
DICE Embeddings

Release 0.1.3.2

Caglar Demir

Nov 25, 2025

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	186
14.3 Classes	186
14.4 Functions	187
14.5 Package Contents	189
Python Module Index	235

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

1 Dicee Manual

Version: dicee 0.2.0

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

Publisher and maintainer: Caglar Demir²

Contact: caglar.demir@upb.de

License: OSI Approved :: MIT License

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

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

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

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

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

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

Why 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
```

(continues on next page)

(continued from previous page)

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

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

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

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

# (2) Two-hop query answering
# Query: ?D : \exist E.Married(D, E) \land hasSibling(E, F9M167)
# Question: To whom a sibling of F9M167 is married to?
# Answer: [F9F158, F9M142] as (F9M157 #married F9F158) and (F9F141 #married F9M142)

predictions = pre_trained_kge.answer_multi_hop_query(query_type="2p",
                                                      query="http://www.benchmark.org/↪family#F9M167",
                                                      ("http://www.benchmark.
                                                       ↪org/family#hasSibling",
                                                       "http://www.benchmark.
                                                       ↪org/family#married")),
                                                       tnorm="min", k=3)

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

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

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

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

For more, please refer to examples/multi_hop_query_answering.

8 Predicting Missing Links

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

9 Downloading Pretrained Models

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

- For more please look at dice-research.org/projects/DiceEmbeddings/¹¹

10 How to Deploy

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

11 Docker

To build the Docker image:

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

To test the Docker image:

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

12 Coverage Report

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

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

(continues on next page)

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

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

(continued from previous page)

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

(continues on next page)

(continued from previous page)

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

13 How to cite

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

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

(continues on next page)

(continued from previous page)

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

(continues on next page)

(continued from previous page)

```
@inproceedings{demir2021convolutional,
  title={Convolutional Complex Knowledge Graph Embeddings},
  author={Caglar Demir and Axel-Cyrille Ngonga Ngomo},
  booktitle={Eighteenth Extended Semantic Web Conference - Research Track},
  year={2021},
  url={https://openreview.net/forum?id=6T45-4TFqaX}
# Shallom
@inproceedings{demir2021shallow,
  title={A shallow neural model for relation prediction},
  author={Demir, Caglar and 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.

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

dicee.config

Classes

Namespace	Simple object for storing attributes.
-----------	---------------------------------------

Module Contents

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

    Simple object for storing attributes.

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

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

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

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

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

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

    sparql_endpoint = None
        An endpoint of a triple store.

    model: str = 'Keci'
        KGE model

    optim: str = 'Adam'
        Optimizer

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

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

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

    lr: float = 0.1
        Learning rate

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

    gpus = None
        Number GPUs to be used during training

    callbacks
        10} }

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

    Type
        { "last_percent_to_consider"
```

```

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

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

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

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

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

weight_decay: float = 0.0
    Weight decay for all trainable params

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

init_param: str = None
    xavier_normal or None

gradient_accumulation_steps: int = 0
    Not tested e

num_folds_for_cv: int = 0
    Number of folds for CV

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

Type
    Evaluate trained model choices

save_model_at_every_epoch: int = None
    Not tested

label_smoothing_rate: float = 0.0

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

random_seed: int = 0
    Random Seed

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

read_only_few: int = None
    Read only first few triples

pykeen_model_kwargs
    Additional keyword arguments for pykeen models

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

```

```

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

p: int = 0
    P parameter of Clifford Embeddings

q: int = 1
    Q parameter of Clifford Embeddings

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

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

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

byte_pair_encoding: bool = False
    Byte pair encoding

Type
    WIP

adaptive_swa: bool = False
    Adaptive stochastic weight averaging

swa: bool = False
    Stochastic weight averaging

swag: bool = False
    Stochastic weight averaging - Gaussian

ema: bool = False
    Exponential Moving Average

twa: bool = False
    Trainable weight averaging

block_size: int = None
    block size of LLM

continual_learning = None
    Path of a pretrained model size of LLM

auto_batch_finding = False
    A flag for using auto batch finding

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

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

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

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

```

```

adaptive_lr
    "cca"}]

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

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

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

__iter__()

```

dicee.dataset_classes

Classes

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

Functions

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

Module Contents

```

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

```

Reload the files from disk to construct the Pytorch dataset

```

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

```

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

Bases: torch.utils.data.Dataset

An abstract class representing a Dataset.

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

Note

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

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

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

Bases: torch.utils.data.Dataset

An abstract class representing a Dataset.

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

Note

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

```
train_set  
  
train_indices_target
```

```

target_dim
num_datapoints
torch_ordered_shaped_bpe_entities
collate_fn = None
__len__()
__getitem__(idx)

```

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

Bases: `torch.utils.data.Dataset`

Dataset for the 1vsALL training strategy

Parameters

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

Return type

`torch.utils.data.Dataset`

train_data

```

block_size = 8
num_of_data_points
collate_fn = None
__len____getitem__(idx)

```

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

Bases: `torch.utils.data.Dataset`

Dataset for the 1vsALL training strategy

Parameters

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

Return type
 torch.utils.data.Dataset

```

train_data
target_dim
collate_fn = None

__len__()
__getitem__(idx)

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

Bases: torch.utils.data.Dataset

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

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

or all $y_i = 1$ s.t. $(h, r) \in E$ 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_i : denotes a multi-label vector in $[0,1]^{|\{E\}|}$ is a binary label.

overall $y_{-i} = 1$ 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.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.

or all $y_i = 1$ s.t. $(h, r \in E_i)$ 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 G is a unique h in E and a relation r in R and . collect_fn => Generates negative triples

collect_fn:

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

y:labels are represented in torch.float16

train_set_idx
Indexed triples for the training.

entity_idxs
mapping.

relation_idxs
mapping.

form
?

store
?

label_smoothing_rate

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

label_smoothing_rate

neg_sample_ratio

train_set

length

num_entities

num_relations

__len__()

__getitem__(idx)

collate_fn (batch: List[torch.Tensor])

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

Bases: pytorch_lightning.LightningDataModule

Create a Dataset for cross validation

Parameters

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

Return type

?

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

An iterable or collection of iterables specifying training samples.

For more information about multiple dataloaders, see this section.

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

For data processing use the following pattern:

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

However, the above are only necessary for distributed processing.

⚠ Warning

do not assign state in *prepare_data*

- *fit()*
- *prepare_data()*
- *setup()*

ℹ Note

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

setup(*args, **kwargs)

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

Parameters

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

Example:

```

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

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

        # don't do this
        self.something = else

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

```

`transfer_batch_to_device(*args, **kwargs)`

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

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

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

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

Note

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

Parameters

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

Returns

A reference to the data on the new device.

Example:

```

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

```

(continues on next page)

(continued from previous page)

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

See also

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

`prepare_data(*args, **kwargs)`

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

⚠ Warning

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

Example:

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

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

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

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

Example:

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

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

(continues on next page)

```
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

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

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, normalize_scores: 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

<code>Evaluator</code>	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

KG

Knowledge Graph

Module Contents

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

Knowledge Graph

```
dataset_dir = 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

KGE

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

Module Contents

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

Bases: dicee.abstracts.BaseInteractiveKGE, dicee.abstracts.
InteractiveQueryDecomposition, dicee.abstracts.BaseInteractiveTrainKGE

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

__str__()

to(device: str) → None

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

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

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

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

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

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

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

Parameter

relation: Union[List[str], str]
String representation of selected relations.
tail_entity: Union[List[str], str]
String representation of selected entities.
k: int
Highest ranked k entities.

Returns: Tuple

Highest K scores and entities

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

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

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

Parameter

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

k: int

Highest ranked k entities.

Returns: Tuple

Highest K scores and entities

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

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

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

Parameter

head_entity: List[str]

String representation of selected entities.

tail_entity: List[str]

String representation of selected entities.

Returns: Tuple

scores

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

Parameters

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

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

Predict missing item in a given triple.

Returns

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

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

Predict triple score

Parameter

head_entity: List[str]

String representation of selected entities.

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

Returns: Tuple

pytorch tensor of triple score

```

return_multi_hop_query_results (aggregated_query_for_all_entities, k: int, only_scores)

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

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

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

Find an answer set for EPFO queries including negation and disjunction

Parameter

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

returns

- *List[Tuple[str, torch.Tensor]]*
- *Entities and corresponding scores sorted in the descending order of scores*

```

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

Find missing triples

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

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

Return (e,r,x)

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

```

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

topk: int
Highest ranked k item to select triples with  $f(e,r,x) > \text{confidence}$  .

at_most: int
Stop after finding at_most missing triples

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

otin G

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

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

Module Contents

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

Bases: `torch.optim.optimizer.Optimizer`

ADOPT Optimizer.

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

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

Mathematical formulation:

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

where:

- 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_t²
```

where:

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

Automatic mode selection:

When `foreach` and `fused` are both `None` (default), the function automatically selects the best implementation based on:
- Parameter types and devices
- Whether differentiable mode is enabled
- 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,

```

(continues on next page)

(continued from previous page)

```
...     eps=1e-6,
...     maximize=False,
... )
```

Note

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

See also

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

dicee.models.base_model

Classes

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

Module Contents

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

Bases: `lightning.LightningModule`

Base class for all neural network modules.

Your models should also subclass this class.

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

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

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

(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.

`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()`

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 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 ($B \times 2 \times T$)

```

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

    Parameters
    -----
    init_params_with_sanity_checking()

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

    Parameters
    *
        • x
        • y_idx
        • ordered_bpe_entities

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

    Parameters
    *
        x

    forward_k_vs_all(*args, **kwargs)

    forward_k_vs_sample(*args, **kwargs)

    get_triple_representation(idx_hrt)

    get_head_relation_representation(indexed_triple)

    get_sentence_representation(x: torch.LongTensor)

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

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

    Parameters
    *
        x (B x 2 x T)

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

class dicee.models.base_model.IdentityClass(args=None)
    Bases: torch.nn.Module

    Base class for all neural network modules.

    Your models should also subclass this class.

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

```

```

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

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

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

```

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

Note

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

Variables

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

```

args = None

__call__(x)

static forward(x)

```

dicee.models.clifford

Classes

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

Module Contents

```

class dicee.models.clifford.Keci(args)
Bases: dicee.models.base_model.BaseKGE
Base class for all neural network modules.

Your models should also subclass this class.

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

```

```

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

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

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

```

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

Note

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

Variables

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

```

name = 'Keci'

p
q
r

requires_grad_for_interactions = True

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

```

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

e2e1, e2e2, e2e3, e3e1, e3e2, e3e3

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

```

compute_sigma_qq(hq, rq)
    Compute sigma_{qq} = sum_{j=1}^{p+q-1} sum_{k=j+1}^{p+q} (h_j r_k - h_k r_j) e_j e_k sigma_{q}
    captures the interactions between along q bases For instance, let q e_1, e_2, e_3, we compute interactions
    between e_1 e_2, e_1 e_3 , and e_2 e_3 This can be implemented with a nested two for loops
        results = [] for j in range(q - 1):
            for k in range(j + 1, q):
                results.append(hq[:, :, j] * rq[:, :, k] - hq[:, :, k] * rq[:, :, j])
        sigma_qq = torch.stack(results, dim=2) assert sigma_qq.shape == (b, r, int((q * (q - 1)) / 2))

    Yet, this computation would be quite inefficient. Instead, we compute interactions along all p, e.g., e1e1,
    e1e2, e1e3,
        e2e1, e2e2, e2e3, e3e1, e3e2, e3e3
    Then select the triangular matrix without diagonals: e1e2, e1e3, e2e3.

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

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

clifford_multiplication(h0, hp, hq, r0, rp, rq)
    Compute our CL multiplication

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

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

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

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

```

Parameter

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

returns

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

forward_k_vs_with_explicit (x: torch.Tensor)

k_vs_all_score (bpe_head_ent_emb, bpe_rel_ent_emb, E)

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

Kvsall training

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

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

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

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

Parameter

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

returns

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

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

Parameter

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

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

rtype

torch.FloatTensor with (n, k) shape

score (h, r, t)

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

Parameter

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

rtype

torch.FloatTensor with (n) shape

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

Bases: *Keci*

Without learning dimension scaling

```
name = 'CKeci'
```

```
requires_grad_for_interactions = False
```

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

Bases: *dicee.models.base_model.BaseKGE*

Base class for all neural network modules.

Your models should also subclass this class.

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

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

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

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

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

Note

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

Variables

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

```
name = 'DeCaL'
```

```
entity_embeddings
```

```
relation_embeddings
```

```


p



q



r



re



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


```

Parameter

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

rtype

torch.FloatTensor with (n) shape

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

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

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

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

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

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

and return:

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

compute_sigmas_multivect (*list_h_emb*, *list_r_emb*)

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

For same bases vectors interaction we have

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

For different base vector interactions, we have

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

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

Kvsall training

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

(3) Perform Cl multiplication

(4) Inner product of (3) and all entity embeddings

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

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

Multiplying a base vector with its scalar coefficient

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

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

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

Parameter

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

returns

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

compute_sigma_pp (hp, rp)

Compute .. math:

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Compute

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

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

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

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

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

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

Compute

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

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

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

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

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

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

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

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

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

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

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

dicee.models.complex

Classes

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

Module Contents

`class dicee.models.complex.ConEx(args)`

Bases: `dicee.models.base_model.BaseKGE`

Convolutional ComplEx Knowledge Graph Embeddings

`name = 'ConEx'`

`conv2d`

`fc_num_input`

`fc1`

`norm_fc1`

`bn_conv2d`

`feature_map_dropout`

`residual_convolution(C_1: Tuple[torch.Tensor, torch.Tensor], C_2: Tuple[torch.Tensor, torch.Tensor]) → torch.FloatTensor`

Compute residual score of two complex-valued embeddings. :param C_1: a tuple of two pytorch tensors that corresponds complex-valued embeddings :param C_2: a tuple of two pytorch tensors that corresponds complex-valued embeddings :return:

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

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

Parameters

`x`

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

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

Bases: `dicee.models.base_model.BaseKGE`

Additive Convolutional ComplEx Knowledge Graph Embeddings

`name = 'AConEx'`

`conv2d`

`fc_num_input`

`fc1`

`norm_fc1`

```

bn_conv2d

feature_map_dropout

residual_convolution(C_1: Tuple[torch.Tensor, torch.Tensor],  

C_2: Tuple[torch.Tensor, torch.Tensor]) → torch.FloatTensor

Compute residual score of two complex-valued embeddings. :param C_1: a tuple of two pytorch tensors  

that corresponds complex-valued embeddings :param C_2: a tuple of two pytorch tensors that corresponds  

complex-valued embeddings :return:

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

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

Parameters
    x

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

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

Base class for all neural network modules.

Your models should also subclass this class.

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

```

```

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

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

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

```

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

Note

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

Variables

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

```
name = 'ComplEx'
```

```

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

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

```

Parameters

- **emb_h**
- **emb_r**
- **emb_E**

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

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

dicee.models.duale

Classes

Duale

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

Module Contents

```

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

```

Input

x: torch.LongTensor with (n,) shape

Output

torch.FloatTensor with (n) shape

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

Negative Sampling forward pass:

Input

x: torch.LongTensor with (n,) shape

Output

torch.FloatTensor with (n) shape

forward_k_vs_all (x)

KvsAll forward pass

Input

x: torch.LongTensor with (n,) shape

Output

torch.FloatTensor with (n) shape

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

Transpose function

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

dicee.models.ensemble

Classes

EnsembleKGE

Module Contents

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

    name

    train_mode = True

    args

    named_children()

    property example_input_array

    parameters()

    modules()

    __iter__()

    __len__()

    eval()
```

```

to (device)

state_dict ()

Return the state dict of the ensemble.

load_state_dict (state_dict, strict=True)

Load the state dict into the ensemble.

mem_of_model ()

__call__ (x_batch)

step ()

get_embeddings ()

__str__ ()

```

dicee.models.function_space

Classes

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

Module Contents

```

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

Learning Knowledge Neural Graphs

name = 'FMult'

entity_embeddings

relation_embeddings

k

num_sample = 50

gamma

roots

weights

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

chain_func (weights, x: torch.FloatTensor)

```

```

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

    Parameters
        x

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

    Parameters
        x

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

```

```

trapezoid(list_W, list_b)

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

    Parameters
        x

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

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

        name = 'LFMult1'

        entity_embeddings

        relation_embeddings

        forward_triples(idx_triple)

    Parameters
        x

        tri_score(h, r, t)

        vtp_score(h, r, t)

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

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

        name = 'LFMult'

        entity_embeddings

        relation_embeddings

        degree

        m

        x_values

        forward_triples(idx_triple)

    Parameters
        x

        construct_multi_coeff(x)

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

        linear(x, w, b)

```

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

tri_score(*coeff_h, coeff_r, coeff_t*)

this part implement the trilinear scoring techniques:

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

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

vtp_score(*h, r, t*)

this part implement the vector triple product scoring techniques:

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

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

comp_func(*h, r, t*)

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

polynomial(*coeff, x, degree*)

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

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

pop(*coeff, x, degree*)

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

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

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

dicee.models.literal

Classes

LiteralEmbeddings

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

Module Contents

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

Bases: `torch.nn.Module`

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

num_of_data_properties

Number of data properties (attributes).

Type

`int`

embedding_dims

Dimension of the embeddings.

Type

`int`

entity_embeddings

Pre-trained entity embeddings.

Type

`torch.tensor`

dropout

Dropout rate for regularization.

Type

`float`

gate_residual

Whether to use gated residual connections.

Type

`bool`

freeze_entity_embeddings

Whether to freeze the entity embeddings during training.

Type

`bool`

embedding_dim

num_of_data_properties

hidden_dim

gate_residual = True

freeze_entity_embeddings = True

entity_embeddings

data_property_embeddings

fc

fc_out

dropout

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

Parameters

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

Returns

scalar predictions.

Return type

Tensor

property device

dicee.models.octonion

Classes

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

Functions

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

Module Contents

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

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

(continues on next page)

```

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

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

```

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

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 = 'OMult'

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

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

k_vs_all_score(bpe_head_ent_emb, bpe_rel_ent_emb, E)

forward_k_vs_all(x)

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

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

Bases: `dicee.models.base_model.BaseKGE`

Base class for all neural network modules.

Your models should also subclass this class.

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

```

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

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

```

(continues on next page)

(continued from previous page)

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

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

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

Note

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

Variables

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

```
name = 'ConvO'

conv2d

fc_num_input

fc1

bn_conv2d

norm_fc1

feature_map_dropout

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

residual_convolution(O_1, O_2)

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

Parameters

`x`

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

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

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

Bases: `dicee.models.base_model.BaseKGE`

Additive Convolutional Octonion Knowledge Graph Embeddings

`name = 'AConvO'`

`conv2d`

```

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

```

Parameters

x

forward_k_vs_all(x: torch.Tensor)

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

dicee.models.pykeen_models

Classes

PykeenKGE

A class for using knowledge graph embedding models implemented in Pykeen

Module Contents

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

Bases: *dicee.models.base_model.BaseKGE*

A class for using knowledge graph embedding models implemented in Pykeen

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

model_kwargs

name

model

loss_history = []

args

entity_embeddings = None

relation_embeddings = None

```

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

    else:
        t = self.entity_embeddings.weight

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

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

abstract forward_k_vs_sample(x: torch.LongTensor, target_entity_idx)

```

dicee.models.quaternion

Classes

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

Functions

<i>quaternion_mul_with_unit_norm</i> (*, Q_1, Q_2)
--

Module Contents

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

class dicee.models.quaternion.QMult(args)

Bases: `dicee.models.base_model.BaseKGE`

Base class for all neural network modules.

Your models should also subclass this class.

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

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

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

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

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

Note

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

Variables

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

```
name = 'QMult'

explicit = True

quaternion_multiplication_followed_by_inner_product(h, r, t)
```

Parameters

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

Returns

Triple scores.

```
static quaternion_normalizer(x: torch.FloatTensor) -> torch.FloatTensor
```

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

Absolute value of a quaternion

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

L2 norm of quaternion vector:

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

Parameters

x – The vector.

Returns

The normalized vector.

```
score (head_ent_emb: torch.FloatTensor, rel_ent_emb: torch.FloatTensor,
        tail_ent_emb: torch.FloatTensor)
k_vs_all_score (bpe_head_ent_emb, bpe_rel_ent_emb, E)
```

Parameters

- **bpe_head_ent_emb**
- **bpe_rel_ent_emb**
- **E**

```
forward_k_vs_all (x)
```

Parameters

x

```
forward_k_vs_sample (x, target_entity_idx)
```

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

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

Bases: *dicee.models.base_model.BaseKGE*

Convolutional Quaternion Knowledge Graph Embeddings

```
name = 'ConvQ'
```

```
entity_embeddings
```

```
relation_embeddings
```

```
conv2d
```

```
fc_num_input
```

```
fc1
```

```
bn_conv1
```

```
bn_conv2
```

```
feature_map_dropout
```

```
residual_convolution (Q_1, Q_2)
```

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

Parameters

x

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

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

```

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

Additive Convolutional Quaternion Knowledge Graph Embeddings

name = 'AConvQ'

entity_embeddings

relation_embeddings

conv2d

fc_num_input

fc1

bn_conv1

bn_conv2

feature_map_dropout

residual_convolution (Q_1, Q_2)

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

Parameters
    x

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

```

dicee.models.real

Classes

<i>DistMult</i>	Embedding Entities and Relations for Learning and Inference in Knowledge Bases
<i>TransE</i>	Translating Embeddings for Modeling
<i>Shallow</i>	A shallow neural model for relation prediction (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

<code>quaternion_mul</code> (→ 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

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

Module Contents

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

Bases: `dicee.models.base_model.BaseKGE`

Base class for all neural network modules.

Your models should also subclass this class.

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

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

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

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

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

Note

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

Variables

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

```
name = 'BytE'

config

temperature = 0.5

topk = 2

transformer

lm_head

loss_function(yhat_batch, y_batch)
```

Parameters

- `yhat_batch`
- `y_batch`

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

Parameters

x (B by T tensor)

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

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

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

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

Parameters

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

Returns

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

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

Example:

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

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

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

(continues on next page)

```
...  
opt2.step()
```

Note

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

class dicee.models.transformers.**LayerNorm** (*ndim, bias*)

Bases: `torch.nn.Module`

LayerNorm but with an optional bias. PyTorch doesn't support simply `bias=False`

weight

bias

forward (*input*)

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

Bases: `torch.nn.Module`

Base class for all neural network modules.

Your models should also subclass this class.

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

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

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

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

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

Note

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

Variables

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

```

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

```

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

Bases: torch.nn.Module

Base class for all neural network modules.

Your models should also subclass this class.

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

```

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

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

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

```

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

Note

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

Variables

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

`c_fc`

```

gelu
c_proj
dropout
forward(x)

class dicee.models.transformers.Block(config)

```

Bases: `torch.nn.Module`

Base class for all neural network modules.

Your models should also subclass this class.

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

```

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

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

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

```

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

Note

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

Variables

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

```

ln_1
attn
ln_2
mlp
forward(x)

class dicee.models.transformers.GPTConfig

block_size: int = 1024
```

```

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

class dicee.models.transformers.GPT(config)

```

Bases: torch.nn.Module

Base class for all neural network modules.

Your models should also subclass this class.

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

```

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

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

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

```

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

Note

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

Variables

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

`config`

`transformer`

`lm_head`

```

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

forward (idx, targets=None)
crop_block_size (block_size)
classmethod from_pretrained (model_type, override_args=None)
configure_optimizers (weight_decay, learning_rate, betas, device_type)
estimate_mfu (fwdbwd_per_iter, dt)
    estimate model flops utilization (MFU) in units of A100 bfloat16 peak FLOPS

```

Classes

<i>ADOPT</i>	ADOPT Optimizer.
<i>BaseKGELightning</i>	Base class for all neural network modules.
<i>BaseKGE</i>	Base class for all neural network modules.
<i>IdentityClass</i>	Base class for all neural network modules.
<i>BaseKGE</i>	Base class for all neural network modules.
<i>Block</i>	Base class for all neural network modules.
<i>DistMult</i>	Embedding Entities and Relations for Learning and Inference in Knowledge Bases
<i>TransE</i>	Translating Embeddings for Modeling
<i>Shallom</i>	A shallow neural model for relation prediction (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.

continues on next page

Table 1 – continued from previous page

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

Functions

```

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

octonion_mul(*, O_1, O_2)

octonion_mul_norm(*, O_1, O_2)

```

Package Contents

```

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

```

Bases: *torch.optim.optimizer.Optimizer*

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

Raises

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

Example

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

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

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

i Note

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

`clip_lambda`

`__setstate__(state)`

Restore optimizer state from a checkpoint.

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

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

Parameters

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

i Note

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

`step (closure=None)`

Perform a single optimization step.

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

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

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

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

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

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

Parameters

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

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

Default: None

Returns

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

Return type

Optional[Tensor]

Example

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

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

Note

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

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

Bases: lightning.LightningModule

Base class for all neural network modules.

Your models should also subclass this class.

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

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

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

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

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

Note

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

Variables

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

`training_step_outputs` = []

`mem_of_model()` → Dict

Size of model in MB and number of params

`training_step`(batch, batch_idx=None)

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

Parameters

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

Returns

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

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

Example:

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

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

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

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

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

Note

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

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

Parameters

- `yhat_batch`
- `y_batch`

`on_train_epoch_end(*args, **kwargs)`

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

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

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

    def training_step(self):
        loss = ...
```

(continues on next page)

(continued from previous page)

```
    self.training_step_outputs.append(loss)
    return loss

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

`test_epoch_end(outputs: List[Any])`

`test_dataloader() → None`

An iterable or collection of iterables specifying test samples.

For more information about multiple dataloaders, see this section.

For data processing use the following pattern:

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

However, the above are only necessary for distributed processing.

⚠ Warning

do not assign state in `prepare_data`

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

ℹ Note

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

ℹ Note

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

`val_dataloader() → None`

An iterable or collection of iterables specifying validation samples.

For more information about multiple dataloaders, see this section.

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

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

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

Note

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

Note

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

`predict_dataloader() → None`

An iterable or collection of iterables specifying prediction samples.

For more information about multiple dataloaders, see this section.

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

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

Note

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

Returns

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

`train_dataloader() → None`

An iterable or collection of iterables specifying training samples.

For more information about multiple dataloaders, see this section.

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

For data processing use the following pattern:

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

However, the above are only necessary for distributed processing.

⚠ Warning

do not assign state in prepare_data

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

ℹ Note

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

`configure_optimizers(parameters=None)`

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

Returns

Any of these 6 options.

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

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

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

(continues on next page)

(continued from previous page)

```
# is available when the scheduler is updated, thus stopping
# training if not found. If set to `False`, it will only produce a warning
"strict": True,
# If using the `LearningRateMonitor` callback to monitor the
# learning rate progress, this keyword can be used to specify
# a custom logged name
"name": None,
}
```

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

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

Note

Some things to know:

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

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

Bases: `BaseKG``Lightning`

Base class for all neural network modules.

Your models should also subclass this class.

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

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

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

(continues on next page)

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

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

Note

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

Variables

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

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

loss
selected_optimizer = None
normalizer_class = None
normalize_head_entity_embeddings
normalize_relation_embeddings
normalize_tail_entity_embeddings
hidden_normalizer
```

```

param_init
input_dp_ent_real
input_dp_rel_real
hidden_dropout
loss_history = []
byte_pair_encoding
max_length_subword_tokens
block_size

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

forward(x: torch.LongTensor | Tuple[torch.LongTensor, torch.LongTensor],
  y_idx: torch.LongTensor = None)
Parameters
  • x
  • y_idx
  • ordered_bpe_entities
forward_triples(x: torch.LongTensor) → torch.Tensor
Parameters
  x
forward_k_vs_all(*args, **kwargs)
forward_k_vs_sample(*args, **kwargs)
get_triple_representation(idx_hrt)
get_head_relation_representation(indexed_triple)
get_sentence_representation(x: torch.LongTensor)
Parameters
  • (b (x shape)
  • 3
  • t)

```

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

Parameters

x (B x 2 x T)

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

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

Bases: torch.nn.Module

Base class for all neural network modules.

Your models should also subclass this class.

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

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

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

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

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

Note

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

Variables

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

```
args = None

__call__(x)

static forward(x)

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

Bases: `BaseKGLightning`

Base class for all neural network modules.

Your models should also subclass this class.

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

```

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

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

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

```

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

Note

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

Variables

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

`args`

```

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

```

```

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

Parameters
x (B x 2 x T)

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

Parameters
-----
init_params_with_sanity_checking()

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

Parameters
• x
• y_idx
• ordered_bpe_entities

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

Parameters
x
forward_k_vs_all(*args, **kwargs)

forward_k_vs_sample(*args, **kwargs)
get_triple_representation(idx_hrt)

```

```

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

Parameters

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

```

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

Parameters

- **x** (*B x 2 x T*)

```

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

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

Bases: *torch.nn.Module*

Base class for all neural network modules.

Your models should also subclass this class.

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

```

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

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

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

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

Note

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

Variables

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

ln_1

```

attn
ln_2
mlp
forward(x)
```

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

```

name = 'DistMult'
k_vs_all_score(emb_h: torch.FloatTensor, emb_r: torch.FloatTensor, emb_E: torch.FloatTensor)
```

Parameters

- **emb_h**
- **emb_r**
- **emb_E**

```

forward_k_vs_all(x: torch.LongTensor)
forward_k_vs_sample(x: torch.LongTensor, target_entity_idx: torch.LongTensor)
score(h, r, t)
```

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

```

name = 'TransE'
margin = 4
score(head_ent_emb, rel_ent_emb, tail_ent_emb)
forward_k_vs_all(x: torch.Tensor) → torch.FloatTensor
```

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

```

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

```

forward_triples(x) → torch.FloatTensor

Parameters
    x

Returns

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

dist_func

margin = 1.0

forward_triples(x: torch.LongTensor)

Parameters
    x

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

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

vocab_size
    Total vocabulary size (num_entities + num_relations)

n_layer
    Number of transformer layers

n_head
    Number of attention heads per layer

n_embd
    Embedding dimension (set to match model embedding_dim)

dropout
    Dropout rate applied throughout the model

bias
    Whether to use bias in linear layers

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

block_size: int = 3

vocab_size: int = None

n_layer: int = 6

n_head: int = 8

n_embd: int = None

```

```

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

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

```

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

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

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

```

name = 'CoKE'

config

pos_emb

mask_emb

blocks

ln_f

coke_dropout

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

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

```

```

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

```

Base class for all neural network modules.

Your models should also subclass this class.

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

```

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

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

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

```

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

Note

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

Variables

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

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

loss
selected_optimizer = None
normalizer_class = None
normalize_head_entity_embeddings
normalize_relation_embeddings
normalize_tail_entity_embeddings
hidden_normalizer
param_init
input_dp_ent_real
input_dp_rel_real
```

```

hidden_dropout
loss_history = []
byte_pair_encoding
max_length_subword_tokens
block_size

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

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

  forward_triples(x: torch.LongTensor) → torch.Tensor
    Parameters
      x
    forward_k_vs_all(*args, **kwargs)
    forward_k_vs_sample(*args, **kwargs)
    get_triple_representation(idx_hrt)
    get_head_relation_representation(indexed_triple)
    get_sentence_representation(x: torch.LongTensor)
    Parameters
      • (b (x shape)
      • 3
      • t)
    get_bpe_head_and_relation_representation(x: torch.LongTensor)
      → Tuple[torch.FloatTensor, torch.FloatTensor]
    Parameters
      x (B × 2 × T)

```

```

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

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

    Convolutional ComplEx Knowledge Graph Embeddings

    name = 'ConEx'

    conv2d

    fc_num_input

    fc1

    norm_fc1

    bn_conv2d

    feature_map_dropout

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

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

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

    Parameters
        x

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

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

    Additive Convolutional ComplEx Knowledge Graph Embeddings

    name = 'AConEx'

    conv2d

    fc_num_input

    fc1

    norm_fc1

    bn_conv2d

    feature_map_dropout

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

```

```

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

Parameters
    x

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

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

```

Base class for all neural network modules.

Your models should also subclass this class.

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

```

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

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

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

```

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

Note

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

Variables

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

```

name = 'ComplEx'

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

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

```

Parameters

- `emb_h`
- `emb_r`

- `emb_E`

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

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

`dicee.models.quaternion_mul`(**Q_1, Q_2*)
 → `Tuple[torch.Tensor, torch.Tensor, torch.Tensor, torch.Tensor]`

Perform quaternion multiplication :param *Q_1*: :param *Q_2*: :return:

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

Bases: `BaseKGELightning`

Base class for all neural network modules.

Your models should also subclass this class.

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

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

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

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

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

Note

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

Variables

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

args

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

```

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

Parameters
  x (B x 2 x T)

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

Parameters
-----
init_params_with_sanity_checking()

```

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

Parameters

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

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

Parameters

x

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

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

```
get_triple_representation(idx_hrt)
```

```
get_head_relation_representation(indexed_triple)
```

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

Parameters

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

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

Parameters

x (B x 2 x T)

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

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

Bases: torch.nn.Module

Base class for all neural network modules.

Your models should also subclass this class.

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

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

(continues on next page)

(continued from previous page)

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

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

Note

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

Variables

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

```
args = None

__call__(x)

static forward(x)

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

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

Base class for all neural network modules.

Your models should also subclass this class.

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

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

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

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

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

Note

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

Variables

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

```
name = 'QMult'

explicit = True

quaternion_multiplication_followed_by_inner_product(h, r, t)
```

Parameters

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

Returns

Triple scores.

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

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

Absolute value of a quaternion

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

L2 norm of quaternion vector:

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

Parameters

`x` – The vector.

Returns

The normalized vector.

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

`k_vs_all_score(bpe_head_ent_emb, bpe_rel_ent_emb, E)`

Parameters

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

`forward_k_vs_all(x)`

Parameters

`x`

`forward_k_vs_sample(x, target_entity_idx)`

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

```

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

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

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

Parameters
x

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

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

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

```

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

Parameters

x

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

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

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

Bases: *BaseKGLightning*

Base class for all neural network modules.

Your models should also subclass this class.

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

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

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

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

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

Note

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

Variables

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

`args`

`embedding_dim` = None

`num_entities` = None

`num_relations` = None

`num_tokens` = None

`learning_rate` = None

```

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

Parameters
  x (B x 2 x T)

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

Parameters
-----
init_params_with_sanity_checking()

```

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

Parameters

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

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

Parameters

x

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

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

```
get_triple_representation(idx_hrt)
```

```
get_head_relation_representation(indexed_triple)
```

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

Parameters

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

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

Parameters

x (B x 2 x T)

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

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

Bases: `torch.nn.Module`

Base class for all neural network modules.

Your models should also subclass this class.

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

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

(continues on next page)

(continued from previous page)

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

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

Note

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

Variables

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

```
args = None

__call__(x)

static forward(x)

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

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

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

Bases: `dicee.models.base_model.BaseKGE`

Base class for all neural network modules.

Your models should also subclass this class.

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

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

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

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

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

Note

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

Variables

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

`name = 'OMult'`

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

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

`k_vs_all_score(bpe_head_ent_emb, bpe_rel_ent_emb, E)`

`forward_k_vs_all(x)`

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

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

Bases: `dicee.models.base_model.BaseKGE`

Base class for all neural network modules.

Your models should also subclass this class.

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

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

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

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

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

Note

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

Variables

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

```
name = 'ConvO'

conv2d

fc_num_input

fc1

bn_conv2d

norm_fc1

feature_map_dropout

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

residual_convolution(O_1, O_2)

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

Parameters

`x`

`forward_k_vs_all(x: torch.Tensor)`

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

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

Bases: `dicee.models.base_model.BaseKGE`

Additive Convolutional Octonion Knowledge Graph Embeddings

`name = 'AConvO'`

`conv2d`

`fc_num_input`

`fc1`

`bn_conv2d`

`norm_fc1`

`feature_map_dropout`

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

`residual_convolution(O_1, O_2)`

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

Parameters

`x`

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

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

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

Bases: *dicee.models.base_model.BaseKGE*

Base class for all neural network modules.

Your models should also subclass this class.

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

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

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

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

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

i Note

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

Variables

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

```
name = 'Keci'
```

```
p
```

```
q
```

```
r
```

```
requires_grad_for_interactions = True
```

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

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

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

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

$$ei^2 = +1 \text{ for } i <= p \quad ej^2 = -1 \text{ for } p < j <= p+q \quad ei ej = -ejei \text{ for } i$$

`eq j`

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

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

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

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

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

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

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

dicee.weight_averaging

Classes

<code>SWA</code>	Stochastic Weight Averaging callbacks.
<code>SWAG</code>	Stochastic Weight Averaging - Gaussian (SWAG).
<code>EMA</code>	Exponential Moving Average (EMA) callback.
<code>TWA</code>	Train with Weight Averaging (TWA) using subspace projection + averaging.

Module Contents

```
class dicee.weight_averaging.SWA(swa_start_epoch, swa_c_epochs: int = 1, lr_init: float = 0.1,
                                  swa_lr: float = 0.05, max_epochs: int = None)
Bases: dicee.abtracts.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. Math: # SWA update: # θ_swa ← (1 - alpha) * θ_swa + alpha * θ # alpha = 1 / (n + 1), where n = number of models already averaged # alpha is tracked via self.swa_n in code

    on_train_epoch_start(trainer, model)
        Update learning rate according to SWA schedule.

    on_train_epoch_end(trainer, model)
        Apply SWA averaging if conditions are met.

    on_fit_end(trainer, model)
        Replace main model with SWA model at the end of training.

class dicee.weight_averaging.SWAG(swa_start_epoch, swa_c_epochs: int = 1, lr_init: float = 0.1,
                                  swa_lr: float = 0.05, max_epochs: int = None, max_num_models: int = 20,
                                  var_clamp: float = 1e-30)
Bases: dicee.abtracts.AbstractCallback

Stochastic Weight Averaging - Gaussian (SWAG).

    swa_start_epoch
```

```

swa_c_epochs = 1
swa_lr = 0.05
lr_init = 0.1
max_epochs = None
max_num_models = 20
var_clamp = 1e-30
mean = None
sq_mean = None
deviations = []
gswa_n = 0
current_epoch = -1
get_mean_and_var()
    Return mean + variance (diagonal part).
sample(base_model, scale=0.5)
    Sample new model from SWAG posterior distribution.
    Math: # From SWAG, posterior is approximated as: #  $\theta \sim N(\text{mean}, \Sigma)$  # where  $\Sigma \approx \text{diag}(\text{var}) + (1/(K-1)) * D D^T$  # - mean = running average of weights # - var = elementwise variance (sq_mean - mean^2) # - D = [dev_1, dev_2, ..., dev_K], deviations from mean (low-rank approx) # - K = number of collected models
    # Sampling step: # 1.  $\theta_{\text{diag}} = \text{mean} + \text{scale} * \text{std} \odot \varepsilon$ , where  $\varepsilon \sim N(0, I)$  # 2.  $\theta_{\text{lowrank}} = \theta_{\text{diag}} + (D z) / \sqrt{K-1}$ , where  $z \sim N(0, I_K)$  # Final sample =  $\theta_{\text{lowrank}}$ 
on_train_epoch_start(trainer, model)
    Update LR schedule (same as SWA).
on_train_epoch_end(trainer, model)
    Collect Gaussian stats at the end of epochs after swa_start.
on_fit_end(trainer, model)
    Set model weights to the collected SWAG mean at the end of training.
class dicee.weight_averaging.EMA(ema_start_epoch: int, decay: float = 0.999,
                                 max_epochs: int = None, ema_c_epochs: int = 1)
Bases: dicee.abstracts.AbstractCallback
Exponential Moving Average (EMA) callback.

ema_start_epoch
decay = 0.999
max_epochs = None
ema_c_epochs = 1
ema_model = None

```

```

current_epoch = -1

static ema_update(ema_model, running_model, decay: float)
    Update EMA model with exponential moving average of current model. Math: # EMA update: #  $\theta_{\text{ema}} \leftarrow (1 - \text{alpha}) * \theta_{\text{ema}} + \text{alpha} * \theta$  # alpha = 1 - decay, where decay is the EMA smoothing factor (typical 0.99 - 0.999) # alpha controls how much of the current model  $\theta$  contributes to the EMA # decay is fixed in code -> can be extended to scheduled

on_train_epoch_start(trainer, model)
    Track current epoch.

on_train_epoch_end(trainer, model)
    Update EMA if past start epoch.

on_fit_end(trainer, model)
    Replace main model with EMA model at the end of training.

class dicee.weight_averaging.TWA(twa_start_epoch: int, lr_init: float, num_samples: int = 5,
    reg_lambda: float = 0.0, max_epochs: int = None, twa_c_epochs: int = 1)
    Bases: dicee.abstracts.AbstractCallback
    Train with Weight Averaging (TWA) using subspace projection + averaging.

twa_start_epoch
    num_samples = 5
    reg_lambda = 0.0
    max_epochs = None
    lr_init
    twa_c_epochs = 1
    current_epoch = -1
    weight_samples = []
    twa_model = None
    base_weights = None
    P = None
    beta = None

sample_weights(model)
    Collect sampled weights from the current model and maintain rolling buffer.

build_projection(weight_samples, k=None)
    Build projection subspace from collected weight samples. :param weight_samples: list of flat weight tensors [(D,), ...] :param k: number of basis vectors to keep. Defaults to min(N, D).

Returns
    (D,) base weight vector (average) P: (D, k) projection matrix with top-k basis directions

Return type
    mean_w

```

```

on_train_epoch_start (trainer, model)
    Track epoch.

on_train_epoch_end (trainer, model)
    Main TWA logic: build subspace and update in  $\beta$  space.

    # Math: # TWA weight update:  $w_{twa} = mean_w + P * beta$  #  $mean_w = (1/n) * sum_i w_i$  (SWA baseline)
    #  $\beta \leftarrow (1 - \eta * \lambda) * \beta - \eta * P^T * g$  #  $g$  = gradient of training loss w.r.t. full model weights
    #  $\eta$  = learning rate,  $\lambda$  = ridge regularization #  $P$  = orthonormal basis spanning sampled checkpoints
    { $w_i$ }

on_fit_end (trainer, model)
    Replace with TWA model at the end.

```

14.2 Attributes

version

14.3 Classes

<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.

continues on next page

Table 3 – continued from previous page

<code>PykeenKGE</code>	A class for using knowledge graph embedding models implemented in Pykeen
<code>ByteE</code>	Base class for all neural network modules.
<code>BaseKGE</code>	Base class for all neural network modules.
<code>EnsembleKGE</code>	
<code>DICE_Trainer</code>	DICE_Trainer implement
<code>KGE</code>	Knowledge Graph Embedding Class for interactive usage of pre-trained models
<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.
<code>QueryGenerator</code>	

14.4 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

continues on next page

Table 4 – continued from previous page

<code>load_model_ensemble(...)</code>	Construct Ensemble Of weights and initialize pytorch module from namespace arguments
<code>save_numpy_ndarray(*, data, file_path)</code>	
<code>numpy_data_type_changer(→ numpy.ndarray)</code>	Detect most efficient data type for a given triples
<code>save_checkpoint_model(→ None)</code>	Store Pytorch model into disk
<code>store(→ None)</code>	
<code>add_noisy_triples(→ pandas.DataFrame)</code>	Add randomly constructed triples
<code>read_or_load_kg(args, cls)</code>	
<code>intialize_model(→ Tuple[object, str])</code>	
<code>load_json(→ dict)</code>	
<code>save_embeddings(→ None)</code>	Save it as CSV if memory allows.
<code>random_prediction(pre_trained_kge)</code>	
<code>deploy_triple_prediction(pre_trained_kge, str_subject, ...)</code>	
<code>deploy_tail_entity_prediction(pre_trained_kge, ...)</code>	
<code>deploy_head_entity_prediction(pre_trained_kge, ...)</code>	
<code>deploy_relation_prediction(pre_trained_kge, ...)</code>	
<code>vocab_to_parquet(vocab_to_idx, name, ...)</code>	
<code>create_experiment_folder([folder_name])</code>	
<code>continual_training_setup_executor(→ None)</code>	
<code>exponential_function(→ torch.FloatTensor)</code>	
<code>load_numpy(→ numpy.ndarray)</code>	
<code>evaluate(entity_to_idx, scores, easy_answers, # @TODO: CD: Renamed this function hard_answers)</code>	
<code>download_file(url[, destination_folder])</code>	
<code>download_files_from_url(→ None)</code>	
<code>download_pretrained_model(→ str)</code>	
<code>write_csv_from_model_parallel(path)</code>	Create
<code>from_pretrained_model_write_embeddings_int(→ None)</code>	
<code>mapping_from_first_two_cols_to_third(train_se</code>	
<code>timeit(func)</code>	

continues on next page

Table 4 – continued from previous page

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

14.5 Package Contents

`class dicee.Pyke(args)`

Bases: `dicee.models.base_model.BaseKGE`

A Physical Embedding Model for Knowledge Graphs

`name = 'Pyke'`

`dist_func`

`margin = 1.0`

`forward_triples(x: torch.LongTensor)`

Parameters

`x`

`class dicee.DistMult(args)`

Bases: `dicee.models.base_model.BaseKGE`

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

`name = 'DistMult'`

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

Parameters

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

`forward_k_vs_all(x: torch.LongTensor)`

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

`score(h, r, t)`

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

σ_{pp} captures the interactions between along p bases. For instance, let $p = 3$, 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 $i \leq p$ $ej^2 = -1$ for $p < j \leq p+q$ $ei ej = -ejei$ for $i \neq j$

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

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

(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 $C_{\{p,q\}}(R)^d$

Parameter

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

returns

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

forward_k_vs_with_explicit (x: torch.Tensor)

k_vs_all_score (bpe_head_ent_emb, bpe_rel_ent_emb, E)

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

Kvsall training

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

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

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

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

Parameter

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

returns

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

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

Parameter

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

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

rtype

torch.FloatTensor with (n, k) shape

score (h, r, t)

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

Parameter

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

rtype

torch.FloatTensor with (n) shape

```
class dicee.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

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

For different base vector interactions, we have

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

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

forward_k_vs_with_explicit and this 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])
```

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

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.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)

    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.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 differents scoring function as in the paper to evaluate the score.
We also consider combining with Neural Networks.

`name = 'LFMult'`

`entity_embeddings`

`relation_embeddings`

`degree`

`m`

`x_values`

`forward_triples(idx_triple)`

Parameters

`x`

```

construct_multi_coeff(x)

poly_NN(x, coefh, coefr, coeft)
    Constructing a 2 layers NN to represent the embeddings. h = 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} dfrac{a_i*b_j*c_k}{1+(i+j+k)%d}
    1. generate the range for i,j and k from [0 d-1]
    2. perform dfrac{a_i*b_j*c_k}{1+(i+j+k)%d} in parallel for every batch
    3. take the sum over each batch

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

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

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

$\text{argmax}_{\{r \text{ in } R\}} f(h, r, t)$, 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]], ...]
tnorm: str The t-norm operator.
neg_norm: str The negation norm.
lambda_: float lambda parameter for sugeno and yager negation norms
k: int The top-k substitutions for intermediate variables.

returns

- *List[Tuple[str, torch.Tensor]]*
- *Entities and corresponding scores sorted in the descending order of scores*

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

Find missing triples

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

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

Return (e,r,x)

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

confidence: float

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

topk: int

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

at_most: int

Stop after finding at_most missing triples

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

otin G

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 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 `__getitem__(idx)`, 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 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.AllvsAll(train_set_idx: numpy.ndarray, entity_idxs, relation_idxs, label_smoothing_rate=0.0)
Bases: torch.utils.data.Dataset

```

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

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

overall $y_{i,j} = 1$ s.t. $(h, r) \in E_j$ 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.

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

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

|new_y| << |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):

```

(continues on next page)

```

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

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

```

This is called before requesting the dataloaders:

```

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

```

```
class dicee.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: 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.__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, 28
 dicee.dataset_classes, 32
 dicee.eval_static_funcs, 46
 dicee.evaluator, 47
 dicee.executer, 49
 dicee.knowledge_graph, 51
 dicee.knowledge_graph_embeddings, 52
 dicee.models, 56
 dicee.models.adopt, 56
 dicee.models.base_model, 65
 dicee.models.clifford, 74
 dicee.models.complex, 81
 dicee.models.duale, 84
 dicee.models.ensemble, 85
 dicee.models.function_space, 86
 dicee.models.literal, 89
 dicee.models.octonion, 91
 dicee.models.pykeen_models, 94
 dicee.models.quaternion, 95
 dicee.models.real, 98
 dicee.models.static_funcs, 101
 dicee.models.transformers, 101
 dicee.query_generator, 160
 dicee.read_preprocess_save_load_kg, 162
 dicee.read_preprocess_save_load_kg.preprocess,
 162
 dicee.read_preprocess_save_load_kg.read_from_disk,
 163
 dicee.read_preprocess_save_load_kg.save_load_disk,
 163
 dicee.read_preprocess_save_load_kg.util,
 164
 dicee.sanity_checkers, 168
 dicee.scripts, 169
 dicee.scripts.index_serve, 169
 dicee.scripts.run, 171
 dicee.static_funcs, 171
 dicee.static_funcs_training, 174
 dicee.static_preprocess_funcs, 175
 dicee.trainer, 176
 dicee.trainer.dice_trainer, 176
 dicee.trainer.model_parallelism, 178
 dicee.trainer.torch_trainer, 178
 dicee.trainer.torch_trainer_ddp, 180

Index

Non-alphabetical

`__call__()` (*dicee.EnsembleKGE method*), 213
`__call__()` (*dicee.models.base_model.IdentityClass method*), 74
`__call__()` (*dicee.models.ensemble.EnsembleKGE method*), 86
`__call__()` (*dicee.models.IdentityClass method*), 121, 135, 141
`getitem__()` (*dicee.AllvsAll method*), 223
`getitem__()` (*dicee.BPE_NegativeSamplingDataset method*), 220
`getitem__()` (*dicee.dataset_classes.AllvsAll method*), 36
`getitem__()` (*dicee.dataset_classes.BPE_NegativeSamplingDataset method*), 33
`getitem__()` (*dicee.dataset_classes.KvsAll method*), 35
`getitem__()` (*dicee.dataset_classes.KvsSampleDataset method*), 39
`getitem__()` (*dicee.dataset_classes.LiteralDataset method*), 45
`getitem__()` (*dicee.dataset_classes.MultiClassClassificationDataset method*), 34
`getitem__()` (*dicee.dataset_classes.MultiLabelDataset method*), 34
`getitem__()` (*dicee.dataset_classes.NegSampleDataset method*), 39
`getitem__()` (*dicee.dataset_classes.OnevsAllDataset method*), 35
`getitem__()` (*dicee.dataset_classes.OnevsSample method*), 37
`getitem__()` (*dicee.dataset_classes.TriplePredictionDataset method*), 40
`getitem__()` (*dicee.KvsAll method*), 223
`getitem__()` (*dicee.KvsSampleDataset method*), 226
`getitem__()` (*dicee.LiteralDataset method*), 232
`getitem__()` (*dicee.MultiClassClassificationDataset method*), 221
`getitem__()` (*dicee.MultiLabelDataset method*), 221
`getitem__()` (*dicee.NegSampleDataset method*), 226
`getitem__()` (*dicee.OnevsAllDataset method*), 222
`getitem__()` (*dicee.OnevsSample method*), 225
`getitem__()` (*dicee.TriplePredictionDataset method*), 227
`iter__()` (*dicee.config.Namespace method*), 32
`iter__()` (*dicee.EnsembleKGE method*), 213
`iter__()` (*dicee.knowledge_graph.KG method*), 52
`iter__()` (*dicee.models.ensemble.EnsembleKGE method*), 85
`len__()` (*dicee.AllvsAll method*), 223
`len__()` (*dicee.BPE_NegativeSamplingDataset method*), 220
`len__()` (*dicee.dataset_classes.AllvsAll method*), 36
`len__()` (*dicee.dataset_classes.BPE_NegativeSamplingDataset method*), 33
`len__()` (*dicee.dataset_classes.KvsAll method*), 35
`len__()` (*dicee.dataset_classes.KvsSampleDataset method*), 39
`len__()` (*dicee.dataset_classes.LiteralDataset method*), 45
`len__()` (*dicee.dataset_classes.MultiClassClassificationDataset method*), 34
`len__()` (*dicee.dataset_classes.MultiLabelDataset method*), 34
`len__()` (*dicee.dataset_classes.NegSampleDataset method*), 39
`len__()` (*dicee.dataset_classes.OnevsAllDataset method*), 35
`len__()` (*dicee.dataset_classes.OnevsSample method*), 37
`len__()` (*dicee.dataset_classes.TriplePredictionDataset method*), 40
`len__()` (*dicee.EnsembleKGE method*), 213
`len__()` (*dicee.knowledge_graph.KG method*), 52
`len__()` (*dicee.KvsAll method*), 223
`len__()` (*dicee.KvsSampleDataset method*), 226
`len__()` (*dicee.LiteralDataset method*), 232
`len__()` (*dicee.models.ensemble.EnsembleKGE method*), 85
`len__()` (*dicee.MultiClassClassificationDataset method*), 221
`len__()` (*dicee.MultiLabelDataset method*), 221
`len__()` (*dicee.NegSampleDataset method*), 226
`len__()` (*dicee.OnevsAllDataset method*), 222
`len__()` (*dicee.OnevsSample method*), 225
`len__()` (*dicee.TriplePredictionDataset method*), 227
`setstate__()` (*dicee.models.ADOPT method*), 111
`setstate__()` (*dicee.models.adopt.ADOPT method*), 60
`str__()` (*dicee.EnsembleKGE method*), 213
`str__()` (*dicee.KGE method*), 216
`str__()` (*dicee.knowledge_graph_embeddings.KGE method*), 53
`str__()` (*dicee.models.ensemble.EnsembleKGE method*), 86
`version__` (*in module dicee*), 234

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*), 161
achieve_answer () (*dicee.QueryGenerator method*), 233
AConEx (*class in dicee*), 198
AConEx (*class in dicee.models*), 130
AConEx (*class in dicee.models.complex*), 82
AConvO (*class in dicee*), 199
AConvO (*class in dicee.models*), 143
AConvO (*class in dicee.models.octonion*), 93
AConvQ (*class in dicee*), 199
AConvQ (*class in dicee.models*), 137
AConvQ (*class in dicee.models.quaternion*), 97
adaptive_lr (*dicee.config.Namespace attribute*), 31
adaptive_swa (*dicee.config.Namespace attribute*), 31
add_new_entity_embeddings () (*dicee.abstracts.BaseInteractiveKGE method*), 15
add_noise_rate (*dicee.config.Namespace attribute*), 29
add_noise_rate (*dicee.knowledge_graph.KG attribute*), 51
add_noisy_triples () (*in module dicee*), 214
add_noisy_triples () (*in module dicee.static_funcs*), 173
add_noisy_triples_into_training () (*dicee.read_preprocess_save_load_kg.read_from_disk.ReadFromDisk method*), 163
add_noisy_triples_into_training () (*dicee.read_preprocess_save_load_kg.ReadFromDisk method*), 168
add_reciprocal (*dicee.knowledge_graph.KG attribute*), 51
ADOPT (*class in dicee.models*), 109
ADOPT (*class in dicee.models.adopt*), 58
adopt () (*in module dicee.models.adopt*), 61
AllvsAll (*class in dicee*), 223
AllvsAll (*class in dicee.dataset_classes*), 35
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*), 218
answer_multi_hop_query () (*dicee.knowledge_graph_embeddings.KGE method*), 55
app (*in module dicee.scripts.index_server*), 170
apply_coefficients () (*dicee.DeCaL method*), 195
apply_coefficients () (*dicee.Keci method*), 191
apply_coefficients () (*dicee.models.clifford.DeCaL method*), 80
apply_coefficients () (*dicee.models.clifford.Keci method*), 76
apply_coefficients () (*dicee.models.DeCaL method*), 149
apply_coefficients () (*dicee.models.Keci method*), 145
apply_reciprocal_or_noise () (*in module dicee.read_preprocess_save_load_kg.util*), 166
apply_semantic_constraint (*dicee.abstracts.BaseInteractiveKGE attribute*), 14
apply_unit_norm (*dicee.BaseKGE attribute*), 211
apply_unit_norm (*dicee.models.base_model.BaseKGE attribute*), 72
apply_unit_norm (*dicee.models.BaseKGE attribute*), 119, 122, 128, 132, 138, 151, 155
args (*dicee.BaseKGE attribute*), 211
args (*dicee.DICE_Trainer attribute*), 215
args (*dicee.EnsembleKGE attribute*), 212
args (*dicee.evaluator.Evaluator attribute*), 48
args (*dicee.executor.Execute attribute*), 49
args (*dicee.models.base_model.BaseKGE attribute*), 71
args (*dicee.models.base_model.IdentityClass attribute*), 74
args (*dicee.models.BaseKGE attribute*), 119, 122, 128, 132, 138, 151, 154
args (*dicee.models.ensemble.EnsembleKGE attribute*), 85
args (*dicee.models.IdentityClass attribute*), 121, 135, 141
args (*dicee.models.pykeen_models.PykeenKGE attribute*), 94
args (*dicee.models.PykeenKGE attribute*), 153
args (*dicee.PykeenKGE attribute*), 207
args (*dicee.trainer.DICE_Trainer attribute*), 181
args (*dicee.trainer.dice_trainer.DICE_Trainer attribute*), 176
ASWA (*class in dicee.callbacks*), 24
aswa (*dicee.analyse_experiments.Experiment attribute*), 19
attn (*dicee.models.Block attribute*), 124
attn (*dicee.models.transformers.Block attribute*), 106
attn_dropout (*dicee.models.transformers.SelfAttention attribute*), 105

attributes (*dicee.abstracts.AbstractTrainer* attribute), 13
auto_batch_finding (*dicee.config.Namespace* attribute), 31

B

backend (*dicee.config.Namespace* attribute), 29
backend (*dicee.knowledge_graph.KG* attribute), 52
base_weights (*dicee.weight_averaging.TWA* attribute), 185
BaseInteractiveKGE (*class in dicee.abstracts*), 14
BaseInteractiveTrainKGE (*class in dicee.abstracts*), 18
BaseKGE (*class in dicee*), 210
BaseKGE (*class in dicee.models*), 118, 121, 127, 132, 138, 150, 154
BaseKGE (*class in dicee.models.base_model*), 71
BaseKGELightning (*class in dicee.models*), 112
BaseKGELightning (*class in dicee.models.base_model*), 65
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), 29
batch_size (*dicee.CVDataModule* attribute), 228
batch_size (*dicee.dataset_classes.CVDataModule* attribute), 41
batches_per_epoch (*dicee.callbacks.LRScheduler* attribute), 28
beta (*dicee.weight_averaging.TWA* attribute), 185
bias (*dicee.models.CoKEConfig* attribute), 126, 127
bias (*dicee.models.real.CoKEConfig* attribute), 100
bias (*dicee.models.transformers.GPTConfig* attribute), 107
bias (*dicee.models.transformers.LayerNorm* attribute), 104
Block (*class in dicee.models*), 124
Block (*class in dicee.models.transformers*), 106
block_size (*dicee.BaseKGE* attribute), 211
block_size (*dicee.config.Namespace* attribute), 31
block_size (*dicee.dataset_classes.MultiClassClassificationDataset* attribute), 34
block_size (*dicee.models.base_model.BaseKGE* attribute), 72
block_size (*dicee.models.BaseKGE* attribute), 120, 123, 129, 133, 139, 152, 155
block_size (*dicee.models.CoKEConfig* attribute), 126
block_size (*dicee.models.real.CoKEConfig* attribute), 100
block_size (*dicee.models.transformers.GPTConfig* attribute), 106
block_size (*dicee.MultiClassClassificationDataset* attribute), 221
blocks (*dicee.CoKE* attribute), 207
blocks (*dicee.models.CoKE* attribute), 127
blocks (*dicee.models.real.CoKE* attribute), 101
bn_conv1 (*dicee.AConvQ* attribute), 200
bn_conv1 (*dicee.ConvQ* attribute), 200
bn_conv1 (*dicee.models.AConvQ* attribute), 137
bn_conv1 (*dicee.models.ConvQ* attribute), 137
bn_conv1 (*dicee.models.quaternion.AConvQ* attribute), 98
bn_conv1 (*dicee.models.quaternion.ConvQ* attribute), 97
bn_conv2 (*dicee.AConvQ* attribute), 200
bn_conv2 (*dicee.ConvQ* attribute), 200
bn_conv2 (*dicee.models.AConvQ* attribute), 137
bn_conv2 (*dicee.models.ConvQ* attribute), 137
bn_conv2 (*dicee.models.quaternion.AConvQ* attribute), 98
bn_conv2 (*dicee.models.quaternion.ConvQ* attribute), 97
bn_conv2d (*dicee.AConEx* attribute), 199
bn_conv2d (*dicee.AConvO* attribute), 199
bn_conv2d (*dicee.ConEx* attribute), 202
bn_conv2d (*dicee.ConvO* attribute), 201
bn_conv2d (*dicee.models.AConEx* attribute), 130
bn_conv2d (*dicee.models.AConvO* attribute), 143
bn_conv2d (*dicee.models.complex.AConEx* attribute), 82
bn_conv2d (*dicee.models.complex.ConEx* attribute), 82
bn_conv2d (*dicee.models.ConEx* attribute), 130
bn_conv2d (*dicee.models.ConvO* attribute), 143
bn_conv2d (*dicee.models.octonion.AConvO* attribute), 94
bn_conv2d (*dicee.models.octonion.ConvO* attribute), 93
BPE_NegativeSamplingDataset (*class in dicee*), 220
BPE_NegativeSamplingDataset (*class in dicee.dataset_classes*), 32
build_chain_funcs () (*dicee.models.FMult2* method), 158

```

build_chain_funcs() (dicee.models.function_space.FMult2 method), 87
build_func() (dicee.models.FMult2 method), 158
build_func() (dicee.models.function_space.FMult2 method), 87
build_projection() (dicee.weight_averaging.TWA method), 185
Byte (class in dicee), 208
Byte (class in dicee.models.transformers), 102
byte_pair_encoding (dicee.analyse_experiments.Experiment attribute), 19
byte_pair_encoding (dicee.BaseKGE attribute), 211
byte_pair_encoding (dicee.config.Namespace attribute), 31
byte_pair_encoding (dicee.knowledge_graph.KG attribute), 51
byte_pair_encoding (dicee.models.base_model.BaseKGE attribute), 72
byte_pair_encoding (dicee.models.BaseKGE attribute), 120, 123, 129, 133, 139, 152, 155

```

C

```

c_attn (dicee.models.transformers.SelfAttention attribute), 104
c_fc (dicee.models.transformers.MLP attribute), 105
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), 29
callbacks (dicee.trainer.torch_trainer_ddp.NodeTrainer attribute), 181
causal (dicee.models.CoKEConfig attribute), 126, 127
causal (dicee.models.real.CoKEConfig attribute), 100
causal (dicee.models.transformers.GPTConfig attribute), 107
causal (dicee.models.transformers.SelfAttention attribute), 105
chain_func() (dicee.models.FMult method), 157
chain_func() (dicee.models.function_space.FMult method), 86
chain_func() (dicee.models.function_space.GFMult method), 87
chain_func() (dicee.models.GFMult method), 157
CKeci (class in dicee), 189
CKeci (class in dicee.models), 147
CKeci (class in dicee.models.clifford), 78
cl_pqr() (dicee.DeCaL method), 194
cl_pqr() (dicee.models.clifford.DeCaL method), 79
cl_pqr() (dicee.models.DeCaL method), 148
cleanup() (dicee.executer.Execute method), 49
clifford_multiplication() (dicee.Keci method), 191
clifford_multiplication() (dicee.models.clifford.Keci method), 76
clifford_multiplication() (dicee.models.Keci method), 145
clip_lambda (dicee.models.ADOPT attribute), 111
clip_lambda (dicee.models.adopt.ADOPT attribute), 60
CoKE (class in dicee), 206
CoKE (class in dicee.models), 127
CoKE (class in dicee.models.real), 100
coke_dropout (dicee.CoKE attribute), 207
coke_dropout (dicee.models.CoKE attribute), 127
coke_dropout (dicee.models.real.CoKE attribute), 101
CoKEConfig (class in dicee.models), 126
CoKEConfig (class in dicee.models.real), 100
collate_fn (dicee.AllvsAll attribute), 223
collate_fn (dicee.dataset_classes.AllvsAll attribute), 36
collate_fn (dicee.dataset_classes.KvsAll attribute), 35
collate_fn (dicee.dataset_classes.KvsSampleDataset attribute), 39
collate_fn (dicee.dataset_classes.MultiClassClassificationDataset attribute), 34
collate_fn (dicee.dataset_classes.MultiLabelDataset attribute), 34
collate_fn (dicee.dataset_classes.OnevsAllDataset attribute), 35
collate_fn (dicee.dataset_classes.OnevsSample attribute), 37
collate_fn (dicee.KvsAll attribute), 223
collate_fn (dicee.KvsSampleDataset attribute), 226
collate_fn (dicee.MultiClassClassificationDataset attribute), 221
collate_fn (dicee.MultiLabelDataset attribute), 221
collate_fn (dicee.OnevsAllIDataset attribute), 222
collate_fn (dicee.OnevsSample attribute), 224, 225
collate_fn() (dicee.BPE_NegativeSamplingDataset method), 220
collate_fn() (dicee.dataset_classes.BPE_NegativeSamplingDataset method), 33
collate_fn() (dicee.dataset_classes.TriplePredictionDataset method), 40

```

collate_fn() (*dicee.TriplePredictionDataset* method), 227
 collection_name (*dicee.scripts.index_serve.NeuralSearcher* attribute), 170
 comp_func() (*dicee.LFMult* method), 206
 comp_func() (*dicee.models.function_space.LFMult* method), 89
 comp_func() (*dicee.models.LFMult* method), 159
 ComplEx (*class in dicee*), 197
 ComplEx (*class in dicee.models*), 131
 ComplEx (*class in dicee.models.complex*), 83
 compute_convergence() (*in module dicee.callbacks*), 24
 compute_func() (*dicee.models.FMult* method), 157
 compute_func() (*dicee.models.FMult2* method), 158
 compute_func() (*dicee.models.function_space.FMult* method), 86
 compute_func() (*dicee.models.function_space.FMult2* method), 87
 compute_func() (*dicee.models.function_space.GFMult* method), 87
 compute_func() (*dicee.models.GFMult* method), 157
 compute_mrr() (*dicee.callbacks.ASWA* static method), 24
 compute_sigma_pp() (*dicee.DeCaL* method), 195
 compute_sigma_pp() (*dicee.Keci* method), 190
 compute_sigma_pp() (*dicee.models.clifford.DeCaL* method), 80
 compute_sigma_pp() (*dicee.models.clifford.Keci* method), 75
 compute_sigma_pp() (*dicee.models.DeCaL* method), 149
 compute_sigma_pp() (*dicee.models.Keci* method), 144
 compute_sigma_pq() (*dicee.DeCaL* method), 196
 compute_sigma_pq() (*dicee.Keci* method), 191
 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), 150
 compute_sigma_pq() (*dicee.models.Keci* method), 145
 compute_sigma_pr() (*dicee.DeCaL* method), 196
 compute_sigma_pr() (*dicee.models.clifford.DeCaL* method), 81
 compute_sigma_pr() (*dicee.models.DeCaL* method), 150
 compute_sigma_qq() (*dicee.DeCaL* method), 195
 compute_sigma_qq() (*dicee.Keci* method), 191
 compute_sigma_qq() (*dicee.models.clifford.DeCaL* method), 80
 compute_sigma_qq() (*dicee.models.clifford.Keci* method), 75
 compute_sigma_qq() (*dicee.models.DeCaL* method), 149
 compute_sigma_qq() (*dicee.models.Keci* method), 145
 compute_sigma_qr() (*dicee.DeCaL* method), 196
 compute_sigma_qr() (*dicee.models.clifford.DeCaL* method), 81
 compute_sigma_qr() (*dicee.models.DeCaL* method), 150
 compute_sigma_rr() (*dicee.DeCaL* method), 196
 compute_sigma_rr() (*dicee.models.clifford.DeCaL* method), 81
 compute_sigma_rr() (*dicee.models.DeCaL* method), 150
 compute_sigma_rr() (*dicee.DeCaL* method), 194
 compute_sigmas_multivect() (*dicee.DeCaL* method), 79
 compute_sigmas_multivect() (*dicee.models.clifford.DeCaL* method), 148
 compute_sigmas_multivect() (*dicee.models.DeCaL* method), 144
 compute_sigmas_single() (*dicee.DeCaL* method), 194
 compute_sigmas_single() (*dicee.models.clifford.DeCaL* method), 79
 compute_sigmas_single() (*dicee.models.DeCaL* method), 148
 ConEx (*class in dicee*), 202
 ConEx (*class in dicee.models*), 130
 ConEx (*class in dicee.models.complex*), 82
 config (*dicee.BytE* attribute), 208
 config (*dicee.CoKE* attribute), 207
 config (*dicee.models.CoKE* attribute), 127
 config (*dicee.models.real.CoKE* attribute), 101
 config (*dicee.models.transformers.BytE* attribute), 102
 config (*dicee.models.transformers.GPT* attribute), 107
 configs (*dicee.abstracts.BaseInteractiveKGE* attribute), 14
 configure_optimizers() (*dicee.models.base_model.BaseKGELighting* method), 70
 configure_optimizers() (*dicee.models.BaseKGELighting* method), 117
 configure_optimizers() (*dicee.models.transformers.GPT* method), 108
 construct_batch_selected_cl_multivector() (*dicee.Keci* method), 192
 construct_batch_selected_cl_multivector() (*dicee.models.clifford.Keci* method), 77
 construct_batch_selected_cl_multivector() (*dicee.models.Keci* method), 146
 construct_cl_multivector() (*dicee.DeCaL* method), 195
 construct_cl_multivector() (*dicee.Keci* method), 191
 construct_cl_multivector() (*dicee.models.clifford.DeCaL* method), 80

construct_cl_multivector() (*dicee.models.clifford.Keci method*), 76
 construct_cl_multivector() (*dicee.models.DeCaL method*), 149
 construct_cl_multivector() (*dicee.models.Keci method*), 146
 construct_dataset() (*in module dicee*), 220
 construct_dataset() (*in module dicee.dataset_classes*), 32
 construct_ensemble(*dicee.abstracts.BaseInteractiveKGE attribute*), 14
 construct_graph() (*dicee.query_generator.QueryGenerator method*), 161
 construct_graph() (*dicee.QueryGenerator method*), 233
 construct_input_and_output() (*dicee.abstracts.BaseInteractiveKGE method*), 16
 construct_multi_coeff() (*dicee.LFMult method*), 205
 construct_multi_coeff() (*dicee.models.function_space.LFMult method*), 88
 construct_multi_coeff() (*dicee.models.LFMult method*), 159
 continual_learning(*dicee.config.Namespace attribute*), 31
 continual_start() (*dicee.DICE_Trainer method*), 215
 continual_start() (*dicee.executer.ContinuousExecute method*), 50
 continual_start() (*dicee.trainer.DICE_Trainer method*), 181
 continual_start() (*dicee.trainer.dice_trainer.DICE_Trainer method*), 177
 continual_training_setup_executor() (*in module dicee*), 214
 continual_training_setup_executor() (*in module dicee.static_funcs*), 174
 ContinuousExecute (*class in dicee.executer*), 50
 conv2d(*dicee.AConEx attribute*), 198
 conv2d(*dicee.AConvO attribute*), 199
 conv2d(*dicee.AConvQ attribute*), 200
 conv2d(*dicee.ConEx attribute*), 202
 conv2d(*dicee.ConvO attribute*), 201
 conv2d(*dicee.ConvQ attribute*), 200
 conv2d(*dicee.models.AConEx attribute*), 130
 conv2d(*dicee.models.AConvO attribute*), 143
 conv2d(*dicee.models.AConvQ attribute*), 137
 conv2d(*dicee.models.complex.AConEx attribute*), 82
 conv2d(*dicee.models.complex.ConEx attribute*), 82
 conv2d(*dicee.models.ConEx attribute*), 130
 conv2d(*dicee.models.ConvO attribute*), 143
 conv2d(*dicee.models.ConvQ attribute*), 137
 conv2d(*dicee.models.octonion.AConvO attribute*), 93
 conv2d(*dicee.models.octonion.ConvO attribute*), 93
 conv2d(*dicee.models.quaternion.AConvQ attribute*), 98
 conv2d(*dicee.models.quaternion.ConvQ attribute*), 97
 ConvO (*class in dicee*), 201
 ConvO (*class in dicee.models*), 142
 ConvO (*class in dicee.models.octonion*), 92
 ConvQ (*class in dicee*), 200
 ConvQ (*class in dicee.models*), 136
 ConvQ (*class in dicee.models.quaternion*), 97
 count_triples() (*in module dicee.read_preprocess_save_load_kg.util*), 166
 create_and_store_kg() (*dicee.executer.Execute method*), 49
 create_constraints() (*in module dicee.read_preprocess_save_load_kg.util*), 166
 create_constraints() (*in module dicee.static_preprocess_funcs*), 175
 create_experiment_folder() (*in module dicee*), 214
 create_experiment_folder() (*in module dicee.static_funcs*), 174
 create_random_data() (*dicee.callbacks.PseudoLabellingCallback method*), 24
 create_reciprocal_triples() (*in module dicee*), 213
 create_reciprocal_triples() (*in module dicee.read_preprocess_save_load_kg.util*), 167
 create_reciprocal_triples() (*in module dicee.static_funcs*), 172
 create_vector_database() (*dicee.KGE method*), 216
 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*), 181
 current_epoch(*dicee.weight_averaging.EMA attribute*), 184
 current_epoch(*dicee.weight_averaging.SWA attribute*), 183
 current_epoch(*dicee.weight_averaging.SWAG attribute*), 184
 current_epoch(*dicee.weight_averaging.TWA attribute*), 185
 CVDataModule (*class in dicee*), 227
 CVDataModule (*class in dicee.dataset_classes*), 40
 cycle_length(*dicee.callbacks.LRScheduler attribute*), 28

D

data_module (*dicee.callbacks.PseudoLabellingCallback attribute*), 24

```

data_property_embeddings (dicee.models.literal.LiteralEmbeddings attribute), 90
data_property_to_idx (dicee.dataset_classes.LiteralDataset attribute), 45
data_property_to_idx (dicee.LiteralDataset attribute), 232
dataset_dir (dicee.config.Namespace attribute), 29
dataset_dir (dicee.knowledge_graph.KG attribute), 51
dataset_sanity_checking () (in module dicee.read_preprocess_save_load_kg.util), 167
DeCaL (class in dicee), 193
DeCaL (class in dicee.models), 147
DeCaL (class in dicee.models.clifford), 78
decay (dicee.weight_averaging.EMA attribute), 184
decide () (dicee.callbacks.ASWA method), 24
default_eval_model (dicee.callbacks.PeriodicEvalCallback attribute), 27
degree (dicee.LFMult attribute), 205
degree (dicee.models.function_space.LFMult attribute), 88
degree (dicee.models.LFMult attribute), 158
denormalize () (dicee.dataset_classes.LiteralDataset static method), 45
denormalize () (dicee.LiteralDataset static method), 232
deploy () (dicee.KGE method), 219
deploy () (dicee.knowledge_graph_embeddings.KGE method), 56
deploy_head_entity_prediction () (in module dicee), 214
deploy_head_entity_prediction () (in module dicee.static_funcs), 173
deploy_relation_prediction () (in module dicee), 214
deploy_relation_prediction () (in module dicee.static_funcs), 174
deploy_tail_entity_prediction () (in module dicee), 214
deploy_tail_entity_prediction () (in module dicee.static_funcs), 173
deploy_triple_prediction () (in module dicee), 214
deploy_triple_prediction () (in module dicee.static_funcs), 173
describe () (dicee.knowledge_graph.KG method), 52
description_of_input (dicee.knowledge_graph.KG attribute), 52
deviations (dicee.weight_averaging.SWAG attribute), 184
device (dicee.models.literal.LiteralEmbeddings property), 91
DICE_Trainer (class in dicee), 215
DICE_Trainer (class in dicee.trainer), 181
DICE_Trainer (class in dicee.trainer.dice_trainer), 176
dicee
    module, 12
dicee.__main__
    module, 12
dicee.abstracts
    module, 12
dicee.analyse_experiments
    module, 19
dicee.callbacks
    module, 20
dicee.config
    module, 28
dicee.dataset_classes
    module, 32
dicee.eval_static_funcs
    module, 46
dicee.evaluator
    module, 47
dicee.executor
    module, 49
dicee.knowledge_graph
    module, 51
dicee.knowledge_graph_embeddings
    module, 52
dicee.models
    module, 56
dicee.models.adopt
    module, 56
dicee.models.base_model
    module, 65
dicee.models.clifford
    module, 74
dicee.models.complex
    module, 81

```

```

dicee.models.dualE
    module, 84
dicee.models.ensemble
    module, 85
dicee.models.function_space
    module, 86
dicee.models.literal
    module, 89
dicee.models.octonion
    module, 91
dicee.models.pykeen_models
    module, 94
dicee.models.quaternion
    module, 95
dicee.models.real
    module, 98
dicee.models.static_funcs
    module, 101
dicee.models.transformers
    module, 101
dicee.query_generator
    module, 160
dicee.read_preprocess_save_load_kg
    module, 162
dicee.read_preprocess_save_load_kg.preprocess
    module, 162
dicee.read_preprocess_save_load_kg.read_from_disk
    module, 163
dicee.read_preprocess_save_load_kg.save_load_disk
    module, 163
dicee.read_preprocess_save_load_kg.util
    module, 164
dicee.sanity_checkers
    module, 168
dicee.scripts
    module, 169
dicee.scripts.index_serve
    module, 169
dicee.scripts.run
    module, 171
dicee.static_funcs
    module, 171
dicee.static_funcs_training
    module, 174
dicee.static_preprocess_funcs
    module, 175
dicee.trainer
    module, 176
dicee.trainer.dice_trainer
    module, 176
dicee.trainer.model_parallelism
    module, 178
dicee.trainer.torch_trainer
    module, 178
dicee.trainer.torch_trainer_ddp
    module, 180
dicee.weight_averaging
    module, 183
discrete_points (dicee.models.FMult2 attribute), 157
discrete_points (dicee.models.function_space.FMult2 attribute), 87
dist_func (dicee.models.Pyke attribute), 126
dist_func (dicee.models.real.Pyke attribute), 99
dist_func (dicee.Pyke attribute), 189
DistMult (class in dicee), 189
DistMult (class in dicee.models), 125
DistMult (class in dicee.models.real), 98
distributed (dicee.executer.Execute attribute), 49
download_file () (in module dicee), 214

```

download_file() (*in module dicee.static_funcs*), 174
 download_files_from_url() (*in module dicee*), 214
 download_files_from_url() (*in module dicee.static_funcs*), 174
 download_pretrained_model() (*in module dicee*), 214
 download_pretrained_model() (*in module dicee.static_funcs*), 174
 dropout (*dicee.models.CoKEConfig attribute*), 126
 dropout (*dicee.models.literal.LiteralEmbeddings attribute*), 90
 dropout (*dicee.models.real.CoKEConfig attribute*), 100
 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*), 196
 DualE (*class in dicee.models*), 159
 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*), 175
 EMA (*class in dicee.weight_averaging*), 184
 ema (*dicee.config.Namespace attribute*), 31
 ema_c_epochs (*dicee.weight_averaging.EMA attribute*), 184
 ema_model (*dicee.weight_averaging.EMA attribute*), 184
 ema_start_epoch (*dicee.weight_averaging.EMA attribute*), 184
 ema_update() (*dicee.weight_averaging.EMA static method*), 185
 embedding_dim (*dicee.analyse_experiments.Experiment attribute*), 19
 embedding_dim (*dicee.BaseKGE attribute*), 211
 embedding_dim (*dicee.config.Namespace attribute*), 29
 embedding_dim (*dicee.models.base_model.BaseKGE attribute*), 72
 embedding_dim (*dicee.models.BaseKGE attribute*), 119, 122, 128, 132, 138, 151, 155
 embedding_dim (*dicee.models.literal.LiteralEmbeddings attribute*), 90
 embedding_dims (*dicee.models.literal.LiteralEmbeddings attribute*), 90
 enable_log (*in module dicee.static_preprocess_funcs*), 175
 enc (*dicee.knowledge_graph.KG attribute*), 52
 end() (*dicee.executer.Execute method*), 50
 EnsembleKGE (*class in dicee*), 212
 EnsembleKGE (*class in dicee.models.ensemble*), 85
 ent2id (*dicee.query_generator.QueryGenerator attribute*), 161
 ent2id (*dicee.QueryGenerator attribute*), 233
 ent_in (*dicee.query_generator.QueryGenerator attribute*), 161
 ent_in (*dicee.QueryGenerator attribute*), 233
 ent_out (*dicee.query_generator.QueryGenerator attribute*), 161
 ent_out (*dicee.QueryGenerator attribute*), 233
 entities_str (*dicee.knowledge_graph.KG property*), 52
 entity_embeddings (*dicee.AConvQ attribute*), 200
 entity_embeddings (*dicee.ConvQ attribute*), 200
 entity_embeddings (*dicee.DeCaL attribute*), 193
 entity_embeddings (*dicee.DualE attribute*), 197
 entity_embeddings (*dicee.LFMult attribute*), 205
 entity_embeddings (*dicee.models.AConvQ attribute*), 137
 entity_embeddings (*dicee.models.clifford.DeCaL attribute*), 78
 entity_embeddings (*dicee.models.ConvQ attribute*), 137
 entity_embeddings (*dicee.models.DeCaL attribute*), 147
 entity_embeddings (*dicee.models.DualE attribute*), 160
 entity_embeddings (*dicee.models.dualE.DualE attribute*), 84
 entity_embeddings (*dicee.models.FMult attribute*), 156
 entity_embeddings (*dicee.models.FMult2 attribute*), 157
 entity_embeddings (*dicee.models.function_space.FMult attribute*), 86
 entity_embeddings (*dicee.models.function_space.FMult2 attribute*), 87
 entity_embeddings (*dicee.models.function_space.GFMult attribute*), 87
 entity_embeddings (*dicee.models.function_space.LFMult attribute*), 88
 entity_embeddings (*dicee.models.function_space.LFMult1 attribute*), 88
 entity_embeddings (*dicee.models.GFMult attribute*), 157
 entity_embeddings (*dicee.models.LFMult attribute*), 158
 entity_embeddings (*dicee.models.LFMult1 attribute*), 158

entity_embeddings (*dicee.models.literal.LiteralEmbeddings* attribute), 90
 entity_embeddings (*dicee.models.pykeen_models.PykeenKGE* attribute), 94
 entity_embeddings (*dicee.models.PykeenKGE* attribute), 153
 entity_embeddings (*dicee.models.quaternion.AConvQ* attribute), 98
 entity_embeddings (*dicee.models.quaternion.ConvQ* attribute), 97
 entity_embeddings (*dicee.PykeenKGE* attribute), 207
 entity_to_idx (*dicee.dataset_classes.LiteralDataset* attribute), 44, 45
 entity_to_idx (*dicee.knowledge_graph.KG* attribute), 51
 entity_to_idx (*dicee.LiteralDataset* attribute), 231, 232
 entity_to_idx (*dicee.scripts.index_serve.NeuralSearcher* attribute), 170
 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), 213
 eval() (*dicee.evaluator.Evaluator* method), 48
 eval() (*dicee.models.ensemble.EnsembleKGE* method), 85
 eval_at_epochs (*dicee.config.Namespace* attribute), 31
 eval_epochs (*dicee.callbacks.PeriodicEvalCallback* attribute), 27
 eval_every_n_epochs (*dicee.config.Namespace* attribute), 31
 eval_lp_performance() (*dicee.KGE* method), 216
 eval_lp_performance() (*dicee.knowledge_graph_embeddings.KGE* method), 53
 eval_model (*dicee.config.Namespace* attribute), 30
 eval_model (*dicee.knowledge_graph.KG* attribute), 51
 eval_rank_of_head_and_tail_byte_pair_encoded_entity() (*dicee.evaluator.Evaluator* method), 48
 eval_rank_of_head_and_tail_entity() (*dicee.evaluator.Evaluator* method), 48
 eval_with_bpe_vs_all() (*dicee.evaluator.Evaluator* method), 48
 eval_with_byte() (*dicee.evaluator.Evaluator* method), 48
 eval_with_data() (*dicee.evaluator.Evaluator* method), 49
 eval_with_vs_all() (*dicee.evaluator.Evaluator* method), 48
 evaluate() (in module *dicee*), 214
 evaluate() (in module *dicee.static_funcs*), 174
 evaluate_bpe_lp() (in module *dicee.static_funcs_training*), 175
 evaluate_ensemble_link_prediction_performance() (in module *dicee.eval_static_funcs*), 47
 evaluate_link_prediction_performance() (in module *dicee.eval_static_funcs*), 46
 evaluate_link_prediction_performance_with_bpe() (in module *dicee.eval_static_funcs*), 46
 evaluate_link_prediction_performance_with_bpe_reciprocals() (in module *dicee.eval_static_funcs*), 46
 evaluate_link_prediction_performance_with_reciprocals() (in module *dicee.eval_static_funcs*), 46
 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*), 174
 evaluate_lp_bpe_k_vs_all() (*dicee.evaluator.Evaluator* method), 48
 evaluate_lp_bpe_k_vs_all() (in module *dicee.eval_static_funcs*), 46
 evaluate_lp_k_vs_all() (*dicee.evaluator.Evaluator* method), 48
 evaluate_lp_with_byte() (*dicee.evaluator.Evaluator* method), 48
 Evaluator (class in *dicee.evaluator*), 48
 evaluator (*dicee.DICE_Trainer* attribute), 215
 evaluator (*dicee.executer.Execute* attribute), 49
 evaluator (*dicee.trainer.DICE_Trainer* attribute), 181
 evaluator (*dicee.trainer.dice_trainer.DICE_Trainer* attribute), 177
 every_x_epoch (*dicee.callbacks.KGESaveCallback* attribute), 23
 example_input_array (*dicee.EnsembleKGE* property), 213
 example_input_array (*dicee.models.ensemble.EnsembleKGE* property), 85
 Execute (class in *dicee.executer*), 49
 exists() (*dicee.knowledge_graph.KG* method), 52
 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), 136
 explicit (*dicee.models.quaternion.QMult* attribute), 96
 explicit (*dicee.QMult* attribute), 203
 exponential_function() (in module *dicee*), 214

`exponential_function()` (*in module dicee.static_funcs*), 174
`extract_input_outputs()` (*dicee.trainer.torch_trainer_ddp.NodeTrainer method*), 181
`extract_input_outputs()` (*in module dicee.trainer.model_parallelism*), 178
`extract_input_outputs_set_device()` (*dicee.trainer.torch_trainer.TorchTrainer method*), 179

F

`f` (*dicee.callbacks.KronE attribute*), 26
`fc` (*dicee.models.literal.LiteralEmbeddings attribute*), 90
`fc1` (*dicee.AConEx attribute*), 199
`fc1` (*dicee.AConvO attribute*), 199
`fc1` (*dicee.AConvQ attribute*), 200
`fc1` (*dicee.ConEx attribute*), 202
`fc1` (*dicee.ConvO attribute*), 201
`fc1` (*dicee.ConvQ attribute*), 200
`fc1` (*dicee.models.AConEx attribute*), 130
`fc1` (*dicee.models.AConvO attribute*), 143
`fc1` (*dicee.models.AConvQ attribute*), 137
`fc1` (*dicee.models.complex.AConEx attribute*), 82
`fc1` (*dicee.models.complex.ConEx attribute*), 82
`fc1` (*dicee.models.ConEx attribute*), 130
`fc1` (*dicee.models.ConvO attribute*), 143
`fc1` (*dicee.models.ConvQ attribute*), 137
`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*), 97
`fc_num_input` (*dicee.AConEx attribute*), 198
`fc_num_input` (*dicee.AConvO attribute*), 199
`fc_num_input` (*dicee.AConvQ attribute*), 200
`fc_num_input` (*dicee.ConEx attribute*), 202
`fc_num_input` (*dicee.ConvO attribute*), 201
`fc_num_input` (*dicee.ConvQ attribute*), 200
`fc_num_input` (*dicee.models.AConEx attribute*), 130
`fc_num_input` (*dicee.models.AConvO attribute*), 143
`fc_num_input` (*dicee.models.AConvQ attribute*), 137
`fc_num_input` (*dicee.models.complex.AConEx attribute*), 82
`fc_num_input` (*dicee.models.complex.ConEx attribute*), 82
`fc_num_input` (*dicee.models.ConEx attribute*), 130
`fc_num_input` (*dicee.models.ConvO attribute*), 143
`fc_num_input` (*dicee.models.ConvQ attribute*), 137
`fc_num_input` (*dicee.models.octonion.AConvO attribute*), 93
`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*), 97
`fc_out` (*dicee.models.literal.LiteralEmbeddings attribute*), 90
`feature_map_dropout` (*dicee.AConEx attribute*), 199
`feature_map_dropout` (*dicee.AConvO attribute*), 199
`feature_map_dropout` (*dicee.AConvQ attribute*), 200
`feature_map_dropout` (*dicee.ConEx attribute*), 202
`feature_map_dropout` (*dicee.ConvO attribute*), 201
`feature_map_dropout` (*dicee.ConvQ attribute*), 200
`feature_map_dropout` (*dicee.models.AConEx attribute*), 130
`feature_map_dropout` (*dicee.models.AConvO attribute*), 143
`feature_map_dropout` (*dicee.models.AConvQ attribute*), 137
`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*), 130
`feature_map_dropout` (*dicee.models.ConvO attribute*), 143
`feature_map_dropout` (*dicee.models.ConvQ attribute*), 137
`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*), 97
`feature_map_dropout_rate` (*dicee.BaseKGE attribute*), 211
`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*), 119, 122, 128, 133, 139, 151, 155

```

fetch_worker() (in module dicee.read_preprocess_save_load_kg.util), 166
fill_query() (dicee.query_generator.QueryGenerator method), 161
fill_query() (dicee.QueryGenerator method), 233
find_good_batch_size() (in module dicee.trainer.model_parallelism), 178
find_missing_triples() (dicee.knowledge_graph_embeddings.KGE method), 55
fit() (dicee.trainer.model_parallelism.TensorParallel method), 178
fit() (dicee.trainer.torch_trainer_ddp.TorchDDPTrainer method), 180
fit() (dicee.trainer.torch_trainer.TorchTrainer method), 179
flash (dicee.models.transformers.SelfAttention attribute), 105
FMult (class in dicee.models), 156
FMult (class in dicee.models.function_space), 86
FMult2 (class in dicee.models), 157
FMult2 (class in dicee.models.function_space), 87
form_of_labelling (dicee.DICE_Trainer attribute), 215
form_of_labelling (dicee.trainer.DICE_Trainer attribute), 181
form_of_labelling (dicee.trainer.dice_trainer.DICE_Trainer attribute), 177
forward() (dicee.BaseKGE method), 212
forward() (dicee.BytE method), 209
forward() (dicee.models.base_model.BaseKGE method), 73
forward() (dicee.models.base_model.IdentityClass static method), 74
forward() (dicee.models.BaseKGE method), 120, 123, 129, 133, 139, 152, 156
forward() (dicee.models.Block method), 125
forward() (dicee.models.IdentityClass static method), 121, 135, 141
forward() (dicee.models.literal.LiteralEmbeddings method), 91
forward() (dicee.models.transformers.Block method), 106
forward() (dicee.models.transformers.BytE method), 102
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), 179
forward_backward_update_loss() (in module dicee.trainer.model_parallelism), 178
forward_byte_pair_encoded_k_vs_all() (dicee.BaseKGE method), 211
forward_byte_pair_encoded_k_vs_all() (dicee.models.base_model.BaseKGE method), 72
forward_byte_pair_encoded_k_vs_all() (dicee.models.BaseKGE method), 120, 123, 129, 133, 139, 152, 155
forward_byte_pair_encoded_triple() (dicee.BaseKGE method), 212
forward_byte_pair_encoded_triple() (dicee.models.base_model.BaseKGE method), 72
forward_byte_pair_encoded_triple() (dicee.models.BaseKGE method), 120, 123, 129, 133, 139, 152, 155
forward_k_vs_all() (dicee.AConEx method), 199
forward_k_vs_all() (dicee.AConvO method), 199
forward_k_vs_all() (dicee.ACovQ method), 200
forward_k_vs_all() (dicee.BaseKGE method), 212
forward_k_vs_all() (dicee.CoKE method), 207
forward_k_vs_all() (dicee.ComplEx method), 198
forward_k_vs_all() (dicee.ConEx method), 202
forward_k_vs_all() (dicee.ConvO method), 202
forward_k_vs_all() (dicee.ConvQ method), 201
forward_k_vs_all() (dicee.DeCaL method), 194
forward_k_vs_all() (dicee.DistMult method), 189
forward_k_vs_all() (dicee.DualE method), 197
forward_k_vs_all() (dicee.Keci method), 192
forward_k_vs_all() (dicee.models.AConEx method), 130
forward_k_vs_all() (dicee.models.AConvO method), 143
forward_k_vs_all() (dicee.models.ACovQ method), 138
forward_k_vs_all() (dicee.models.base_model.BaseKGE method), 73
forward_k_vs_all() (dicee.models.BaseKGE method), 120, 123, 129, 134, 140, 153, 156
forward_k_vs_all() (dicee.models.clifford.DeCaL method), 79
forward_k_vs_all() (dicee.models.clifford.Keci method), 77
forward_k_vs_all() (dicee.models.CoKE method), 127
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), 130
forward_k_vs_all() (dicee.models.ConvO method), 143
forward_k_vs_all() (dicee.models.ConvQ method), 137
forward_k_vs_all() (dicee.models.DeCaL method), 148

```

forward_k_vs_all() (*dicee.models.DistMult method*), 125
 forward_k_vs_all() (*dicee.models.DualE method*), 160
 forward_k_vs_all() (*dicee.models.dualE.DualE method*), 85
 forward_k_vs_all() (*dicee.models.Keci method*), 146
 forward_k_vs_all() (*dicee.models.octonion.AConvO method*), 94
 forward_k_vs_all() (*dicee.models.octonion.ConvO method*), 93
 forward_k_vs_all() (*dicee.models.octonion.OMult method*), 92
 forward_k_vs_all() (*dicee.models.OMult method*), 142
 forward_k_vs_all() (*dicee.models.pykeen_models.PykeenKGE method*), 94
 forward_k_vs_all() (*dicee.models.PykeenKGE method*), 153
 forward_k_vs_all() (*dicee.models.QMult method*), 136
 forward_k_vs_all() (*dicee.models.quaternion.AConvQ method*), 98
 forward_k_vs_all() (*dicee.models.quaternion.ConvQ method*), 97
 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*), 99
 forward_k_vs_all() (*dicee.models.real.TransE method*), 99
 forward_k_vs_all() (*dicee.models.Shallom method*), 125
 forward_k_vs_all() (*dicee.models.TransE method*), 125
 forward_k_vs_all() (*dicee.OMult method*), 205
 forward_k_vs_all() (*dicee.PykeenKGE method*), 207
 forward_k_vs_all() (*dicee.QMult method*), 204
 forward_k_vs_all() (*dicee.Shallom method*), 205
 forward_k_vs_all() (*dicee.TransE method*), 193
 forward_k_vs_sample() (*dicee.AConEx method*), 199
 forward_k_vs_sample() (*dicee.BaseKGE method*), 212
 forward_k_vs_sample() (*dicee.CoKE method*), 207
 forward_k_vs_sample() (*dicee.ComplEx method*), 198
 forward_k_vs_sample() (*dicee.ConEx method*), 202
 forward_k_vs_sample() (*dicee.DistMult method*), 189
 forward_k_vs_sample() (*dicee.Keci method*), 192
 forward_k_vs_sample() (*dicee.models.AConEx method*), 131
 forward_k_vs_sample() (*dicee.models.base_model.BaseKGE method*), 73
 forward_k_vs_sample() (*dicee.models.BaseKGE method*), 120, 123, 129, 134, 140, 153, 156
 forward_k_vs_sample() (*dicee.models.clifford.Keci method*), 77
 forward_k_vs_sample() (*dicee.models.CoKE method*), 127
 forward_k_vs_sample() (*dicee.models.ComplEx method*), 132
 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*), 82
 forward_k_vs_sample() (*dicee.models.ConEx method*), 130
 forward_k_vs_sample() (*dicee.models.DistMult method*), 125
 forward_k_vs_sample() (*dicee.models.Keci method*), 146
 forward_k_vs_sample() (*dicee.models.pykeen_models.PykeenKGE method*), 95
 forward_k_vs_sample() (*dicee.models.PykeenKGE method*), 154
 forward_k_vs_sample() (*dicee.models.QMult method*), 136
 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*), 208
 forward_k_vs_sample() (*dicee.QMult method*), 204
 forward_k_vs_with_explicit() (*dicee.Keci method*), 192
 forward_k_vs_with_explicit() (*dicee.models.clifford.Keci method*), 77
 forward_k_vs_with_explicit() (*dicee.models.Keci method*), 146
 forward_triples() (*dicee.AConEx method*), 199
 forward_triples() (*dicee.AConvO method*), 199
 forward_triples() (*dicee.AConvQ method*), 200
 forward_triples() (*dicee.BaseKGE method*), 212
 forward_triples() (*dicee.ConEx method*), 202
 forward_triples() (*dicee.ConvO method*), 202
 forward_triples() (*dicee.ConvQ method*), 200
 forward_triples() (*dicee.DeCaL method*), 194
 forward_triples() (*dicee.DualE method*), 197
 forward_triples() (*dicee.Keci method*), 192
 forward_triples() (*dicee.LFMult method*), 205
 forward_triples() (*dicee.models.AConEx method*), 131
 forward_triples() (*dicee.models.AConvO method*), 143

```

forward_triples() (dicee.models.AConvQ method), 137
forward_triples() (dicee.models.base_model.BaseKGE method), 73
forward_triples() (dicee.models.BaseKGE method), 120, 123, 129, 134, 140, 152, 156
forward_triples() (dicee.models.clifford.DeCaL method), 79
forward_triples() (dicee.models.clifford.Keci method), 77
forward_triples() (dicee.models.complex.AConEx method), 83
forward_triples() (dicee.models.complex.ConEx method), 82
forward_triples() (dicee.models.ConEx method), 130
forward_triples() (dicee.models.ConvO method), 143
forward_triples() (dicee.models.ConvQ method), 137
forward_triples() (dicee.models.DeCaL method), 148
forward_triples() (dicee.models.DualE method), 160
forward_triples() (dicee.models.dualE.DualE method), 84
forward_triples() (dicee.models.FMult method), 157
forward_triples() (dicee.models.FMult2 method), 158
forward_triples() (dicee.models.function_space.FMult method), 86
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), 88
forward_triples() (dicee.models.function_space.LFMult1 method), 88
forward_triples() (dicee.models.GFMult method), 157
forward_triples() (dicee.models.Keci method), 147
forward_triples() (dicee.models.LFMult method), 158
forward_triples() (dicee.models.LFMult1 method), 158
forward_triples() (dicee.models.octonion.AConvO method), 94
forward_triples() (dicee.models.octonion.ConvO method), 93
forward_triples() (dicee.models.Pyke method), 126
forward_triples() (dicee.models.pykeen_models.PykeenKGE method), 95
forward_triples() (dicee.models.PykeenKGE method), 154
forward_triples() (dicee.models.quaternion.AConvQ method), 98
forward_triples() (dicee.models.quaternion.ConvQ method), 97
forward_triples() (dicee.models.real.Pyke method), 99
forward_triples() (dicee.models.real.Shallom method), 99
forward_triples() (dicee.models.Shallom method), 125
forward_triples() (dicee.Pyke method), 189
forward_triples() (dicee.PykeenKGE method), 208
forward_triples() (dicee.Shallom method), 205
freeze_entity_embeddings (dicee.models.literal.LiteralEmbeddings attribute), 90
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), 215
from_pretrained_model_write_embeddings_into_csv() (in module dicee.static_funcs), 174
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), 52
function() (dicee.models.FMult2 method), 158
function() (dicee.models.function_space.FMult2 method), 87

```

G

```

gamma (dicee.models.FMult attribute), 157
gamma (dicee.models.function_space.FMult attribute), 86
gate_residual (dicee.models.literal.LiteralEmbeddings attribute), 90
gated_residual_proj (dicee.models.literal.LiteralEmbeddings attribute), 90
gelu (dicee.models.transformers.MLP attribute), 105
gen_test (dicee.query_generator.QueryGenerator attribute), 161
gen_test (dicee.QueryGenerator attribute), 233
gen_valid (dicee.query_generator.QueryGenerator attribute), 161
gen_valid (dicee.QueryGenerator attribute), 233
generate() (dicee.BytE method), 209
generate() (dicee.KGE method), 216
generate() (dicee.knowledge_graph_embeddings.KGE method), 53
generate() (dicee.models.transformers.BytE method), 103
generate_queries() (dicee.query_generator.QueryGenerator method), 161
generate_queries() (dicee.QueryGenerator method), 233
get_aswa_state_dict() (dicee.callbacks.ASWA method), 24
get_bpe_head_and_relation_representation() (dicee.BaseKGE method), 212
get_bpe_head_and_relation_representation() (dicee.models.base_model.BaseKGE method), 73

```

get_bpe_head_and_relation_representation() (*dicee.models.BaseKGE method*), 120, 124, 129, 134, 140, 153, 156
 get_bpe_token_representation() (*dicee.abstracts.BaseInteractiveKGE method*), 14
 get_callbacks() (*in module dicee.trainer.dice_trainer*), 176
 get_default_arguments() (*in module dicee.analyse_experiments*), 19
 get_default_arguments() (*in module dicee.scripts.index_serve*), 170
 get_default_arguments() (*in module dicee.scripts.run*), 171
 get_ee_vocab() (*in module dicee*), 213
 get_ee_vocab() (*in module dicee.read_preprocess_save_load_kg.util*), 166
 get_ee_vocab() (*in module dicee.static_funcs*), 172
 get_ee_vocab() (*in module dicee.static_preprocess_funcs*), 175
 get_embeddings() (*dicee.BaseKGE method*), 212
 get_embeddings() (*dicee.EnsembleKGE method*), 213
 get_embeddings() (*dicee.models.base_model.BaseKGE method*), 73
 get_embeddings() (*dicee.models.BaseKGE method*), 121, 124, 129, 134, 140, 153, 156
 get_embeddings() (*dicee.models.ensemble.EnsembleKGE method*), 86
 get_embeddings() (*dicee.models.real.Shallom method*), 99
 get_embeddings() (*dicee.models.Shallom method*), 125
 get_embeddings() (*dicee.Shallom method*), 205
 get_entity_embeddings() (*dicee.abstracts.BaseInteractiveKGE method*), 15
 get_entity_index() (*dicee.abstracts.BaseInteractiveKGE method*), 15
 get_er_vocab() (*in module dicee*), 213
 get_er_vocab() (*in module dicee.read_preprocess_save_load_kg.util*), 166
 get_er_vocab() (*in module dicee.static_funcs*), 172
 get_er_vocab() (*in module dicee.static_preprocess_funcs*), 175
 get_eval_report() (*dicee.abstracts.BaseInteractiveKGE method*), 14
 get_head_relation_representation() (*dicee.BaseKGE method*), 212
 get_head_relation_representation() (*dicee.models.base_model.BaseKGE method*), 73
 get_head_relation_representation() (*dicee.models.BaseKGE method*), 120, 123, 129, 134, 140, 153, 156
 get_kronecker_triple_representation() (*dicee.callbacks.KronE method*), 26
 get_mean_and_var() (*dicee.weight_averaging.SWAG method*), 184
 get_num_params() (*dicee.models.transformers.GPT method*), 107
 get_padded_bpe_triple_representation() (*dicee.abstracts.BaseInteractiveKGE method*), 14
 get_queries() (*dicee.query_generator.QueryGenerator method*), 162
 get_queries() (*dicee.QueryGenerator method*), 234
 get_re_vocab() (*in module dicee*), 213
 get_re_vocab() (*in module dicee.read_preprocess_save_load_kg.util*), 166
 get_re_vocab() (*in module dicee.static_funcs*), 172
 get_re_vocab() (*in module dicee.static_preprocess_funcs*), 175
 get_relation_embeddings() (*dicee.abstracts.BaseInteractiveKGE method*), 15
 get_relation_index() (*dicee.abstracts.BaseInteractiveKGE method*), 15
 get_sentence_representation() (*dicee.BaseKGE method*), 212
 get_sentence_representation() (*dicee.models.base_model.BaseKGE method*), 73
 get_sentence_representation() (*dicee.models.BaseKGE method*), 120, 124, 129, 134, 140, 153, 156
 get_transductive_entity_embeddings() (*dicee.KGE method*), 216
 get_transductive_entity_embeddings() (*dicee.knowledge_graph_embeddings.KGE method*), 53
 get_triple_representation() (*dicee.BaseKGE method*), 212
 get_triple_representation() (*dicee.models.base_model.BaseKGE method*), 73
 get_triple_representation() (*dicee.models.BaseKGE method*), 120, 123, 129, 134, 140, 153, 156
 GFMult (*class in dicee.models*), 157
 GFMult (*class in dicee.models.function_space*), 87
 global_rank (*dicee.abstracts.AbstractTrainer attribute*), 13
 global_rank (*dicee.trainer.torch_trainer_ddp.NodeTrainer attribute*), 180
 GPT (*class in dicee.models.transformers*), 107
 GPTConfig (*class in dicee.models.transformers*), 106
 gpus (*dicee.config.Namespace attribute*), 29
 gradient_accumulation_steps (*dicee.config.Namespace attribute*), 30
 ground_queries() (*dicee.query_generator.QueryGenerator method*), 161
 ground_queries() (*dicee.QueryGenerator method*), 233
 gswa_n (*dicee.weight_averaging.SWAG attribute*), 184

H

hidden_dim (*dicee.models.literal.LiteralEmbeddings attribute*), 90
 hidden_dropout (*dicee.BaseKGE attribute*), 211
 hidden_dropout (*dicee.models.base_model.BaseKGE attribute*), 72
 hidden_dropout (*dicee.models.BaseKGE attribute*), 120, 123, 128, 133, 139, 152, 155
 hidden_dropout_rate (*dicee.BaseKGE attribute*), 211
 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), 119, 122, 128, 133, 139, 151, 155
 hidden_normalizer (*dicee.BaseKGE* attribute), 211
 hidden_normalizer (*dicee.models.base_model.BaseKGE* attribute), 72
 hidden_normalizer (*dicee.models.BaseKGE* attribute), 119, 123, 128, 133, 139, 152, 155

|

IdentityClass (*class in dicee.models*), 121, 134, 140
 IdentityClass (*class in dicee.models.base_model*), 73
 idx_entity_to_bpe_shaped (*dicee.knowledge_graph.KG* attribute), 52
 index() (*in module dicee.scripts.index_serve*), 170
 index_triple() (*dicee.abstracts.BaseInteractiveKGE* method), 15
 init_dataloader() (*dicee.DICE_Trainer* method), 215
 init_dataloader() (*dicee.trainer.DICE_Trainer* method), 182
 init_dataloader() (*dicee.trainer.dice_trainer.DICE_Trainer* method), 177
 init_dataset() (*dicee.DICE_Trainer* method), 215
 init_dataset() (*dicee.trainer.DICE_Trainer* method), 182
 init_dataset() (*dicee.trainer.dice_trainer.DICE_Trainer* method), 177
 init_param (*dicee.config.Namespace* attribute), 30
 init_params_with_sanity_checking() (*dicee.BaseKGE* method), 212
 init_params_with_sanity_checking() (*dicee.models.base_model.BaseKGE* method), 73
 init_params_with_sanity_checking() (*dicee.models.BaseKGE* method), 120, 123, 129, 133, 139, 152, 156
 initial_eval_setting (*dicee.callbacks.ASWA* attribute), 24
 initialize_or_load_model() (*dicee.DICE_Trainer* method), 215
 initialize_or_load_model() (*dicee.trainer.DICE_Trainer* method), 182
 initialize_or_load_model() (*dicee.trainer.dice_trainer.DICE_Trainer* method), 177
 initialize_trainer() (*dicee.DICE_Trainer* method), 215
 initialize_trainer() (*dicee.trainer.DICE_Trainer* method), 182
 initialize_trainer() (*dicee.trainer.dice_trainer.DICE_Trainer* method), 177
 initialize_trainer() (*in module dicee.trainer.dice_trainer*), 176
 input_dp_ent_real (*dicee.BaseKGE* attribute), 211
 input_dp_ent_real (*dicee.models.base_model.BaseKGE* attribute), 72
 input_dp_ent_real (*dicee.models.BaseKGE* attribute), 120, 123, 128, 133, 139, 152, 155
 input_dp_rel_real (*dicee.BaseKGE* attribute), 211
 input_dp_rel_real (*dicee.models.base_model.BaseKGE* attribute), 72
 input_dp_rel_real (*dicee.models.BaseKGE* attribute), 120, 123, 128, 133, 139, 152, 155
 input_dropout_rate (*dicee.BaseKGE* attribute), 211
 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), 119, 122, 128, 133, 139, 151, 155
 InteractiveQueryDecomposition (*class in dicee.abstracts*), 16
 initialize_model() (*in module dicee*), 214
 initialize_model() (*in module dicee.static_funcs*), 173
 is_continual_training (*dicee.DICE_Trainer* attribute), 215
 is_continual_training (*dicee.evaluator.Evaluator* attribute), 48
 is_continual_training (*dicee.executer.Execute* attribute), 49
 is_continual_training (*dicee.trainer.DICE_Trainer* attribute), 181
 is_continual_training (*dicee.trainer.dice_trainer.DICE_Trainer* attribute), 176
 is_global_zero (*dicee.abstracts.AbstractTrainer* attribute), 13
 is_rank_zero() (*dicee.executer.Execute* method), 49
 is_seen() (*dicee.abstracts.BaseInteractiveKGE* method), 15
 is_sparql_endpoint_alive() (*in module dicee.sanity_checkers*), 169

K

k (*dicee.models.FMult* attribute), 156
 k (*dicee.models.FMult2* attribute), 157
 k (*dicee.models.function_space.FMult* attribute), 86
 k (*dicee.models.function_space.FMult2* attribute), 87
 k (*dicee.models.function_space.GFMult* attribute), 87
 k (*dicee.models.GFMult* attribute), 157
 k_fold_cross_validation() (*dicee.DICE_Trainer* method), 216
 k_fold_cross_validation() (*dicee.trainer.DICE_Trainer* method), 182
 k_fold_cross_validation() (*dicee.trainer.dice_trainer.DICE_Trainer* method), 177
 k_vs_all_score() (*dicee.ComplEx* static method), 198
 k_vs_all_score() (*dicee.DistMult* method), 189
 k_vs_all_score() (*dicee.Keci* method), 192
 k_vs_all_score() (*dicee.models.clifford.Keci* method), 77

k_vs_all_score() (*dicee.models.ComplEx static method*), 131
 k_vs_all_score() (*dicee.models.complex.ComplEx static method*), 84
 k_vs_all_score() (*dicee.models.DistMult method*), 125
 k_vs_all_score() (*dicee.models.Keci method*), 146
 k_vs_all_score() (*dicee.models.octonion.OMult method*), 92
 k_vs_all_score() (*dicee.models.OMult method*), 142
 k_vs_all_score() (*dicee.models.QMult method*), 136
 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*), 205
 k_vs_all_score() (*dicee.QMult method*), 204
 Keci (*class in dicee*), 189
 Keci (*class in dicee.models*), 144
 Keci (*class in dicee.models.clifford*), 74
 kernel_size (*dicee.BaseKGE attribute*), 211
 kernel_size (*dicee.config.Namespace attribute*), 30
 kernel_size (*dicee.models.base_model.BaseKGE attribute*), 72
 kernel_size (*dicee.models.BaseKGE attribute*), 119, 122, 128, 133, 139, 151, 155
 KG (*class in dicee.knowledge_graph*), 51
 kg (*dicee.callbacks.PseudoLabellingCallback attribute*), 24
 kg (*dicee.read_preprocess_save_load_kg.LoadSaveToDisk attribute*), 168
 kg (*dicee.read_preprocess_save_load_kg.PreprocessKG attribute*), 167
 kg (*dicee.read_preprocess_save_load_kg.preprocess.PreprocessKG attribute*), 162
 kg (*dicee.read_preprocess_save_load_kg.read_from_disk.ReadFromDisk attribute*), 163
 kg (*dicee.read_preprocess_save_load_kg.ReadFromDisk attribute*), 168
 kg (*dicee.read_preprocess_save_load_kg.save_load_disk.LoadSaveToDisk attribute*), 163
 KGE (*class in dicee*), 216
 KGE (*class in dicee.knowledge_graph_embeddings*), 53
 KGESaveCallback (*class in dicee.callbacks*), 22
 knowledge_graph (*dicee.executer.Execute attribute*), 49
 KronE (*class in dicee.callbacks*), 26
 KvsAll (*class in dicee*), 222
 KvsAll (*class in dicee.dataset_classes*), 35
 kvsall_score() (*dicee.DualE method*), 197
 kvsall_score() (*dicee.models.DualE method*), 160
 kvsall_score() (*dicee.models.dualE.DualE method*), 84
 KvsSampleDataset (*class in dicee*), 225
 KvsSampleDataset (*class in dicee.dataset_classes*), 38

L

label_smoothing_rate (*dicee.AllvsAll attribute*), 223
 label_smoothing_rate (*dicee.config.Namespace attribute*), 30
 label_smoothing_rate (*dicee.dataset_classes.AllvsAll attribute*), 36
 label_smoothing_rate (*dicee.dataset_classes.KvsAll attribute*), 35
 label_smoothing_rate (*dicee.dataset_classes.KvsSampleDataset attribute*), 39
 label_smoothing_rate (*dicee.dataset_classes.OnevsSample attribute*), 37
 label_smoothing_rate (*dicee.dataset_classes.TriplePredictionDataset attribute*), 40
 label_smoothing_rate (*dicee.KvsAll attribute*), 223
 label_smoothing_rate (*dicee.KvsSampleDataset attribute*), 226
 label_smoothing_rate (*dicee.OnevsSample attribute*), 224, 225
 label_smoothing_rate (*dicee.TriplePredictionDataset attribute*), 227
 labels (*dicee.dataset_classes.NegSampleDataset attribute*), 39
 labels (*dicee.NegSampleDataset attribute*), 226
 layer_norm (*dicee.models.literal.LiteralEmbeddings attribute*), 91
 LayerNorm (*class in dicee.models.transformers*), 104
 learning_rate (*dicee.BaseKGE attribute*), 211
 learning_rate (*dicee.models.base_model.BaseKGE attribute*), 72
 learning_rate (*dicee.models.BaseKGE attribute*), 119, 122, 128, 132, 138, 151, 155
 length (*dicee.dataset_classes.NegSampleDataset attribute*), 39
 length (*dicee.dataset_classes.TriplePredictionDataset attribute*), 40
 length (*dicee.NegSampleDataset attribute*), 226
 length (*dicee.TriplePredictionDataset attribute*), 227
 level (*dicee.callbacks.Perturb attribute*), 27
 LFMult (*class in dicee*), 205
 LFMult (*class in dicee.models*), 158
 LFMult (*class in dicee.models.function_space*), 88
 LFMult1 (*class in dicee.models*), 158

LFMult1 (class in dicee.models.function_space), 88
 linear() (dicee.LFMult method), 206
 linear() (dicee.models.function_space.LFMult method), 88
 linear() (dicee.models.LFMult method), 159
 list2tuple() (dicee.query_generator.QueryGenerator method), 161
 list2tuple() (dicee.QueryGenerator method), 233
 LiteralDataset (class in dicee), 231
 LiteralDataset (class in dicee.dataset_classes), 44
 LiteralEmbeddings (class in dicee.models.literal), 89
 lm_head (dicee.BytE attribute), 209
 lm_head (dicee.models.transformers.BytE attribute), 102
 lm_head (dicee.models.transformers.GPT attribute), 107
 ln_1 (dicee.models.Block attribute), 124
 ln_1 (dicee.models.transformers.Block attribute), 106
 ln_2 (dicee.models.Block attribute), 125
 ln_2 (dicee.models.transformers.Block attribute), 106
 ln_f (dicee.CoKE attribute), 207
 ln_f (dicee.models.CoKE attribute), 127
 ln_f (dicee.models.real.CoKE attribute), 101
 load() (dicee.read_preprocess_save_load_kg.LoadSaveToDisk method), 168
 load() (dicee.read_preprocess_save_load_kg.save_load_disk.LoadSaveToDisk method), 163
 load_and_validate_literal_data() (dicee.dataset_classes.LiteralDataset static method), 45
 load_and_validate_literal_data() (dicee.LiteralDataset static method), 232
 load_from_memmap() (dicee.executor.Execute method), 50
 load_json() (in module dicee), 214
 load_json() (in module dicee.static_funcs), 173
 load_model() (in module dicee), 213
 load_model() (in module dicee.static_funcs), 173
 load_model_ensemble() (in module dicee), 213
 load_model_ensemble() (in module dicee.static_funcs), 173
 load_numpy() (in module dicee), 214
 load_numpy() (in module dicee.static_funcs), 174
 load_numpy_ndarray() (in module dicee.read_preprocess_save_load_kg.util), 167
 load_pickle() (in module dicee), 213
 load_pickle() (in module dicee.read_preprocess_save_load_kg.util), 167
 load_pickle() (in module dicee.static_funcs), 173
 load_queries() (dicee.query_generator.QueryGenerator method), 162
 load_queries() (dicee.QueryGenerator method), 234
 load_queries_and_answers() (dicee.query_generator.QueryGenerator static method), 162
 load_queries_and_answers() (dicee.QueryGenerator static method), 234
 load_state_dict() (dicee.EnsembleKGE method), 213
 load_state_dict() (dicee.models.ensemble.EnsembleKGE method), 86
 load_term_mapping() (in module dicee), 213, 220
 load_term_mapping() (in module dicee.static_funcs), 173
 load_term_mapping() (in module dicee.trainer.dice_trainer), 176
 load_with_pandas() (in module dicee.read_preprocess_save_load_kg.util), 167
 loader_backend (dicee.dataset_classes.LiteralDataset attribute), 45
 loader_backend (dicee.LiteralDataset attribute), 232
 LoadSaveToDisk (class in dicee.read_preprocess_save_load_kg), 168
 LoadSaveToDisk (class in dicee.read_preprocess_save_load_kg.save_load_disk), 163
 local_rank (dicee.abstracts.AbstractTrainer attribute), 13
 local_rank (dicee.trainer.torch_trainer_ddp.NodeTrainer attribute), 180
 loss (dicee.BaseKGE attribute), 211
 loss (dicee.models.base_model.BaseKGE attribute), 72
 loss (dicee.models.BaseKGE attribute), 119, 122, 128, 133, 139, 152, 155
 loss_func (dicee.trainer.torch_trainer_ddp.NodeTrainer attribute), 181
 loss_function (dicee.trainer.torch_trainer.TorchTrainer attribute), 179
 loss_function() (dicee.BytE method), 209
 loss_function() (dicee.models.base_model.BaseKGELightning method), 67
 loss_function() (dicee.models.BaseKGELightning method), 114
 loss_function() (dicee.models.transformers.BytE method), 102
 loss_history (dicee.BaseKGE attribute), 211
 loss_history (dicee.models.base_model.BaseKGE attribute), 72
 loss_history (dicee.models.BaseKGE attribute), 120, 123, 129, 133, 139, 152, 155
 loss_history (dicee.models.pykeen_models.PykeenKGE attribute), 94
 loss_history (dicee.models.PykeenKGE attribute), 153
 loss_history (dicee.PykeenKGE attribute), 207
 loss_history (dicee.trainer.torch_trainer_ddp.NodeTrainer attribute), 181

```

lr (dicee.analyse_experiments.Experiment attribute), 19
lr (dicee.config.Namespace attribute), 29
lr_init (dicee.weight_averaging.SWA attribute), 183
lr_init (dicee.weight_averaging.SWAG attribute), 184
lr_init (dicee.weight_averaging.TWA attribute), 185
lr_lambda (dicee.callbacks.LRScheduler attribute), 28
LRScheduler (class in dicee.callbacks), 27

M

m (dicee.LFMult attribute), 205
m (dicee.models.function_space.LFMult attribute), 88
m (dicee.models.LFMult attribute), 158
main () (in module dicee.scripts.index_serve), 171
main () (in module dicee.scripts.run), 171
make_iterable_verbose () (in module dicee.static_funcs_training), 174
make_iterable_verbose () (in module dicee.trainer.torch_trainer_ddp), 180
mapping_from_first_two_cols_to_third () (in module dicee), 220
mapping_from_first_two_cols_to_third () (in module dicee.static_preprocess_funcs), 176
margin (dicee.models.Pyke attribute), 126
margin (dicee.models.real.Pyke attribute), 99
margin (dicee.models.real.TransE attribute), 99
margin (dicee.models.TransE attribute), 125
margin (dicee.Pyke attribute), 189
margin (dicee.TransE attribute), 193
mask_emb (dicee.CoKE attribute), 207
mask_emb (dicee.models.CoKE attribute), 127
mask_emb (dicee.models.real.CoKE attribute), 101
max_ans_num (dicee.query_generator.QueryGenerator attribute), 161
max_ans_num (dicee.QueryGenerator attribute), 233
max_epochs (dicee.callbacks.KGESaveCallback attribute), 23
max_epochs (dicee.callbacks.PeriodicEvalCallback attribute), 27
max_epochs (dicee.weight_averaging.EMA attribute), 184
max_epochs (dicee.weight_averaging.SWA attribute), 183
max_epochs (dicee.weight_averaging.SWAG attribute), 184
max_epochs (dicee.weight_averaging.TWA attribute), 185
max_length_subword_tokens (dicee.BaseKGE attribute), 211
max_length_subword_tokens (dicee.knowledge_graph.KG attribute), 52
max_length_subword_tokens (dicee.models.base_model.BaseKGE attribute), 72
max_length_subword_tokens (dicee.models.BaseKGE attribute), 120, 123, 129, 133, 139, 152, 155
max_num_models (dicee.weight_averaging.SWAG attribute), 184
max_num_of_classes (dicee.dataset_classes.KvsSampleDataset attribute), 39
max_num_of_classes (dicee.KvsSampleDataset attribute), 226
mean (dicee.weight_averaging.SWAG attribute), 184
mem_of_model () (dicee.EnsembleKGE method), 213
mem_of_model () (dicee.models.base_model.BaseKGELightning method), 66
mem_of_model () (dicee.models.BaseKGELightning method), 113
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), 125
mlp (dicee.models.transformers.Block attribute), 106
mode (dicee.query_generator.QueryGenerator attribute), 161
mode (dicee.QueryGenerator attribute), 233
model (dicee.config.Namespace attribute), 29
model (dicee.models.pykeen_models.PykeenKGE attribute), 94
model (dicee.models.PykeenKGE attribute), 153
model (dicee.PykeenKGE attribute), 207
model (dicee.trainer.torch_trainer_ddp.NodeTrainer attribute), 181
model (dicee.trainer.torch_trainer.TorchTrainer attribute), 179
model_kwarg (dicee.models.pykeen_models.PykeenKGE attribute), 94
model_kwarg (dicee.models.PykeenKGE attribute), 153
model_kwarg (dicee.PykeenKGE attribute), 207
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, 28
dicee.dataset_classes, 32
dicee.eval_static_funcs, 46
dicee.evaluator, 47
dicee.executer, 49
dicee.knowledge_graph, 51
dicee.knowledge_graph_embeddings, 52
dicee.models, 56
dicee.models.adopt, 56
dicee.models.base_model, 65
dicee.models.clifford, 74
dicee.models.complex, 81
dicee.models.dualE, 84
dicee.models.ensemble, 85
dicee.models.function_space, 86
dicee.models.literal, 89
dicee.models.octonion, 91
dicee.models.pykeen_models, 94
dicee.models.quaternion, 95
dicee.models.real, 98
dicee.models.static_funcs, 101
dicee.models.transformers, 101
dicee.query_generator, 160
dicee.read_preprocess_save_load_kg, 162
dicee.read_preprocess_save_load_kg.preprocess, 162
dicee.read_preprocess_save_load_kg.read_from_disk, 163
dicee.read_preprocess_save_load_kg.save_load_disk, 163
dicee.read_preprocess_save_load_kg.util, 164
dicee.sanity_checkers, 168
dicee.scripts, 169
dicee.scripts.index_serve, 169
dicee.scripts.run, 171
dicee.static_funcs, 171
dicee.static_funcs_training, 174
dicee.static_preprocess_funcs, 175
dicee.trainer, 176
dicee.trainer.dice_trainer, 176
dicee.trainer.model_parallelism, 178
dicee.trainer.torch_trainer, 178
dicee.trainer.torch_trainer_ddp, 180
dicee.weight_averaging, 183
modules() (dicee.EnsembleKGE method), 213
modules() (dicee.models.ensemble.EnsembleKGE method), 85
moving_average() (dicee.weight_averaging.SWA static method), 183
MultiClassClassificationDataset (class in dicee), 221
MultiClassClassificationDataset (class in dicee.dataset_classes), 34
MultiLabelDataset (class in dicee), 220
MultiLabelDataset (class in dicee.dataset_classes), 33

```

N

```

n (dicee.models.FMult2 attribute), 157
n (dicee.models.function_space.FMult2 attribute), 87
n_embd (dicee.models.CoKEConfig attribute), 126
n_embd (dicee.models.real.CoKEConfig attribute), 100
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), 31
n_head (dicee.models.CoKEConfig attribute), 126
n_head (dicee.models.real.CoKEConfig attribute), 100
n_head (dicee.models.transformers.GPTConfig attribute), 107
n_head (dicee.models.transformers.SelfAttention attribute), 105
n_layer (dicee.models.CoKEConfig attribute), 126
n_layer (dicee.models.real.CoKEConfig attribute), 100
n_layer (dicee.models.transformers.GPTConfig attribute), 107

```

n_layers (*dicee.models.FMult2 attribute*), 157
 n_layers (*dicee.models.function_space.FMult2 attribute*), 87
 name (*dicee.abtracts.BaseInteractiveKGE property*), 15
 name (*dicee.AConEx attribute*), 198
 name (*dicee.AConvO attribute*), 199
 name (*dicee.AConvQ attribute*), 200
 name (*dicee.BytE attribute*), 208
 name (*dicee.CKeci attribute*), 189
 name (*dicee.CoKE attribute*), 207
 name (*dicee.ComplEx attribute*), 198
 name (*dicee.ConEx attribute*), 202
 name (*dicee.ConvO attribute*), 201
 name (*dicee.ConvQ attribute*), 200
 name (*dicee.DeCaL attribute*), 193
 name (*dicee.DistMult attribute*), 189
 name (*dicee.DualE attribute*), 197
 name (*dicee.EnsembleKGE attribute*), 212
 name (*dicee.Keci attribute*), 190
 name (*dicee.LFMult attribute*), 205
 name (*dicee.models.AConEx attribute*), 130
 name (*dicee.models.AConvO attribute*), 143
 name (*dicee.models.AConvQ attribute*), 137
 name (*dicee.models.CKeci attribute*), 147
 name (*dicee.models.clifford.CKeci attribute*), 78
 name (*dicee.models.clifford.DeCaL attribute*), 78
 name (*dicee.models.clifford.Keci attribute*), 75
 name (*dicee.models.CoKE attribute*), 127
 name (*dicee.models.ComplEx attribute*), 131
 name (*dicee.models.complex.AConEx attribute*), 82
 name (*dicee.models.complex.ComplEx attribute*), 83
 name (*dicee.models.complex.ConEx attribute*), 82
 name (*dicee.models.ConEx attribute*), 130
 name (*dicee.models.ConvO attribute*), 143
 name (*dicee.models.ConvQ attribute*), 137
 name (*dicee.models.DeCaL attribute*), 147
 name (*dicee.models.DistMult attribute*), 125
 name (*dicee.models.DualE attribute*), 159
 name (*dicee.models.dualE.DualE attribute*), 84
 name (*dicee.models.ensemble.EnsembleKGE attribute*), 85
 name (*dicee.models.FMult attribute*), 156
 name (*dicee.models.FMult2 attribute*), 157
 name (*dicee.models.function_space.FMult attribute*), 86
 name (*dicee.models.function_space.FMult2 attribute*), 87
 name (*dicee.models.function_space.GFMult attribute*), 87
 name (*dicee.models.function_space.LFMult attribute*), 88
 name (*dicee.models.function_space.LFMult1 attribute*), 88
 name (*dicee.models.GFMult attribute*), 157
 name (*dicee.models.Keci attribute*), 144
 name (*dicee.models.LFMult attribute*), 158
 name (*dicee.models.LFMult1 attribute*), 158
 name (*dicee.models.octonion.AConvO attribute*), 93
 name (*dicee.models.octonion.ConvO attribute*), 93
 name (*dicee.models.octonion.OMult attribute*), 92
 name (*dicee.models.OMult attribute*), 142
 name (*dicee.models.Pyke attribute*), 126
 name (*dicee.models.pykeen_models.PykeenKGE attribute*), 94
 name (*dicee.models.PykeenKGE attribute*), 153
 name (*dicee.models.QMult attribute*), 136
 name (*dicee.models.quaternion.AConvQ attribute*), 98
 name (*dicee.models.quaternion.ConvQ attribute*), 97
 name (*dicee.models.quaternion.QMult attribute*), 96
 name (*dicee.models.real.CoKE attribute*), 100
 name (*dicee.models.real.DistMult attribute*), 98
 name (*dicee.models.real.Pyke attribute*), 99
 name (*dicee.models.real.Shallom attribute*), 99
 name (*dicee.models.real.TransE attribute*), 99
 name (*dicee.models.Shallom attribute*), 125
 name (*dicee.models.TransE attribute*), 125

name (*dicee.models.transformers.BytE attribute*), 102
 name (*dicee.OMult attribute*), 205
 name (*dicee.Pyke attribute*), 189
 name (*dicee.PykeenKGE attribute*), 207
 name (*dicee.QMult attribute*), 203
 name (*dicee.Shallom attribute*), 205
 name (*dicee.TransE attribute*), 193
 named_children () (*dicee.EnsembleKGE method*), 212
 named_children () (*dicee.models.ensemble.EnsembleKGE method*), 85
 Namespace (*class in dicee.config*), 29
 neg_ratio (*dicee.BPE_NegativeSamplingDataset attribute*), 220
 neg_ratio (*dicee.config.Namespace attribute*), 30
 neg_ratio (*dicee.dataset_classes.BPE_NegativeSamplingDataset attribute*), 33
 neg_ratio (*dicee.dataset_classes.KvsSampleDataset attribute*), 38
 neg_ratio (*dicee.KvsSampleDataset attribute*), 226
 neg_sample_ratio (*dicee.CVDataModule attribute*), 228
 neg_sample_ratio (*dicee.dataset_classes.CVDataModule attribute*), 41
 neg_sample_ratio (*dicee.dataset_classes.NegSampleDataset attribute*), 39
 neg_sample_ratio (*dicee.dataset_classes.OnesVsSample attribute*), 37
 neg_sample_ratio (*dicee.dataset_classes.TriplePredictionDataset attribute*), 40
 neg_sample_ratio (*dicee.NegSampleDataset attribute*), 226
 neg_sample_ratio (*dicee.OnesVsSample attribute*), 224, 225
 neg_sample_ratio (*dicee.TriplePredictionDataset attribute*), 227
 negnorm () (*dicee.abstracts.InteractiveQueryDecomposition method*), 16
 NegSampleDataset (*class in dicee*), 226
 NegSampleDataset (*class in dicee.dataset_classes*), 39
 neural_searcher (*in module dicee.scripts.index_serve*), 170
 NeuralSearcher (*class in dicee.scripts.index_serve*), 170
 NodeTrainer (*class in dicee.trainer.torch_trainer_ddp*), 180
 norm_fc1 (*dicee.AConEx attribute*), 199
 norm_fc1 (*dicee.AConvO attribute*), 199
 norm_fc1 (*dicee.ConEx attribute*), 202
 norm_fc1 (*dicee.ConvO attribute*), 201
 norm_fc1 (*dicee.models.AConEx attribute*), 130
 norm_fc1 (*dicee.models.AConvO attribute*), 143
 norm_fc1 (*dicee.models.complex.AConEx attribute*), 82
 norm_fc1 (*dicee.models.complex.ConEx attribute*), 82
 norm_fc1 (*dicee.models.ConEx attribute*), 130
 norm_fc1 (*dicee.models.ConvO attribute*), 143
 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*), 44
 normalization (*dicee.LiteralDataset attribute*), 231
 normalization_params (*dicee.dataset_classes.LiteralDataset attribute*), 44, 45
 normalization_params (*dicee.LiteralDataset attribute*), 231, 232
 normalization_type (*dicee.dataset_classes.LiteralDataset attribute*), 45
 normalization_type (*dicee.LiteralDataset attribute*), 232
 normalize_head_entity_embeddings (*dicee.BaseKGE attribute*), 211
 normalize_head_entity_embeddings (*dicee.models.base_model.BaseKGE attribute*), 72
 normalize_head_entity_embeddings (*dicee.models.BaseKGE attribute*), 119, 123, 128, 133, 139, 152, 155
 normalize_relation_embeddings (*dicee.BaseKGE attribute*), 211
 normalize_relation_embeddings (*dicee.models.base_model.BaseKGE attribute*), 72
 normalize_relation_embeddings (*dicee.models.BaseKGE attribute*), 119, 123, 128, 133, 139, 152, 155
 normalize_tail_entity_embeddings (*dicee.BaseKGE attribute*), 211
 normalize_tail_entity_embeddings (*dicee.models.base_model.BaseKGE attribute*), 72
 normalize_tail_entity_embeddings (*dicee.models.BaseKGE attribute*), 119, 123, 128, 133, 139, 152, 155
 normalizer_class (*dicee.BaseKGE attribute*), 211
 normalizer_class (*dicee.models.base_model.BaseKGE attribute*), 72
 normalizer_class (*dicee.models.BaseKGE attribute*), 119, 123, 128, 133, 139, 152, 155
 num_bpe_entities (*dicee.BPE_NegativeSamplingDataset attribute*), 220
 num_bpe_entities (*dicee.dataset_classes.BPE_NegativeSamplingDataset attribute*), 33
 num_bpe_entities (*dicee.knowledge_graph.KG attribute*), 52
 num_core (*dicee.config.Namespace attribute*), 30
 num_data_properties (*dicee.dataset_classes.LiteralDataset attribute*), 45
 num_data_properties (*dicee.LiteralDataset attribute*), 232
 num_datapoints (*dicee.BPE_NegativeSamplingDataset attribute*), 220

num_datapoints (*dicee.dataset_classes.BPE_NegativeSamplingDataset* attribute), 33
 num_datapoints (*dicee.dataset_classes.MultiLabelDataset* attribute), 34
 num_datapoints (*dicee.MultiLabelDataset* attribute), 221
 num_ent (*dicee.DualE* attribute), 197
 num_ent (*dicee.models.DualE* attribute), 160
 num_ent (*dicee.models.dualE.DualE* attribute), 84
 num_entities (*dicee.BaseKGE* attribute), 211
 num_entities (*dicee.CVDataModule* attribute), 228
 num_entities (*dicee.dataset_classes.CVDataModule* attribute), 41
 num_entities (*dicee.dataset_classes.KvsSampleDataset* attribute), 38
 num_entities (*dicee.dataset_classes.LiteralDataset* attribute), 44, 45
 num_entities (*dicee.dataset_classes.NegSampleDataset* attribute), 39
 num_entities (*dicee.dataset_classes.OnevsSample* attribute), 37
 num_entities (*dicee.dataset_classes.TriplePredictionDataset* attribute), 40
 num_entities (*dicee.evaluator.Evaluator* attribute), 48
 num_entities (*dicee.knowledge_graph.KG* attribute), 51
 num_entities (*dicee.KvsSampleDataset* attribute), 226
 num_entities (*dicee.LiteralDataset* attribute), 231, 232
 num_entities (*dicee.models.base_model.BaseKGE* attribute), 72
 num_entities (*dicee.models.BaseKGE* attribute), 119, 122, 128, 132, 138, 151, 155
 num_entities (*dicee.NegSampleDataset* attribute), 226
 num_entities (*dicee.OnevsSample* attribute), 224
 num_entities (*dicee.TriplePredictionDataset* attribute), 227
 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), 29
 num_epochs (*dicee.trainer.torch_trainer_ddp.NodeTrainer* attribute), 181
 num_folds_for_cv (*dicee.config.Namespace* attribute), 30
 num_of_data_points (*dicee.dataset_classes.MultiClassClassificationDataset* attribute), 34
 num_of_data_points (*dicee.MultiClassClassificationDataset* attribute), 221
 num_of_data_properties (*dicee.models.literal.LiteralEmbeddings* attribute), 90
 num_of_epochs (*dicee.callbacks.PseudoLabellingCallback* attribute), 24
 num_of_output_channels (*dicee.BaseKGE* attribute), 211
 num_of_output_channels (*dicee.config.Namespace* attribute), 30
 num_of_output_channels (*dicee.models.base_model.BaseKGE* attribute), 72
 num_of_output_channels (*dicee.models.BaseKGE* attribute), 119, 122, 128, 133, 139, 152, 155
 num_params (*dicee.analyse_experiments.Experiment* attribute), 19
 num_relations (*dicee.BaseKGE* attribute), 211
 num_relations (*dicee.CVDataModule* attribute), 228
 num_relations (*dicee.dataset_classes.CVDataModule* attribute), 41
 num_relations (*dicee.dataset_classes.NegSampleDataset* attribute), 39
 num_relations (*dicee.dataset_classes.OnevsSample* attribute), 37
 num_relations (*dicee.dataset_classes.TriplePredictionDataset* attribute), 40
 num_relations (*dicee.evaluator.Evaluator* attribute), 48
 num_relations (*dicee.knowledge_graph.KG* attribute), 51
 num_relations (*dicee.models.base_model.BaseKGE* attribute), 72
 num_relations (*dicee.models.BaseKGE* attribute), 119, 122, 128, 132, 138, 151, 155
 num_relations (*dicee.NegSampleDataset* attribute), 226
 num_relations (*dicee.OnevsSample* attribute), 224
 num_relations (*dicee.TriplePredictionDataset* attribute), 227
 num_sample (*dicee.models.FMult* attribute), 156
 num_sample (*dicee.models.function_space.FMult* attribute), 86
 num_sample (*dicee.models.function_space.GFMult* attribute), 87
 num_sample (*dicee.models.GFMult* attribute), 157
 num_samples (*dicee.weight_averaging.TWA* attribute), 185
 num_tokens (*dicee.BaseKGE* attribute), 211
 num_tokens (*dicee.knowledge_graph.KG* attribute), 52
 num_tokens (*dicee.models.base_model.BaseKGE* attribute), 72
 num_tokens (*dicee.models.BaseKGE* attribute), 119, 122, 128, 132, 138, 151, 155
 num_workers (*dicee.CVDataModule* attribute), 228
 num_workers (*dicee.dataset_classes.CVDataModule* attribute), 41
 numpy_data_type_changer () (*in module dicee*), 214
 numpy_data_type_changer () (*in module dicee.static_funcs*), 173

O

octonion_mul () (*in module dicee.models*), 141

octonion_mul() (in module dicee.models.octonion), 91
 octonion_mul_norm() (in module dicee.models), 141
 octonion_mul_norm() (in module dicee.models.octonion), 91
 octonion_normalizer() (dicee.AConvO static method), 199
 octonion_normalizer() (dicee.ConvO static method), 202
 octonion_normalizer() (dicee.models.AConvO static method), 143
 octonion_normalizer() (dicee.models.ConvO static method), 143
 octonion_normalizer() (dicee.models.octonion.AConvO static method), 94
 octonion_normalizer() (dicee.models.octonion.ConvO static method), 93
 octonion_normalizer() (dicee.models.octonion.OMult static method), 92
 octonion_normalizer() (dicee.models.OMult static method), 142
 octonion_normalizer() (dicee.OMult static method), 205
 OMult (class in dicee), 204
 OMult (class in dicee.models), 141
 OMult (class in dicee.models.octonion), 91
 on_epoch_end() (dicee.callbacks.KGESaveCallback method), 23
 on_epoch_end() (dicee.callbacks.PseudoLabellingCallback method), 24
 on_fit_end() (dicee.abstracts.AbstractCallback method), 17
 on_fit_end() (dicee.abstracts.AbstractPPECallback method), 18
 on_fit_end() (dicee.abstracts.AbstractTrainer method), 13
 on_fit_end() (dicee.callbacks.AccumulateEpochLossCallback method), 21
 on_fit_end() (dicee.callbacks.ASWA method), 24
 on_fit_end() (dicee.callbacks.Eval method), 25
 on_fit_end() (dicee.callbacks.KGESaveCallback method), 23
 on_fit_end() (dicee.callbacks.LRScheduler method), 28
 on_fit_end() (dicee.callbacks.PeriodicEvalCallback method), 27
 on_fit_end() (dicee.callbacks.PrintCallback method), 22
 on_fit_end() (dicee.weight_averaging.EMA method), 185
 on_fit_end() (dicee.weight_averaging.SWA method), 183
 on_fit_end() (dicee.weight_averaging.SWAG method), 184
 on_fit_end() (dicee.weight_averaging.TWA method), 186
 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), 26
 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), 27
 on_train_epoch_end() (dicee.callbacks.PrintCallback method), 22
 on_train_epoch_end() (dicee.models.base_model.BaseKGELighting method), 67
 on_train_epoch_end() (dicee.models.BaseKGELighting method), 114
 on_train_epoch_end() (dicee.weight_averaging.EMA method), 185
 on_train_epoch_end() (dicee.weight_averaging.SWA method), 183
 on_train_epoch_end() (dicee.weight_averaging.SWAG method), 184
 on_train_epoch_end() (dicee.weight_averaging.TWA method), 186
 on_train_epoch_start() (dicee.abstracts.AbstractTrainer method), 13
 on_train_epoch_start() (dicee.weight_averaging.EMA method), 185
 on_train_epoch_start() (dicee.weight_averaging.SWA method), 183
 on_train_epoch_start() (dicee.weight_averaging.SWAG method), 184
 on_train_epoch_start() (dicee.weight_averaging.TWA method), 185
 on_train_start() (dicee.callbacks.LRScheduler method), 28
 OnevsAllDataset (class in dicee), 221
 OnevsAllDataset (class in dicee.dataset_classes), 34

OnevsSample (*class in dicee*), 223
 OnevsSample (*class in dicee.dataset_classes*), 36
 optim (*dicee.config.Namespace attribute*), 29
 optimizer (*dicee.trainer.torch_trainer_ddp.NodeTrainer attribute*), 180
 optimizer (*dicee.trainer.torch_trainer.TorchTrainer attribute*), 179
 optimizer_name (*dicee.BaseKGE attribute*), 211
 optimizer_name (*dicee.models.base_model.BaseKGE attribute*), 72
 optimizer_name (*dicee.models.BaseKGE attribute*), 119, 122, 128, 133, 139, 151, 155
 ordered_bpe_entities (*dicee.BPE_NegativeSamplingDataset attribute*), 220
 ordered_bpe_entities (*dicee.dataset_classes.BPE_NegativeSamplingDataset attribute*), 33
 ordered_bpe_entities (*dicee.knowledge_graph.KG attribute*), 52
 ordered_shaped_bpe_tokens (*dicee.knowledge_graph.KG attribute*), 51

P

p (*dicee.config.Namespace attribute*), 31
 p (*dicee.DeCaL attribute*), 194
 p (*dicee.Keci attribute*), 190
 p (*dicee.models.clifford.DeCaL attribute*), 78
 p (*dicee.models.clifford.Keci attribute*), 75
 p (*dicee.models.DeCaL attribute*), 148
 p (*dicee.models.Keci attribute*), 144
 P (*dicee.weight_averaging.TWA attribute*), 185
 padding (*dicee.knowledge_graph.KG attribute*), 52
 pandas_dataframe_indexer () (*in module dicee.read_preprocess_save_load_kg.util*), 165
 param_init (*dicee.BaseKGE attribute*), 211
 param_init (*dicee.models.base_model.BaseKGE attribute*), 72
 param_init (*dicee.models.BaseKGE attribute*), 119, 123, 128, 133, 139, 152, 155
 parameters () (*dicee.abstracts.BaseInteractiveKGE method*), 16
 parameters () (*dicee.EnsembleKGE method*), 213
 parameters () (*dicee.models.ensemble.EnsembleKGE method*), 85
 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*), 51
 path_for_serialization (*dicee.knowledge_graph.KG attribute*), 51
 path_single_kg (*dicee.config.Namespace attribute*), 29
 path_single_kg (*dicee.knowledge_graph.KG attribute*), 51
 path_to_store_single_run (*dicee.config.Namespace attribute*), 29
 PeriodicEvalCallback (*class in dicee.callbacks*), 27
 Perturb (*class in dicee.callbacks*), 26
 polars_dataframe_indexer () (*in module dicee.read_preprocess_save_load_kg.util*), 164
 poly_NN () (*dicee.LFMult method*), 206
 poly_NN () (*dicee.models.function_space.LFMult method*), 88
 poly_NN () (*dicee.models.LFMult method*), 159
 polynomial () (*dicee.LFMult method*), 206
 polynomial () (*dicee.models.function_space.LFMult method*), 89
 polynomial () (*dicee.models.LFMult method*), 159
 pop () (*dicee.LFMult method*), 206
 pop () (*dicee.models.function_space.LFMult method*), 89
 pop () (*dicee.models.LFMult method*), 159
 pos_emb (*dicee.CoKE attribute*), 207
 pos_emb (*dicee.models.CoKE attribute*), 127
 pos_emb (*dicee.models.real.CoKE attribute*), 101
 pq (*dicee.analyse_experiments.Experiment attribute*), 20
 predict () (*dicee.KGE method*), 217
 predict () (*dicee.knowledge_graph_embeddings.KGE method*), 54
 predict_dataloader () (*dicee.models.base_model.BaseKGELightning method*), 69
 predict_dataloader () (*dicee.models.BaseKGELightning method*), 116
 predict_literals () (*dicee.KGE method*), 219
 predict_literals () (*dicee.knowledge_graph_embeddings.KGE method*), 56
 predict_missing_head_entity () (*dicee.KGE method*), 216
 predict_missing_head_entity () (*dicee.knowledge_graph_embeddings.KGE method*), 53
 predict_missing_relations () (*dicee.KGE method*), 217
 predict_missing_relations () (*dicee.knowledge_graph_embeddings.KGE method*), 53

```

predict_missing_tail_entity() (dicee.KGE method), 217
predict_missing_tail_entity() (dicee.knowledge_graph_embeddings.KGE method), 54
predict_topk() (dicee.KGE method), 218
predict_topk() (dicee.knowledge_graph_embeddings.KGE method), 54
prepare_data() (dicee.CVDataModule method), 230
prepare_data() (dicee.dataset_classes.CVDataModule method), 43
preprocess_with_byte_pair_encoding() (dicee.read_preprocess_save_load_kg.PreprocessKG method), 167
preprocess_with_byte_pair_encoding() (dicee.read_preprocess_save_load_kg.preprocess.PreprocessKG method), 162
preprocess_with_byte_pair_encoding_with_padding() (dicee.read_preprocess_save_load_kg.PreprocessKG method), 168
preprocess_with_byte_pair_encoding_with_padding() (dicee.read_preprocess_save_load_kg.preprocess.PreprocessKG method), 162
preprocess_with_pandas() (dicee.read_preprocess_save_load_kg.PreprocessKG method), 168
preprocess_with_pandas() (dicee.read_preprocess_save_load_kg.preprocess.PreprocessKG method), 162
preprocess_with_polars() (dicee.read_preprocess_save_load_kg.PreprocessKG method), 168
preprocess_with_polars() (dicee.read_preprocess_save_load_kg.preprocess.PreprocessKG method), 162
preprocesses_input_args() (in module dicee.static_funcs), 175
PreprocessKG (class in dicee.read_preprocess_save_load_kg), 167
PreprocessKG (class in dicee.read_preprocess_save_load_kg.preprocess), 162
PrintCallback (class in dicee.callbacks), 21
process (dicee.trainer.torch_trainer.TorchTrainer attribute), 179
PseudoLabellingCallback (class in dicee.callbacks), 23
Pyke (class in dicee), 189
Pyke (class in dicee.models), 126
Pyke (class in dicee.models.real), 99
pykeen_model_kwarg (dicee.config.Namespace attribute), 30
PykeenKGE (class in dicee), 207
PykeenKGE (class in dicee.models), 153
PykeenKGE (class in dicee.models.pykeen_models), 94

```

Q

```

q (dicee.config.Namespace attribute), 31
q (dicee.DeCaL attribute), 194
q (dicee.Keci attribute), 190
q (dicee.models.clifford.DeCaL attribute), 79
q (dicee.models.clifford.Keci attribute), 75
q (dicee.models.DeCaL attribute), 148
q (dicee.models.Keci attribute), 144
qdant_client (dicee.scripts.index_serve.NeuralSearcher attribute), 170
QMult (class in dicee), 202
QMult (class in dicee.models), 135
QMult (class in dicee.models.quaternion), 95
quaternion_mul() (in module dicee.models), 132
quaternion_mul() (in module dicee.models.static_funcs), 101
quaternion_mul_with_unit_norm() (in module dicee.models), 135
quaternion_mul_with_unit_norm() (in module dicee.models.quaternion), 95
quaternion_multiplication_followed_by_inner_product() (dicee.models.QMult method), 136
quaternion_multiplication_followed_by_inner_product() (dicee.models.quaternion.QMult method), 96
quaternion_multiplication_followed_by_inner_product() (dicee.QMult method), 203
quaternion_normalizer() (dicee.models.QMult static method), 136
quaternion_normalizer() (dicee.models.quaternion.QMult static method), 96
quaternion_normalizer() (dicee.QMult static method), 203
queries (dicee.scripts.index_serve.StringListRequest attribute), 170
query_name_to_struct (dicee.query_generator.QueryGenerator attribute), 161
query_name_to_struct (dicee.QueryGenerator attribute), 233
QueryGenerator (class in dicee), 233
QueryGenerator (class in dicee.query_generator), 161

```

R

```

r (dicee.DeCaL attribute), 194
r (dicee.Keci attribute), 190
r (dicee.models.clifford.DeCaL attribute), 79
r (dicee.models.clifford.Keci attribute), 75
r (dicee.models.DeCaL attribute), 148
r (dicee.models.Keci attribute), 144
random_prediction() (in module dicee), 214
random_prediction() (in module dicee.static_funcs), 173
random_seed (dicee.config.Namespace attribute), 30
ratio (dicee.callbacks.Perturb attribute), 27

```

re (*dicee.DeCaL* attribute), 194
 re (*dicee.models.clifford.DeCaL* attribute), 79
 re (*dicee.models.DeCaL* attribute), 148
 re_vocab (*dicee.evaluator.Evaluator* attribute), 48
 read_from_disk() (in module *dicee.read_preprocess_save_load_kg.util*), 166
 read_from_triple_store_with_pandas() (in module *dicee.read_preprocess_save_load_kg.util*), 166
 read_from_triple_store_with_polars() (in module *dicee.read_preprocess_save_load_kg.util*), 166
 read_only_few (*dicee.config.Namespace* attribute), 30
 read_only_few (*dicee.knowledge_graph.KG* attribute), 51
 read_or_load_kg() (in module *dicee*), 214
 read_or_load_kg() (in module *dicee.static_funcs*), 173
 read_with_pandas() (in module *dicee.read_preprocess_save_load_kg.util*), 166
 read_with_polars() (in module *dicee.read_preprocess_save_load_kg.util*), 166
 ReadFromDisk (class in *dicee.read_preprocess_save_load_kg*), 168
 ReadFromDisk (class in *dicee.read_preprocess_save_load_kg.read_from_disk*), 163
 reducer (*dicee.scripts.index_serve.StringListRequest* attribute), 170
 reg_lambda (*dicee.weight_averaging.TWA* attribute), 185
 rel2id (*dicee.query_generator.QueryGenerator* attribute), 161
 rel2id (*dicee.QueryGenerator* attribute), 233
 relation_embeddings (*dicee.AConvQ* attribute), 200
 relation_embeddings (*dicee.ConvQ* attribute), 200
 relation_embeddings (*dicee.DeCaL* attribute), 194
 relation_embeddings (*dicee.DualE* attribute), 197
 relation_embeddings (*dicee.LFMult* attribute), 205
 relation_embeddings (*dicee.models.AConvQ* attribute), 137
 relation_embeddings (*dicee.models.clifford.DeCaL* attribute), 78
 relation_embeddings (*dicee.models.ConvQ* attribute), 137
 relation_embeddings (*dicee.models.DeCaL* attribute), 148
 relation_embeddings (*dicee.models.DualE* attribute), 160
 relation_embeddings (*dicee.models.dualE.DualE* attribute), 84
 relation_embeddings (*dicee.models.FMult* attribute), 156
 relation_embeddings (*dicee.models.FMult2* attribute), 158
 relation_embeddings (*dicee.models.function_space.FMult* attribute), 86
 relation_embeddings (*dicee.models.function_space.FMult2* attribute), 87
 relation_embeddings (*dicee.models.function_space.GFMult* attribute), 87
 relation_embeddings (*dicee.models.function_space.LFMult* attribute), 88
 relation_embeddings (*dicee.models.function_space.LFMult1* attribute), 88
 relation_embeddings (*dicee.models.GFMult* attribute), 157
 relation_embeddings (*dicee.models.LFMult* attribute), 158
 relation_embeddings (*dicee.models.LFMult1* attribute), 158
 relation_embeddings (*dicee.models.pykeen_models.PykeenKGE* attribute), 94
 relation_embeddings (*dicee.models.PykeenKGE* attribute), 153
 relation_embeddings (*dicee.models.quaternion.AConvQ* attribute), 98
 relation_embeddings (*dicee.models.quaternion.ConvQ* attribute), 97
 relation_embeddings (*dicee.PykeenKGE* attribute), 207
 relation_to_idx (*dicee.knowledge_graph.KG* attribute), 52
 relations_str (*dicee.knowledge_graph.KG* property), 52
 reload_dataset() (in module *dicee*), 220
 reload_dataset() (in module *dicee.dataset_classes*), 32
 report (*dicee.DICE_Trainer* attribute), 215
 report (*dicee.evaluator.Evaluator* attribute), 48
 report (*dicee.executor.Execute* attribute), 49
 report (*dicee.trainer.DICE_Trainer* attribute), 181
 report (*dicee.trainer.dice_trainer.DICE_Trainer* attribute), 176
 reports (*dicee.callbacks.Eval* attribute), 25
 reports (*dicee.callbacks.PeriodicEvalCallback* attribute), 27
 requires_grad_for_interactions (*dicee.CKeci* attribute), 189
 requires_grad_for_interactions (*dicee.Keci* attribute), 190
 requires_grad_for_interactions (*dicee.models.CKeci* attribute), 147
 requires_grad_for_interactions (*dicee.models.clifford.CKeci* attribute), 78
 requires_grad_for_interactions (*dicee.models.clifford.Keci* attribute), 75
 requires_grad_for_interactions (*dicee.models.Keci* attribute), 144
 resid_dropout (*dicee.models.transformers.SelfAttention* attribute), 105
 residual_convolution() (*dicee.AConEx* method), 199
 residual_convolution() (*dicee.AConvO* method), 199
 residual_convolution() (*dicee.AConvQ* method), 200
 residual_convolution() (*dicee.ConEx* method), 202
 residual_convolution() (*dicee.ConvO* method), 202

```

residual_convolution() (dicee.ConvQ method), 200
residual_convolution() (dicee.models.AConEx method), 130
residual_convolution() (dicee.models.AConvO method), 143
residual_convolution() (dicee.models.AConvQ method), 137
residual_convolution() (dicee.models.complex.AConEx method), 83
residual_convolution() (dicee.models.complex.ConEx method), 82
residual_convolution() (dicee.models.ConEx method), 130
residual_convolution() (dicee.models.ConvO method), 143
residual_convolution() (dicee.models.ConvQ method), 137
residual_convolution() (dicee.models.octonion.AConvO method), 94
residual_convolution() (dicee.models.octonion.ConvO method), 93
residual_convolution() (dicee.models.quaternion.AConvQ method), 98
residual_convolution() (dicee.models.quaternion.ConvQ method), 97
retrieve_embedding() (dicee.scripts.index_serve.NeuralSearcher method), 170
retrieve_embeddings() (in module dicee.scripts.index_serve), 170
return_multi_hop_query_results() (dicee.KGE method), 218
return_multi_hop_query_results() (dicee.knowledge_graph_embeddings.KGE method), 55
root() (in module dicee.scripts.index_serve), 170
roots (dicee.models.FMult attribute), 157
roots (dicee.models.function_space.FMult attribute), 86
roots (dicee.models.function_space.GFMult attribute), 87
roots (dicee.models.GFMult attribute), 157
runtime (dicee.analyse_experiments.Experiment attribute), 20

```

S

```

sample() (dicee.weight_averaging.SWAG method), 184
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), 30
sample_triples_ratio (dicee.knowledge_graph.KG attribute), 51
sample_weights() (dicee.weight_averaging.TWA method), 185
sampling_ratio (dicee.dataset_classes.LiteralDataset attribute), 44, 45
sampling_ratio (dicee.LiteralDataset attribute), 231, 232
sanity_check_callback_args() (in module dicee.sanity_checkers), 169
sanity_checking_with_arguments() (in module dicee.sanity_checkers), 169
save() (dicee.abstracts.BaseInteractiveKGE method), 15
save() (dicee.read_preprocess_save_load_kg.LoadSaveToDisk method), 168
save() (dicee.read_preprocess_save_load_kg.save_load_disk.LoadSaveToDisk method), 163
save_checkpoint() (dicee.abstracts.AbstractTrainer static method), 14
save_checkpoint_model() (in module dicee), 214
save_checkpoint_model() (in module dicee.static_funcs), 173
save_embeddings() (in module dicee), 214
save_embeddings() (in module dicee.static_funcs), 173
save_embeddings_as_csv (dicee.config.Namespace attribute), 29
save_every_n_epochs (dicee.config.Namespace attribute), 31
save_experiment() (dicee.analyse_experiments.Experiment method), 20
save_model_at_every_epoch (dicee.config.Namespace attribute), 30
save_model_every_n_epoch (dicee.callbacks.PeriodicEvalCallback attribute), 27
save_numpy_ndarray() (in module dicee), 214
save_numpy_ndarray() (in module dicee.read_preprocess_save_load_kg.util), 167
save_numpy_ndarray() (in module dicee.static_funcs), 173
save_pickle() (in module dicee), 213
save_pickle() (in module dicee.read_preprocess_save_load_kg.util), 167
save_pickle() (in module dicee.static_funcs), 173
save_queries() (dicee.query_generator.QueryGenerator method), 162
save_queries() (dicee.QueryGenerator method), 234
save_queries_and_answers() (dicee.query_generator.QueryGenerator static method), 162
save_queries_and_answers() (dicee.QueryGenerator static method), 234
save_trained_model() (dicee.executer.Execute method), 50
scalar_batch_NN() (dicee.LFMult method), 206
scalar_batch_NN() (dicee.models.function_space.LFMult method), 88
scalar_batch_NN() (dicee.models.LFMult method), 159
scaler (dicee.callbacks.Perturb attribute), 27
scaler (dicee.trainer.torch_trainer_ddp.NodeTrainer attribute), 181
scheduler (dicee.callbacks.LRScheduler attribute), 28
score() (dicee.CoKE method), 207

```

score() (*dicee.ComplEx static method*), 198
 score() (*dicee.DistMult method*), 189
 score() (*dicee.Keci method*), 192
 score() (*dicee.models.clifford.Keci method*), 77
 score() (*dicee.models.CoKE method*), 127
 score() (*dicee.models.ComplEx static method*), 131
 score() (*dicee.models.complex.ComplEx static method*), 83
 score() (*dicee.models.DistMult method*), 125
 score() (*dicee.models.Keci method*), 146
 score() (*dicee.models.octonion.OMult method*), 92
 score() (*dicee.models.OMult method*), 142
 score() (*dicee.models.QMult method*), 136
 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*), 99
 score() (*dicee.models.TransE method*), 125
 score() (*dicee.OMult method*), 205
 score() (*dicee.QMult method*), 204
 score() (*dicee.TransE method*), 193
 score_func (*dicee.models.FMult2 attribute*), 157
 score_func (*dicee.models.function_space.FMult2 attribute*), 87
 scoring_technique (*dicee.analyse_experiments.Experiment attribute*), 20
 scoring_technique (*dicee.config.Namespace attribute*), 30
 search() (*dicee.scripts.index_serve.NeuralSearcher method*), 170
 search_embeddings() (*in module dicee.scripts.index_serve*), 170
 search_embeddings_batch() (*in module dicee.scripts.index_serve*), 170
 seed (*dicee.query_generator.QueryGenerator attribute*), 161
 seed (*dicee.QueryGenerator attribute*), 233
 select_model() (*in module dicee*), 213
 select_model() (*in module dicee.static_funcs*), 173
 selected_optimizer (*dicee.BaseKGE attribute*), 211
 selected_optimizer (*dicee.models.base_model.BaseKGE attribute*), 72
 selected_optimizer (*dicee.models.BaseKGE attribute*), 119, 122, 128, 133, 139, 152, 155
 SelfAttention (*class in dicee.models.transformers*), 104
 separator (*dicee.config.Namespace attribute*), 30
 separator (*dicee.knowledge_graph.KG attribute*), 52
 sequential_vocabulary_construction() (*dicee.read_preprocess_save_load_kg.PreprocessKG method*), 168
 sequential_vocabulary_construction() (*dicee.read_preprocess_save_load_kg.preprocess.PreprocessKG method*), 162
 serve() (*in module dicee.scripts.index_serve*), 171
 set_global_seed() (*dicee.query_generator.QueryGenerator method*), 161
 set_global_seed() (*dicee.QueryGenerator method*), 233
 set_model_eval_mode() (*dicee.abstracts.BaseInteractiveKGE method*), 15
 set_model_train_mode() (*dicee.abstracts.BaseInteractiveKGE method*), 14
 setup() (*dicee.CVDataModule method*), 228
 setup() (*dicee.dataset_classes.CVDataModule method*), 41
 setup_executor() (*dicee.executer.Execute method*), 49
 Shallom (*class in dicee*), 205
 Shallom (*class in dicee.models*), 125
 Shallom (*class in dicee.models.real*), 99
 shallom (*dicee.models.real.Shallom attribute*), 99
 shallom (*dicee.models.Shallom attribute*), 125
 shallom (*dicee.Shallom attribute*), 205
 single_hop_query_answering() (*dicee.KGE method*), 218
 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*), 29
 sparql_endpoint (*dicee.knowledge_graph.KG attribute*), 51
 sq_mean (*dicee.weight_averaging.SWAG attribute*), 184
 start() (*dicee.DICE_Trainer method*), 216
 start() (*dicee.executer.Execute method*), 50
 start() (*dicee.read_preprocess_save_load_kg.PreprocessKG method*), 167
 start() (*dicee.read_preprocess_save_load_kg.preprocess.PreprocessKG method*), 162
 start() (*dicee.read_preprocess_save_load_kg.read_from_disk.ReadFromDisk method*), 163
 start() (*dicee.read_preprocess_save_load_kg.ReadFromDisk method*), 168
 start() (*dicee.trainer.DICE_Trainer method*), 182
 start() (*dicee.trainer.dice_trainer.DICE_Trainer method*), 177

```

start_time (dicee.callbacks.PrintCallback attribute), 22
start_time (dicee.executer.Execute attribute), 49
state_dict () (dicee.EnsembleKGE method), 213
state_dict () (dicee.models.ensemble.EnsembleKGE method), 86
step () (dicee.EnsembleKGE method), 213
step () (dicee.models.ADOPT method), 111
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), 215
storage_path (dicee.trainer.DICE_Trainer attribute), 181
storage_path (dicee.trainer.dice_trainer.DICE_Trainer attribute), 177
store () (in module dicee), 214
store () (in module dicee.static_funcs), 173
store_ensemble () (dicee.abstracts.AbstractPPECallback method), 18
strategy (dicee.abstracts.AbstractTrainer attribute), 13
StringListRequest (class in dicee.scripts.index_serve), 170
SWA (class in dicee.weight_averaging), 183
swa (dicee.config.Namespace attribute), 31
swa_c_epochs (dicee.config.Namespace attribute), 32
swa_c_epochs (dicee.weight_averaging.SWA attribute), 183
swa_c_epochs (dicee.weight_averaging.SWAG attribute), 183
swa_lr (dicee.weight_averaging.SWA attribute), 183
swa_lr (dicee.weight_averaging.SWAG attribute), 184
swa_model (dicee.weight_averaging.SWA attribute), 183
swa_n (dicee.weight_averaging.SWA attribute), 183
swa_start_epoch (dicee.config.Namespace attribute), 32
swa_start_epoch (dicee.weight_averaging.SWA attribute), 183
swa_start_epoch (dicee.weight_averaging.SWAG attribute), 183
SWAG (class in dicee.weight_averaging), 183
swag (dicee.config.Namespace attribute), 31

```

T

```

T () (dicee.DualE method), 197
T () (dicee.models.DualE method), 160
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), 223
target_dim (dicee.dataset_classes.AllvsAll attribute), 36
target_dim (dicee.dataset_classes.MultiLabelDataset attribute), 33
target_dim (dicee.dataset_classes.OnevsAllDataset attribute), 35
target_dim (dicee.knowledge_graph.KG attribute), 52
target_dim (dicee.MultiLabelDataset attribute), 221
target_dim (dicee.OnevsAllDataset attribute), 222
temperature (dicee.BytE attribute), 208
temperature (dicee.models.transformers.BytE attribute), 102
tensor_t_norm () (dicee.abstracts.InteractiveQueryDecomposition method), 16
TensorParallel (class in dicee.trainer.model_parallelism), 178
test_dataloader () (dicee.models.base_model.BaseKGELightning method), 67
test_dataloader () (dicee.models.BaseKGELightning method), 115
test_epoch_end () (dicee.models.base_model.BaseKGELightning method), 67
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), 161
test_path (dicee.QueryGenerator attribute), 233
timeit () (in module dicee), 213, 220
timeit () (in module dicee.read_preprocess_save_load_kg.util), 166
timeit () (in module dicee.static_funcs), 172
timeit () (in module dicee.static_preprocess_funcs), 175
to () (dicee.EnsembleKGE method), 213
to () (dicee.KGE method), 216
to () (dicee.knowledge_graph_embeddings.KGE method), 53

```

`to()` (*dicee.models.ensemble.EnsembleKGE* method), 85
`to_df()` (*dicee.analyse_experiments.Experiment* method), 20
`topk` (*dicee.BytE* attribute), 208
`topk` (*dicee.models.transformers.BytE* attribute), 102
`topk` (*dicee.scripts.index_serve.NeuralSearcher* attribute), 170
`torch_ordered_shaped_bpe_entities` (*dicee.dataset_classes.MultiLabelDataset* attribute), 34
`torch_ordered_shaped_bpe_entities` (*dicee.MultiLabelDataset* attribute), 221
`TorchDDPTrainer` (class in *dicee.trainer.torch_trainer_ddp*), 180
`TorchTrainer` (class in *dicee.trainer.torch_trainer*), 179
`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), 181
`train_data` (*dicee.AllvsAll* attribute), 223
`train_data` (*dicee.dataset_classes.AllvsAll* attribute), 36
`train_data` (*dicee.dataset_classes.KvsAll* attribute), 35
`train_data` (*dicee.dataset_classes.KvsSampleDataset* attribute), 38
`train_data` (*dicee.dataset_classes.MultiClassClassificationDataset* attribute), 34
`train_data` (*dicee.dataset_classes.OnevsAllDataset* attribute), 35
`train_data` (*dicee.dataset_classes.OnevsSample* attribute), 37
`train_data` (*dicee.KvsAll* attribute), 222
`train_data` (*dicee.KvsSampleDataset* attribute), 226
`train_data` (*dicee.MultiClassClassificationDataset* attribute), 221
`train_data` (*dicee.OnevsAllDataset* attribute), 222
`train_data` (*dicee.OnevsSample* attribute), 224
`train_dataloader()` (*dicee.CVDataModule* method), 228
`train_dataloader()` (*dicee.dataset_classes.CVDataModule* method), 41
`train_dataloader()` (*dicee.models.base_model.BaseKGELightning* method), 69
`train_dataloader()` (*dicee.models.BaseKGELightning* method), 116
`train_dataloaders` (*dicee.trainer.torch_trainer.TorchTrainer* attribute), 179
`train_dataset_loader` (*dicee.trainer.torch_trainer_ddp.NodeTrainer* attribute), 181
`train_file_path` (*dicee.dataset_classes.LiteralDataset* attribute), 44, 45
`train_file_path` (*dicee.LiteralDataset* attribute), 231, 232
`train_h1` (*dicee.analyse_experiments.Experiment* attribute), 20
`train_h3` (*dicee.analyse_experiments.Experiment* attribute), 20
`train_h10` (*dicee.analyse_experiments.Experiment* attribute), 20
`train_indices_target` (*dicee.dataset_classes.MultiLabelDataset* attribute), 33
`train_indices_target` (*dicee.MultiLabelDataset* attribute), 221
`train_k_vs_all()` (*dicee.abstracts.BaseInteractiveTrainKGE* method), 18
`train_literals()` (*dicee.abstracts.BaseInteractiveTrainKGE* method), 18
`train_mode` (*dicee.EnsembleKGE* attribute), 212
`train_mode` (*dicee.models.ensemble.EnsembleKGE* attribute), 85
`train_mrr` (*dicee.analyse_experiments.Experiment* attribute), 20
`train_path` (*dicee.query_generator.QueryGenerator* attribute), 161
`train_path` (*dicee.QueryGenerator* attribute), 233
`train_set` (*dicee.BPE_NegativeSamplingDataset* attribute), 220
`train_set` (*dicee.dataset_classes.BPE_NegativeSamplingDataset* attribute), 33
`train_set` (*dicee.dataset_classes.MultiLabelDataset* attribute), 33
`train_set` (*dicee.dataset_classes.NegSampleDataset* attribute), 39
`train_set` (*dicee.dataset_classes.TriplePredictionDataset* attribute), 40
`train_set` (*dicee.MultiLabelDataset* attribute), 221
`train_set` (*dicee.NegSampleDataset* attribute), 226
`train_set` (*dicee.TriplePredictionDataset* attribute), 227
`train_set_idx` (*dicee.CVDataModule* attribute), 228
`train_set_idx` (*dicee.dataset_classes.CVDataModule* attribute), 40
`train_set_target` (*dicee.knowledge_graph.KG* attribute), 52
`train_target` (*dicee.AllvsAll* attribute), 223
`train_target` (*dicee.dataset_classes.AllvsAll* attribute), 36
`train_target` (*dicee.dataset_classes.KvsAll* attribute), 35
`train_target` (*dicee.dataset_classes.KvsSampleDataset* attribute), 38
`train_target` (*dicee.KvsAll* attribute), 223
`train_target` (*dicee.KvsSampleDataset* attribute), 226
`train_target_indices` (*dicee.knowledge_graph.KG* attribute), 52
`train_triples` (*dicee.dataset_classes.NegSampleDataset* attribute), 39
`train_triples` (*dicee.NegSampleDataset* attribute), 226
`train_triples()` (*dicee.abstracts.BaseInteractiveTrainKGE* method), 18
`trained_model` (*dicee.executer.Execute* attribute), 49
`trainer` (*dicee.config.Namespace* attribute), 30

trainer (*dicee.DICE_Trainer* attribute), 215
 trainer (*dicee.executer.Execute* attribute), 49
 trainer (*dicee.trainer.DICE_Trainer* attribute), 181
 trainer (*dicee.trainer.dice_trainer.DICE_Trainer* attribute), 176
 trainer (*dicee.trainer.torch_trainer_ddp.NodeTrainer* attribute), 180
 training_step (*dicee.trainer.torch_trainer.TorchTrainer* attribute), 179
 training_step () (*dicee.BytE* method), 209
 training_step () (*dicee.models.base_model.BaseKGELightning* method), 66
 training_step () (*dicee.models.BaseKGELightning* method), 113
 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), 113
 training_technique (*dicee.knowledge_graph.KG* attribute), 52
 TransE (*class in dicee*), 193
 TransE (*class in dicee.models*), 125
 TransE (*class in dicee.models.real*), 99
 transfer_batch_to_device () (*dicee.CVDataModule* method), 229
 transfer_batch_to_device () (*dicee.dataset_classes.CVDataModule* method), 42
 transformer (*dicee.BytE* attribute), 209
 transformer (*dicee.models.transformers.BytE* attribute), 102
 transformer (*dicee.models.transformers.GPT* attribute), 107
 trapezoid() (*dicee.models.FMult2* method), 158
 trapezoid() (*dicee.models.function_space.FMult2* method), 87
 tri_score() (*dicee.LFMult* method), 206
 tri_score() (*dicee.models.function_space.LFMult* method), 89
 tri_score() (*dicee.models.function_space.LFMult1* method), 88
 tri_score() (*dicee.models.LFMult* method), 159
 tri_score() (*dicee.models.LFMult1* method), 158
 triple_score() (*dicee.KGE* method), 218
 triple_score() (*dicee.knowledge_graph_embeddings.KGE* method), 54
 TriplePredictionDataset (*class in dicee*), 226
 TriplePredictionDataset (*class in dicee.dataset_classes*), 39
 tuple2list () (*dicee.query_generator.QueryGenerator* method), 161
 tuple2list () (*dicee.QueryGenerator* method), 233
 TWA (*class in dicee.weight_averaging*), 185
 twa (*dicee.config.Namespace* attribute), 31
 twa_c_epochs (*dicee.weight_averaging.TWA* attribute), 185
 twa_model (*dicee.weight_averaging.TWA* attribute), 185
 twa_start_epoch (*dicee.weight_averaging.TWA* attribute), 185

U

unlabelled_size (*dicee.callbacks.PseudoLabellingCallback* attribute), 24
 unmap () (*dicee.query_generator.QueryGenerator* method), 161
 unmap () (*dicee.QueryGenerator* method), 233
 unmap_query () (*dicee.query_generator.QueryGenerator* method), 161
 unmap_query () (*dicee.QueryGenerator* method), 233

V

val_aswa (*dicee.callbacks.ASWA* attribute), 24
 val_dataloader () (*dicee.models.base_model.BaseKGELightning* method), 68
 val_dataloader () (*dicee.models.BaseKGELightning* method), 115
 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), 161
 val_path (*dicee.QueryGenerator* attribute), 233
 validate_knowledge_graph () (*in module dicee.sanity_checkers*), 169
 var_clamp (*dicee.weight_averaging.SWAG* attribute), 184
 vocab_preparation () (*dicee.evaluator.Evaluator* method), 48
 vocab_size (*dicee.models.CoKEConfig* attribute), 126
 vocab_size (*dicee.models.real.CoKEConfig* attribute), 100
 vocab_size (*dicee.models.transformers.GPTConfig* attribute), 106
 vocab_to_parquet () (*in module dicee*), 214
 vocab_to_parquet () (*in module dicee.static_funcs*), 174
 vtp_score () (*dicee.LFMult* method), 206
 vtp_score () (*dicee.models.function_space.LFMult* method), 89

vtp_score() (*dicee.models.function_space.LFMult1 method*), 88
vtp_score() (*dicee.models.LFMult method*), 159
vtp_score() (*dicee.models.LFMult1 method*), 158

W

warmup_steps (*dicee.callbacks.LRScheduler attribute*), 28
weight (*dicee.models.transformers.LayerNorm attribute*), 104
weight_decay (*dicee.BaseKGE attribute*), 211
weight_decay (*dicee.config.Namespace attribute*), 30
weight_decay (*dicee.models.base_model.BaseKGE attribute*), 72
weight_decay (*dicee.models.BaseKGE attribute*), 119, 122, 128, 133, 139, 152, 155
weight_samples (*dicee.weight_averaging.TWA attribute*), 185
weights (*dicee.models.FMult attribute*), 157
weights (*dicee.models.function_space.FMult attribute*), 86
weights (*dicee.models.function_space.GFMult attribute*), 87
weights (*dicee.models.GFMult attribute*), 157
write_csv_from_model_parallel() (*in module dicee*), 215
write_csv_from_model_parallel() (*in module dicee.static_funcs*), 174
write_links() (*dicee.query_generator.QueryGenerator method*), 161
write_links() (*dicee.QueryGenerator method*), 233
write_report() (*dicee.executer.Execute method*), 50

X

x_values (*dicee.LFMult attribute*), 205
x_values (*dicee.models.function_space.LFMult attribute*), 88
x_values (*dicee.models.LFMult attribute*), 158