, 156
 num_entities (*dicee.NegSampleDataset attribute*), 224
 num_entities (*dicee.OnevsSample attribute*), 221, 222
 num_entities (*dicee.TriplePredictionDataset attribute*), 225
 num_epochs (*dicee.abstracts.AbstractPPECallback attribute*), 17
 num_epochs (*dicee.analyse_experiments.Experiment attribute*), 19

num_epochs (*dicee.callbacks.ASWA attribute*), 24
 num_epochs (*dicee.config.Namespace attribute*), 30
 num_epochs (*dicee.trainer.torch_trainer_ddp.NodeTrainer attribute*), 182
 num_folds_for_cv (*dicee.config.Namespace attribute*), 31
 num_of_data_points (*dicee.dataset_classes.MultiClassClassificationDataset attribute*), 35
 num_of_data_points (*dicee.MultiClassClassificationDataset attribute*), 219
 num_of_data_properties (*dicee.models.literal.LiteralEmbeddings attribute*), 90, 91
 num_of_epochs (*dicee.callbacks.PseudoLabellingCallback attribute*), 24
 num_of_output_channels (*dicee.BaseKGE attribute*), 209
 num_of_output_channels (*dicee.config.Namespace attribute*), 31
 num_of_output_channels (*dicee.models.base_model.BaseKGE attribute*), 72
 num_of_output_channels (*dicee.models.BaseKGE attribute*), 120, 123, 129, 134, 140, 153, 156
 num_params (*dicee.analyse_experiments.Experiment attribute*), 19
 num_relations (*dicee.BaseKGE attribute*), 208
 num_relations (*dicee.CVDataModule attribute*), 225
 num_relations (*dicee.dataset_classes.CVDataModule attribute*), 41
 num_relations (*dicee.dataset_classes.NegSampleDataset attribute*), 40
 num_relations (*dicee.dataset_classes.OnevsSample attribute*), 38
 num_relations (*dicee.dataset_classes.TriplePredictionDataset attribute*), 41
 num_relations (*dicee.evaluator.Evaluator attribute*), 48
 num_relations (*dicee.knowledge_graph.KG attribute*), 52
 num_relations (*dicee.models.base_model.BaseKGE attribute*), 72
 num_relations (*dicee.models.BaseKGE attribute*), 120, 123, 129, 133, 139, 152, 156
 num_relations (*dicee.NegSampleDataset attribute*), 224
 num_relations (*dicee.OnevsSample attribute*), 222
 num_relations (*dicee.TriplePredictionDataset attribute*), 225
 num_sample (*dicee.models.FMult attribute*), 157
 num_sample (*dicee.models.function_space.FMult attribute*), 87
 num_sample (*dicee.models.function_space.GFMult attribute*), 87
 num_sample (*dicee.models.GFMult attribute*), 158
 num_tokens (*dicee.BaseKGE attribute*), 208
 num_tokens (*dicee.knowledge_graph.KG attribute*), 52
 num_tokens (*dicee.models.base_model.BaseKGE attribute*), 72
 num_tokens (*dicee.models.BaseKGE attribute*), 120, 123, 129, 133, 139, 152, 156
 num_workers (*dicee.CVDataModule attribute*), 225
 num_workers (*dicee.dataset_classes.CVDataModule attribute*), 41
 numpy_data_type_changer () (*in module dicee*), 211
 numpy_data_type_changer () (*in module dicee.static_funcs*), 174

O

octonion_mul () (*in module dicee.models*), 142
 octonion_mul () (*in module dicee.models.octonion*), 92
 octonion_mul_norm () (*in module dicee.models*), 142
 octonion_mul_norm () (*in module dicee.models.octonion*), 92
 octonion_normalizer () (*dicee.AConvO static method*), 197
 octonion_normalizer () (*dicee.ConvO static method*), 199
 octonion_normalizer () (*dicee.models.AConvO static method*), 144
 octonion_normalizer () (*dicee.models.ConvO static method*), 144
 octonion_normalizer () (*dicee.models.octonion.AConvO static method*), 94
 octonion_normalizer () (*dicee.models.octonion.ConvO static method*), 94
 octonion_normalizer () (*dicee.models.octonion.OMult static method*), 92
 octonion_normalizer () (*dicee.models.OMult static method*), 143
 octonion_normalizer () (*dicee.OMult static method*), 202
 OMult (*class in dicee*), 201
 OMult (*class in dicee.models*), 142
 OMult (*class in dicee.models.octonion*), 92
 on_epoch_end () (*dicee.callbacks.KGESaveCallback method*), 24
 on_epoch_end () (*dicee.callbacks.PseudoLabellingCallback method*), 24
 on_fit_end () (*dicee.abstracts.AbstractCallback method*), 17
 on_fit_end () (*dicee.abstracts.AbstractPPECallback method*), 18
 on_fit_end () (*dicee.abstracts.AbstractTrainer method*), 13
 on_fit_end () (*dicee.callbacks.AccumulateEpochLossCallback method*), 21
 on_fit_end () (*dicee.callbacks.ASWA method*), 24
 on_fit_end () (*dicee.callbacks.Eval method*), 26
 on_fit_end () (*dicee.callbacks.KGESaveCallback method*), 23
 on_fit_end () (*dicee.callbacks.LRScheduler method*), 28
 on_fit_end () (*dicee.callbacks.PeriodicEvalCallback method*), 28

on_fit_end() (*dicee.callbacks.PrintCallback* method), 22
 on_fit_end() (*dicee.callbacks.SWA* method), 29
 on_fit_start() (*dicee.abstracts.AbstractCallback* method), 16
 on_fit_start() (*dicee.abstracts.AbstractPPECallback* method), 18
 on_fit_start() (*dicee.abstracts.AbstractTrainer* method), 13
 on_fit_start() (*dicee.callbacks.Eval* method), 25
 on_fit_start() (*dicee.callbacks.KGESaveCallback* method), 23
 on_fit_start() (*dicee.callbacks.KronE* method), 27
 on_fit_start() (*dicee.callbacks.PrintCallback* method), 22
 on_init_end() (*dicee.abstracts.AbstractCallback* method), 16
 on_init_start() (*dicee.abstracts.AbstractCallback* method), 16
 on_train_batch_end() (*dicee.abstracts.AbstractCallback* method), 17
 on_train_batch_end() (*dicee.abstracts.AbstractTrainer* method), 13
 on_train_batch_end() (*dicee.callbacks.Eval* method), 26
 on_train_batch_end() (*dicee.callbacks.KGESaveCallback* method), 23
 on_train_batch_end() (*dicee.callbacks.LRScheduler* method), 28
 on_train_batch_end() (*dicee.callbacks.PrintCallback* method), 22
 on_train_batch_start() (*dicee.callbacks.Perturb* method), 27
 on_train_epoch_end() (*dicee.abstracts.AbstractCallback* method), 17
 on_train_epoch_end() (*dicee.abstracts.AbstractTrainer* method), 13
 on_train_epoch_end() (*dicee.callbacks.ASWA* method), 25
 on_train_epoch_end() (*dicee.callbacks.Eval* method), 26
 on_train_epoch_end() (*dicee.callbacks.KGESaveCallback* method), 23
 on_train_epoch_end() (*dicee.callbacks.PeriodicEvalCallback* method), 28
 on_train_epoch_end() (*dicee.callbacks.PrintCallback* method), 22
 on_train_epoch_end() (*dicee.callbacks.SWA* method), 29
 on_train_epoch_end() (*dicee.models.base_model.BaseKGELightning* method), 68
 on_train_epoch_end() (*dicee.models.BaseKGELightning* method), 115
 on_train_epoch_start() (*dicee.abstracts.AbstractTrainer* method), 13
 on_train_epoch_start() (*dicee.callbacks.SWA* method), 29
 on_train_start() (*dicee.callbacks.LRScheduler* method), 28
 OnevsAllDataset (*class in dicee*), 219
 OnevsAllDataset (*class in dicee.dataset_classes*), 35
 OnevsSample (*class in dicee*), 221
 OnevsSample (*class in dicee.dataset_classes*), 37
 optim (*dicee.config.Namespace* attribute), 30
 optimizer (*dicee.trainer.torch_trainer_ddp.NodeTrainer* attribute), 181
 optimizer (*dicee.trainer.torch_trainer.TorchTrainer* attribute), 180
 optimizer_name (*dicee.BaseKGE* attribute), 208
 optimizer_name (*dicee.models.base_model.BaseKGE* attribute), 72
 optimizer_name (*dicee.models.BaseKGE* attribute), 120, 123, 129, 134, 140, 152, 156
 ordered_bpe_entities (*dicee.BPE_NegativeSamplingDataset* attribute), 218
 ordered_bpe_entities (*dicee.dataset_classes.BPE_NegativeSamplingDataset* attribute), 34
 ordered_bpe_entities (*dicee.knowledge_graph.KG* attribute), 53
 ordered_shaped_bpe_tokens (*dicee.knowledge_graph.KG* attribute), 52

P

p (*dicee.config.Namespace* attribute), 31
 p (*dicee.DeCaL* attribute), 191
 p (*dicee.Keci* attribute), 188
 p (*dicee.models.clifford.DeCaL* attribute), 79
 p (*dicee.models.clifford.Keci* attribute), 75
 p (*dicee.models.DeCaL* attribute), 149
 p (*dicee.models.Keci* attribute), 145
 padding (*dicee.knowledge_graph.KG* attribute), 52
 pandas_dataframe_indexer() (*in module dicee.read_preprocess_save_load_kg.util*), 166
 param_init (*dicee.BaseKGE* attribute), 209
 param_init (*dicee.models.base_model.BaseKGE* attribute), 73
 param_init (*dicee.models.BaseKGE* attribute), 120, 124, 129, 134, 140, 153, 156
 parameters() (*dicee.abstracts.BaseInteractiveKGE* method), 16
 parameters() (*dicee.EnsembleKGE* method), 210
 parameters() (*dicee.models.ensemble.EnsembleKGE* method), 86
 path (*dicee.abstracts.AbstractPPECallback* attribute), 17
 path (*dicee.callbacks.AccumulateEpochLossCallback* attribute), 21
 path (*dicee.callbacks.ASWA* attribute), 24
 path (*dicee.callbacks.Eval* attribute), 25
 path (*dicee.callbacks.KGESaveCallback* attribute), 23

path_dataset_folder (*dicee.analyse_experiments.Experiment* attribute), 19
 path_for_deserialization (*dicee.knowledge_graph.KG* attribute), 52
 path_for_serialization (*dicee.knowledge_graph.KG* attribute), 52
 path_single_kg (*dicee.config.Namespace* attribute), 30
 path_single_kg (*dicee.knowledge_graph.KG* attribute), 52
 path_to_store_single_run (*dicee.config.Namespace* attribute), 29
 PeriodicEvalCallback (*class* in *dicee.callbacks*), 27
 Perturb (*class* in *dicee.callbacks*), 27
 polars_dataframe_indexer () (*in module dicee.read_preprocess_save_load_kg.util*), 165
 poly_NN () (*dicee.LFMult* method), 203
 poly_NN () (*dicee.models.function_space.LFMult* method), 89
 poly_NN () (*dicee.models.LFMult* method), 160
 polynomial () (*dicee.LFMult* method), 204
 polynomial () (*dicee.models.function_space.LFMult* method), 89
 polynomial () (*dicee.models.LFMult* method), 160
 pop () (*dicee.LFMult* method), 204
 pop () (*dicee.models.function_space.LFMult* method), 90
 pop () (*dicee.models.LFMult* method), 160
 pos_emb (*dicee.CoKE* attribute), 204
 pos_emb (*dicee.models.CoKE* attribute), 128
 pos_emb (*dicee.models.real.CoKE* attribute), 101
 pq (*dicee.analyse_experiments.Experiment* attribute), 20
 predict () (*dicee.KGE* method), 215
 predict () (*dicee.knowledge_graph_embeddings.KGE* method), 55
 predict_dataloader () (*dicee.models.base_model.BaseKGELightning* method), 69
 predict_dataloader () (*dicee.models.BaseKGELightning* method), 117
 predict_literals () (*dicee.KGE* method), 217
 predict_literals () (*dicee.knowledge_graph_embeddings.KGE* method), 56
 predict_missing_head_entity () (*dicee.KGE* method), 214
 predict_missing_head_entity () (*dicee.knowledge_graph_embeddings.KGE* method), 53
 predict_missing_relations () (*dicee.KGE* method), 214
 predict_missing_relations () (*dicee.knowledge_graph_embeddings.KGE* method), 54
 predict_missing_tail_entity () (*dicee.KGE* method), 215
 predict_missing_tail_entity () (*dicee.knowledge_graph_embeddings.KGE* method), 54
 predict_topk () (*dicee.KGE* method), 215
 predict_topk () (*dicee.knowledge_graph_embeddings.KGE* method), 55
 prepare_data () (*dicee.CVDataModule* method), 227
 prepare_data () (*dicee.dataset_classes.CVDataModule* method), 43
 preprocess_with_byte_pair_encoding () (*dicee.read_preprocess_save_load_kg.PreprocessKG* method), 168
 preprocess_with_byte_pair_encoding () (*dicee.read_preprocess_save_load_kg.preprocess.PreprocessKG* method), 163
 preprocess_with_byte_pair_encoding_with_padding () (*dicee.read_preprocess_save_load_kg.PreprocessKG* method), 169
 preprocess_with_byte_pair_encoding_with_padding () (*dicee.read_preprocess_save_load_kg.preprocess.PreprocessKG* method), 163
 preprocess_with_pandas () (*dicee.read_preprocess_save_load_kg.PreprocessKG* method), 169
 preprocess_with_pandas () (*dicee.read_preprocess_save_load_kg.preprocess.PreprocessKG* method), 163
 preprocess_with_polars () (*dicee.read_preprocess_save_load_kg.PreprocessKG* method), 169
 preprocess_with_polars () (*dicee.read_preprocess_save_load_kg.preprocess.PreprocessKG* method), 163
 preprocesses_input_args () (*in module dicee.static_preprocess_funcs*), 176
 PreprocessKG (*class* in *dicee.read_preprocess_save_load_kg*), 168
 PreprocessKG (*class* in *dicee.read_preprocess_save_load_kg.preprocess*), 163
 PrintCallback (*class* in *dicee.callbacks*), 21
 process (*dicee.trainer.torch_trainer.TorchTrainer* attribute), 180
 PseudoLabellingCallback (*class* in *dicee.callbacks*), 24
 Pyke (*class* in *dicee*), 186
 Pyke (*class* in *dicee.models*), 126
 Pyke (*class* in *dicee.models.real*), 100
 pykeen_model_kwarg (*dicee.config.Namespace* attribute), 31
 PykeenKGE (*class* in *dicee*), 204
 PykeenKGE (*class* in *dicee.models*), 154
 PykeenKGE (*class* in *dicee.models.pykeen_models*), 95

Q

q (*dicee.config.Namespace* attribute), 31
 q (*dicee.DeCaL* attribute), 191
 q (*dicee.Keci* attribute), 188
 q (*dicee.models.clifford.DeCaL* attribute), 79
 q (*dicee.models.clifford.Keci* attribute), 76
 q (*dicee.models.DeCaL* attribute), 149

`q (dicee.models.Keci attribute), 145`
`qdraft_client (dicee.scripts.index_serve.NeuralSearcher attribute), 171`
`QMult (class in dicee), 200`
`QMult (class in dicee.models), 136`
`QMult (class in dicee.models.quaternion), 96`
`quaternion_mul () (in module dicee.models), 133`
`quaternion_mul () (in module dicee.models.static_funcs), 102`
`quaternion_mul_with_unit_norm () (in module dicee.models), 136`
`quaternion_mul_with_unit_norm () (in module dicee.models.quaternion), 96`
`quaternion_multiplication_followed_by_inner_product () (dicee.models.QMult method), 137`
`quaternion_multiplication_followed_by_inner_product () (dicee.models.quaternion.QMult method), 97`
`quaternion_multiplication_followed_by_inner_product () (dicee.QMult method), 201`
`quaternion_normalizer () (dicee.models.QMult static method), 137`
`quaternion_normalizer () (dicee.models.quaternion.QMult static method), 97`
`quaternion_normalizer () (dicee.QMult static method), 201`
`queries (dicee.scripts.index_serve.StringListRequest attribute), 171`
`query_name_to_struct (dicee.query_generator.QueryGenerator attribute), 162`
`query_name_to_struct (dicee.QueryGenerator attribute), 231`
`QueryGenerator (class in dicee), 230`
`QueryGenerator (class in dicee.query_generator), 162`

R

`r (dicee.DeCaL attribute), 191`
`r (dicee.Keci attribute), 188`
`r (dicee.models.clifford.DeCaL attribute), 79`
`r (dicee.models.clifford.Keci attribute), 76`
`r (dicee.models.DeCaL attribute), 149`
`r (dicee.models.Keci attribute), 145`
`random_prediction () (in module dicee), 212`
`random_prediction () (in module dicee.static_funcs), 174`
`random_seed (dicee.config.Namespace attribute), 31`
`ratio (dicee.callbacks.Perturb attribute), 27`
`re (dicee.DeCaL attribute), 191`
`re (dicee.models.clifford.DeCaL attribute), 79`
`re (dicee.models.DeCaL attribute), 149`
`re_vocab (dicee.evaluator.Evaluator attribute), 48`
`read_from_disk () (in module dicee.read_preprocess_save_load_kg.util), 167`
`read_from_triple_store_with_pandas () (in module dicee.read_preprocess_save_load_kg.util), 167`
`read_from_triple_store_with_polars () (in module dicee.read_preprocess_save_load_kg.util), 167`
`read_only_few (dicee.config.Namespace attribute), 31`
`read_only_few (dicee.knowledge_graph.KG attribute), 52`
`read_or_load_kg () (in module dicee), 211`
`read_or_load_kg () (in module dicee.static_funcs), 174`
`read_with_pandas () (in module dicee.read_preprocess_save_load_kg.util), 167`
`read_with_polars () (in module dicee.read_preprocess_save_load_kg.util), 167`
`ReadFromDisk (class in dicee.read_preprocess_save_load_kg), 169`
`ReadFromDisk (class in dicee.read_preprocess_save_load_kg.read_from_disk), 164`
`reducer (dicee.scripts.index_serve.StringListRequest attribute), 171`
`rel2id (dicee.query_generator.QueryGenerator attribute), 162`
`rel2id (dicee.QueryGenerator attribute), 230`
`relation_embeddings (dicee.AConvQ attribute), 197`
`relation_embeddings (dicee.ConvQ attribute), 198`
`relation_embeddings (dicee.DeCaL attribute), 191`
`relation_embeddings (dicee.DualE attribute), 194`
`relation_embeddings (dicee.LFMult attribute), 203`
`relation_embeddings (dicee.models.AConvQ attribute), 138`
`relation_embeddings (dicee.models.clifford.DeCaL attribute), 79`
`relation_embeddings (dicee.models.ConvQ attribute), 138`
`relation_embeddings (dicee.models.DeCaL attribute), 149`
`relation_embeddings (dicee.models.DualE attribute), 161`
`relation_embeddings (dicee.models.dualE.DualE attribute), 85`
`relation_embeddings (dicee.models.FMult attribute), 157`
`relation_embeddings (dicee.models.FMult2 attribute), 159`
`relation_embeddings (dicee.models.function_space.FMult attribute), 87`
`relation_embeddings (dicee.models.function_space.FMult2 attribute), 88`
`relation_embeddings (dicee.models.function_space.GFMult attribute), 87`
`relation_embeddings (dicee.models.function_space.LFMult attribute), 89`

relation_embeddings (*dicee.models.function_space.LFMult1 attribute*), 88
 relation_embeddings (*dicee.models.GFMult attribute*), 158
 relation_embeddings (*dicee.models.LFMult attribute*), 159
 relation_embeddings (*dicee.models.LFMult1 attribute*), 159
 relation_embeddings (*dicee.models.pykeen_models.PykeenKGE attribute*), 95
 relation_embeddings (*dicee.models.PykeenKGE attribute*), 154
 relation_embeddings (*dicee.models.quaternion.AConvQ attribute*), 98
 relation_embeddings (*dicee.models.quaternion.ConvQ attribute*), 98
 relation_embeddings (*dicee.PykeenKGE attribute*), 205
 relation_to_idx (*dicee.knowledge_graph.KG attribute*), 52
 relations_str (*dicee.knowledge_graph.KG property*), 53
 reload_dataset () (*in module dicee*), 217
 reload_dataset () (*in module dicee.dataset_classes*), 33
 report (*dicee.DICE_Trainer attribute*), 212
 report (*dicee.evaluator.Evaluator attribute*), 48
 report (*dicee.executer.Execute attribute*), 50
 report (*dicee.trainer.DICE_Trainer attribute*), 182
 report (*dicee.trainer.dice_trainer.DICE_Trainer attribute*), 177
 reports (*dicee.callbacks.Eval attribute*), 25
 reports (*dicee.callbacks.PeriodicEvalCallback attribute*), 27
 requires_grad_for_interactions (*dicee.CKeci attribute*), 187
 requires_grad_for_interactions (*dicee.Keci attribute*), 188
 requires_grad_for_interactions (*dicee.models.CKeci attribute*), 148
 requires_grad_for_interactions (*dicee.models.clifford.CKeci attribute*), 78
 requires_grad_for_interactions (*dicee.models.clifford.Keci attribute*), 76
 requires_grad_for_interactions (*dicee.models.Keci attribute*), 145
 resid_dropout (*dicee.models.transformers.SelfAttention attribute*), 105
 residual_convolution () (*dicee.AConEx method*), 196
 residual_convolution () (*dicee.AConvO method*), 197
 residual_convolution () (*dicee.AConvQ method*), 197
 residual_convolution () (*dicee.ConEx method*), 200
 residual_convolution () (*dicee.ConvO method*), 199
 residual_convolution () (*dicee.ConvQ method*), 198
 residual_convolution () (*dicee.models.AConEx method*), 131
 residual_convolution () (*dicee.models.AConvO method*), 144
 residual_convolution () (*dicee.models.AConvQ method*), 138
 residual_convolution () (*dicee.models.complex.AConEx method*), 83
 residual_convolution () (*dicee.models.complex.ConEx method*), 82
 residual_convolution () (*dicee.models.ConEx method*), 131
 residual_convolution () (*dicee.models.ConvO method*), 144
 residual_convolution () (*dicee.models.ConvQ method*), 138
 residual_convolution () (*dicee.models.octonion.AConvO method*), 94
 residual_convolution () (*dicee.models.octonion.ConvO method*), 94
 residual_convolution () (*dicee.models.quaternion.AConvQ method*), 98
 residual_convolution () (*dicee.models.quaternion.ConvQ method*), 98
 retrieve_embedding () (*dicee.scripts.index_serve.NeuralSearcher method*), 171
 retrieve_embeddings () (*in module dicee.scripts.index_serve*), 171
 return_multi_hop_query_results () (*dicee.KGE method*), 216
 return_multi_hop_query_results () (*dicee.knowledge_graph_embeddings.KGE method*), 55
 root () (*in module dicee.scripts.index_serve*), 171
 roots (*dicee.models.FMult attribute*), 158
 roots (*dicee.models.function_space.FMult attribute*), 87
 roots (*dicee.models.function_space.GFMult attribute*), 87
 roots (*dicee.models.GFMult attribute*), 158
 runtime (*dicee.analyse_experiments.Experiment attribute*), 20

S

sample_counter (*dicee.abstracts.AbstractPPECallback attribute*), 17
 sample_entity () (*dicee.abstracts.BaseInteractiveKGE method*), 15
 sample_relation () (*dicee.abstracts.BaseInteractiveKGE method*), 15
 sample_triples_ratio (*dicee.config.Namespace attribute*), 31
 sample_triples_ratio (*dicee.knowledge_graph.KG attribute*), 52
 sampling_ratio (*dicee.dataset_classes.LiteralDataset attribute*), 45, 46
 sampling_ratio (*dicee.LiteralDataset attribute*), 229, 230
 sanity_check_callback_args () (*in module dicee.sanity_checkers*), 170
 sanity_checking_with_arguments () (*in module dicee.sanity_checkers*), 170
 save () (*dicee.abstracts.BaseInteractiveKGE method*), 15

save() (*dicee.read_preprocess_save_load_kg.LoadSaveToDisk method*), 169
 save() (*dicee.read_preprocess_save_load_kg.save_load_disk.LoadSaveToDisk method*), 164
 save_checkpoint() (*dicee.abstracts.AbstractTrainer static method*), 14
 save_checkpoint_model() (*in module dicee*), 211
 save_checkpoint_model() (*in module dicee.static_funcs*), 174
 save_embeddings() (*in module dicee*), 212
 save_embeddings() (*in module dicee.static_funcs*), 174
 save_embeddings_as_csv (*dicee.config.Namespace attribute*), 29
 save_every_n_epochs (*dicee.config.Namespace attribute*), 32
 save_experiment() (*dicee.analyse_experiments.Experiment method*), 20
 save_model_at_every_epoch (*dicee.config.Namespace attribute*), 31
 save_model_every_n_epoch (*dicee.callbacks.PeriodicEvalCallback attribute*), 27
 save_numpy_ndarray() (*in module dicee*), 211
 save_numpy_ndarray() (*in module dicee.read_preprocess_save_load_kg.util*), 168
 save_numpy_ndarray() (*in module dicee.static_funcs*), 174
 save_pickle() (*in module dicee*), 211
 save_pickle() (*in module dicee.read_preprocess_save_load_kg.util*), 168
 save_pickle() (*in module dicee.static_funcs*), 174
 save_queries() (*dicee.query_generator.QueryGenerator method*), 163
 save_queries() (*dicee.QueryGenerator method*), 231
 save_queries_and_answers() (*dicee.query_generator.QueryGenerator static method*), 163
 save_queries_and_answers() (*dicee.QueryGenerator static method*), 231
 save_trained_model() (*dicee.executer.Execute method*), 50
 scalar_batch_NN() (*dicee.LFMult method*), 203
 scalar_batch_NN() (*dicee.models.function_space.LFMult method*), 89
 scalar_batch_NN() (*dicee.models.LFMult method*), 160
 scaler (*dicee.callbacks.Perturb attribute*), 27
 scaler (*dicee.trainer.torch_trainer_ddp.NodeTrainer attribute*), 182
 scheduler (*dicee.callbacks.LRScheduler attribute*), 28
 score() (*dicee.CoKE method*), 204
 score() (*dicee.ComplEx static method*), 196
 score() (*dicee.DistMult method*), 187
 score() (*dicee.Keci method*), 190
 score() (*dicee.models.clifford.Keci method*), 78
 score() (*dicee.models.CoKE method*), 128
 score() (*dicee.models.ComplEx static method*), 132
 score() (*dicee.models.complex.ComplEx static method*), 84
 score() (*dicee.models.DistMult method*), 126
 score() (*dicee.models.Keci method*), 147
 score() (*dicee.models.octonion.OMult method*), 92
 score() (*dicee.models.OMult method*), 143
 score() (*dicee.models.QMult method*), 137
 score() (*dicee.models.quaternion.QMult method*), 97
 score() (*dicee.models.real.CoKE method*), 101
 score() (*dicee.models.real.DistMult method*), 99
 score() (*dicee.models.real.TransE method*), 100
 score() (*dicee.models.TransE method*), 126
 score() (*dicee.OMult method*), 202
 score() (*dicee.QMult method*), 201
 score() (*dicee.TransE method*), 190
 score_func (*dicee.models.FMult2 attribute*), 158
 score_func (*dicee.models.function_space.FMult2 attribute*), 88
 scoring_technique (*dicee.analyse_experiments.Experiment attribute*), 20
 scoring_technique (*dicee.config.Namespace attribute*), 30
 search() (*dicee.scripts.index_serve.NeuralSearcher method*), 171
 search_embeddings() (*in module dicee.scripts.index_serve*), 171
 search_embeddings_batch() (*in module dicee.scripts.index_serve*), 171
 seed (*dicee.query_generator.QueryGenerator attribute*), 162
 seed (*dicee.QueryGenerator attribute*), 230
 select_model() (*in module dicee*), 211
 select_model() (*in module dicee.static_funcs*), 174
 selected_optimizer (*dicee.BaseKGE attribute*), 209
 selected_optimizer (*dicee.models.base_model.BaseKGE attribute*), 73
 selected_optimizer (*dicee.models.BaseKGE attribute*), 120, 123, 129, 134, 140, 153, 156
 SelfAttention (*class in dicee.models.transformers*), 104
 separator (*dicee.config.Namespace attribute*), 30
 separator (*dicee.knowledge_graph.KG attribute*), 53
 sequential_vocabulary_construction() (*dicee.read_preprocess_save_load_kg.PreprocessKG method*), 169

```

sequential_vocabulary_construction() (dicee.read_preprocess_save_load_kg.preprocess.PreprocessKG method), 163
serve() (in module dicee.scripts.index_serve), 172
set_global_seed() (dicee.query_generator.QueryGenerator method), 162
set_global_seed() (dicee.QueryGenerator method), 231
set_model_eval_mode() (dicee.abstracts.BaseInteractiveKGE method), 15
set_model_train_mode() (dicee.abstracts.BaseInteractiveKGE method), 14
setup() (dicee.CVDataModule method), 226
setup() (dicee.dataset_classes.CVDataModule method), 42
setup_executor() (dicee.executer.Execute method), 50
Shallom (class in dicee), 202
Shallom (class in dicee.models), 126
Shallom (class in dicee.models.real), 100
shallom (dicee.models.real.Shallom attribute), 100
shallom (dicee.models.Shallom attribute), 126
shallom (dicee.Shallom attribute), 202
single_hop_query_answering() (dicee.KGE method), 216
single_hop_query_answering() (dicee.knowledge_graph_embeddings.KGE method), 55
snapshot_dir (dicee.callbacks.LRScheduler attribute), 28
snapshot_loss (dicee.callbacks.LRScheduler attribute), 28
sparql_endpoint (dicee.config.Namespace attribute), 30
sparql_endpoint (dicee.knowledge_graph.KG attribute), 52
start() (dicee.DICE_Trainer method), 213
start() (dicee.executer.Execute method), 51
start() (dicee.read_preprocess_save_load_kg.PreprocessKG method), 168
start() (dicee.read_preprocess_save_load_kg.preprocess.PreprocessKG method), 163
start() (dicee.read_preprocess_save_load_kg.read_from_disk.ReadFromDisk method), 164
start() (dicee.read_preprocess_save_load_kg.ReadFromDisk method), 169
start() (dicee.trainer.DICE_Trainer method), 183
start() (dicee.trainer.dice_trainer.DICE_Trainer method), 178
start_time (dicee.callbacks.PrintCallback attribute), 22
start_time (dicee.executer.Execute attribute), 50
state_dict() (dicee.EnsembleKGE method), 210
state_dict() (dicee.models.ensemble.EnsembleKGE method), 86
step() (dicee.EnsembleKGE method), 211
step() (dicee.models.ADOPT method), 112
step() (dicee.models.adopt.ADOPT method), 60
step() (dicee.models.ensemble.EnsembleKGE method), 86
step_count (dicee.callbacks.LRScheduler attribute), 28
storage_path (dicee.config.Namespace attribute), 29
storage_path (dicee.DICE_Trainer attribute), 213
storage_path (dicee.trainer.DICE_Trainer attribute), 182
storage_path (dicee.trainer.dice_trainer.DICE_Trainer attribute), 178
store() (in module dicee), 211
store() (in module dicee.static_funcs), 174
store_ensemble() (dicee.abstracts.AbstractPPECallback method), 18
strategy (dicee.abstracts.AbstractTrainer attribute), 13
StringListRequest (class in dicee.scripts.index_serve), 171
SWA (class in dicee.callbacks), 28
swa (dicee.config.Namespace attribute), 32
swa_c_epochs (dicee.callbacks.SWA attribute), 29
swa_lr (dicee.callbacks.SWA attribute), 29
swa_model (dicee.callbacks.SWA attribute), 29
swa_n (dicee.callbacks.SWA attribute), 29
swa_start_epoch (dicee.callbacks.SWA attribute), 29
swa_start_epoch (dicee.config.Namespace attribute), 32

```

T

```

T() (dicee.DualE method), 195
T() (dicee.models.DualE method), 161
T() (dicee.models.dualE.DualE method), 85
t_conorm() (dicee.abstracts.InteractiveQueryDecomposition method), 16
t_norm() (dicee.abstracts.InteractiveQueryDecomposition method), 16
target_dim (dicee.AllvsAll attribute), 221
target_dim (dicee.dataset_classes.AllvsAll attribute), 37
target_dim (dicee.dataset_classes.MultiLabelDataset attribute), 34
target_dim (dicee.dataset_classes.OnevsAllDataset attribute), 35
target_dim (dicee.knowledge_graph.KG attribute), 52

```

target_dim (*dicee.MultiLabelDataset* attribute), 218
target_dim (*dicee.OnevsAllDataset* attribute), 219
temperature (*dicee.BytE* attribute), 206
temperature (*dicee.models.transformers.BytE* attribute), 103
tensor_t_norm () (*dicee.abstracts.InteractiveQueryDecomposition* method), 16
TensorParallel (class in *dicee.trainer.model_parallelism*), 179
test_dataloader () (*dicee.models.base_model.BaseKGELightning* method), 68
test_dataloader () (*dicee.models.BaseKGELightning* method), 116
test_epoch_end () (*dicee.models.base_model.BaseKGELightning* method), 68
test_epoch_end () (*dicee.models.BaseKGELightning* method), 115
test_h1 (*dicee.analyse_experiments.Experiment* attribute), 20
test_h3 (*dicee.analyse_experiments.Experiment* attribute), 20
test_h10 (*dicee.analyse_experiments.Experiment* attribute), 20
test_mrr (*dicee.analyse_experiments.Experiment* attribute), 20
test_path (*dicee.query_generator.QueryGenerator* attribute), 162
test_path (*dicee.QueryGenerator* attribute), 230
timeit () (in module *dicee*), 211, 217
timeit () (in module *dicee.read_preprocess_save_load_kg.util*), 167
timeit () (in module *dicee.static_funcs*), 173
timeit () (in module *dicee.static_preprocess_funcs*), 176
to () (*dicee.EnsembleKGE* method), 210
to () (*dicee.KGE* method), 214
to () (*dicee.knowledge_graph_embeddings.KGE* method), 53
to () (*dicee.models.ensemble.EnsembleKGE* method), 86
to_df () (*dicee.analyse_experiments.Experiment* method), 20
topk (*dicee.BytE* attribute), 206
topk (*dicee.models.transformers.BytE* attribute), 103
topk (*dicee.scripts.index_serve.NeuralSearcher* attribute), 171
torch_ordered_shaped_bpe_entities (*dicee.dataset_classes.MultiLabelDataset* attribute), 34
torch_ordered_shaped_bpe_entities (*dicee.MultiLabelDataset* attribute), 218
TorchDDPTrainer (class in *dicee.trainer.torch_trainer_ddp*), 181
TorchTrainer (class in *dicee.trainer.torch_trainer*), 180
total_epochs (*dicee.callbacks.LRScheduler* attribute), 28
total_steps (*dicee.callbacks.LRScheduler* attribute), 28
train () (*dicee.abstracts.BaseInteractiveTrainKGE* method), 18
train () (*dicee.trainer.torch_trainer_ddp.NodeTrainer* method), 182
train_data (*dicee.AllvsAll* attribute), 221
train_data (*dicee.dataset_classes.AllvsAll* attribute), 37
train_data (*dicee.dataset_classes.KvsAll* attribute), 36
train_data (*dicee.dataset_classes.KvsSampleDataset* attribute), 39
train_data (*dicee.dataset_classes.MultiClassClassificationDataset* attribute), 35
train_data (*dicee.dataset_classes.OnevsAllDataset* attribute), 35
train_data (*dicee.dataset_classes.OnevsSample* attribute), 37, 38
train_data (*dicee.KvsAll* attribute), 220
train_data (*dicee.KvsSampleDataset* attribute), 223
train_data (*dicee.MultiClassClassificationDataset* attribute), 219
train_data (*dicee.OnevsAllDataset* attribute), 219
train_data (*dicee.OnevsSample* attribute), 221, 222
train_dataloader () (*dicee.CVDataModule* method), 225
train_dataloader () (*dicee.dataset_classes.CVDataModule* method), 41
train_dataloader () (*dicee.models.base_model.BaseKGELightning* method), 69
train_dataloader () (*dicee.models.BaseKGELightning* method), 117
train_dataloaders (*dicee.trainer.torch_trainer.TorchTrainer* attribute), 180
train_dataset_loader (*dicee.trainer.torch_trainer_ddp.NodeTrainer* attribute), 182
train_file_path (*dicee.dataset_classes.LiteralDataset* attribute), 45
train_file_path (*dicee.LiteralDataset* attribute), 229
train_h1 (*dicee.analyse_experiments.Experiment* attribute), 20
train_h3 (*dicee.analyse_experiments.Experiment* attribute), 20
train_h10 (*dicee.analyse_experiments.Experiment* attribute), 20
train_indices_target (*dicee.dataset_classes.MultiLabelDataset* attribute), 34
train_indices_target (*dicee.MultiLabelDataset* attribute), 218
train_k_vs_all () (*dicee.abstracts.BaseInteractiveTrainKGE* method), 18
train_literals () (*dicee.abstracts.BaseInteractiveTrainKGE* method), 18
train_mode (*dicee.EnsembleKGE* attribute), 210
train_mode (*dicee.models.ensemble.EnsembleKGE* attribute), 86
train_mrr (*dicee.analyse_experiments.Experiment* attribute), 20
train_path (*dicee.query_generator.QueryGenerator* attribute), 162
train_path (*dicee.QueryGenerator* attribute), 230

`train_set (dicee.BPE_NegativeSamplingDataset attribute), 218`
`train_set (dicee.dataset_classes.BPE_NegativeSamplingDataset attribute), 34`
`train_set (dicee.dataset_classes.MultiLabelDataset attribute), 34`
`train_set (dicee.dataset_classes.NegSampleDataset attribute), 40`
`train_set (dicee.dataset_classes.TriplePredictionDataset attribute), 41`
`train_set (dicee.MultiLabelDataset attribute), 218`
`train_set (dicee.NegSampleDataset attribute), 224`
`train_set (dicee.TriplePredictionDataset attribute), 225`
`train_set_idx (dicee.CVDataModule attribute), 225`
`train_set_idx (dicee.dataset_classes.CVDataModule attribute), 41`
`train_set_target (dicee.knowledge_graph.KG attribute), 52`
`train_target (dicee.AllvsAll attribute), 221`
`train_target (dicee.dataset_classes.AllvsAll attribute), 37`
`train_target (dicee.dataset_classes.KvsAll attribute), 36`
`train_target (dicee.dataset_classes.KvsSampleDataset attribute), 39`
`train_target (dicee.KvsAll attribute), 220`
`train_target (dicee.KvsSampleDataset attribute), 223`
`train_target_indices (dicee.knowledge_graph.KG attribute), 53`
`train_triples (dicee.dataset_classes.NegSampleDataset attribute), 40`
`train_triples (dicee.NegSampleDataset attribute), 224`
`train_triples () (dicee.abstracts.BaseInteractiveTrainKGE method), 18`
`trained_model (dicee.executer.Execute attribute), 50`
`trainer (dicee.config.Namespace attribute), 30`
`trainer (dicee.DICE_Trainer attribute), 213`
`trainer (dicee.executer.Execute attribute), 50`
`trainer (dicee.trainer.DICE_Trainer attribute), 182`
`trainer (dicee.trainer.dice_trainer.DICE_Trainer attribute), 177`
`trainer (dicee.trainer.torch_trainer_ddp.NodeTrainer attribute), 181`
`training_step (dicee.trainer.torch_trainer.TorchTrainer attribute), 180`
`training_step () (dicee.BytE method), 206`
`training_step () (dicee.models.base_model.BaseKGELightning method), 66`
`training_step () (dicee.models.BaseKGELightning method), 114`
`training_step () (dicee.models.transformers.BytE method), 103`
`training_step_outputs (dicee.models.base_model.BaseKGELightning attribute), 66`
`training_step_outputs (dicee.models.BaseKGELightning attribute), 114`
`training_technique (dicee.knowledge_graph.KG attribute), 52`
`TransE (class in dicee), 190`
`TransE (class in dicee.models), 126`
`TransE (class in dicee.models.real), 99`
`transfer_batch_to_device () (dicee.CVDataModule method), 226`
`transfer_batch_to_device () (dicee.dataset_classes.CVDataModule method), 42`
`transformer (dicee.BytE attribute), 206`
`transformer (dicee.models.transformers.BytE attribute), 103`
`transformer (dicee.models.transformers.GPT attribute), 108`
`trapezoid() (dicee.models.FMult2 method), 159`
`trapezoid() (dicee.models.function_space.FMult2 method), 88`
`tri_score() (dicee.LFMult method), 203`
`tri_score() (dicee.models.function_space.LFMult method), 89`
`tri_score() (dicee.models.function_space.LFMult1 method), 88`
`tri_score() (dicee.models.LFMult method), 160`
`tri_score() (dicee.models.LFMult1 method), 159`
`triple_score() (dicee.KGE method), 215`
`triple_score() (dicee.knowledge_graph_embeddings.KGE method), 55`
`TriplePredictionDataset (class in dicee), 224`
`TriplePredictionDataset (class in dicee.dataset_classes), 40`
`tuple2list () (dicee.query_generator.QueryGenerator method), 162`
`tuple2list () (dicee.QueryGenerator method), 231`

U

`unlabelled_size (dicee.callbacks.PseudoLabellingCallback attribute), 24`
`unmap () (dicee.query_generator.QueryGenerator method), 162`
`unmap () (dicee.QueryGenerator method), 231`
`unmap_query () (dicee.query_generator.QueryGenerator method), 162`
`unmap_query () (dicee.QueryGenerator method), 231`

V

`val_aswa (dicee.callbacks.ASWA attribute), 24`

val_dataloader() (*dicee.models.base_model.BaseKGE**Lightning method*), 69
val_dataloader() (*dicee.models.BaseKGE**Lightning method*), 116
val_h1 (*dicee.analyse_experiments.Experiment* attribute), 20
val_h3 (*dicee.analyse_experiments.Experiment* attribute), 20
val_h10 (*dicee.analyse_experiments.Experiment* attribute), 20
val_mrr (*dicee.analyse_experiments.Experiment* attribute), 20
val_path (*dicee.query_generator.QueryGenerator* attribute), 162
val_path (*dicee.QueryGenerator* attribute), 230
validate_knowledge_graph() (*in module dicee.sanity_checkers*), 170
vocab_preparation() (*dicee.evaluator.Evaluator* method), 49
vocab_size (*dicee.models.CoKEConfig* attribute), 127
vocab_size (*dicee.models.real.CoKEConfig* attribute), 100, 101
vocab_size (*dicee.models.transformers.GPTConfig* attribute), 107
vocab_to_parquet() (*in module dicee*), 212
vocab_to_parquet() (*in module dicee.static_funcs*), 175
vtp_score() (*dicee.LFMult* method), 203
vtp_score() (*dicee.models.function_space.LFMult* method), 89
vtp_score() (*dicee.models.function_space.LFMult1* method), 88
vtp_score() (*dicee.models.LFMult* method), 160
vtp_score() (*dicee.models.LFMult1* method), 159

W

warmup_steps (*dicee.callbacks.LRScheduler* attribute), 28
weight (*dicee.models.transformers.LayerNorm* attribute), 104
weight_decay (*dicee.BaseKGE* attribute), 209
weight_decay (*dicee.config.Namespace* attribute), 30
weight_decay (*dicee.models.base_model.BaseKGE* attribute), 72
weight_decay (*dicee.models.BaseKGE* attribute), 120, 123, 129, 134, 140, 153, 156
weights (*dicee.models.FMult* attribute), 158
weights (*dicee.models.function_space.FMult* attribute), 87
weights (*dicee.models.function_space.GFMult* attribute), 87
weights (*dicee.models.GFMult* attribute), 158
write_csv_from_model_parallel() (*in module dicee*), 212
write_csv_from_model_parallel() (*in module dicee.static_funcs*), 175
write_links() (*dicee.query_generator.QueryGenerator* method), 162
write_links() (*dicee.QueryGenerator* method), 231
write_report() (*dicee.executer.Execute* method), 51

X

x_values (*dicee.LFMult* attribute), 203
x_values (*dicee.models.function_space.LFMult* attribute), 89
x_values (*dicee.models.LFMult* attribute), 159